OAK RIDGE
NATIONAL LABORATORY
MANAGED BY UT-BATTELLE
FOR THE DEPARTMENT OF ENERGY

ORNL/TM-9179/R7
ENDF-364/R1

UPDATED USERS' GUIDE FOR SAMMY: MULTILEVEL R-MATRIX FITS TO NEUTRON DATA USING BAYES' EQUATIONS

September 2006

Prepared by
Nancy M. Larson

UT-BATTELLE
ORNL-27 (4-00)

DOCUMENT AVAILABILITY

Reports produced after January 1, 1996, are generally available free via the U.S. Department of Energy (DOE) Information Bridge:

Web site: http://www.osti.gov/bridge

Reports produced before January 1, 1996, may be purchased by members of the public from the following source:

National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Telephone: 703-605-6000 (1-800-553-6847)
TDD: 703-487-4639
Fax: 703-605-6900
E-mail: info@ntis.fedworld.gov
Web site: http://www.ntis.gov/support/ordernowabout.htm

Reports are available to DOE employees, DOE contractors, Energy Technology Data Exchange (ETDE) representatives, and International Nuclear Information System (INIS) representatives from the following source:

Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831
Telephone: 865-576-8401
Fax: 865-576-5728
E-mail: reports@adonis.osti.gov
Web site: http://www.osti.gov/contact.html

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

ORNL/TM-9179/R7
ENDF-364/R1

Nuclear Science and Technology Division

UPDATED USERS' GUIDE FOR SAMMY: MULTILEVEL R-MATRIX FITS TO NEUTRON DATA USING BAYES' EQUATIONS

Nancy M. Larson

Date of First Publication: August 1984
Date of Revision 1: April 1985
Date of Revision 2: June 1989
Date of Revision 3: September 1996
Date of Revision 4: December 1998
Date of Revision 5: October 2000
Date of Revision 6: July 2003
Date of Revision 7: September 2006

Prepared by the
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, TN 37831
managed by
UT-BATTELLE, LLC
for the
U.S. DEPARTMENT OF ENERGY
under contract DE-AC05-00R22725

CONTENTS

LIST OF TABLES ix
LIST OF FIGURES xiii
ACKNOWLEDGMENTS xv
ABSTRACT xvii

I. INTRODUCTION 1
A. MODIFICATIONS AND ADDITIONS IN REVISION 7 3

II. SCATTERING THEORY 9

A. EQUATIONS FOR SCATTERING THEORY 11
1. R-Matrix and A-Matrix Equations 15
2. Derivation of Scattering Theory Equations 19
a. Relating the scattering matrix to the cross sections 27
B. VERSIONS OF MULTILEVEL R-MATRIX THEORY 29
1. Reich-Moore Approximation to Multilevel R-Matrix Theory 31
a. Energy-differential cross sections 33
i. One-level two-channel case 35
b. Angular distributions 39
c. Specifying individual reaction types 43
d. External R-function 45
2. Simulation of Full R-Matrix 47
3. Breit-Wigner Approximation 49
a. Single and multilevel Breit-Wigner cross sections 51
4. Direct Capture Component 53
C. DETAILS AND CONVENTIONS USED IN SAMMY 55
1. Spin and Angular Momentum Conventions 57
a. Quantum vector algebra 61
2. Kinematics 63
a. Derivation of kinematics equations 67
b. Kinematics for elastic scattering 73
3. Evaluation of Hard-Sphere Phase Shift 75
4. Modifications for Charged Particles 77
a. Charged-particle initial states 79
5. Inverse Reactions (Reciprocity) 81
D. DERIVATIVES 85
1. Derivatives for Reich-Moore Approximation 87
a. Derivatives with respect to R-matrix 89
b. Derivatives with respect to resonance parameters 93
c. Derivatives with respect to channel radius 95
d. Derivatives of logarithmic external R-function 99
e. Derivatives with respect to *p*-parameters 101
2. Derivatives for MLBW and SLBW Approximations 107
3. Details Involving Derivatives 109

III. CORRECTIONS FOR EXPERIMENTAL CONDITIONS 113

A. THEORETICAL FOUNDATION FOR NUMERICAL BROADENING 115
1. Analyst's Responsibility for Auxiliary Energy Grid 117
2. Choose Auxiliary Energy Grid 119
3. Perform Numerical Integration 123

B. DOPPLER BROADENING 127
1. Free-Gas Model of Doppler Broadening 129
a. Derivatives with respect to effective temperature *T* 131
2. Leal-Hwang Doppler Broadening 133
3. High-Energy Gaussian Approximation to Doppler Broadening 137
4. Crystal-Lattice Model of Doppler Broadening 139

C. RESOLUTION BROADENING 141
1. Gaussian plus Exponential Resolution Broadening 143
a. Resolution broadening: Gaussian 145
b. Resolution broadening: exponential 151
c. Resolution broadening: convolution of Gaussian and exponential 153
2. Oak Ridge Resolution Function (ORR) 155
a. Individual components of the ORR resolution function 157
b. Converting length to time dependence 161
c. Convolution of components of ORR resolution function 163
3. RPI (and GELINA and nTOF) Resolution Broadening 165
a. Components of the RPI/GELINA/nTOF resolution function 167
b. Input for the RPI/GELINA/nTOF resolution function 171
4. Straight-Line Energy Average 175
5. User-Defined Numerical Resolution Function 177

D. SELF-SHIELDING AND MULTIPLE-SCATTERING CORRECTIONS 179

E. OTHER EXPERIMENTAL CORRECTIONS 185
1. Transmission Experiments 187
2. Combining Several Nuclides in a Single Sample 189
3. Data-Reduction Parameters 191
a. Explicit normalization and/or background functions 193
b. User-supplied data-reduction parameters 197
4. Paramagnetic Cross Section 199
5. Detector Efficiency 201
6. Self-Indication Measurements 203
7. Corrections for Angular Distributions 205
8. Energy Scale Dependence on t_0 and L 207

IV. THE FITTING PROCEDURE 211

A. DERIVATION OF BAYES' EQUATIONS 213
1. Derivation of SAMMY's Solution Schemes 217
2. Chi-Squared and Weighted Residuals 221
3. Iteration Scheme 225
B. IMPLEMENTATION OF BAYES' EQUATIONS 229
1. Solving Bayes' Equations: N+V Inversion Scheme 231
2. Solving Bayes' Equations: I+Q Inversion Scheme 233
3. Solving Bayes' Equations: M+W Inversion Scheme 235
C. CONSTRUCTING THE PARAMETER SET 237
D. TREATMENT OF DATA COVARIANCE MATRICES 239
1. Derivation of Data Covariance Matrix Equation 243
2. Propagated Uncertainty Parameters 253
3. Implicit Data Covariance Matrix 257
E. MISCELLANEOUS TOPICS RELATED TO COVARIANCES 261
1. Simultaneous Fitting to Several Data Sets 263
2. Retroactive Parameter Covariance Matrix Method 265
3. Least Squares and Other Extensions of SAMMY's Methodology 267
4. Covariances for Calculated Cross Sections 269
5. Calculating Average Values and Uncertainties for Resonance Widths 271
6. Modifying the Parameter Uncertainties 273

V. POST-PROCESSORS AND OTHER MISCELLANEOUS TOPICS 277

A. RECONSTRUCTING POINT-WISE CROSS SECTIONS 279
B. INTEGRAL QUANTITIES 281
1. User-Supplied Flux for Watt Spectrum Average 285
C. AVERAGING THE CROSS SECTIONS 289
1. Energy- or Time-Weighted Averages for Experimental Data 291
2. Bondarenko-Weighted Averages 293
3. Unweighted Energy Average 295
D. STELLAR-AVERAGED CAPTURE CROSS SECTIONS 297
E. PSEUDO CROSS SECTIONS FOR TESTING 301
F. SUMMED STRENGTH FUNCTION 303

VI. INPUT TO SAMMY 305

A. THE INPut FILE 307
1. Alphanumeric Commands 327
B. THE PARameter FILE 377
C. THE DATa AND Data CoVariance FILES 425
1. Experimental Data 427
2. Explicit Data Covariance Matrices 429
3. Implicit Data Covariance (IDC) Matrices.....431
a. Input for propagated uncertainty parameters.....433
b. User-supplied implicit data covariance matrix.....435
c. Implicit data covariance for normalization and background 437
D. INTEGRAL DATA FILE 439
E. INTERACTIVE INPUT TO SAMMY 441
F. OTHER INPUT FILES FOR SAMMY 443
1. The AVeraGe File.....445
2. Input to Produce Files in ENDF File 2 or File 32 Format 449
3. Using ENDF File 2 as input to SAMMY.....455
4. Format of the MXW file 457
5. Crystal-Lattice Model File.....459

VII. OUTPUT FROM SAMMY 461

A. LINE-PRINTER OUTPUT 465
B. OUTPUT TO BE USED AS INPUT 467
C. PLOT OUTPUT 471
D. COMPLETE SET OF PARTIAL DERIVATIVES FOR RESONANCE PARAMETERS.....475
E. COMPACT FORMAT FOR PARAMETER COVARIANCE INFORMATION 477
F. PUBLICATION AIDS 479

VIII. UNRESOLVED RESONANCE REGION 481

A. EQUATIONS FOR UNRESOLVED RESONANCE REGION 483
1. Derivation of Non-Elastic Average Cross Section 489
B. INPUT FOR ANALYSIS OF DATA IN UNRESOLVED RESONANCE REGION 495
C. OUTPUT FROM ANALYSIS IN UNRESOLVED RESONANCE REGION 509
D. CONVERTING SAMMY/URR PARAMETERS TO ENDF/B PARAMETERS 511
1. Relation of SAMMY/URR Radius to ENDF/B Radius 513

IX. THE ENDF CONNECTION 517

A. CSEWG CONSTANTS 521

X. AUXILIARY PROGRAMS 523

A. ANGODF: CONVERT FROM ENERGY/ANGLE TO ANGLE/ENERGY 527
B. CONVRT: CONVERT FROM REFIT INPUT TO SAMMY OR VICE VERSA 529
C. SAMAMR: ADD, MIX, OR RECOVER VARIABLES 531
D. SAMAMX: MODIFY A SINGLE VALUE 543
E. SAMCPR: COMPARE RESULTS 545
F. SAMDIS: STATISTICAL DISTRIBUTIONS 547
G. SAMFTZ: FIX TZERO 549
H. SAMORT: PLOT THE OAK RIDGE RESOLUTION FUNCTION 551
I. SAMPLT: ALTERNATIVE FORM FOR PLOT FILES 553
J SAMQUA: RESONANCE QUANTUM NUMBERS 555
K. SAMRPT: PLOT RPI RESOLUTION FUNCTION 559
L. SAMRST: PLOT RESOLUTION FUNCTION 561
M. SAMSMC: MONTE CARLO MULTIPLE SCATTERING 563
N. SAMSTA: STAIRCASE PLOTS 565
O. SAMTHN: THINNING DATA 567
P. SUGGEL: ESTIMATING *L* AND *J* 569
Q. SAMRML: CALCULATE CROSS SECTIONS FROM ENDF FILE 2 573

XI. HELPFUL HINTS FOR RUNNING SAMMY 575

A. STRATEGY FOR DATA EVALUATION WITH SAMMY 577
B. PROCEDURES TO FOLLOW WHEN YOU HAVE PROBLEMS 585
C. MISCELLANEOUS COMMENTS AND SUGGESTIONS 589

XII. EXAMPLES 595

A. TUTORIAL 597
B. TEST CASES 599
C. MONTE CARLO SIMULATIONS OF MULTIPLE-SCATTERING CORRECTIONS 609

XIII. DESCRIPTION OF THE COMPUTER CODE SAMMY 611

A. DYNAMIC ALLOCATION OF ARRAY STORAGE 613
B. USE OF TEMPORARY DATA FILES TO STORE INTERMEDIATE RESULTS 617
C. DIVISION OF THE PROGRAM INTO AUTONOMOUS SEGMENTS 627
D. COMPUTER-SPECIFIC FEATURES 637
E. ORELA DATA FORMAT 639
F. CONFIGURATION AND DISTRIBUTION SYSTEM 641

REFERENCES 647

APPENDIX A. VERSIONS OF THIS MANUAL 655

A.1 MODIFICATIONS AND ADDITIONS IN REVISION 1 657
A.2 MODIFICATIONS AND ADDITIONS IN REVISION 2 659
A.3 MODIFICATIONS AND ADDITIONS IN REVISION 3 661
A.4 MODIFICATIONS AND ADDITIONS IN REVISION 4 663
A.5 MODIFICATIONS AND ADDITIONS IN REVISION 5 667
A.6 MODIFICATIONS AND ADDITIONS IN REVISION 6 669

APPENDIX B. ACKNOWLEDGMENTS FROM EARLIER VERSIONS 673

LIST OF TABLES

Table **Page**

II A.1 Hard-sphere penetrability (penetration factor) P, level shift factors S, and potential-scattering phase shifts φ for orbital angular momentum l, wave number k, and channel radius a_c, with $\rho = ka_c$ 13

II B2.1 Parameter values used to illustrate Reich-Moore vs. full R-matrix calculations 48

II C1.1 Spin and angular momentum conventions used in SAMMY 58

II C1 a.1 Allowed values for the sum of two quantized vectors 62

III C1.1 Resolution-broadening input parameters 144

III C3 b.1 Default values for parameters for RPI resolution function. 173

III C3 b.2 Parameters suitable for use with experimental data from GELINA at IRMM and from nTOF at CERN. 174

III C5.1 Format for numerical UDR function file. 177

III E4.1 Default parameter values for paramagnetic cross sections. 199

IV D2.1 Types of parameters that may be PUP'd 253

VI.1 SAMMY input files 305

VI A.1 Format of the INPut file 309

VI A1.1 Categories for alphanumeric commands 328

VI A1.2 Alphanumeric statements for use in the INPut file, card set 3 330

VI A1.3 Alphabetical list of acceptable commands for card set 3 367

VI B.1 Header line for card sets in the PARameter file 379

VI B.2 Format of the PARameter file 383

VI B.3 Format of the PARameter file when spin group information is included here 423

VI C1.1 MULTI-style format for the DATa file 428

VI C2.1 Format of the data covariance file 430

LIST OF TABLES (continued)

Table **Page**

VI C3 b.1 Format for user-supplied IDC file....436

VI D.1 Types of integral data....439

VI D.2 Format of the NTG file....440

VI E.1 Input for a typical SAMMY run starting with a new PARameter file....441

VI F1.1 Format of the AVG file....446

VI F1.2 Format of the BONdarenko file....447

VI F2.1 File needed for generated ENDF File 2 output....451

VI F2.2 Key-word-based file needed for generating ENDF File 2 output....452

VI F4.1 Format for File 3 cross sections to be added for stellar averages....458

VI F5.1 Format of the SAMMY CLM file (Crystal-Lattice Model)....459

VII.1 SAMMY output files....461

VII B.1 Binary COVariance file....468

VII C.1 Sections of the ODF file generated by SAMMY, for transmission or total cross-section data....471

VII C.2 Sections of the ODF file generated by SAMMY, for energy-differential data that are neither transmission nor total cross section....472

VII C.3 Sections of SAMMY.ODF when data are angular distributions....473

VII C.4 Sections of the ODF file SAMMY.DAT generated by SAMMY when data are angular distributions....473

VII D.1 Contents of the output file SAMMY.PDS....476

VII E.1 Map from true correlation coefficient *C* to integer *M* and back to approximate coefficient *c* for compact format....478

VII F.1 Columns of SAMMY.PUB file....479

VII F.2 Converting SAMMY.PUB into a spreadsheet....480

LIST OF TABLES (continued)

Table **Page**

VIII B.1 Formats for original PARameter file for treatment of the unresolved resonance region 499

VIII B.2 Formats for annotated PARameter file for treatment of the unresolved resonance region 501

VIII B.3 Energy ranges encountered in the unresolved resonance region 506

IX.1 Key-word-based file needed for generating ENDF File 3 output 519

IX A.1 Exact values of constants as used in the current version of SAMMY 522

X.1 SAMMY auxiliary codes 523

X A.1 Contents of the ODF file SAMMY.DAT 527

X A.2 Contents of the ODF file SAMMY.ODF for angular distribution data 527

X A.3 Contents of the ODF file created by program ANGODF 528

X C.1 Commands to analyze data from three samples of different thicknesses at two different temperatures 535

X C.2 The initial PARameter file t007a.par for the example of Section X.C 538

X C.3 Intermediate PARameter file raa.par 538

X C.4 Intermediate PARameter file rcc.par 538

X C.5 Intermediate PARameter file rdd.par 539

X C.6 Intermediate PARameter file ree.par 539

X C.7 Intermediate PARameter file rff.par 539

X C.8 Intermediate PARameter file rgg.par 540

X C.9 PARameter file rhh.par, containing final results for the example of Section X.C 540

X C.10 PARameter file rii.par, which is a permutation of the file rhh.par 540

X C.11 PARameter file rkk.par, which is a permutation of the file rhh.par 541

LIST OF TABLES (continued)

Table **Page**

X C.12 The PARameter file r1l.par, which is a permutation of the file hh.par.....541

X F.1 Input for program SAMDIS.....548

X J.1 Input options for SAMQUA in particle-pair mode.....556

X N.1 Input for Program SAMSTA 565

X P.1 Variables appearing in the “suggel.inp” file 570

XI B.1 Possible solutions to some common problems 587

XII A.1 Computer exercises for the student.....598

XII B.1 SAMMY test cases 600

XII C.1 Sample Monte Carlo simulations.....609

XIII A.1 Illustration of dynamic allocation of array storage 613

XIII B.1 Files used by SAMMY 618

XIII C.1 Segments of the code SAMMY 628

XIII E.1 Arguments for ODF subroutines.....640

XIII F.1 Installation instructions for SAMMY, as given in the INSTALL file.....642

LIST OF FIGURES

Figure **Page**

II.1 Schematic of entrance and exit channels as used in scattering theory.....10

II B2.1 Reich-Moore approximation vs. full R-matrix for artificial example of test case tr110 48

II C2.1 Schematic of particle pairs for kinematics calculation 63

II C5.1 Schematic of kinematics for inverse reactions..... 82

III A1.1 Unbroadened cross section calculated with too few points in the auxiliary grid 117

III A1.2 Incorrect Doppler-broadened cross section calculated with too few points in the auxiliary grid.....117

III A1.3 Unbroadened cross section calculated with an adequate number of points in the auxiliary grid.....118

III A1.4 Doppler-broadened cross section calculated with an adequate number of points in the auxiliary grid 118

III D.1 Geometry for the single-scattering correction to capture or fission yield, for a neutron incident on the flat surface of a cylindrical sample.....181

XIII C.1 Flow chart for commonly used SAMMY modules.....635

ACKNOWLEDGMENTS FOR REVISION 7

Nearly three decades of my life have been devoted to the development of the SAMMY code. This endeavor has proven to be often challenging, sometimes exciting, seldom boring, occasionally frustrating, frequently bewildering, but always worthwhile. This revision of the SAMMY manual will likely be the final one for which I am sole author. While the code is expected to remain in widespread use, future development will require ventures into arenas foreign to my innate abilities and training: graphical user interfaces, modern programming languages, sophisticated data storage and retrieval systems, and other unforeseeable innovations. People younger and more energetic than I will become involved in those ventures.

Enough about the future. With regard to the present work, ideas from many people have contributed to this effort. Special thanks go to the members of the ORNL Nuclear Data Group, who have never shied from asking for new or upgraded features in the code and who willingly and happily accept the responsibility of testing those features after they are implemented. In alphabetical order, members of the ORNL NDG are Goran Arbanas, Herve Derrien, Mike Dunn, Maurice Greene, Klaus Guber, Liuz Leal, Royce Sayer, and Dorothea Wiarda.

There is one other group whose joint contribution must be acknowledged. During the past several years, I was privileged to serve as a member of the IAEA Coordinated Research Project on Light Element Standards; my contribution to this effort was primarily to use SAMMY's treatment of covariances to facilitate comparison between the two R-matrix codes used for the light-element evaluations. The lively discussions and interactions among the group members provided significant insight into the use and propagation of measurement uncertainties throughout the data-fitting process. Many of the innovations described in Section IV of this manual owe their conception to ideas discussed during meetings of this group.

Reviewing a document like this one is a formidable task, and the author is deeply indebted to everyone who participated in that effort. David Davis, who carefully read the first draft of Section II and politely pointed out my mistakes, has earned my gratitude (as well as my admiration for his endless patience). Official peer reviews of the various pieces of this document were performed by the following ORNL personnel (in alphabetical order): Goran Arbanas, Jeff Blackmon, Herve Derrien, Maurice Greene, Paul Koehler, Luiz Leal, Royce Sayer, and Dorothea Wiarda. Each of these people offered valuable suggestions which have improved the accuracy, legibility, and usefulness of this document, and I am grateful for their conscientiousness. Thanks also go to Joyce Echols, who carefully checked all the links in the pdf file; any remaining problems with the links were introduced by this author after Joyce completed her testing. Finally, thanks to technical editors Debbie Stevens and Marsha Savage, whose advice and assistance were invaluable in producing a high-quality document.

Support from the National Nuclear Security Administration (NNSA) Nuclear Criticality Safety Program (NCSP) for both the SAMMY software development and preparation of the manual is gratefully acknowledged.

Acknowledgments from previous revisions of this manual are found in Appendix B.

ABSTRACT

In 1980 the multilevel multichannel R-matrix code SAMMY was released for use in analysis of neutron-induced cross section data at the Oak Ridge Electron Linear Accelerator. Since that time, SAMMY has evolved to the point where it is now in use around the world for analysis of many different types of data. With the incorporation of charged-particle capabilities, SAMMY is no longer limited to incident neutrons, but can also be used for incident protons, alpha particles, or other charged particles; likewise, Coulomb exit channels can be included. Corrections for a wide variety of experimental conditions are available in the code: Doppler and resolution broadening, multiple-scattering corrections for capture or reaction yields, normalizations and backgrounds, to name but a few. The fitting procedure is Bayes' method, and data and parameter covariance matrices are properly treated within the code. Pre- and post-processing capabilities are also available, including (but not limited to) connections with the Evaluated Nuclear Data Files. Though originally designed for use in the resolved resonance region, SAMMY also includes a treatment for data analysis in the unresolved resonance region.

This document serves as a users' guide for SAMMY and many of its auxiliary codes.

Citations:

Citations for use of the SAMMY code should refer to this manual as

N. M. Larson, *Updated Users' Guide for SAMMY: Multilevel R-Matrix Fits to Neutron Data Using Bayes' Equations*, ORNL/TM-9179/R7, Oak Ridge National Laboratory, Oak Ridge, TN, USA (2006). Also available as ENDF-364/R1.

In addition, the paper presented at the ND2004 Nuclear Data Conference may be cited as

N. M. Larson, "Upgrades to the R-Matrix Code SAMMY," ND2004 (International Conference on Nuclear Data for Science and Technology, Sept. 26–Oct. 1, 2004).

I. INTRODUCTION

This document serves as a users' guide to the multilevel multichannel R-matrix code SAMMY. Beginning with Revision 6, the organization of this manual has been redesigned in an effort to make it more legible, logical, and useful. A summary of the structure of this document is given here.

Versions of this manual issued prior to Revision 6 included a guide to additions and modifications from previous versions; this information is now moved to the end of the manual, in Appendix A. An introduction specifically for release 7, describing recent modifications and additions to the code and the manual, is found immediately following this general introduction, in Section I.A. All SAMMY users are encouraged to read that section for an overview of recent developments.

Analysis of neutron cross-section data in the resolved resonance region (RRR) has three distinct aspects, each of which must be included in any analysis code: First, an appropriate formalism is needed for generating theoretical cross sections. Second, a plausible mathematical description must be provided for every experimental condition that affects the values of the quantities being measured. Third, a fitting procedure must be available to determine the parameter values which provide the "best" fit of theoretical to experimental numbers. These three aspects of the SAMMY code are described in Sections II, III, and IV of this manual, respectively.

Calculation of the cross sections in the RRR is described in Section II, with emphasis on the Reich-Moore approximation to R-matrix theory. Explicit equations are given for the various types of energy-differential cross sections (total, elastic, capture, fission, other reaction) and for the angle- and energy-differential cross sections (elastic, reaction). Both Coulomb and non-Coulomb (neutron) formulae are shown.

Experimental modifications to the theoretical cross sections in the RRR are described in Section III. Included here are such effects as Doppler and resolution broadening, normalization and backgrounds, finite-size corrections, and treatment of more than one nuclide in the target sample.

SAMMY's fitting procedure is described in Section IV. Bayes' equations are derived from Bayes' theorem plus assumptions about normality and linearity. The relationship between Bayes' equations and the more familiar least squares equations is described. Emphasis is placed on methodologies for properly including all measurement uncertainty in the analysis process, including the many SAMMY options for inclusion of data covariance information.

Section V describes such topics as post-processor options (calculating multigroup cross sections or other averages) and other miscellaneous features.

The input to SAMMY is detailed in Section VI. Output is described in Section VII.

SAMMY's treatment of the unresolved resonance region (URR) is discussed in Section VIII. The theoretical treatment was borrowed directly from Fritz Fröhner's FITACS program; subsequently, input/output and certain details of the calculation have been augmented to increase the utility of this code.

Section IX describes the relationship of SAMMY to the Evaluated Nuclear Data Files (ENDF). Certain types of ENDF files can be used to provide resonance parameters, parameter covariance matrices, or experimental data as input to SAMMY. Likewise, SAMMY can produce files containing resonance parameters, point-wise cross sections, or uncertainty information.

A number of auxiliary programs are available for use with SAMMY input or output. Section X contains a brief description of those for which this author has maintenance responsibility.

Advice for running SAMMY is presented in Section XI. Even experienced SAMMY users are encouraged to read this section, as it contains information about recent developments that may be unfamiliar (but potentially useful) to long-time users. Novices are likely to find valuable suggestions in this section. Anyone requesting the author's help is expected to have read and followed the procedures outlined in Section XI.B.

Sample runs are described in Section XII. These include (1) tutorial exercises (designed to familiarize a novice user with running the code), (2) test cases (designed for quality control, to ensure that the code gives consistent answers from one platform to another and from one version to another, but also useful as examples of input for specific features of the code), and (3) simulations (Monte Carlo simulations of multiple-scattering corrections, designed to test the accuracy of the SAMMY treatment for those corrections).

Section XIII provides an introduction to the computer code itself, for the benefit of the code managers at various sites. The casual user will probably not need the information from this section.

I.A. MODIFICATIONS AND ADDITIONS IN REVISION 7

Modifications, additions, and improvements to SAMMY subsequent to the publication of Revision 6 of this manual are summarized here.

<u>New or expanded options in the resolved resonance region (RRR)</u>

1. The ability to quickly and efficiently generate and use the data covariance matrix (DCM) has been greatly enhanced with the development of two features:
   a. The Propagated Uncertainty Parameter (PUP) option allows the uncertainty associated with any parameter to be incorporated into the data covariance matrix, while holding the value for that parameter constant. Sections IV.D.1 and IV.D.2 give details; input is described in Section VI.C.3.a.
   b. The User-Supplied Implicit Data Covariance (IDC) option allows the components of the DCM to be generated external to SAMMY. See Sections IV.D.3 and VI.C.3.b.
2. Covariances associated with point-wise cross sections can now be calculated and printed; see Section IV.E.4 for details.
3. Techniques have been improved for simultaneous fitting using the M+W scheme for solution of Bayes' Equations. For example, either explicit or implicit data covariance matrices may be used for the individual data sets. Details regarding simultaneous fitting are in Section IV.E.1.
4. Options have been introduced to perform true least-squares fitting (as opposed to Bayes techniques, which require estimation of finite prior parameter uncertainties). Least-squares fitting implicitly assumes infinite prior parameter uncertainties. See Section IV.E.3.
5. The "retroactive covariance method" has received considerable attention to ensure that it is working properly. Also, it is now possible to make a SAMMY run using the original parameter values together with the retroactive covariance matrix to test whether the combination is reasonable. See Section IV.E.2 for details.
6. Ad hoc methods have been created for modifying the output uncertainties in the parameter covariance matrix, in order to report more realistic uncertainties in ENDF files or other publications. These methods are discussed in Section IV.E.6.
7. The RPI resolution function has been extended in order to provide capabilities to simulate the GELINA and nTOF resolution functions. Extensions include a continuously varying time-channel width. Thanks to Frank Gunsing for providing appropriate forms and parameter values for those. Details are given in Section III.C.3.
8. An option has been created to efficiently calculate unweighted energy-averaged cross sections (Section V.C.3).
9. As an alternative to the energy dependence of the flux used in the Watt spectrum average [Section V.B, Eq. (V B.7)], the user may specify the flux numerically on an energy grid. Details are given in Section V.B.1.

10. An optional correction for neutron sensitivity has been added to the multiple-scattering correction for capture yields. See Section III.B for details.

11. An externally generated direct capture component may be added to the R-matrix cross section, with a variable normalization on this component. See Section II.B.4.

12. The ENDF connection has been strengthened:

    a. A new ENDF format for File 2 resonance parameters (LRU = 1, LRF = 7, titled "R-Matrix Limited") was developed by the SAMMY author and approved by the Cross Section Evaluation Working Group in November of 2004. This format provides capability for reporting virtually any SAMMY R-matrix parameterization (for incident neutrons) into the evaluated nuclear data files. SAMMY can both read and write this format. Sections VI.F.2, VI.F.3, and IX discuss this and other ENDF formats.

    b. To facilitate use of the new R-matrix format, the auxiliary code SAMRML was developed as an aid to processor-code developers. This code calculates cross sections and derivatives from the R-matrix parameters, much as SAMMY itself does, but does not contain any of the measurement-related capabilities (e.g., Doppler or resolution broadening, multiple-scattering corrections) found in SAMMY. See Section X.Q for details.

    c. A second new ENDF format, for File 32 (covariances for resonance parameters), was developed by the SAMMY author and approved by CSEWG in 2004. This format (denoted the Compact Covariance Format, and defined by parameter LCOMP = 2 allows the parameter uncertainties and an abbreviated correlation matrix to be stored in the ENDF file. Again, SAMMY can both read and write this format; see Sections VI.F.2, VI.F.3, and IX.

    d. SAMMY can also read and write other ENDF File 32 covariance formats (LCOMP = 0 for Breit Wigner; LCOMP = 1 for any of the Breit Wigner, Reich Moore, and R-matrix limited formats), though not in all possible permutations. See Section IX for details.

    e. For comparison purposes, it is now possible to read and write ENDF File 2 (resonance parameters) in either of the Breit-Wigner formats (LRF = 1 or 2). SAMMY users are reminded, however, that these crude approximations should *not* be used for new evaluations.

<u>Input and output improvements in RRR</u>

1. Most of the data-related parameters (e.g., abundances, Doppler temperature, resolution-broadening parameters) can now be specified in the INPut file rather than the PARameter file. See the end of Table VI A.1 for a list of parameter types (card sets) that can be moved to the INPut file.

2. A flag to include the uncertainty on a parameter while holding the parameter fixed (i.e., to treat the parameter as a PUP, as described in Section IV.D.2) will be acknowledged in either the INPut file or the PARameter file. A flag to vary a parameter will be ignored in the INPut file. The option to PUP a parameter in the INPut file makes it far easier for the user to organize a sequence of SAMMY runs involving several different data sets.

3. To specify reactions such as inelastic or (n,p), the input has been somewhat cumbersome. With this release, a more intuitive key-word-based input is available. See Section II.B.1.c and card sets 4 and 8 of Table VIA.1 for details.
4. The PUBLISH command was updated to include spins J and L. See Section VII.F for details.
5. Simpler options have been created for the input of prior uncertainties for various classes of resonance parameters. See card set "Last D" in Table VI B.2.
6. Simpler options have been created for input of prior uncertainties for broadening parameters (card set 4 of the PARameter file) and for channel radii (card set 7a).

Streamlining and modernization changes

1. A new distribution system was created for SAMMY by Dorothea Wiarda. For details, see Section XIII.F.
2. The use of temporary data files has been substantially lessened but not yet completely eliminated. The functions previously performed by "reads to" and "writes from" the temporary files are now performed within the code.
3. Array sizes have been reduced where possible.
4. Modifications were introduced to make it easy to use extremely large arrays, for those rare situations in which those modifications are necessary. Thanks to Goran Arbanas for his work on this feature. For details, see Section XIII.A.
5. Sections II, III, and IV of this manual have been reorganized into a more sensible and legible ordering with greatly expanded descriptions.
6. Section XI of this manual, "Helpful Hints for Running SAMMY," has been completely rewritten. Both novice and experienced users are encouraged to read this section.

Bugs eliminated in the RRR

1. The conversion of the covariance matrix from *u*-parameters to *p*-parameters had previously ignored the dependence of the neutron (or other) widths on the resonance energy. This deficiency has now been corrected; details are in Section II.D.1.e.
2. The RPI resolution function (Section III.C.3) has been corrected to work properly at low energy.
3. Bondarenko averaging (Section V.C.2) now works with "make no corrections," that is, when the unaveraged cross sections were not Doppler- or resolution-broadened prior to averaging.
4. For average cross sections:
   a. The energy- or time-weighted average (Section V.C.1) had been working correctly but also had great potential for abuse: The implementation of this feature assumed that the "unaveraged" cross sections had been averaged over the time-channel width –that is, the implementation assumed that these are measured values, not theoretical cross sections.

Therefore this method should not be used when accurate averages of theoretical cross sections are wanted.

b. To obtain accurate averages of theoretical cross sections, one can use the Bondarenko averaging technique (Section V.C.2). However, for more efficient calculations of unweighted (weighted with a constant) averages, the new unweighted energy average described in Section V.C.3 is the method of choice.

5. The Watt spectrum average (Section V.B) was previously calculated incorrectly; this has been fixed.
6. Kinematics equations for angular distributions with non-zero Q value have been derived and implemented in the code. (See Section II.C.2.b.) It therefore is now possible to properly calculate angular distribution reaction cross sections. (Previously, these cross sections had been calculated incorrectly.)
7. In some cases, especially those involving high orbital angular momentum, elastic scattering angular distributions for incident charged particles (Section II.C.4.a) had been calculated incorrectly. This is now corrected.
8. A bug affecting very-low-energy cross sections has been eliminated from the Leal-Hwang Doppler-broadening method (Section III.B.2). This method now produces virtually the same results as does the free-gas model of Section III.B.1.
9. A bug has been corrected in the "`RECONSTRUCT CROSS SEctions from resonance parameters`" option, so that fission cross sections are also correctly generated.

<u>Auxiliary programs</u>

1. The SAMQUA program has been enhanced to additional information, useful in determining whether a particular spin group and/or channel must be included. See Section X.J.
2. Input for and output from the SAMMY run which prepares input for the Monte Carlo simulation code SAMSMC has been changed, to eliminate redundancies and reduce mistakes; see Section X.M for details.
3. The SUGGEL program is now portable to LINUX systems. See Section X.P.
4. A code SAMRML was developed to calculate cross sections and partial derivatives at any specified energy, starting from ENDF File 2. See Section X.Q.

<u>Improvements in the unresolved resonance region (URR)</u>

1. Elastic data may be fitted. Previously, only total, inelastic, fission, or capture were allowed.
2. The ability to perform a "no-Bayes" run (calculation of cross section with no fitting to data) was added.
3. Calculation of the Dresner integration was upgraded.
4. The Moldauer prescription for width fluctuations was implemented. Previously, it had been inadvertently disabled in the coding.

5. Options were added to include direct capture and/or direct inelastic.
6. Options for interfacing with ENDF were enhanced.
7. The interior of the code was redesigned (modernized) a bit.
8. Bugs related to sequential runs were found and eliminated.
9. Previously, the value of $\langle \Gamma_f \rangle$ would occasionally become negative during an analysis; when this happens, the value is now set to the absolute value of $\langle \Gamma_f \rangle$.
10. The PARameter file has been modified for increased human legibility. Spin and orbital angular momentum may be added to the listing of $\langle \Gamma_f \rangle$ to reduce possibilities for confusion.
11. Usage of the parameter covariance matrix has been generalized to include features previously available only in the RRR.

Prognostication

Though it is never possible to precisely predict the path forward, it is possible to itemize options under consideration for future implementation into the code. Below are listed some of these options for the resolved resonance region. (For a similar list in the unresolved resonance region, see Section VIII.) Comments on these options, suggestions for prioritization, and proposals for additional items are always welcome.

1. Put each nuclide's R-matrix information into a separate file. Analysis of measurements with multiple nuclides in the sample would then use multiple PARameter files rather than one combined file.
2. Provide measurement-related information (e.g., thickness, temperature, resolution function, background) in a separate file for each data set. Information concerning the measurement would then be thoroughly isolated from information concerning the R-matrix.
3. Implement a technique for analyzing inverse reaction data without rewriting the resonance parameters or the experimental data. This would allow, for example, n+^{16}O data to be analyzed simultaneously with α + ^{13}C data.
4. Implement convergence criteria when iterating for non linearity (Section IV.A.3).
5. Simplify the simultaneous fitting of more than one data set (Section IV.E.1) and the use of least-squares (Section IV.E.3).
6. Invent methodologies for incorporating uncertainty in the *theory* into the analysis. For example, what is the effect of our limited knowledge of spin assignments for the very small resonances?
7. When two mostly independent measurements are marginally related (e.g., by having used the same physical sample), provide options for incorporating uncertainties from that relationship into the analysis.
8. Currently, the auxiliary grid (Section III.A) is generated only once during the fitting procedure. When resonance energies are varied, and the values change significantly in early iterations, the

original auxiliary grid may not be adequate. Implement an option to regenerate this grid for each iteration.

9. Currently, corrections for experimental effects in angular-distribution data are rather unsophisticated. Is there a need for improvement here?
10. Create a graphical user interface.
11. Introduce a modern configuration control and archival system for the code.
12. Introduce modern matrix-manipulation techniques, especially for very large runs. Preliminary studies have indicated that this will significantly reduce the time requirements for extremely large runs.

II. SCATTERING THEORY

Details of scattering theory have been well understood since the middle of the previous century, when they were summarized in a review article by Lane and Thomas [AL58]. A wealth of additional reference material is available to the student of scattering theory; only a few are listed here. The text by Foderaro [AF71] provides a more elementary introduction to the subject. One publication by Fröhner [FF80] is based on lectures presented at the International Centre for Theoretical Physics (ICTP) Winter Courses on Nuclear Physics and Reactors, 1978; this is a comprehensive and useful guide to applied neutron resonance theory. It includes a variety of topics, including preparation of data, various approximations to scattering theory, Doppler broadening, experimental complications, data-fitting procedures, and statistical tests. Another Fröhner paper [FF00] is somewhat more theoretical, and covers many aspects of data fitting in the resonance region.

The particular aspect of scattering theory with which we are concerned is the R-matrix formalism. A summary of the underlying principles is given here.

R-matrix theory is a mathematically rigorous phenomenological description of what is actually seen in an experiment (i.e., the measured cross section). The theory is not a model of neutron-nucleus interaction, in the sense that it makes no assumptions about the underlying physics of the interaction. Instead it parameterizes the measurement in terms of quantities such as the interaction radii and boundary conditions, resonance energies and widths, and quantum numbers; values for these parameters may be determined by fitting theoretical calculations to observed data. The theory is mathematically correct, in that it is analytic, unitary, and rigorous; nevertheless, in practical applications, the theory is always approximated in some fashion.

R-matrix theory is based on the following assumptions: (1) the applicability of non-relativistic quantum mechanics; (2) the absence or unimportance of all processes in which more than two product nuclei are formed; (3) the absence or unimportance of all processes of creation or destruction; and (4) the existence of a finite radial separation beyond which no nuclear interactions occur, although Coulomb interactions are given special treatment. [In practical applications two of these four assumptions may be violated in one degree or another: (1) The theory may be used for relativistic neutron energies, and corrected for relativistic effects; nevertheless, non-relativistic quantum mechanics is assumed. (2) A fission experiment with more than two final products is treated as a two-step process. That is, the immediate result of the neutron-nuclide interaction is assumed to be limited to two final products, at least one of which decays prior to detection.]

R-matrix theory is expressed in terms of channels, where a channel is defined as a pair of (incoming or outgoing) particles, plus specific information relevant to the interaction between the two particles. A schematic depicting entrance and exit channels is shown in Figure II.1. Note that entrance channels can also occur as exit channels, but some exit channels (e.g., fission channels) do not occur as entrance channels. Two interacting particles are shown in the portion of the figure that is labeled “Interior Region”; here the particles are separated by less than the interaction radius *a*.

In Section II.A, general equations of scattering theory are presented and their derivations discussed. The fundamental R-matrix equations are presented. Section II.A.1 gives a detailed derivation of the equations for a simple case. Section II.A.2 shows the relationship between the R-matrix and the A-matrix, which is another common representation of scattering theory.

The approximations to R-matrix theory available in the SAMMY code are detailed in Section II.B. The recommended choice for most applications is the Reich-Moore approximation, described in Section II.B.1. For some applications, the Reich-Moore approximation is inadequate; for those cases, a method for using SAMMY's Reich-Moore approximation to mimic the full (exact) R-matrix is presented Section II.B.2. Two historically useful but now obsolete approximations are single-level and multilevel Breit Wigner (SLBW and MLBW), discussed in Section II.B.3. Provisions for including non-compound (direct) effects are discussed in Section II.B.4.

In Section II.C, details are given for the SAMMY nomenclature and other conventions, for transformations to the center-of-momentum system, and for the calculation of penetrability, shift factors, and hard-sphere phase shifts in both Coulomb and non-Coulomb cases.

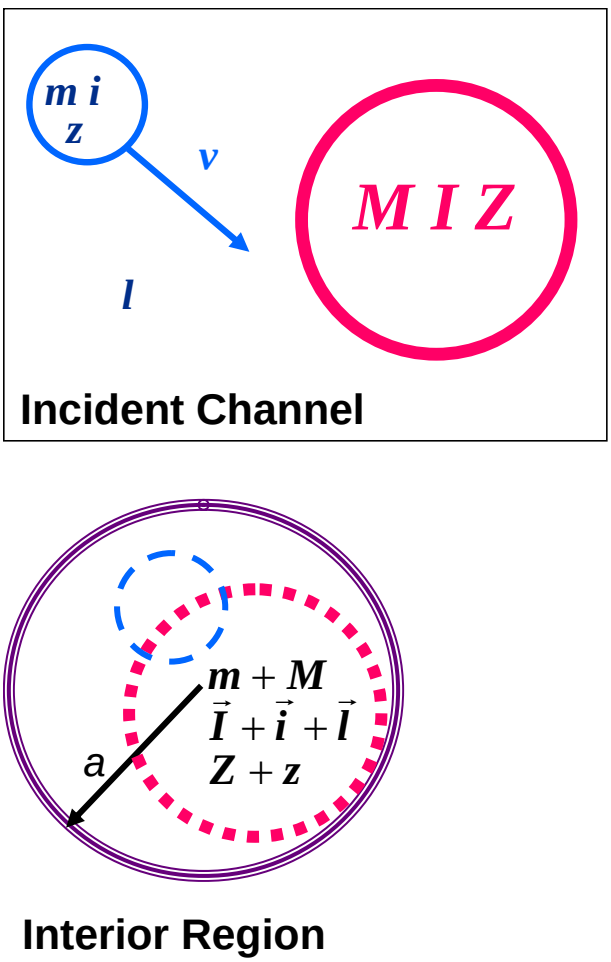
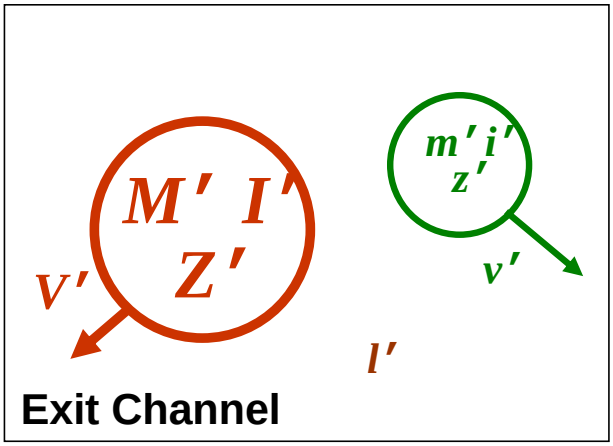


Figure II.1. Schematic of entrance and exit channels as used in scattering theory. For the interior region (with separation distance $r < a$), no assumptions are made about the nature of the interaction. In the figure, m, i, and z refer to the mass, spin, and charge of the incident particle while M, I and Z refer to the target particle. Orbital angular momentum is denoted by l and velocity by v. Primes are used for post-collision quantities.



II. A. EQUATIONS FOR SCATTERING THEORY

In this section, equations for scattering theory are presented but not derived. Specifics for the R-matrix formulation of scattering theory are presented in Section II.A.1, which provides a discussion of an alternative formulation (the A-matrix). Readers interested in the derivation of the equations for scattering theory are referred to the Lane and Thomas article [AL58] for a detailed derivation in the general case, or to Section II.A.2 of this document for a simplified version.

In scattering theory, a channel may be defined by $c = (\alpha, l, s, J)$, where the following definitions apply:

- α represents the two particles making up the channel; α includes mass (m and M), charge (z and Z), spin (i and I) with associated parities, and all other quantum numbers for each of the two particles, plus the Q-value (equivalent to the negative of the threshold energy in the center of momentum system).

- l is the orbital angular momentum of the pair, and the associated parity is given by $(-1)^l$.

- s represents the channel spin (including the associated parity); that is, s is the quantized vector sum of the spins of the two particles of the pair: $\vec{\boldsymbol{s}} = \vec{\boldsymbol{i}} + \vec{\boldsymbol{I}}$.

- J is the total angular momentum (and associated parity); that is, J is the quantized vector sum of l and s: $\vec{\boldsymbol{J}} = \vec{\boldsymbol{l}} + \vec{\boldsymbol{s}}$.

Only J and its associated parity π are conserved for any given interaction. The other quantum numbers may differ from channel to channel, as long as the sum rules for spin and parity are obeyed. Within this document and within the SAMMY code, the set of all channels with the same J and π are called a "spin group."

In all formulae given below, spin quantum numbers (e.g., J) are implicitly assumed to include the associated parity. Quantized vector sum rules are implicitly assumed to be obeyed. Readers unfamiliar with these sum rules are referred to Section II.C.1.a for a mini-tutorial on the subject.

Let the angle-integrated cross sections from entrance channel c to exit channel c' with total angular momentum J be represented by $\sigma_{cc'}$. This cross section is given in terms of the scattering matrix $U_{cc'}$ as

$$\sigma_{cc'} = \frac{\pi}{k_a^2} g_{J\alpha} \left| e^{2iw_c} \delta_{cc'} - U_{cc'} \right|^2 \delta_{JJ'} \quad , \qquad \text{(II A.1)}$$

where k_α is the wave number (and $K_\alpha = \hbar k_\alpha =$ center-of-mass momentum) associated with incident particle pair α, $g_{J\alpha}$ is the spin statistical factor, and w_c is the Coulomb phase-shift

difference. Note that w_c is zero for non-Coulomb channels. (Details for the charged-particle case are presented in Section II.C.4.) The spin statistical factor g is given by

$$g_{J\alpha} = \frac{2J+1}{(2i+1)\,(2I+1)} \quad , \tag{II A.2}$$

and center-of-mass momentum K_α by

$$K_\alpha^2 = \left(\hbar k_\alpha\right)^2 = \frac{2m\,M^2}{\left(m+M\right)^2} E \quad . \tag{II A.3}$$

Here E is the laboratory kinetic energy of the incident (moving) particle. A derivation of this value for K_α is given in Section II.C.2.

The scattering matrix U can be written in terms of matrix W as

$$U_{cc'} = \Omega_c\, W_{cc'}\, \Omega_{c'} \quad , \tag{II A.4}$$

where Ω is given by

$$\Omega_c = e^{i\,(w_c - \varphi_c)} \quad . \tag{II A.5}$$

Here again, w_c is zero for non-Coulomb channels, and the potential scattering phase shifts for non-Coulomb interactions φ_c are defined in many references (e.g., [AL58]) and shown in Table II A.1. The matrix W in Eq. (II A.4) is related to the R-matrix (in matrix notation with indices suppressed) via

$$W = P^{1/2}(I - RL)^{-1}(I - RL^*)P^{-1/2} \quad . \tag{II A.6}$$

The quantity I in this equation represents the identity matrix. The form of the R-matrix is given in Section II.A.1 in general and in Section II.B for the versions used in SAMMY. The quantity L in Eq. (II A.6) is given by

$$L = (S - B) + iP \quad , \tag{II A.7}$$

with P being the penetration factor (penetrability) S the shift factor, and B the arbitrary boundary constant at the channel radius a_c. P and S are functions of energy E, and also depend on the orbital angular momentum l and the channel radius a_c. Formulae for P and S are found in many references (see, for example, Eq. (2.9) in [JL58]).

For non-Coulomb interactions, the penetrability and shift factor have the form

$$P \rightarrow P_l\left(\rho\right) \quad \text{and} \quad S \rightarrow S_l\left(\rho\right) \quad , \tag{II A.8}$$

where ρ is related to the center-of-mass momentum which in turn is related to the laboratory energy of the incident particle (E). For arbitrary channel c with particle pair α, orbital angular momentum l, and channel radius a_c, ρ has the form

$$\rho = k_\alpha\, a_c = \frac{1}{\hbar}\sqrt{\frac{2m_\alpha M_\alpha}{\left(m_\alpha + M_\alpha\right)}\frac{M}{(m+M)}}\sqrt{\left(E - \Xi_\alpha\right)}\;\; a_c \quad , \qquad \text{(II A.9)}$$

as shown in Section II.C.2. Here Ξ_α is the energy threshold for particle pair α, m_α and M_α are the masses of the two particles of particle pair α, and m and M are the masses of the incident particle and target nuclide, respectively.

Appropriate formulae for P, S, and φ in the non-Coulomb case are shown in Table IIA.1. For two charged particles, formulae for the penetrabilities are given in Section II.C.4.

The energy dependence of fission and capture widths is negligible over the energy range of these calculations. Therefore, a penetrability of unity may be used.

Table II A.1. Hard-sphere penetrability (penetration factor) *P*, level shift factor *S*, and potential-scattering phase shift *φ* for orbital angular momentum *l*, wave number *k*, and channel radius a_c, with ρ = ka_c

l	P_l	S_l	φ_l
0	ρ	0	ρ
1	$\rho^3/(1 + \rho^2)$	$-1 / (1 + \rho^2)$	$\rho - \tan^{-1}\rho$
2	$\rho^5 / (9 + 3\rho^2 + \rho^4)$	$-(18 + 3\rho^2) / (9 + 3\rho^2 + \rho^4)$	$\rho - \tan^{-1}[3\rho / (3 - \rho^2)]$
3	$\rho^7 / (225 + 45\rho^2) + 6\rho^4 + \rho^6)$	$-(675 + 90\rho^2 + 6\rho^4) / (225 + 45\rho^2 + 6\rho^4 + \rho^6)$	$\rho - \tan^{-1}[\rho(15-\rho^2) / (15-6\rho^2)]$
4	$\rho^9 / (11025 + 1575\rho^2 + 135\rho^4 + 10\rho^6 + \rho^8$	$-(44100 + 4725\rho^2 + 270\rho^4 + 10\rho^6) / (11025 + 1575\rho^2 + 135\rho^4 + 10\rho^6 + \rho^8)$	$\rho - \tan^{-1}[\rho(105 - 10\rho^2) / (105 - 45\rho^2 + \rho^4)]$
l	$\dfrac{\rho^2 P_{l-1}}{\left(l - S_{l-1}\right)^2 + P_{l-1}^2}$	$\dfrac{\rho^2 (l - S_{l-1})}{(l - S_{l-1})^2 + P_{l-1}^2} - l$	$\varphi_{l-1} - \tan^{-1}\left((P_{l-1}/(l - S_{l-1})\right)$ or $B_l = (B_{l-1} + X_l) / (1 - B_{l-1}X_l)$ with $B_l = \tan(\rho - \varphi_l)$ and $X_l = (P_{l-1})/(l - S_{l-1})$

Formulae for a particular cross section type can be derived by summing over the terms in Eq. (II A.1). For the total cross section, the sum over all possible exit channels and all spin groups gives

$$\begin{aligned}\sigma^{total} &= \sum_{\substack{incident\\channels\\c}} \sum_{\substack{all\\channels\\c'}} \sum_{J} \frac{\pi}{k_\alpha^2} g_\alpha \left|\delta_{cc'} - U_{cc'}\right|^2 \\ &= \frac{\pi}{k_\alpha^2} \sum_{J} g_J \sum_{\substack{incident\\channels\\c}} \sum_{\substack{all\\channels\\c'}} \left(\delta_{cc'} - U_{cc'}\delta_{cc'} - U_{cc'}^{*}\delta_{cc'} + \left|U_{cc'}\right|^2\right) \qquad \text{(II A.10)} \\ &= \frac{2\pi}{k_\alpha^2} \sum_{J} g_J \sum_{\substack{incident\\channels\\c}} \left(1 - \mathrm{Re}\left(U_{cc}\right)\right) \quad .\end{aligned}$$

For non-charged incident particles, the elastic (or scattering) cross section is given by

$$\sigma_{\alpha\alpha} = \frac{\pi}{k_\alpha^2} \sum_{J} g_J \sum_{\substack{c=incident\\channel}} \left(1 - 2\,\mathrm{Re}\left(U_{cc}\right) + \sum_{\substack{c'=incident\\channel}} \left|U_{cc'}\right|^2\right) \quad . \qquad \text{(II A.11)}$$

Similarly, the cross section for any non-elastic reaction can be written

$$\sigma_\alpha^{reaction} = \frac{\pi}{k_\alpha^2} \sum_{J} g_J \sum_{\substack{c=incident\\channel}} \sum_{\substack{c'=reaction\\channel}} \left|U_{cc'}\right|^2 \quad . \qquad \text{(II A.12)}$$

In particular, the capture cross section could be written as the difference between the total and all other cross sections,

$$\sigma^{capture} = \frac{\pi}{k_\alpha^2} \sum_{J} g_J \sum_{\substack{c=incident\\channel}} \left(1 - \sum_{\substack{c'=all\ channels\\except\ capture}} \left|U_{cc'}\right|^2\right) \quad . \qquad \text{(II A.13)}$$

(This form will be used later, in Section II.B.1.a, when the capture channels are treated in an approximate fashion.)

II.A.1. R-Matrix and A-Matrix Equations

The R-matrix was introduced in Eq. (II A.6) as

$$W = P^{1/2}(I - RL)^{-1}(I - RL^{*})P^{-1/2} \quad , \tag{II A1.1}$$

but the formula for the R-matrix was not given there. If λ represents a particular resonance (or level), then the general form for the R-matrix is

$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c}\, \gamma_{\lambda c'}}{E_{\lambda} - E}\, \delta_{J J'} \quad , \tag{II A1.2}$$

where E_{λ} represents the energy of the resonance, and the reduced width amplitude γ is related to the partial width Γ by

$$\Gamma_{\lambda \boldsymbol{c}} = 2\, \boldsymbol{P_c}\, \gamma_{\lambda \boldsymbol{c}}^{2} \quad . \tag{II A1.3}$$

The sum in Eq. (II A1.2) contains an infinite number of levels. All channels, including the "gamma channel" for which one of the particles is a photon, are represented by the channel indices.

The R-matrix is not the only possibility for parameterization of the scattering matrix. In the R-matrix formulation, equations are expressed in terms of channel-channel interactions. It is also possible to formulate scattering theory in terms of level-level interactions; this formulation uses what is called the A-matrix, which is defined as

$$A_{\mu\lambda}^{-1} = \left(E_{\lambda} - E\right)\delta_{\mu\lambda} - \sum_{c} \gamma_{\mu c}\, L_{c}\, \gamma_{\lambda c} \quad . \tag{II A1.4}$$

To see the relationship of the A-matrix to the R-matrix, we begin by multiplying both sides of Eq. (II A1.4) by A and summing over λ:

$$\sum_{\lambda} A_{\mu\lambda}^{-1} A_{\lambda\nu} = \sum_{\lambda}\left(E_{\lambda} - E\right)\delta_{\mu\lambda} A_{\lambda\nu} - \sum_{c} \gamma_{\mu c}\, L_{c} \sum_{\lambda} \gamma_{\lambda c}\, A_{\lambda\nu} \quad ,$$

or

$$\delta_{\mu\nu} = \left(E_{\mu} - E\right) A_{\mu\nu} - \sum_{c} \gamma_{\mu c}\, L_{c} \sum_{\lambda} \gamma_{\lambda c}\, A_{\lambda\nu} \quad . \tag{II A1.5}$$

Dividing by $\left(E_{\mu} - E\right)$, multiplying on the left by $\gamma_{\mu c'}$ and on the right by $\gamma_{\nu c''}$, and summing over μ puts this equation into the form

$$\begin{aligned} \sum_{\mu} \gamma_{\mu c'} \left(E_{\mu} - E\right)^{-1} \delta_{\mu\nu}\, \gamma_{\nu c''} &= \sum_{\mu} \gamma_{\mu c'} \left(E_{\mu} - E\right)^{-1} \left(E_{\mu} - E\right) A_{\mu\nu}\, \gamma_{\nu c''} \\ &\quad - \sum_{\mu} \gamma_{\mu c'} \left(E_{\mu} - E\right)^{-1} \sum_{c} \gamma_{\mu c}\, L_{c} \sum_{\lambda} \gamma_{\lambda c} A_{\lambda\nu}\, \gamma_{\nu c''} \quad , \end{aligned} \tag{II A1.6}$$

which can be reduced to

$$\gamma_{\nu c'} \left(E_\nu - E\right)^{-1} \gamma_{\nu c''} = \sum_\mu \gamma_{\mu c'} A_{\mu\nu} \gamma_{\nu c''} - \sum_c \left[\sum_\mu \gamma_{\mu c'} \left(E_\mu - E\right)^{-1} \gamma_{\mu c} \right] L_c \sum_\lambda \gamma_{\lambda c} A_{\lambda\nu} \gamma_{\nu c''} \quad . \tag{II A1.7}$$

Summing over ν puts this into the form

$$\left[\sum_\nu \gamma_{\nu c'} \left(E_\nu - E\right)^{-1} \gamma_{\nu c''} \right] = \sum_{\mu\nu} \gamma_{\mu c'} A_{\mu\nu} \gamma_{\nu c''} - \sum_c \left[\sum_\mu \gamma_{\mu c'} \left(E_\mu - E\right)^{-1} \gamma_{\mu c} \right] L_c \sum_{\lambda\nu} \gamma_{\lambda c} A_{\lambda\nu} \gamma_{\nu c''} \quad , \tag{II A1.8}$$

in which we can replace the quantities in square brackets by the R-matrix, giving

$$\begin{aligned} R_{c'c''} &= \sum_{\mu\nu} \gamma_{\mu c'} A_{\mu\nu} \gamma_{\nu c''} - \sum_c R_{c'c} L_c \sum_{\lambda\nu} \gamma_{\lambda c} A_{\lambda\nu} \gamma_{\nu c''} \\ &= \sum_c \left[\delta_{c'c} - R_{c'c} L_c \right] \sum_{\lambda\nu} \gamma_{\lambda c} A_{\lambda\nu} \gamma_{\nu c''} \quad . \end{aligned} \tag{II A1.9}$$

Solving for the summation, this equation can be rewritten as

$$\left[\left(I - RL\right)^{-1} R \right]_{cc''} = \sum_{\lambda\nu} \gamma_{\lambda c} A_{\lambda\nu} \gamma_{\nu c''} \quad . \tag{II A1.10}$$

To relate this to the scattering matrix, we note that Eq. (II A.6) can be rewritten using Eq. (II A.7) into the form

$$\begin{aligned} W &= P^{1/2} \left(I - RL\right)^{-1} \left(I - RL^*\right) P^{-1/2} \\ &= P^{1/2} \left(I - RL\right)^{-1} \left(I - RL + 2iRP\right) P^{-1/2} \\ &= P^{1/2} \left[\left(I - RL\right)^{-1} \left(I - RL\right) + 2i \left(I - RL\right)^{-1} RP \right] P^{-1/2} \\ &= P^{1/2} P^{-1/2} + 2iP^{1/2} \left(I - RL\right)^{-1} RPP^{-1/2} \\ &= I + 2iP^{1/2} \left(I - RL\right)^{-1} RP^{1/2} \quad . \end{aligned} \tag{II A1.11}$$

Comparing Eq. (II A1.10) to Eq. (II A1.11) gives, in matrix form,

$$W = I + 2iP^{1/2} \gamma A \gamma P^{1/2} \quad . \tag{II A1.12}$$

These equations are exact; no approximations have been made.

One common approximation should be discussed here: the "eliminated channel" approximation, for which one particular type of channel is treated in aggregate and assumed to not interfere from level to level. This is most easily understood in the A-matrix definition, Eq. (II A1.4); assuming no level-level interference for the gamma channels (for example), this equation can be approximated as

$$A^{-1}_{\mu\lambda} \approx \left(E_\lambda - E\right)\delta_{\mu\lambda} - \left[\sum_{\substack{\gamma=\text{gamma}\\ \text{channels}}} \gamma_{\mu\gamma}\, L_\gamma\, \gamma_{\lambda\gamma}\right]\delta_{\mu\lambda} - \sum_{\substack{c=\text{particle}\\ \text{channels}}} \gamma_{\mu c}\, L_c\, \gamma_{\lambda c} \quad . \qquad \text{(II A1.13)}$$

The quantity in square brackets corresponds to those channels for which the level-level interference is to be neglected; that is, only the interactions within one level are important. For gamma channels, $L = S+iP$ reduces to $L= i$, so Eq. (II A1.13) becomes

$$A^{-1}_{\mu\lambda} \approx \left(E_\lambda - E - i\overline{\Gamma}_{\lambda\gamma}/2\right)\delta_{\mu\lambda} - \sum_{\substack{c=\text{particle}\\ \text{channels}}} \gamma_{\mu c}\, L_c\, \gamma_{\lambda c} \quad . \qquad \text{(II A1.14)}$$

The bar over $\overline{\Gamma}_{\lambda\gamma}$ is used to indicate the special treatment for this channel.

In this form, our expression for A is analogous to the exact expression in Eq. (II A1.4) with two modifications: the additional imaginary term is added to the energy difference, and the sum over the channels includes only the "particle channels" (non-eliminated channels). It is therefore possible to immediately write the R-matrix formula for the eliminated-channel approximation as

$$R_{cc'} = \sum_\lambda \frac{\gamma_{\lambda c}\, \gamma_{\lambda c'}}{E_\lambda - E - i\overline{\Gamma}_{\lambda\gamma}/2}\, \delta_{JJ'} \quad , \qquad \text{(II A1.15)}$$

where the channel indices c and c' refer only to particle channels, not to the gamma channels. This formula for the R-matrix is the Reich-Moore approximation and is the form which is used in the SAMMY code. See Section II.B.1 for more about this formulation of R-matrix theory.

II.A.2. Derivation of Scattering Theory Equations

Many authors have given derivations of the equations for the scattering matrix in terms of the R-matrix. Sources for the derivation shown here are unpublished lecture notes of Fröhner [FF02], presented at the SAMMY workshop in Paris in 2002, and Foderaro [AF71]. This derivation is valid for only the simple case of spinless projectiles and target nuclei, assuming only elastic scattering and absorption. For the general case, the reader is referred to Lane and Thomas [AL58].

Schrödinger equation

The Schrödinger equation with a complex potential is

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + V + iW\right)\psi = E\psi \quad , \tag{II A2.1}$$

in which one can consider that V causes scattering and W causes absorption. The wave function can be expanded in the usual fashion,

$$\psi(r,\cos\theta) \;=\; \sum_{l=0}^{\infty}\frac{u_l(r)}{r}P_l(\cos\theta) \quad , \tag{II A2.2}$$

for which the radial portion obeys the equation

$$\frac{d^2u_l}{dr^2} \;+\; \left[k^2 - \frac{2m}{\hbar^2}(V+iW) - \frac{l(l+1)}{r^2}\right]u_l \;=\; 0 \quad , \tag{II A2.3}$$

subject to the conditions that $|\psi|^2$ is everywhere finite and that

$$u_l(r=0) = 0 \quad . \tag{II A2.4}$$

In the external region, $r > a$, the nuclear forces are zero ($V = W = 0$), so the solution has the form

$$u_l(r) \;=\; I_l(r) - U_l\,O_l(r) \quad . \tag{II A2.5}$$

I_l represents an incoming free wave, and O_l represents an outgoing free wave. U_l is the "collision function" or "S function" that describes the effects of the nuclear interaction, giving both the attenuation and the phase shift of the outgoing wave:

$$|U_l|^2 = 1 \;\text{ for } W = 0 \quad ,$$

and

$$|U_l|^2 < 1 \;\text{ for } W \neq 0 \quad . \tag{II A2.6}$$

Our goal is to determine an appropriate analytic form for U_l.

Orthogonal eigenvectors in interior region

For the interior region $r < a$, we define eigenfunctions $w_{\lambda l}(r)$ and eigenvalues E_λ,

$$E_\lambda = \frac{\hbar^2 k_\lambda^2}{2m} \quad , \tag{II A2.7}$$

for the wave equation without absorption ($W = 0$),

$$\frac{d^2 w_{\lambda l}}{dr^2} + \left[k_\lambda^{\,2} - \frac{2m}{\hbar^2} V - \frac{l(l+1)}{r^2} \right] w_{\lambda l} = 0 \quad , \tag{II A2.8}$$

for which the boundary conditions are

$$w_{\lambda l}(r=0) = 0 \qquad \text{and} \qquad \frac{a}{w_{\lambda l}(a)} \left. \frac{d w_{\lambda l}}{dr} \right|_{r=a} = B_l \quad . \tag{II A2.9}$$

Note that $w_{\lambda l}(r)$ is real if the boundary parameter B_l is chosen to be real. The eigenfunctions are orthogonal, since

$$\begin{aligned} \int_0^a \left(\frac{d^2 w_{\lambda l}}{dr^2} w_{\mu l} - w_{\lambda l} \frac{d^2 w_{\mu l}}{dr^2} \right) dr &= \int_0^a \frac{d}{dr} \left(\frac{d w_{\lambda l}}{dr} w_{\mu l} - w_{\lambda l} \frac{d w_{\mu l}}{dr} \right) dr \\ &= \left[\frac{d w_{\lambda l}}{dr} w_{\mu l} - w_{\lambda l} \frac{d w_{\mu l}}{dr} \right]_0^a \\ &= \left. \frac{d w_{\lambda l}}{dr} \right|_{r=a} w_{\mu l}(a) \; - \; w_{\lambda l}(a) \left. \frac{d w_{\mu l}}{dr} \right|_{r=a} - \; [0] \\ &= \frac{B_l}{a} \left[w_{\lambda l}(a) w_{\mu l}(a) - w_{\lambda l}(a) w_{\mu l}(a) \right] \; = \; 0 \quad , \end{aligned} \tag{II A2.10}$$

in which both equations of (II A2.9) have been invoked. The integral in Eq. (II A2.10) can also be evaluated using Eq. (II A2.8), giving

$$
\begin{aligned}
&\int_0^a \left(\frac{d^2 w_{\lambda l}}{d r^2} w_{\mu l} - w_{\lambda l} \frac{d^2 w_{\mu l}}{d r^2} \right) dr \\
&\quad = \int_0^a \left(\left[-k_\lambda^2 - \frac{2mV}{\hbar^2} \right] w_{\lambda l} w_{\mu l} - w_{\lambda l} \left[-k_\mu^2 - \frac{2mV}{\hbar^2} \right] w_{\lambda l} \right) dr \\
&\quad = \int_0^a \left(-k_\lambda^2 w_{\lambda l} w_{\mu l} + k_\mu^2 w_{\lambda l} w_{\mu l} \right) dr \\
&\quad = -\left(k_\lambda^2 - k_\mu^2 \right) \int_0^a w_{\lambda l} w_{\mu l} \, dr \quad .
\end{aligned}
\tag{II A2.11}
$$

Equating Eq. (II A2.10) to Eq. (II A2.11) gives

$$
\left(k_\lambda^2 - k_\mu^2 \right) \int_0^a w_{\lambda l} w_{\mu l} \, dr = 0 \quad . \tag{II A2.12}
$$

For $\lambda \neq \mu$, assuming no degenerate states, it therefore follows that

$$
\int_0^a w_{\lambda l} w_{\mu l} \, dr = 0 \ \text{ if } \lambda \neq \mu \quad . \tag{II A2.13}
$$

The orthogonality of the eigenvectors is therefore established. We assume that these wave functions are normalized such that

$$
\int_0^a w_{\lambda l} \, w_{\mu l} \ dr \ = \ \delta_{\lambda \mu} \quad . \tag{II A2.14}
$$

Matching at the surface

The internal wave function for the true potential (including the imaginary part iW) can be expanded in terms of the eigenfunctions as

$$
u_l(r) = \sum_\lambda c_{\lambda l} \, w_{\lambda l}(r) \quad \text{for } r \leq a \quad , \tag{II A2.15}
$$

with

$$
c_{\lambda l} = \int_0^a u_l \, w_{\lambda l} \ dr \quad . \tag{II A2.16}
$$

This equation for $c_{\lambda l}$ is derived by multiplying Eq. (II A2.15) by $u_{\lambda l}(r)$, integrating, and applying Eq. (II A2.14).

Consider now the integral

$$\int_0^a \left(\frac{d^2 u_l}{dr^2} w_{\lambda l} - u_l \frac{d^2 w_{\lambda l}}{dr^2} \right) dr \quad , \tag{II A2.17}$$

which can be expanded by use of Eqs. (II A2.3) and (II A2.8) to give

$$\begin{aligned} &\int_0^a \left(\frac{d^2 u_l}{dr^2} w_{\lambda l} - u_l \frac{d^2 w_{\lambda l}}{dr^2} \right) dr \\ &= \int_0^a \left(-\left[k^2 - \frac{2m}{\hbar^2}(V + iW) - \frac{l(l+1)}{r^2} \right] u_l \, w_{\lambda l} + u_l \left[k_\lambda{}^2 - \frac{2m}{\hbar^2} V - \frac{l(l+1)}{r^2} \right] w_{\lambda l} \right) dr \\ &= \left(k_\lambda{}^2 - k^2 \right) \int_0^a u_l w_{\lambda l} \, dr \quad + \quad \frac{2m}{\hbar^2} \int_0^a W \, u_l w_{\lambda l} \, dr \quad . \end{aligned} \tag{II A2.18}$$

Defining $\overline{W}_{\lambda l}$ as

$$\overline{W}_{\lambda l} \quad = \quad \int_0^a W \, u_l \, w_{\lambda l} \, dr \Big/ \int_0^a u_l \, w_{\lambda l} \, dr \tag{II A2.19}$$

permits rewriting Eq. (II A2.18) in the form

$$\int_0^a \left(\frac{d^2 u_l}{dr^2} w_{\lambda l} - u_l \frac{d^2 w_{\lambda l}}{dr^2} \right) dr = \left(k_\lambda{}^2 - k^2 + i \frac{2m}{\hbar^2} \overline{W}_{\lambda l} \right) \int_0^a u_l \, w_{\lambda l} \, dr \quad . \tag{II A2.20}$$

Integrating the left-hand side of this equation gives

$$\begin{aligned} \int_0^a \left(\frac{d^2 u_l}{dr^2} w_{\lambda l} - u_l \frac{d^2 w_{\lambda l}}{dr^2} \right) dr \; &= \left[\frac{du_l}{dr} w_{\lambda l} - u_l \frac{dw_{\lambda l}}{dr} \right]_0^a \; = \left[\frac{du_l}{dr} w_{\lambda l} - u_l \frac{dw_{\lambda l}}{dr} \right]_{r=a} \\ &= \left[\frac{du_l}{dr} w_{\lambda l} - u_l \frac{B_l}{a} w_{\lambda l} \right]_{r=a} = \left[a \frac{du_l}{dr} - u_l B_l \right]_{r=a} \frac{w_{\lambda l}(a)}{a} \quad , \end{aligned} \tag{II A2.21}$$

in which we have again made use of the boundary condition of Eq. (II A2.9). Integrating the right-hand side of Eq. (II A2.20) by applying Eq. (II A2.16) gives

$$\left(k_\lambda{}^2 - k^2 + i\frac{2m}{\hbar^2}\bar{W}_{\lambda l}\right)\int_0^a u_l\, w_{\lambda l}\, dr \;=\; \left(k_\lambda{}^2 - k^2 + i\frac{2m}{\hbar^2}\bar{W}_{\lambda l}\right)c_{\lambda l} \quad . \qquad \text{(II A2.22)}$$

Equating Eqs. (II A2.21) and (II A2.22) therefore gives

$$\begin{aligned}\left[a\frac{du_l}{dr} - u_l B_l\right]_{r=a}\frac{w_{\lambda l}}{a} &= \left(k_\lambda{}^2 - k^2 + i\frac{2m}{\hbar^2}\bar{W}_{\lambda l}\right)c_{\lambda l} \quad , \\ \left[a\frac{du_l}{dr} - u_l B_l\right]_{r=a}\frac{w_{\lambda l}}{a} &= \left(E_\lambda - E + i\bar{W}_{\lambda l}\right)\frac{2m\, c_{\lambda l}}{\hbar^2} \quad ,\end{aligned} \qquad \text{(II A2.23)}$$

or

$$c_{\lambda l} = \frac{\hbar^2\, w_{\lambda l}(a)}{2ma\left(E_\lambda - E + i\bar{W}_{\lambda l}\right)}\left[a\frac{du_l}{dr} - u_l B_l\right]_{r=a} \quad . \qquad \text{(II A2.24)}$$

Inserting this into Eq. (II A2.15) gives

$$u_l(r) = \sum_\lambda w_{\lambda l}(r)\frac{\hbar^2 w_{\lambda l}(a)}{2ma\left(E_\lambda - E + i\bar{W}_{\lambda l}\right)}\left[a\frac{du_l}{dr} - u_l B_l\right]_{r=a} \quad , \qquad \text{(II A2.25)}$$

which, when evaluated at $r = a$, becomes

$$u_l(a) = \sum_\lambda \frac{\hbar^2 w_{\lambda l}^2(a)}{2ma\left(E_\lambda - E + i\bar{W}_{\lambda l}\right)}\left[a\frac{du_l}{dr} - u_l B_l\right]_{r=a} \quad . \qquad \text{(II A2.26)}$$

Rearranging, this becomes

$$\begin{aligned}u_l(a) &= \left[a\frac{du_l}{dr} - u_l B_l\right]_{r=a}\sum_\lambda \frac{\left[\hbar^2 w_{\lambda l}^2(a)/2ma\right]}{\left(E_\lambda - E + i\bar{W}_{\lambda l}\right)} \\ &= \left[a\frac{du_l}{dr} - u_l B_l\right]_{r=a}\sum_\lambda \frac{\gamma_{\lambda l}^2}{\left(E_\lambda - E + i\Gamma_{\lambda l}/2\right)} \quad ,\end{aligned} \qquad \text{(II A2.27)}$$

in which the decay amplitude $\gamma_{\lambda l}$ is defined as

$$\gamma_{\lambda l} \equiv \sqrt{\frac{\hbar^2 w_{\lambda l}^2(a)}{2ma}} \qquad \text{(II A2.28)}$$

and the absorption width $\Gamma_{\lambda l}$ as

$$\Gamma_{\lambda l} \equiv 2W_{\lambda l} \quad . \qquad \text{(II A2.29)}$$

If we then define the R-function as

$$R_l = \sum_\lambda \frac{\gamma_{\lambda l}^2}{\left(E_\lambda - E + i\Gamma_{\lambda l}/2\right)} \quad , \qquad \text{(II A2.30)}$$

then Eq. (II A2.27) can be written in the form

$$u_l = \left(a \frac{du_l}{dr} - u_l B_l \right) R_l \quad , \qquad \text{(II A2.31)}$$

in which everything is evaluated at the matching radius *a*.

Scattering matrix in terms of R-matrix (neutrons only)

Equation (II A2.31) can be converted into the usual R-matrix formulae by inserting Eq. (II A2.5),

$$u_l = I_l - U_l O_l \quad , \qquad \text{(II A2.32)}$$

yielding

$$I_l - U_l O_l = \left[a \left(\frac{dI_l}{dr} - U_l \frac{dO_l}{dr} \right) - B_l \left(I_l - U_l O_l \right) \right] R_l \quad , \qquad \text{(II A2.33)}$$

in which everything is again evaluated at the matching radius *a*. Solving Eq. (II A2.33) for *U* gives

$$U_l \left[-O_l + R_l \left(a \frac{dO_l}{dr} - B_l O_l \right) \right] = I_l - R_l \left(a \frac{dI_l}{dr} - B_l I_l \right) \quad , \qquad \text{(II A2.34)}$$

or

$$U_l = \frac{I_l - R_l \left(a \frac{dI_l}{dr} - B_l I_l \right)}{\left[-O_l + R_l \left(a \frac{dO_l}{dr} - B_l O_l \right) \right]} = \frac{I_l}{O_l} \frac{1 - R_l \left(\frac{a}{I_l} \frac{dI_l}{dr} - B_l \right)}{1 - R_l \left(\frac{a}{O_l} \frac{dO_l}{dr} - B_l \right)} \quad . \qquad \text{(II A2.35)}$$

We define L_l as

$$L_l \equiv \frac{a}{O_l(a)} \frac{dO_l}{dr} \bigg|_{r=a} \equiv S_l + i P_l \quad . \qquad \text{(II A2.36)}$$

For spinless particles, $I_l^* = O_l$, so that

$$\frac{a}{I_l(a)} \frac{dI_l}{dr}\bigg|_{r=a} = L_l^* = S_l - iP_l \qquad \text{(II A2.37)}$$

and

$$\frac{I_l}{O_l} = \frac{O_l^*}{O_l} = \frac{|O| e^{-i\varphi}}{|O| e^{i\varphi}} = e^{-2i\varphi} \quad . \qquad \text{(II A2.38)}$$

Therefore Eq. (II A2.34) becomes

$$U_l \;=\; e^{-2i\varphi} \frac{1 - R_l\left(L_l^* - B_l\right)}{1 - R_l\left(L_l - B_l\right)} \quad , \qquad \text{(II A2.39)}$$

which is the usual form for the scattering matrix in terms of the R-matrix in this simple case.

II.A.2.a. Relating the scattering matrix to the cross sections

The relationship between the scattering matrix U and the cross section σ is also described by many authors; see, for example, [AF71]. Here we provide a summary for the simplest case.

The wave function for a spinless particle far from the scattering source can be written as

$$\psi(r,\theta) = e^{ikz} + \frac{e^{ikr}}{r} f(\theta) \quad , \tag{II A2 a.1}$$

where f has the form

$$f(\theta) = \frac{1}{2ik}\sum_l (2l+1)\left[U_l - 1\right] P_l(\cos\theta) \quad . \tag{II A2 a.2}$$

The cross section is then given by

$$\frac{d\sigma}{d\Omega} = \left| f(\theta) \right|^2 \quad . \tag{II A2 a.3}$$

For angle-integrated cross sections, the equation found by inserting Eq. (II A2 a.2) into Eq. (II A2 a.3) can be integrated to give

$$\begin{aligned}
\sigma = \int & \left[-\frac{1}{2ik}\sum_l (2l+1)\left[U_l^* - 1\right] P_l(\cos\theta) \right] \\
& \times \left[\frac{1}{2ik}\sum_{l'} (2l'+1)\left[U_{l'} - 1\right] P_{l'}(\cos\theta) \right] d(\cos\theta)\, d\varphi \\
= & \frac{1}{4k^2}\sum_{ll'} (2l+1)(2l'+1)\left[U_l^* - 1\right]\left[U_{l'} - 1\right] \int_0^{2\pi} d\varphi \int_{-1}^{1} P_l(\cos\theta) P_{l'}(\cos\theta)\, d(\cos\theta) \qquad \text{(II A2 a.4)} \\
= & \frac{1}{4k^2}\sum_{ll'} (2l+1)(2l'+1)\left[U_l^* - 1\right]\left[U_{l'} - 1\right] 2\pi \frac{2}{2l+1}\delta_{ll'} \\
= & \frac{\pi}{k^2}\sum_l (2l+1)\left|U_l - 1\right|^2 \quad .
\end{aligned}$$

This is analogous to the "standard" scattering theory equation shown in Eq. (II A.1).

II. B. VERSIONS OF MULTILEVEL R-MATRIX THEORY

Many representations of multilevel R-matrix theory have been developed over the years. For a summary of the more common versions, the reader is referred to the works of Fröhner [FF80, FF00].

Four versions of R-matrix theory are available in SAMMY: the Reich-Moore approximation (Section II.B.1), the single-level (SLBW) and multilevel Breit-Wigner (MLBW) approximations (Section II.B.3), and a variant on the Reich Moore which mimics the full R-matrix (Section II.B.2). An option to include a direct capture component is also provided (Section II.B.4).

The Reich-Moore approximation is the preferred method for most modern evaluations; it is the default formalism for SAMMY runs.

Fröhner, in fact, suggests that the Reich-Moore approximation is universally applicable to all cases: "Experience has shown that with this approximation [Reich Moore] all resonance cross section data can be described in detail, in the windows as well as in the peaks, even the weirdest multilevel interference patterns . . . It works equally well for light, medium-mass and heavy nuclei, fissile and nonfissile." [FF00, page 60]

For most purposes, Reich Moore is indeed indistinguishable from the exact formulation. Notable exceptions are situations where interference effects exist between capture and other channels. For those cases, small modifications to the SAMMY input will permit the user to mimic the effect of the non-approximated R-matrix; see Section II.B.2 for details.

Occasionally it is not possible to properly describe a cross section within the confines of R-matrix theory, because the reaction includes a direct component. SAMMY has provisions for the user to provide a numerical description of this component; see Section II.B.4 for details.

Also available within SAMMY are both the SLBW and the MLBW formulations (Section II.B.3); these are included for the sake of completeness, for comparison purposes, and because many of the evaluations in the nuclear data files were performed with Breit-Wigner formulae. However, it is strongly recommended that only Reich Moore be used for new evaluations, for several reasons: MLBW is often inadequate; SLBW is almost always inadequate. When it is correct, MLBW gives identical results to Reich Moore. "Ease of Programming" is no longer a valid excuse for using MLBW, since the programming has already been accomplished. Similarly, a slow computer is no longer a legitimate excuse, since modern computers can readily handle the more rigorous formulae.

Finally, it should be noted that SAMMY's implementation of MLBW does not correspond to the usual definition of MLBW. Instead, SAMMY uses the ENDF [ENDF-102] convention in which only the elastic cross section is truly multilevel, and all other types of cross section are single level.

II. B. 1. Reich-Moore Approximation to Multilevel R-Matrix Theory

The Reich-Moore approximation [CR58] is based on the idea that capture channels behave quite differently from particle channels. The particle-pair configuration for a capture channel consists of a gamma "particle" plus a nucleus with one more neutron than the target nucleus. For most physical situations, there are a multitude of such capture channels, whose behavior can be treated in an aggregate or average manner. It is assumed that there is no net interference between the aggregate capture channel and other channels, and the level-level interference of gamma channels is negligible, so that terms describing such interference may be eliminated from the R-matrix formulae. The mathematical derivation of this "eliminated-channel approximation" is discussed in Section II.A.1.

In the eliminated-channel approximation, the R-matrix of Eq. (II A.6) (for the spin group defined by total spin J and implicit parity π) has the form

$$R_{cc'} = \left[\sum_{\lambda} \frac{\gamma_{\lambda c}\, \gamma_{\lambda c'}}{E_{\lambda} - E - i\overline{\Gamma}_{\lambda\gamma} / 2} + R_c^{ext} \delta_{cc'} \right] \delta_{J\,J'} \quad , \qquad \text{(II B1.1)}$$

where all levels (resonances) of that spin group are included in the sum. Subscript λ designates the particular level; subscripts c and c' designate channels (including particle pairs and all the relevant quantum numbers). The width $\overline{\Gamma}_{\lambda\gamma}$ occurring in the denominator corresponds to the "eliminated" non-interfering capture channels of the Reich-Moore approximation; we use the bar to indicate that this width is treated differently from other "particle" widths.

The "external R-function" R_c^{ext} of Eq. (II B1.1) will be discussed in Section II.B.1.d.

The channel width $\Gamma_{\lambda c}$ is given in terms of the reduced-width amplitude $\gamma_{\lambda c}$ by

$$\Gamma_{\lambda c} = 2\, \gamma_{\lambda c}^2\, P_c\left(E\right) \quad , \qquad \text{(II B1.2)}$$

where P_c is the penetrability, whose value is a function of the type of particles in the channel, of the orbital angular momentum l, and of the energy E. The reduced-width amplitude $\gamma_{\lambda c}$ is always independent of energy, but the width $\Gamma_{\lambda c}$ may depend on energy via the penetration factor. For fission and for gamma channels, Eq. (II B1.2) becomes

$$\Gamma_{\lambda c} = 2\, \gamma_{\lambda c}^2 \quad ,$$

that is, the penetrability is effectively 1. (Note: In this manual, the reduced-width amplitude for the eliminated-channel capture width will be denoted by a bar above the symbol γ.)

Cross sections may be calculated by using the above expressions for R, with L given by Eq. (II A.7), to generate W, and from there calculating U and, ultimately, σ. However, while Eq. (II A.6) for W is correct, an equivalent form that is computationally more stable [NL92] is

$$W = I + 2\,i\,X \quad , \tag{II B1.3}$$

where X is given in matrix notation by

$$X = P^{1/2} L^{-1} \left(L^{-1} - R \right)^{-1} R\, P^{1/2} \quad . \tag{II B1.4}$$

When the suppressed indices and implied summations are inserted, the expression for X becomes

$$X_{c\,c'} = P_c^{1/2} L_c^{-1} \sum_{c''} \left[(L^{-1} - R)^{-1} \right]_{c\,c''} R_{c''c'}\; P_{c'}^{1/2}\; \delta_{J\,J'} \quad . \tag{II B1.5}$$

The various cross sections are then written in terms of X.

All calculations internally within SAMMY are expressed in terms of so-called "u-parameters," as distinguished from "p-parameters," which are the input quantities. The u-parameters associated with the resonance p-parameters are as follows:

$$u_{E_\lambda} = \begin{cases} \sqrt{E_\lambda} & \text{for } E_\lambda > 0 \\ -\sqrt{-E_\lambda} & \text{for } E_\lambda < 0 \quad , \end{cases} \tag{II B1.6}$$

and

$$u_{\Gamma_{\lambda c}} = \gamma_{\lambda c} = \begin{cases} \sqrt{\dfrac{\Gamma_{\lambda c}}{2P_l\left(\left|E_\lambda - \Xi_c\right|\right)}} & \text{if } \Gamma_{\lambda c} > 0 \\ -\sqrt{\dfrac{\left|\Gamma_{\lambda c}\right|}{2P_l\left(\left|E_\lambda - \Xi_c\right|\right)}} & \text{if } \Gamma_{\lambda c} < 0 \text{ in the PARameter file} \quad , \end{cases} \tag{II B1.7}$$

in which Ξ_c is the energy threshold for the channel (Section II.C.2).

It is important to note that the partial-width parameter $\Gamma_{\lambda c}$ is always a positive quantity, while the reduced-width amplitude $\gamma_{\lambda c}$ can be either positive or negative. Nevertheless, in the SAMMY input or output PARameter file (and also in the ENDF File 2 formats [ENDF-102]), partial widths may appear with negative signs. The convention is that the sign given in those files is to be associated with the amplitude $\gamma_{\lambda c}$ rather than with the partial width $\Gamma_{\lambda c}$.

II. B. 1. a. Energy-differential cross sections

The observable cross sections are found in terms of X by first substituting Eqs. (II A.4, II A.5, and II B1.3) into Eq. (II A.1), summing over spin groups (i.e., over J^{π}), and then summing over all channels corresponding to those particle pairs and spin groups. If X^r represents the real part and X^i the imaginary part of X, then the angle-integrated (but energy-differential) cross section for the interaction that leads from particle pair α to particle pair α' has the form

$$\sigma_{\alpha,\alpha'}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \Big[\Big(\sin^2\varphi_c \left(1 - 2X_{cc}^i\right) - X_{cc}^r \sin\left(2\varphi_c\right) \Big) \delta_{\alpha,\alpha'} + \sum_{c'} \{ X_{cc'}^{i\,2} + X_{cc'}^{r\,2} \} \Big] \quad . \tag{II B1 a.1}$$

(This formula is accurate only for cases in which one of particles in α is a neutron; however, both particles in α' may be charged.)

In Eq. (II B1 a.1) the summations are over those channels c and c' {of the spin group defined by J^{π}} for which the particle pairs are, respectively, α and α'. More than one "incident channel" $c = (\alpha, l, s, J)$ can contribute to this cross section, for example when both $l = 0$ and $l = 2$ are possible, or when, in the case of incident neutrons and non-zero spin target nuclei, both channel spins are allowed. Similarly, there may be several "exit channels" $c' = \left(\alpha', l', s', J'\right)$, depending on the particular reaction being calculated (e.g., elastic, inelastic, fission).

The total cross section (for non-Coulomb initial states) is the sum of Eq. (II B1 a.1) over all possible final-state particle-pairs α', assuming the scattering matrix is unitary (i.e., assuming that the sum over c' of $\left|U_{cc'}\right|^2 = 1$). Written in terms of the X matrix, the total cross section has the form

$$\sigma_{total}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[\sin^2\varphi_c + X_{cc}^i \cos\,(2\varphi_c) - X_{cc}^r \sin\,(2\varphi_c) \right] \quad , \tag{II B1 a.2}$$

where again the sum over c includes only those channels of the J^{π} spin group for which the particle pair is α.

The angle integrated elastic cross section is given by

$$\sigma_{elastic}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[\sin^2\varphi_c \left(1 - 2X_{cc}^i\right) - X_{cc}^r \sin\left(2\varphi_c\right) + \sum_{c'} \left\{ X_{cc'}^{i\,2} + X_{cc'}^{r\,2} \right\} \right] \quad . \tag{II B1 a.3}$$

In this case, both c and c' are limited to those channels of the J^{π} spin group for which the particle-pair is α; again, there may be more than one such channel for a given spin group.

Similarly, the reaction cross section from particle pair α to particle pair α' (where α' is not equal to α) is

$$\sigma_{reaction}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \sum_{c'} \left[X_{cc'}^{i\ 2} + X_{cc'}^{r\ 2} \right] \quad . \qquad \text{(II B1 a.4)}$$

Here c is restricted to those channels of the J^π spin group from which the particle pair is α, and c' to those channels for which the particle-pair is α'.

The absorption cross section has the form

$$\sigma_{absorption}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[X_{cc}^{i} - \sum_{c'} \left\{ X_{cc'}^{i\ 2} + X_{cc'}^{r\ 2} \right\} \right] \quad . \qquad \text{(II B1 a.5)}$$

Here both the sum over c and the sum over c' include <u>all</u> <u>incident</u> particle channels (i.e., particle pair α only) for the J^π spin group.

The capture cross section for the eliminated radiation channels can be calculated directly as

$$\sigma_{capture}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_{inc\,c} \left[X_{cc}^{i} - \sum_{all\,c'} \left\{ X_{cc'}^{i\ 2} + X_{cc'}^{r\ 2} \right\} \right] \quad , \qquad \text{(II B1 a.6)}$$

or may be found by subtracting the sum of all reaction cross sections from the absorption cross section. In Eq. (II B1 a.6), the sum over c includes all incident particle channels for the J^π spin group, and the sum over c' includes <u>all</u> particle channels, both incident and exit, for that spin group.

II.B.1.a.i. One-level two-channel case

For a simple one-level, two-channel case for which the shift factor is set to zero, the various cross sections defined in Section II.B.1.a can easily be expressed in terms of resonance parameters. Users are reminded that SAMMY is by no means restricted to this simple case and can be used with as many levels and as many channels as are needed to describe the particular physical situation. Nevertheless, it is useful to examine the cross section equations for this simple case: while these equations are a crude over-simplification for most physical situations, there is often physical insight to be gained by examination of these equations.

For this simple case, the X matrix of Eq. (II B1.4) takes the form

$$
\begin{aligned}
X &= \sqrt{P}L^{-1}\left(L^{-1}-R\right)^{-1}R\sqrt{P} \\
&= \begin{bmatrix} \frac{\sqrt{P_1}}{iP_1} & 0 \\ 0 & \frac{\sqrt{P_2}}{iP_2} \end{bmatrix}
\begin{bmatrix} \frac{1}{iP_1}-\frac{\gamma_1^2}{D} & -\frac{\gamma_1\gamma_2}{D} \\ -\frac{\gamma_1\gamma_2}{D} & \frac{1}{iP_2}-\frac{\gamma_2^2}{D} \end{bmatrix}^{-1}
\begin{bmatrix} \frac{\gamma_1^2}{D} & \frac{\gamma_1\gamma_2}{D} \\ \frac{\gamma_1\gamma_2}{D} & \frac{\gamma_2^2}{D} \end{bmatrix}
\begin{bmatrix} \sqrt{P_1} & 0 \\ 0 & \sqrt{P_2} \end{bmatrix} ,
\end{aligned}
\qquad \text{(II B1 ai.1)}
$$

in which the subscript on the penetrabilities denotes the channel number (not the angular momentum), the symbol D has been used for $E_\lambda - E - i\bar{\gamma}_{\lambda\gamma}^2$, and the subscript λ has been omitted from the reduced-width amplitudes for simplicity's sake. This equation can be rewritten as

$$
X = \frac{iP_1P_2D}{iD}\begin{bmatrix} \frac{1}{\sqrt{P_1}} & 0 \\ 0 & \frac{1}{\sqrt{P_2}} \end{bmatrix}
\begin{bmatrix} P_2\left(D-iP_1\gamma_1^2\right) & -iP_1P_2\gamma_1\gamma_2 \\ -iP_1P_2\gamma_1\gamma_2 & P_1\left(D-iP_2\gamma_2^2\right) \end{bmatrix}^{-1}
\begin{bmatrix} \gamma_1^2 & \gamma_1\gamma_2 \\ \gamma_1\gamma_2 & \gamma_2^2 \end{bmatrix}
\begin{bmatrix} \sqrt{P_1} & 0 \\ 0 & \sqrt{P_2} \end{bmatrix}
$$

$$
= \frac{P_1P_2}{P_1P_2\left(D^2-iP_1\gamma_1^2D-iP_2\gamma_2^2D\right)}\begin{bmatrix} \frac{1}{\sqrt{P_1}} & 0 \\ 0 & \frac{1}{\sqrt{P_2}} \end{bmatrix}
\begin{bmatrix} P_1\left(D-iP_2\gamma_2^2\right) & iP_1P_2\gamma_1\gamma_2 \\ iP_1P_2\gamma_1\gamma_2 & P_2\left(D-iP_1\gamma_1^2\right) \end{bmatrix}
$$

$$
\times \begin{bmatrix} \gamma_1^2 & \gamma_1\gamma_2 \\ \gamma_1\gamma_2 & \gamma_2^2 \end{bmatrix}
\begin{bmatrix} \sqrt{P_1} & 0 \\ 0 & \sqrt{P_2} \end{bmatrix} ,
$$

or

$$X = \frac{1}{\left(D^2 - iP_1\gamma_1^2 D - iP_2\gamma_2^2 D\right)} \begin{bmatrix} \frac{1}{\sqrt{P_1}} & 0 \\ 0 & \frac{1}{\sqrt{P_2}} \end{bmatrix}$$

$$\times \begin{bmatrix} P_1\gamma_1^2 D - iP_1P_2\gamma_1^2\gamma_2^2 + iP_1P_2\gamma_1^2\gamma_2^2 & P_1 D\gamma_1\gamma_2 - iP_1P_2\gamma_1\gamma_2^3 + iP_1P_2\gamma_1\gamma_2^3 \\ iP_1P_2\gamma_1^3\gamma_2 + P_2 D\gamma_1\gamma_2 - iP_1P_2\gamma_1^3\gamma_2 & iP_1P_2\gamma_1^2\gamma_2^2 + P_2\gamma_2^2 D - iP_1P_2\gamma_1^2\gamma_2^2 \end{bmatrix} \begin{bmatrix} \sqrt{P_1} & 0 \\ 0 & \sqrt{P_2} \end{bmatrix}$$

$$= \frac{1}{\left(D^2 - iP_1\gamma_1^2 D - iP_2\gamma_2^2 D\right)} \begin{bmatrix} \frac{1}{\sqrt{P_1}} & 0 \\ 0 & \frac{1}{\sqrt{P_2}} \end{bmatrix} \begin{bmatrix} P_1\gamma_1^2 D & P_1 D\gamma_1\gamma_2 \\ P_2 D\gamma_1\gamma_2 & P_2\gamma_2^2 D \end{bmatrix} \begin{bmatrix} \sqrt{P_1} & 0 \\ 0 & \sqrt{P_2} \end{bmatrix}$$

$$= \frac{1}{\left(D - iP_1\gamma_1^2 - iP_2\gamma_2^2\right)} \begin{bmatrix} P_1\gamma_1^2 & \sqrt{P_1P_2}\gamma_1\gamma_2 \\ \sqrt{P_1P_2}\gamma_1\gamma_2 & P_2\gamma_2^2 \end{bmatrix} ,$$

or, finally,

$$\begin{aligned} X &= \frac{1}{\left(E_\lambda - E - i\bar{\gamma}_\gamma^2 - iP_1\gamma_1^2 - iP_2\gamma_2^2\right)} \begin{bmatrix} P_1\gamma_1^2 & \sqrt{P_1P_2}\gamma_1\gamma_2 \\ \sqrt{P_1P_2}\gamma_1\gamma_2 & P_2\gamma_2^2 \end{bmatrix} \\ &= \frac{1}{\left(E_\lambda - E - i\Gamma/2\right)} \begin{bmatrix} \Gamma_1/2 & \sqrt{\Gamma_1\Gamma_2}/2 \\ \sqrt{\Gamma_1\Gamma_2}/2 & \Gamma_2/2 \end{bmatrix} , \end{aligned} \qquad \text{(II B1 ai.2)}$$

in which Γ is the sum of the partial widths $\Gamma_1 + \Gamma_2 + \Gamma_\gamma$.

In this form, X can be substituted into the equations for the various cross sections. Assuming the second channel is a reaction channel, Eq. (II B1 a.2) for the total cross section becomes

$$\begin{aligned} \sigma_{total}(E) &= \frac{4\pi}{k_\alpha^2}\, g_J \left[\sin^2\varphi_c + \frac{\Gamma\Gamma_1}{4d}\cos\,(2\varphi_c) - \frac{\left(E - E_\lambda\right)\Gamma_1}{2d}\sin\,(2\varphi_c) \right] \\ &= \frac{2\pi}{k_\alpha^2}\, g_J \left[1 - \left(1 - \frac{\Gamma\Gamma_1}{2d}\right)\cos\,(2\varphi_c) - \frac{\left(E - E_\lambda\right)\Gamma_1}{d}\sin\,(2\varphi_c) \right] , \end{aligned} \qquad \text{(II B1 ai.3)}$$

in which d has been used to represent $\left|\left(E_\lambda - E - i\Gamma/2\right)\right|^2 = \left(E - E_\lambda\right)^2 + \left(\Gamma/2\right)^2$. Similarly, the elastic cross section, Eq. (II B1 a.3), can be expressed as

$$\sigma_{elastic}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[\sin^2\varphi_c \left(1 - 2\frac{\Gamma\Gamma_1}{4d}\right) - \frac{\left(E - E_\lambda\right)\Gamma_1}{2d}\sin\left(2\varphi_c\right) + \left(\frac{\Gamma\Gamma_1}{4d}\right)^2 + \left(\frac{\left(E - E_\lambda\right)\Gamma_1}{2d}\right)^2 \right] , \qquad \text{(II B1 ai.4)}$$

which reduces to

$$\sigma_{elastic}(E) = \frac{2\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[1 - \cos 2\varphi_c \left(1 - \frac{\Gamma\Gamma_1}{2d}\right) - \sin 2\varphi_c \frac{\left(E - E_\lambda\right)\Gamma_1}{d} - \frac{\Gamma_1\left(\Gamma_\gamma + \Gamma_2\right)}{2d} \right] . \qquad \text{(II B1 ai.5)}$$

The reaction cross section, Eq. (II B1 a.4), becomes

$$\sigma_{reaction}(E) = \frac{4\pi}{k_\alpha^2}\, g \left[\left(\frac{\Gamma\sqrt{\Gamma_1\Gamma_2}}{4d}\right)^2 + \left(\frac{\left(E - E_\lambda\right)\sqrt{\Gamma_1\Gamma_2}}{2d}\right)^2 \right] = \frac{\pi g}{k_\alpha^2}\left[\frac{\Gamma_1\Gamma_2}{d}\right] , \qquad \text{(II B1 ai.6)}$$

and, finally, the capture cross section, Eq. (II B1 a.6), is

$$\sigma_{capture}(E) = \frac{4\pi g}{k_\alpha^2} \left[\frac{\Gamma\Gamma_1}{4d} - \left\{ \left(\frac{\Gamma\Gamma_1}{4d}\right)^2 + \left(\frac{\left(E - E_\lambda\right)\Gamma_1}{2d}\right)^2 + \left(\frac{\Gamma\sqrt{\Gamma_1\Gamma_2}}{4d}\right)^2 + \left(\frac{\left(E - E_\lambda\right)\sqrt{\Gamma_1\Gamma_2}}{2d}\right)^2 \right\} \right] \qquad \text{(II B1 ai.7)}$$

$$= \frac{4\pi g}{k_\alpha^2} \left[\frac{\Gamma\Gamma_1}{4d} - \left\{ \frac{\Gamma_1^{\,2}}{4d} + \frac{\Gamma_1\Gamma_2}{4d} \right\} \right] = \frac{\pi g}{k_\alpha^2}\left[\frac{\Gamma_1\overline{\Gamma}_\gamma}{d}\right] .$$

II.B.1.b. Angular distributions

Angular distributions (elastic, inelastic, or other reaction) cross sections for incident neutrons can be calculated from Reich-Moore resonance parameters. Following Blatt and Biedenharn [JB52] with some notational changes, the angular distribution cross section in the center-of-mass system may be written

$$\frac{d\sigma_{\alpha\alpha'}}{d\Omega_{CM}} = \sum_L B_{L\alpha\alpha'}(E)\, P_L(\cos\beta) \quad , \qquad \text{(II B1 b.1)}$$

in which the subscript $\alpha\alpha'$ indicates which type of cross section is being considered (i.e., α represents the entrance particle pair and α' represents the exit pair). P_L is the Legendre polynomial of degree L, and β is the angle of the outgoing neutron (or other particle) relative to the incoming neutron in the center-of-mass system. The coefficients $B_{L\alpha\alpha'}(E)$ are given by

$$B_{L\alpha\alpha'}(E) = \frac{1}{4k_\alpha^2} \sum_{J_1} \sum_{J_2} \sum_{l_1 s_1} \sum_{l'_1 s'_1} \sum_{l_2 s_2} \sum_{l'_2 s'_2} \frac{1}{(2i+1)(2I+1)} \times G_{\{l_1 s_1 l'_1 s'_1 J_1\}\{l_2 s_2 l'_2 s'_2 J_2\} L} \; \mathrm{Re}\left[(\delta_{c_1 c'_1} - U_{c_1 c'_1})(\delta_{c_2 c'_2} - U^*_{c_2 c'_2})\right] \quad , \qquad \text{(II B1 b.2)}$$

in which the various summations are to be interpreted as follows:

(1) sum over all spin groups defined by spin J_1 and the implicit associated parity

(2) sum over all spin groups defined by spin J_2 and the implicit associated parity

(3) sum over the entrance channels c_1 belonging to the J_1 spin group and having particle pair α, with orbital angular momentum l_1 and channel spin s_1 [i.e., $c_1 = (\alpha, l_1, s_1, J_1)$]

(4) sum over the exit channels c'_1 in J_1 spin group with particle-pair α', orbital angular momentum l'_1, and channel spin s'_1 [i.e., $c'_1 = (\alpha', l'_1, s'_1, J_1)$]

(5) sum over entrance channels c_2 in J_2 spin group where $c_2 = (\alpha, l_2, s_2, J_2)$

(6) sum over exit channels c'_2 in J_2 spin group where $c'_2 = (\alpha', l'_2, s'_2, J_2)$

Also note that i and I are the spins of the two particles (projectile and target nucleus) in particle-pair α.

The geometric factor G can be exactly evaluated as a product of terms

$$G_{\{l_1 s_1 l'_1 s'_1 J_1\}\{l_2 s_2 l'_2 s'_2 J_2\} L} = A_{l_1 s_1 l'_1 s'_1; J_1} \; A_{l_2 s_2 l'_2 s'_2; J_2} \; D_{l_1 s_1 l'_1 s'_1 l_2 s_2 l'_2 s'_2; L J_1 J_2} \quad , \qquad \text{(II B1 b.3)}$$

where the factor $A_{l_1 s_1 l'_1 s'_1; J_1}$ is of the form

$$A_{l_1 s_1 l'_1 s'_1; J_1} = \sqrt{(2l_1+1)\,(2l'_1+1)}\,(2J_1+1)\,\Delta(l_1 J_1 s_1)\,\Delta(l'_1 J_1 s'_1) \quad . \qquad \text{(II B1 b.4)}$$

The expression for D is

$$D_{l_1 s_1 l'_1 s'_1 l_2 s_2 l'_2 s'_2; L J_1 J_2} = (2L+1)\ \Delta^2(J_1 J_2 L)\ \Delta^2(l_1 l_2 L)\ \Delta^2(l'_1 l'_2 L)$$
$$\times\, w(l_1 J_1 l_2 J_2, s_1 L)\ w(l'_1 J_1 l'_2 J_2, s'_1 L)\ \delta_{s_1 s_2}\ \delta_{s'_1 s'_2} (-1)^{s_1 - s'_1} \qquad \text{(II B1 b.5)}$$
$$\times \frac{n!\ (-1)^n}{(n-l_1)!\ (n-l_2)!\ (n-L)!}\ \frac{n'!\ (-1)^{n'}}{(n'-l'_1)!\ (n'-l'_2)!\ (n'-L)!}\ ,$$

in which n is defined by

$$2n = l_1 + l_2 + L\ ; \qquad \text{(II B1 b.6)}$$

D is zero if l_1+l_2+L is an odd number. A similar expression defines n'. The Δ^2 term is given by

$$\Delta^2(abc) = \frac{(a+b-c)!\ (a-b+c)!\ (-a+b+c)!}{(a+b+c+1)!}\ , \qquad \text{(II B1 b.7)}$$

for which the arguments a, b, and c are to be replaced by the appropriate values given in Eqs. (II B1 b.4) and (II B1 b.5). The expression for $\Delta^2(abc)$ implicitly includes a selection rule for the arguments; that is, the quantized vector sum must hold,

$$\vec{a} + \vec{b} = \vec{c} \qquad \text{or} \qquad |a-b| \le c \le a+b \qquad \text{(II B1 b.8)}$$

with c being either integer or half-integer. The quantity w in Eq. (II B1 b.5) is defined as

$$w(l_1 J_1 l_2 J_2, s L) = \sum_{k=kmin}^{kmax} \frac{(-1)^{k+l_1+J_1+l_2+J_2}\ (k+1)!}{(k-(l_1+J_1+s))!\ (k-(l_2+J_2+s))!}$$
$$\times \frac{1}{(k-(l_1+l_2+L))!\ (k-(J_1+J_2+L))!} \qquad \text{(II B1 b.9)}$$
$$\times \frac{1}{(l_1+J_1+l_2+J_2-k)!\ (l_1+J_2+s+L-k)!\ (l_2+J_1+s+L-k)!}$$

(and similarly for the primed expression), where $kmin$ and $kmax$ are chosen such that none of the arguments of the factorials are negative. That is,

$$kmin = \max\{(l_1+J_1+s),\ (l_2+J_2+s),\ (l_1+l_2+L),\ (J_1+J_2+L)\}$$
$$kmax = \min\{(l_1+J_1+l_2+J_2),\ (l_1+J_2+s+L),\ (l_2+J_1+s+L)\}\ . \qquad \text{(II B1 b.10)}$$

Single-channel case

For some situations, these equations can be greatly simplified. When the target spin is zero and there are no possible reactions (no fission, no inelastic, no other reactions), then each spin group will consist of a single channel (the elastic channel). In this case, the coefficients $B_{L\alpha\alpha'}(E)$ reduce to

$$B_{L\alpha\alpha}(E) = \frac{1}{4k_\alpha^2} \sum_{J_1} \sum_{J_2} \sum_{c_1=(\alpha\, l_1 s_1 J_1)} \sum_{c_2=(\alpha\, l_2 s_2 J_2)} G_{\{l_1 s_1 l_1 s_1 J_1\}\{l_2 s_2 l_2 s_2 J_2\} L} \times \frac{1}{(2i_a+1)(2i_b+1)} \operatorname{Re}\left[(1-U_{c_1 c_1})\ (1-U^*_{c_2 c_2}) \right] , \qquad \text{(II B1 b.11)}$$

where the existence of only one channel requires that the primed quantities of Eq.(II B1 b.2) be equal to the unprimed (e.g., $\alpha = \alpha'$). The geometric factor *G* becomes

$$G_{\{l_1 s_1 l_1 s_1 J_1\}\{l_2 s_2 l_2 s_2 J_2\} L} = A_{l_1 s_1 l_1 s_1;\, J_1}\ A_{l_2 s_2 l_2 s_2;\, J_2}\ D_{l_1 s_1 l_1 s_1 l_2 s_2 l_2 s_2;\, L\, J_1 J_2} , \qquad \text{(II B1 b.12)}$$

in which the factor *A* reduces to the simple form

$$A_{l_1 s_1 l_1 s_1;\, J_1} = (2l_1+1)\ (2J_1+1)\ \Delta^2(l_1 J_1 s_1) , \qquad \text{(II B1 b.13)}$$

and the expression for *D* reduces to

$$D_{l_1 s_1 l_1 s_1 l_2 s_2 l_2 s_2;\, L\, J_1 J_2} = (2L+1)\ \Delta^2(J_1 J_2 L)\ \Delta^4(l_1 l_2 L) \times w^2(l_1 J_1 l_2 J_2, s_1 L)\ \delta_{s_1 s_2} \left[\frac{n!}{(n-l_1)!\ (n-l_2)!\ (n-L)!} \right]^2 , \qquad \text{(II B1 b.14)}$$

in which *n* is again defined as in Eq. (II B1 b.6).

II. B.1.c. Specifying individual reaction types

Early versions of SAMMY permitted users to specify “inelastic”, “fission”, and “reaction” data. However, the tacit assumption was that all the exit channels are relevant to the type of data being used. If, for example, three exit channels were specified as (1) inelastic, (2) first fission channel, and (3) second fission channel, then any calculation for “inelastic”, “fission”, or “reaction” data types would automatically include all three exit channels in the final state.

Hence, in early versions of SAMMY, true inelastic cross sections (for example) would be calculated only if <u>all</u> of the following conditions were met:

1. Either “inelastic”, “fission”, or “reaction” was specified as the data type in the INPut file, card set 8.

2. The exit channel description was appropriate for inelastic channels: The INPut file noted that penetrabilities were to be calculated (LPENT = 1 on line 2 of card set 10.1) and also provided a non-zero value for the excitation energy.

3. No fission channel (or other exit channel) was defined in the INPut file (and PARameter file).

Beginning with release M5 of the SAMMY code, it is now possible to include only a subset of the exit channels in the outgoing final state. The third condition in the list above is no longer necessary, but is replaced by another (less restrictive) condition:

3. Exit channels that are not inelastic have a flag (“1” in column 18 of line 2 of card set 10.1 or card set 10.2 of the INPut file), denoting that this channel does not contribute to the final state.

(Similar considerations hold, of course, for any other reaction type, not only for inelastic.)

With release 7.0.0 of the SAMMY code in 2006, a more intuitive input is possible. When channels are specified using either of the particle-pair options (see card set 4 or 4a of Table VIA.1), then the data type line (card set 8 of Table VIA.1) may be used to specify the name(s) of the particle pair(s) to be included in the final-state reaction. Specifically, beginning in the first column of card set 8, include the phrase

FINAL-state particle pairs are

or

PAIRS in final state =

(Only the first five characters are required, the others are optional.) Elsewhere on the same line, give the eight-character designation of the particle pair(s) to be included in the final-state reaction. Only channels involving those particle pairs will be included in the final state; any channels not involving those particle pairs will not be included. (Caution: The particle pair name must be *exactly* as it appears in the INPut file, including capitalization.)

The same two command lines may be used for angular distributions with specific final states, provided the phrase “ANGULar distribution” is given later on the same line.

See test case tr159 for an example which includes three reactions, one being (n,α) and the other two inelastic (n,n'). Various options for input are given in this test case.

Run “k” of test case tr112 shows an example for the angular distribution of a reaction cross section.

II.B.1.d. External R-function

When generating cross sections via R-matrix theory, it is important to include contributions from *all* resonances, even those outside the energy range of the data. Tails from negative-energy resonances (which may correspond to bound states) and from higher-lying resonances can contribute significantly to the "background" of the R-matrix and must therefore not be omitted. There are infinitely many of these resonances, so approximations must be made.

The usual approximation is to use pseudo or dummy resonances to approximate the effect of the infinite number of outlying resonances. The energy associated with a dummy resonance must be outside the energy region for which the analysis is valid.

For discussion regarding two different philosophies for determining appropriate choices of dummy resonances, see Leal et al. [LL99] and Fröhner and Bouland [FF01].

Any number of additional possibilities exist for approximating the contribution of the external resonances to the tail of the R-matrix. A logarithmic parameterization of the R-function is implemented in SAMMY; note that this is properly denoted as a *function* rather than *a matrix*, because it is diagonal with respect to the channels. The form used in the code is

$$R_c^{ext}(E) = \overline{R}_{con,c} + \overline{R}_{lin,c}E + \overline{R}_{q,c}E^2 - s_{lin,c}\left(E_c^{up} - E_c^{down}\right) - \left(s_{con,c} + s_{lin,c}E\right)\ln\left[\frac{E_c^{up} - E}{E - E_c^{down}}\right] \quad . \qquad \text{(II B1 d.1)}$$

Any or all of the seven free parameters may be varied during a SAMMY analysis (see Table VI B.2, card set 3, and card set 3a). Note that R_c^{ext} is strictly real in this parameterization.

The *u*-parameters (i.e., the parameters on which Bayes' equations will operate, as described in Section IV.C) associated with the external R-function are given by

$$\begin{aligned} &u\left(E_c^{down}\right) = E_c^{down} && u\left(E_c^{up}\right) = E_c^{up} && \\ &u\left(\overline{R}_{con,c}\right) = \overline{R}_{con,c} && u\left(\overline{R}_{lin,c}\right) = \overline{R}_{lin,c} && u\left(\overline{R}_{q,c}\right) = \overline{R}_{q,c} \\ &u\left(s_{con,c}\right) = \sqrt{s_{con,c}} && u\left(s_{lin,c}\right) = s_{lin,c} && . \end{aligned} \qquad \text{(II B1 d.2)}$$

Of the current ENDF formats [ENDF-102], only new LRF = 7 format permits this type of parameterization of the R-function. The more commonly used LRF = 3 format (the so-called Reich Moore format) allows only the dummy-resonance option.

II.B.2. Simulation of Full R-Matrix

While SAMMY does not yet have the ability to calculate the full (unapproximated) R-matrix of Lane and Thomas [AL58], it is possible to use the Reich-Moore approximation in such a way that it mimics the full R-matrix with a high degree of accuracy. This is necessary, for example, in cases where there are interference effects between the (incident) neutron channel and the gamma channel – that is, for some low-mass nuclides.

The Reich-Moore approximation involves special treatment ("excluded channels") for the gamma widths (capture widths). Therefore, to approximate the full R-matrix, one sets the Reich-Moore gamma width to a very small number and uses an exit channel to define the actual gamma channel:

1. Set the SAMMY gamma-channel widths to a very small number, perhaps 0.001.

2. Define an exit channel to be the actual capture channel and assign appropriate values for the widths. Quantum numbers for this channel will be the same as those for fission channels (in particular, set LPENT = 0).

3. When calculating capture cross sections, set the IFEXCL flag to 1 for all other (non-gamma) exit channels. (See Section II.B.1.c and card set 10.1 or 10.2 of Table VIA.1 for details.) When calculating other reaction cross sections, set the IFEXCL flag to 0 for the reaction channels of interest, to1 for the capture channels, and to 1 for any other reaction channels to be excluded.

When utilizing this option, SAMMY users should take care that results are not unduly influenced by the approximation in step 1 above. To test this, make radical changes in the value used for the gamma widths (e.g., set the value to 100.0 or 10^{-6}) and recalculate the cross section. Note that it is not possible to set these values to zero; doing so results in numerical overflow problems (because computers do not know how to calculate zero divided by zero).

Comparisons between cross sections calculated by SAMMY and those generated by the R-matrix code EDA [GH75] using the same R-matrix parameters have shown agreement to ~5 significant digits [INDC03]. Some of the runs for those comparisons are now assembled into SAMMY test case tr125.

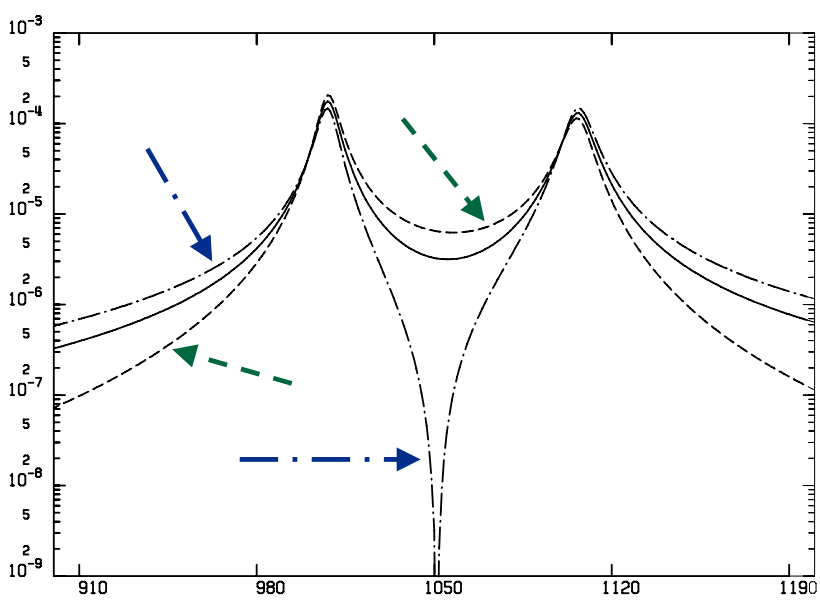
Test case tr110 shows an artificial but extreme example of a situation in which use of the Reich-Moore approximation gives very different results from those obtained via the full R-matrix. For this example, there are two resonances with parameter values as shown in Table II B2.1; plots of the curves calculated with those parameters are shown in Figure II B2.1. As evident from the figure, the Reich-Moore curve lies between the two extreme R-matrix curves which show constructive (dashed curve) and destructive (dot-dash curve) interference.

Table II B2.1. Parameter values used to illustrate Reich-Moore vs. full R-matrix calculations

	λ	Energy (MeV)	$\bar{\Gamma}_{\lambda\gamma}$ (eV)	$\Gamma_{\lambda n}$ (eV)	Sign $\times\,\Gamma_{\lambda\gamma}$ (eV)[a]
Reich Moore	1	1.0	1.0	10000.	
	2	1.1	1.1	11000.	
Pseudo-full R-matrix # 1	1	1.0	10^{-8}	10000.	1.0
	2	1.1	10^{-8}	11000.	1.1
Pseudo-full R-matrix # 2	1	1.0	10^{-8}	10000.	1.0
	2	1.1	10^{-8}	11000.	−1.1

[a] Remember that the value given in the SAMMY PARameter file is not the partial width Γ (which is always a positive number); rather, it is the sign of the reduced-width amplitude γ multiplied by the partial width Γ. Hence, the negative sign in the final entry of this table is actually associated with the reduced-width amplitude for the capture channel. See Section II.B.1 for further discussion.

Figure II B2.1. Reich-Moore approximation vs. full R-matrix for artificial example of test case tr110.



Solid line = Reich Moore
Dot-dash = full R-matrix # 1
Dash = full R-matrix # 2

II.B.3. Breit-Wigner Approximation

In addition to the preferred Reich-Moore formalism, SAMMY also offers the option to calculate cross sections using either the multilevel Breit-Wigner (MLBW) or the single-level Breit-Wigner (SLBW) [GB36]. This has the advantage that the calculation occurs more rapidly because fewer computations are required; however, it also has the disadvantage that unphysical cross sections may be generated. Use of this option is discouraged for new analyses; the option is included within SAMMY for completeness' sake, to permit use of SAMMY with most ENDF resonance parameter information, and to facilitate comparisons with older codes such as SIOB [GD78].

Formulae for MLBW and SLBW cross sections are presented in Section II.B.3.a; these are identical to those used in ENDF files [ENDF-102], although they are not necessarily programmed in this fashion. Formulae for derivatives are given in Section II.D.2.

A note regarding broadening: Historically, the Breit-Wigner formulations had the great advantage that the cross sections could be Doppler broadened analytically, using the high-energy approximation to the free-gas model of Doppler broadening (Section III.B.3). Results were written in terms of χ and ψ functions, and computation was relatively rapid. However, with the advent of modern computers, more accurate cross sections and more accurate Doppler-broadening computations can be accomplished rapidly, without resorting to these rather crude approximations. In SAMMY, Doppler and resolution broadening are accomplished numerically, in the same manner for MLBW and SLBW cross sections as for Reich-Moore cross sections, as described in Section III of this manual.

II.B.3.a. Single and multilevel Breit-Wigner cross sections

The MLBW elastic (scattering) cross section may be written in the form

$$\sigma^{elastic} = \frac{\pi}{k^2}\sum_J g_J \sum_c \left\{ \left(1-\cos 2\varphi\right)\left(2-\sum_\lambda \Gamma_{\lambda c}\Gamma_\lambda / d_\lambda\right) \right.$$
$$+ 2\sin 2\varphi \sum_\lambda \Gamma_{\lambda c}\left(E-E_\lambda\right)/d_\lambda \qquad \text{(II B3 a.1)}$$
$$\left. + \left(\sum_\lambda \Gamma_{\lambda c}\left(E-E_\lambda\right)/d_\lambda\right)^2 + \left(\sum_\lambda \Gamma_{\lambda c}\Gamma_\lambda / 2d_\lambda\right)^2 \right\} \quad ,$$

in which the summation over *c* includes only incident (i.e., neutron) channels. For SLBW, the level-level interference terms in this equation are dropped; that is, the summations over λ in the last line are outside, rather than inside, the parentheses. The total width Γ_λ in Eq. (II B3 a.1) is given by

$$\Gamma_\lambda = \sum_c \Gamma_{\lambda c} + \overline{\Gamma}_{\lambda\gamma} \quad , \qquad \text{(II B3 a.2)}$$

in which the sum over *c* includes **all** particle channels (i.e., over all channels except the eliminated capture channel). Partial widths $\Gamma_{\lambda c}$ and $\overline{\Gamma}_{\lambda\gamma}$ are related to amplitudes $\gamma_{\lambda c}$ and $\overline{\gamma}_\lambda$, as in the Reich-Moore approximation, by

$$\Gamma_{\lambda c}^{neutron} = 2\gamma_{\lambda c}^2 P_c$$
$$\Gamma_{\lambda c}^{fission} = 2\gamma_{\lambda c}^2 \qquad \text{(II B3 a.3)}$$
$$\text{and} \qquad \overline{\Gamma}_{\lambda\gamma} = 2\overline{\gamma}_{\lambda\gamma}^2 \quad .$$

(Note that we have again adopted the convention that the gamma channel be denoted by a bar over the symbol, even though it is not really treated differently from particle channels in the Breit Wigner approximations.) The denominator d_λ in Eq. (II B3 a.1) represents

$$d_\lambda = \left(E-E_\lambda\right)^2 + \left(\Gamma_\lambda / 2\right)^2 \quad . \qquad \text{(II B3 a.4)}$$

For both MLBW and SLBW, the fission cross section is given by

$$\sigma^{fission} = \frac{\pi}{k^2}\sum_J g_J \sum_c \sum_{c'} \sum_\lambda \frac{\Gamma_{\lambda c}\Gamma_{\lambda c'}}{d_\lambda} \quad , \qquad \text{(II B3 a.5)}$$

in which the sum over *c* includes only incident (neutron) channels, d_λ is again given by Eq. (II B3 a.4), and the sum over *c´* includes all exit channels. Caution: In principle, Eq. (II B3 a.5) could be used to describe any reaction channel, where term "reaction" encompasses any non-elastic,

non-capture channel. However, the only reaction channel permitted in ENDF is fission; for SLBW only one fission channel is permitted, and for MLBW two fission channels may be used. In addition, ENDF allows only one neutron channel (i.e., only one entrance channel). Because SAMMY's Breit-Wigner options were created solely for use with ENDF evaluations (for comparison purposes), similar restrictions apply to the use of the Breit-Wigner approximations in SAMMY. (For the more general case involving other reactions such as inelastic, (n,p), (n,α), or fission with more than two channels, use the Reich-Moore approximation as discussed in Section II.B.1.c.)

The Breit-Wigner form for the capture cross section is

$$\sigma^{capture} = \frac{\pi}{k^2} \sum_J g_J \sum_c \sum_\lambda \frac{\Gamma_{\lambda c} \overline{\Gamma}_{\lambda\gamma}}{d_\lambda} \quad , \qquad \text{(II B3 a.6)}$$

where, again, the sum over c includes only incident (neutron) channels. Total and absorption cross sections are given by the appropriate sums of the other three cross sections,

$$\sigma^{total} = \sigma^{elastic} + \sigma^{fission} + \sigma^{capture} \qquad \text{(II B3 a.7)}$$

and

$$\sigma^{absorption} = \sigma^{fission} + \sigma^{capture} \quad . \qquad \text{(II B3 a.8)}$$

As noted in Section IV.C, it is the u-parameters on which Bayes' equations operate. The u-parameters associated with the MLBW and SLBW resonances are defined similarly to those for Reich-Moore resonances:

$$u\left(E_\lambda\right) = \pm\sqrt{\left|E_\lambda\right|} \quad , \qquad \text{(II B3 a.9)}$$

where the negative sign is chosen if $E_\lambda < 0$,

$$u\left(\Gamma_{\lambda c}\right) = \gamma_{\lambda c} \qquad \text{(II B3 a.10)}$$

and

$$u\left(\overline{\Gamma}_{\lambda\gamma}\right) = \overline{\gamma}_{\lambda\gamma} \quad . \qquad \text{(II B3 a.11)}$$

(The reduced-width amplitudes $\gamma_{\lambda c}$ and $\overline{\gamma}_{\lambda\gamma}$ may be either positive or negative. However, the sign is irrelevant in the Breit-Wigner equations, for which the reduced-width amplitudes enter only as squared quantities.)

The matching radius a_c may also be varied (i.e., treated as a u-parameter) with the Breit-Wigner approximations.

II.B.4. Direct Capture Component

An externally generated direct capture component may be added to the appropriate cross section types (capture, absorption, and total) by including the phrase

```
ADD DIRECT CAPTURE Component to capture, total, and absorption cross section
```

in the alphanumeric command section of the INPut file. When this command is present, the direct capture component for at least one of the nuclides is provided as a numerical function of energy, in a separate file (the "DRC file"). SAMMY will linearly interpolate as needed between the energy points given.

The format of the DRC file is as follows:

First line:	key word "NUClide Number", followed by an equal sign "=", followed by the nuclide number as specified in the PARameter file.
Second line:	energy (eV), value of direct capture component (barn), in 2F20 format.
Third line:	repeat second line as many times as needed.
Last line:	blank.

These lines may be repeated for each nuclide as needed. Not all nuclides need to be included, but those which are included should be given in the same order as in the PARameter file. (For example, give the direct capture component for nuclides number 2, 4, and 7, rather than 4, 7, and 2.)

The actual value of the direct capture component added to the capture (and total and absorption) cross section for any given nuclide is the product of the value determined from the DRC file and a constant (energy-independent) coefficient whose value is specified as miscellaneous parameter DRCAP. See Table VI B.2 for details.

Test case tr076 contains examples.

II.C. DETAILS AND CONVENTIONS USED IN SAMMY

Details of cross section evaluation are often a matter of convention: for example, should one use *l-s* or *j-j* coupling for spin assignments? The spin conventions used in SAMMY are described in Section II.C.1.

Section II.C.2 describes the conversion of energy and momentum from the laboratory reference system to the center-of-mass system.

The method used for computing sin2φ and cos2φ, where φ is hard-sphere phase shift, is described in Section II.C.3.

Modifications are needed to the cross section equations when a channel contains two charged particles. These are described in Section II.C.4.

When data from an inverse reaction are used in an evaluation, modifications to either the measured data or the R-matrix parameters are needed. These are described in Section II.C.5.

II.C.1. Spin and Angular Momentum Conventions

For any analysis or evaluation, the analyst bears ultimate responsibility for including the proper spin-group definitions.

This is not the responsibility of the SAMMY program nor of the SAMMY author. SAMMY will issue warnings for obvious errors, but it is the responsibility of the user to notice and heed those warnings. It is also the responsibility of the user to ensure that the set of spin groups is complete; program SAMQUA, described in Section X.J, can be used for guidance in that effort.

It is worthwhile to discuss what is meant by "complete." Clearly, it is neither necessary nor possible to include all legitimate values of all of the quantum numbers (l, s, and J), because an infinite number of spin groups is available. Generally, one should include low values of l, $l = 0$ being always required and $l = 1, 2, 3, \ldots$ being included when the experimental data require their inclusion. For each l, the user should determine (using SAMQUA or by hand) all possible s-values leading to all possible J-values. In general, all such channels and spin groups should be included in the analysis. When the hard-sphere phase shift values are sufficiently large that there is a noticeable contribution to the cross section from the hard-sphere phase shift, all such channels <u>must</u> be included. On rare occasions, there may be one resonance (or several) whose high l-value dictates the presence of a particular channel in a particular spin group, but for which the hard-sphere phase shift is negligible for all energies of interest in this experiment. In this case, it would be reasonable to omit other channels and spin groups with this same l-value, without degrading the quality of the evaluation.

The spin and angular momentum conventions used in SAMMY (and in its predecessor MULTI [GA74]) are described in Table II C1.1. Recall that the word "channel" refers to the physical configuration (e.g., the particular particles involved) as well as to the quantum numbers given here. For example, an incident channel might consist of a neutron (intrinsic spin i = ½) impinging on a target (sample) whose spin is I, so that the channel spin is s, where $\vec{\boldsymbol{s}} = \vec{\boldsymbol{i}} + \vec{\boldsymbol{I}}$. The relative orbital angular momentum of this channel (neutron plus target) is l, and total spin is J, where $\vec{\boldsymbol{J}} = \vec{\boldsymbol{s}} + \vec{\boldsymbol{l}}$. For elastic scattering, the exit channel is the same as the entrance channel. For a reaction such as (n,p), the exit channel contains a proton (spin i' = ½) and another nuclide (spin I'); the channel spin is s', where $\vec{\boldsymbol{s}}' = \vec{\boldsymbol{i}}' + \vec{\boldsymbol{I}}'$. The relative angular momentum proton-nuclide system is $\boldsymbol{l}'$, and the total J must satisfy $\vec{\boldsymbol{J}} = \vec{\boldsymbol{s}}' + \vec{\boldsymbol{l}}'$.

Readers unfamiliar with vector sum rules are referred to Section II.C.1.a for a short summary of the basic principles.

Table II C1.1. Spin and angular momentum conventions used in SAMMY [a]

Symbol	FORTRAN name used in SAMMY	Meaning	Value or range of values
i or i'		Intrinsic spin of incident or outgoing particle	½ for neutron; in general, integer or half-integer
I or I'	SPINI	Spin of target [i.e., sample] or residual nuclei	Integer or half-integer
l or l'	LSPIN (channel 1, group number) *or* LSPIN (whatever channel, group number)	Orbital angular momentum in incident or outgoing channel	Non-negative integer
s or s'	CHSPIN (channel 1, group number) *or* CHSPIN (whatever channel, group number)	Incident or outgoing channel spin, equal to the vector sum of the spins of the two particles in the channel	$\vec{s} = \vec{I} + \vec{i}$ or $\vec{s}' = \vec{I}' + \vec{i}'$
J	SPINJ (group number)	(1) Spin of resonance (2) Spin of excited level in the compound nucleus (3) Total angular momentum quantum number	$\vec{J} = \vec{I} + \vec{s}$ $= \vec{I}' + \vec{s}'$

[a] Note: The channel spin s (s') was denoted by j (j') in early versions of this manual.

The spin statistical factor g_J appearing in the equations for cross section (see Section II.A) is given in terms of the spins *i* and *I* of the two particles in the entrance channel and the total spin *J* of the particular channel; that is

$$g_J = \frac{(2J+1)}{(2i+1)(2I+1)} \qquad \text{(II C1.1)}$$

in the general case, and

$$g_J = \frac{(2J+1)}{2(2I+1)} \qquad \text{(II C1.2)}$$

when the incident particle is a neutron or proton.

A few words of discussion about the use of these quantum numbers in SAMMY are warranted here, to avoid possible confusion:

(1) Values for the spin *i* of the projectile and spin *I* of the target particle are specified in the particle-pair definitions, card set 4 of the INPut file (see Section VI.A). Values for spins i' and I' (for exit particles) are also given in card set 4.

(2) With older input formats, incident spin *i* is assumed to be ½ unless otherwise specified (in card set 3). *I* is given as SPINI in card set 10.1. Values for spins i' and I' are not specified.

(3) Projectile spin *i* and target spin *I* are required for evaluation of the spin statistical factor *g*, and in calculation of the channel spin *s*. Exit particle spins are used to calculate channel spin s' but are otherwise unused.

(4) Channel spins s and s' are used as channel descriptors in the output (LPT or IO file; see Section VII). SAMMY will issue a warning statement (but not abort) if these values are inconsistent (if, for example, $\vec{\boldsymbol{s}} \neq \vec{\boldsymbol{i}} + \vec{\boldsymbol{I}}$).

(5) The orbital angular momentum *l* is used for generating penetrabilities, shift factors, and potential phase shifts.

(6) To the extent that it is possible (depending on which input format is used), SAMMY will warn of inconsistent spin or parity values, and abort when obvious errors occur. Users should read through the SAMMY.LPT file, especially at the beginning of an evaluation, to check for warning messages.

(7) Finally, users are urged to review the discussion in the first two paragraphs of this section, to read and heed the suggestions in Section XI (especially those under the heading “Step 2. Preparation of INPut and PARameter files”), and to make use of the auxiliary code SAMQUA when preparing the spin group information.

II.C.1.a. Quantum vector algebra

For a complete description of sum rules for quantum vectors, the reader is referred to textbooks on elementary quantum mechanics. Here we simply state the vector sum rules without detailed explanation.

Let $\vec{a}$ be a quantized vector. The value of this vector, generally written either *a* or $|\vec{a}|$, is either a positive half-integer or a positive integer. That is to say, *a* can have any of the values 0, 1/2, 1, 3/2, 2, 5/2, etc. For example, the spin of a neutron or proton is 1/2, and the spin of an alpha particle is 0. The orbital angular momentum *l* for a pair of particles is integral, *l* = 0, 1, 2, 3, etc.

Given two quantized vectors $\vec{a}$ and $\vec{b}$, and let $\vec{c} = \vec{a} + \vec{b}$ be the sum of the two vectors. The possible values for *c* are then

$$|a - b| \leq c \leq a + b \quad , \qquad \text{(II C1 a.1)}$$

where the allowed values of c are separated by one unit. Examples are shown in Table II C1 a.1. Values of *a* and *b* are in the left-most column and the uppermost row; values for *c* are in the other cells of the table. Because Eq. (II C1 a.1) is symmetric with respect to *a* and *b*, entries are made only in the lower triangular half of the table.

Each spin vector has an associated parity, which can be positive or negative. For example, protons, neutrons, and alpha particles have positive parity; many nuclides have negative parity. The parity associated with angular momentum *l* is $(-1)^l$. Parity is conserved when two vectors are added; the product of the parities of the two components is the parity of the resulting vector. A vector which is formed as the sum of two positive-parity vectors will have positive parity, a vector which is formed as the sum of two negative-parity vectors will have positive parity, and a vector which is formed as the sum of one positive-parity vector and one negative-parity vector will have negative parity. In other words, if *a* and *b* have the same parity, *c* has positive parity. If f *a* and *b* have different parity, *c* has negative parity.

Table II C1 a.1. Allowed values for the sum of two quantized vectors

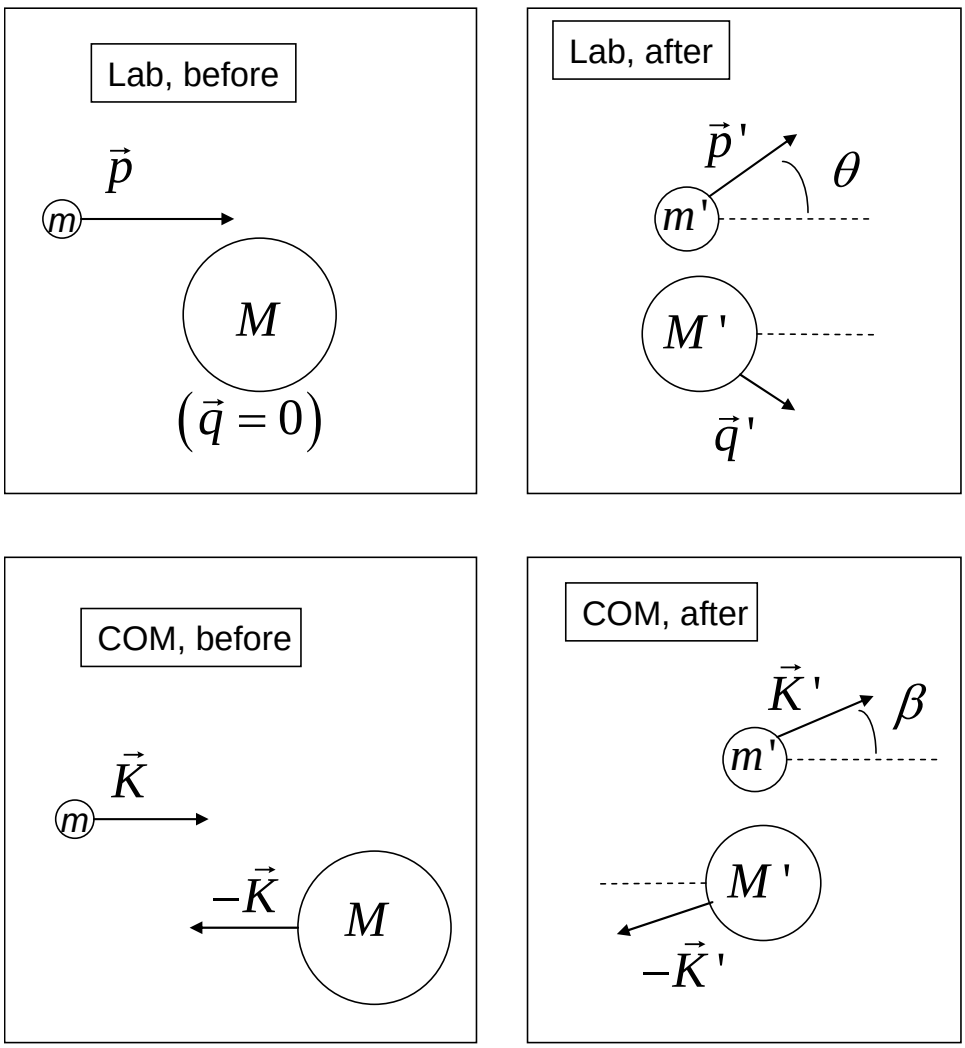
	0	½	1	3/2	2	5/2	3	7/2	4	9/2
0	0									
1/2	1/2	0, 1								
1	1	1/2, 3/2	0, 1, 2							
3/2	3/2	1, 2	1/2, 3/2, 5/2	0, 1, 2, 3						
2	2	3/2, 5/2	1, 2, 3	1/2, 3/2, 5/2, 7/2	0, 1, 2, 3, 4					
5/2	5/2	2, 3	3/2, 5/2, 7/2	1, 2, 3, 4	1/2, 3/2, 5/2, 7/2, 9/2	0, 1, 2, 3, 4, 5				
3	3	5/2, 7/2	2, 3, 4	3/2, 5/2, 7/2, 9/2	1, 2, 3, 4, 5	1/2, 3/2, 5/2, 7/2, 9/2, 11/2	0, 1, 2, 3, 4, 5, 6			
7/2	7/2	3, 4	5/2, 7/2, 9/2	2, 3, 4, 5	3/2, 5/2, 7/2, 9/2, 11/2	1, 2, 3, 4, 5, 6	1/2, 3/2, 5/2, 7/2, 9/2, 11/2, 13/2	0, 1, 2, 3, 4, 5, 6, 7		
4	4	7/2, 9/2	3, 4, 5	5/2, 7/2, 9/2, 11/2	2, 3, 4, 5, 6	3/2, 5/2, 7/2, 9/2, 11/2, 13/2	1, 2, 3, 4, 5, 6, 7	1/2, 3/2, 5/2, 7/2, 9/2, 11/2, 13/2, 15/2	0, 1, 2, 3, 4, 5, 6, 7, 8	
9/2	9/2	4, 5	7/2, 9/2, 11/2	3, 4, 5, 6	5/2, 7/2, 9/2, 11/2, 13/2	2, 3, 4, 5, 6, 7	3/2, 5/2, 7/2, 9/2, 11/2, 13/2, 15/2	1, 2, 3, 4, 5, 6, 7, 8	1/2, 3/2, 5/2, 7/2, 9/2, 11/2, 13/2, 15/2, 17/2	0, 1, 2, 3, 4, 5, 6, 7, 8, 9

II.C.2. Kinematics

The center-of-mass (COM) momenta, $K = \hbar k$ (initial) and $K' = \hbar k'$ (after the interaction), needed in the formulae for cross sections (see Section II.A) may be found in terms of laboratory energies E and E' by utilizing conservation of energy and momentum. The interaction is shown schematically in Figure II C 2.1, in both the laboratory (lab) and COM systems.

In this section we summarize the relevant equations relating the various momenta, energies, and angles involved in the description of the reaction. Details of the derivations are given in Section II.C.2.a.

Figure II C 2.1. Schematic of particle pairs for kinematics calculation.



Nomenclature: The two particles have mass m and M before the interaction (i.e., in the incident channel); the exit channel may contain completely different particles. The initial momentum of the incident particle is $\vec{p}$; the target particle is stationary (momentum $\vec{q}=0$); in the COM, the initial momentum of the incident particle is $\vec{K}=\hbar\vec{k}$, and the target particle's momentum is $-\vec{K}$. Primes refer to values after the interaction (in the exit channel). Quantities measured during an experiment are incident laboratory energy $E=p^2/2m$, laboratory energy of the exiting particle $E'=p'^2/2m'$, and laboratory angle θ relative to the incident direction. All other quantities will be specified in terms of these quantities.

Equation numbers in the rest of this section relate to the derivation in the following section.

The Q-value, Eq. (II C2 a.6), is defined as

$$Q \equiv m+M-m'-M' \tag{II C2.1}$$

and is related to the laboratory threshold energy , Eq. (II C2 a.24), here denoted by Ξ, via

$$\Xi = -\frac{m+M}{M}Q \quad . \tag{II C2.2}$$

The initial momentum K in the COM, Eq. (II C2 a.2), is given by

$$K=\hbar k=\frac{M}{m+M}\sqrt{2mE} \quad , \tag{II C2.3}$$

and the final COM momentum K', Eq. (II C2 a.8), by

$$K'=\sqrt{\frac{2m'M'}{(m'+M')}\frac{M}{(m+M)}\left[E-\Xi\right]} \quad . \tag{II C2.4}$$

The laboratory energy of the outgoing particle, Eq. (II C2 a.25), is equal to

$$E'=\frac{M'}{(m'+M')}\frac{M}{(m+M)}\left\{\gamma\mu+\sqrt{1-\gamma^2\left(1-\mu^2\right)}\right\}^2\left[E-\Xi\right] \quad , \tag{II C2.5}$$

in which $\mu=\cos\theta$, and γ is given in Eq. (II C2 a.26) as

$$\gamma^2 = \frac{m'}{M'}\frac{m}{M}\frac{m'+M'}{m+M}\frac{E}{E-\Xi} \quad . \tag{II C2.6}$$

The relationships between the COM and lab angles are, from Eqs. (II C2 a.29) and (II C2 a.31)

$$\nu = -\gamma\left(1-\mu^2\right) + \mu\sqrt{1-\gamma^2\left(1-\mu^2\right)} \qquad \text{(II C2.7)}$$

and

$$\mu = \frac{\nu+\gamma}{\sqrt{1+\gamma^2+2\gamma\nu}} \quad , \qquad \text{(II C2.8)}$$

where $\nu = \cos\beta$ and β is the COM angle. The transformation of angle-differential cross sections from COM to lab involves the derivative of ν with respect to μ, as given by Eq. (II C2 a.33):

$$\frac{d\nu}{d\mu} = \frac{\left(\mu\gamma + \sqrt{1-\gamma^2\left(1-\mu^2\right)}\right)^2}{\sqrt{1-\gamma^2\left(1-\mu^2\right)}} \quad . \qquad \text{(II C2.9)}$$

See Section II.B.1.b for details on the calculations of angular distributions with the Reich-Moore formulation of R-matrix theory.

In older versions of input to the SAMMY code (when particle-pair input is not used), the excitation energy can be specified either in the laboratory system (as in Eq. (II C2.2)) or in the center-of-mass system (as $-Q$); SAMMY will make the appropriate conversions. The default is laboratory. Users who wish to override the default (or who wish to keep a reminder handy) should include (in INPut file) the phrase

`CM NON-COULOMB EXCITation energies,` or
`LAB NON-COULOMB EXCItation energies`

as needed for the non-Coulomb case and

`CM COULOMB EXCITATIOn energies,` or
`LAB COULOMB EXCITATIon energies`

for use with charged-particle channels.

When using the key-word particle-pair input option (card set 4 of Table VI A.1), it is possible to specify the Q-value (equivalent to the negative of the center-of-mass excitation energy) rather than the excitation energy. It is recommended that Q-value rather than excitation energy be given, to avoid any ambiguity when more than one nuclide is present in the target.

Within SAMMY, the conversion factors from laboratory energy to COM momenta are calculated in subroutine Fixrad in segment/subdirectory “old” (and also used in segment “new”) and stored in an array “Zke” which must then be multiplied by the square root of the energy (minus the adjusted Q value) to give k or k'. Appropriate numerical constants are included to facilitate conversion from units of eV (for energy) to inverse Fermi (for wave number, which is momentum divided by $\hbar$). Values for constants are described in Section IX.A of this report.

II.C.2.a. Derivation of kinematics equations

Let $\vec{V}$ represent the velocity of the center-of-mass (COM) system relative to the laboratory system. Before the interaction, the relationships between the velocities are

$$\frac{\vec{p}}{m} = \frac{\vec{K}}{m} + \vec{V} \quad \text{and} \quad 0 = -\frac{\vec{K}}{M} + \vec{V} \quad , \qquad \text{(II C2 a.1)}$$

from which we can solve for $\vec{V}$ and $\vec{K}$ in terms of $\vec{p}$:

$$\vec{V} = \frac{\vec{K}}{M} \quad \text{and} \quad \vec{K} = \frac{\mathrm{M}}{\mathrm{m+M}}\vec{p} \ , \quad \text{which implies} \quad \vec{V} = \frac{\vec{p}}{(m+M)} \quad . \qquad \text{(II C2 a.2)}$$

The total energy in the lab must equal the energy *in* the COM plus the energy *of* the COM. Before the interaction, this gives us

$$\begin{aligned} E_{\text{lab}} &= E_{\text{of COM}} + E_{\text{in COM}} \\ \frac{p^2}{2m} + m + M &= \frac{(m+M)V^2}{2} + \frac{K^2}{2m} + \frac{K^2}{2M} + m + M \quad , \end{aligned} \qquad \text{(II C2 a.3)}$$

which is clearly true, as can be seen by substitution of the expressions in Eq. (II C2 a.2) into (II C2 a.3). We are using non-relativistic energies but nevertheless including the masses because they may be different before and after the interaction. Within the COM, conservation of energy requires that the initial and final energies are equal:

$$\begin{aligned} E_{\text{in com}} &= E'_{\text{in com}} \\ \frac{K^2}{2m} + \frac{K^2}{2M} + m + M &= \frac{K'^2}{2m'} + \frac{K'^2}{2M'} + m' + M' \quad . \end{aligned} \qquad \text{(II C2 a.4)}$$

Solving for K' in terms of K gives

$$\begin{aligned} \frac{K'^2}{2}\left(\frac{1}{m'} + \frac{1}{M'}\right) &= \frac{K^2}{2}\left(\frac{1}{m} + \frac{1}{M}\right) + \left(m + M - (m' + M')\right) \quad \text{or} \\ \frac{K'^2}{2}\left(\frac{m' + M'}{m'M'}\right) &= \frac{K^2}{2}\left(\frac{m+M}{mM}\right) + (Q) \quad , \end{aligned} \qquad \text{(II C2 a.5)}$$

in which we have defined the Q-value as

$$Q = m + M - m' - M' \quad . \tag{II C2 a.6}$$

Rewriting Eq. (II C2 a.5) using the value for K from Eq. (II C2 a.2) gives

$$\begin{aligned} K'^2 &= \frac{2m'M'}{m'+M'}\left[K^2\left(\frac{m+M}{2mM}\right)+Q\right] \\ &= \frac{2m'M'}{m'+M'}\left[\left\{p\frac{M}{m+M}\right\}^2\left(\frac{m+M}{2mM}\right)+Q\right] \\ &= \frac{2m'M'}{m'+M'}\left[\frac{p^2}{2m}\frac{M}{(m+M)}+Q\right] \quad . \end{aligned} \tag{II C2 a.7}$$

This can also be written as

$$K'^2 = \frac{2m'M'}{m'+M'}\left[E\frac{M}{(m+M)}+Q\right] \quad , \tag{II C2 a.8}$$

in which E is equal to the kinetic energy of the incident particle in the laboratory system,

$$E = \frac{p^2}{2m} \quad . \tag{II C2 a.9}$$

This definition of E is used throughout this manual; cross sections are always specified in terms of this energy unless otherwise noted explicitly.

The transformation from COM to laboratory gives values for momenta after the interaction. Again, we add velocities, similar to Eq. (II C2 a.1), using Eq. (II C2 a.2) for $\vec{V}$:

$$\frac{\vec{p}\,'}{m'} = \frac{\vec{K}\,'}{m'} + \vec{V} = \frac{\vec{K}\,'}{m'} + \frac{\vec{p}}{(m+M)} \quad . \tag{II C2 a.10}$$

(An analogous set of equations holds for the second particle,

$$\frac{\vec{q}\,'}{M'} = -\frac{\vec{K}}{M} + \vec{V} = -\frac{\vec{K}}{M} + \frac{\vec{p}}{(m+M)} \quad , \tag{II C2 a.11}$$

but we shall not be concerned with this particle now.)

Setting $\mu = \cos\theta$ and $\nu = \cos\beta$, we can write Eq. (II C2 a.10) in terms of components

$$\frac{p'\cos\theta}{m'} = \frac{K'\cos\beta}{m'} + \frac{p}{(m+M)} \quad \text{and} \quad \frac{p'\sin q}{m'} = \frac{K'\sin\beta}{m'} + 0 \qquad \text{(II C2 a.12)}$$

or

$$p'\mu = K'\nu + \frac{m'p}{(m+M)} \quad \text{and} \quad p'\sqrt{1-\mu^2} = K'\sqrt{1-\nu^2} \quad , \qquad \text{(II C2 a.13)}$$

in which we have set $\mu = \cos\theta$ and $\nu = \cos\beta$. Squaring and adding the two equations in (II C2 a.13) gives

$$\left(\frac{p'\mu}{m'}\right)^2 + \left(\frac{p'\sqrt{1-\mu^2}}{m'}\right)^2 = \left(\frac{K'\nu}{m'}\right)^2 + \left(\frac{K'\sqrt{1-\nu^2}}{m'}\right)^2 + 2\frac{K'\nu}{m'}\frac{p}{(m+M)} + \left(\frac{p}{(m+M)}\right)^2 , \qquad \text{(II C2 a.14)}$$

or

$$\frac{p'^2}{m'^2} = \frac{K'^2}{m'^2} + \frac{2K'\nu p}{m'(m+M)} + \frac{p^2}{(m+M)^2} \quad . \qquad \text{(II C2 a.15)}$$

Replacing $K'\nu$ with its equivalent from Eq. (II C2 a.13) puts Eq. (II C2 a.15) into the form

$$\frac{p'^2}{m'^2} = \frac{K'^2}{m'^2} + \frac{2p}{m'(m+M)}\left\{p'\mu - \frac{m'p}{m+M}\right\} + \frac{p^2}{(m+M)^2} \quad , \qquad \text{(II C2 a.16)}$$

which can be rearranged as

$$p'^2 = K'^2 + \frac{2m'p\mu}{(m+M)}p' - \frac{m'^2 p^2}{(m+M)^2} \quad . \qquad \text{(II C2 a.17)}$$

Solving for p' in terms of other quantities gives

$$\begin{aligned} p' &= \frac{m'}{m+M}p\mu + \sqrt{\left(\frac{m'}{m+M}\right)^2 p^2\mu^2 - \left(\frac{m'}{m+M}\right)^2 p^2 + K'^2} \\ &= \frac{m'}{m+M}\left\{p\mu + \sqrt{p^2\left(\mu^2-1\right) + \left(\frac{m+M}{m'}\right)^2 K'^2}\right\} \quad . \end{aligned} \qquad \text{(II C2 a.18)}$$

(Consideration of the $p = 0$ limit confirms that this choice of sign for the radical is appropriate.)

From Eq. (II C2 a.7), we know K' in terms of p. Therefore, to simplify Eq. (II C2 a.18), we define ξ as

$$\xi = \left(\frac{m'}{m+M}\right)\frac{p}{K'} \quad . \tag{II C2 a.19}$$

Using this definition of ξ, Eq. (II C2 a.18) can be put into the form

$$\begin{aligned} p' &= \frac{m'}{m+M}\left\{ p\mu + \sqrt{p^2\left(\mu^2-1\right)+\xi^{-2}p^2} \right\} \\ &= \frac{m'}{m+M}\frac{p}{\xi}\left\{ \xi\mu + \sqrt{1-\xi^2\left(1-\mu^2\right)} \right\} \quad . \end{aligned} \tag{II C2 a.20}$$

The quantity outside the curly brackets is exactly equal to K'; making this substitution gives

$$p' = K'\left\{ \xi\mu + \sqrt{1-\xi^2\left(1-\mu^2\right)} \right\} \quad . \tag{II C2 a.21}$$

The laboratory energy of the outgoing particle can then be found as

$$E' = \frac{p'^2}{2m'} = \frac{K'^2}{2m'}\left\{ \xi\mu + \sqrt{1-\xi^2\left(1-\mu^2\right)} \right\}^2 \quad , \tag{II C2 a.22}$$

or, using Eq. (II C2 a.8) for K',

$$E' = \frac{M'}{m'+M'}\left\{ \xi\mu + \sqrt{1-\xi^2\left(1-\mu^2\right)} \right\}^2 \left[E\frac{M}{(m+M)} + Q \right] \quad . \tag{II C2 a.23}$$

It is customary to define the laboratory threshold energy, here denoted by Ξ, as

$$\Xi \equiv -\frac{m+M}{M}Q \quad . \tag{II C2 a.24}$$

In terms of Ξ, Eq. (II C2 a.23) for E' becomes

$$E' = \frac{M'}{m'+M'}\frac{M}{(m+M)}\left\{ \xi\mu + \sqrt{1-\xi^2\left(1-\mu^2\right)} \right\}^2 \left[E-\Xi\right] \quad . \tag{II C2 a.25}$$

Equation (II C2 a.19) for ξ can also be written in terms of Ξ, using Eq. (II C2 a.8), as

$$\xi^2 = \frac{\left(\frac{m'}{m+M}\right)^2 2mE}{\frac{2m'M'}{m'+M'}\left[E\frac{M}{(m+M)}+Q\right]} = \frac{m'}{M'}\frac{m}{M}\frac{m'+M'}{m+M}\frac{E}{E-\Xi} \quad . \qquad \text{(II C2 a.26)}$$

Next, we consider the transformation of angle from laboratory θ to COM β and vice versa. From Eq. (II C2 a.13) we have

$$p'\mu = K'\nu + \frac{m'p}{(m+M)} = K'\nu + K'\xi \quad , \qquad \text{(II C2 a.27)}$$

in which we have made use of Eq. (II C2 a.19). Substituting Eq. (II C2 a.21) into this equation gives

$$p'\mu = K'\left\{\xi\mu + \sqrt{1-\xi^2\left(1-\mu^2\right)}\right\}\mu = K'\nu + K'\xi \quad , \qquad \text{(II C2 a.28)}$$

which reduces to

$$\nu = -\xi\left(1-\mu^2\right) + \mu\sqrt{1-\xi^2\left(1-\mu^2\right)} \quad . \qquad \text{(II C2 a.29)}$$

This equation can be inverted to give μ in terms of ν as follows:

$$\begin{gathered}
\left[\nu + \xi\left(1-\mu^2\right)\right]^2 = \mu^2\left[1-\xi^2\left(1-\mu^2\right)\right] \quad , \\
\nu^2 + 2\xi\nu\left(1-\mu^2\right) + \xi^2\left(1-2\mu^2+\mu^4\right) = \mu^2 - \xi^2\mu^2 + \xi^2\mu^4 \quad , \\
\mu^2\left(1+\xi^2+2\xi\nu\right) = \nu^2 + 2\xi\nu + \xi^2 \quad , \\
\mu^2 = \frac{\nu^2+2\xi\nu+\xi^2}{\left(1+\xi^2+2\xi\nu\right)} \quad ,
\end{gathered} \qquad \text{(II C2 a.30)}$$

or, finally, as

$$\mu = \frac{\nu+\xi}{\sqrt{1+\xi^2+2\xi\nu}} \quad . \qquad \text{(II C2 a.31)}$$

The transformation of cross section from COM to lab requires the derivative of ν with respect to μ; this is found from Eq. (II C2 a.29):

$$\begin{aligned}\frac{d\nu}{d\mu} &= \frac{d}{d\mu}\left\{-\xi\left(1-\mu^2\right)+\mu\sqrt{1-\xi^2\left(1-\mu^2\right)}\ \right\} \\ &= 2\mu\xi+\sqrt{1-\xi^2\left(1-\mu^2\right)}+\frac{\mu\, 2\mu\xi^2\ \frac{1}{2}}{\sqrt{1-\xi^2\left(1-\mu^2\right)}} \\ &= \frac{2\mu\xi\sqrt{1-\xi^2\left(1-\mu^2\right)}+1-\xi^2\left(1-\mu^2\right)+\mu^2\xi^2}{\sqrt{1-\xi^2\left(1-\mu^2\right)}}\quad ,\end{aligned} \tag{II C2 a.32}$$

giving, finally, the expression for the derivative

$$\frac{d\nu}{d\mu} = \frac{\left(\mu\xi+\sqrt{1-\xi^2\left(1-\mu^2\right)}\right)^2}{\sqrt{1-\xi^2\left(1-\mu^2\right)}}\quad . \tag{II C2 a.33}$$

II.C.2.b. Kinematics for elastic scattering

In the case of elastic scattering, primed quantities are exactly equal to unprimed, and the Q-value is zero. The equations of Section II.C.2 therefore simplify to the forms shown here.

The initial momentum K in the center-of-mass (COM) system is found from Eq. (II C2.3) to be

$$K = \hbar k = \frac{M}{m+M}\sqrt{2mE} \quad , \qquad \text{(II C2 b.1)}$$

and the final COM momentum K' is found in Eq. (II C2.4) to be

$$K' = \frac{M}{m+M}\sqrt{2mE} \quad . \qquad \text{(II C2 b.2)}$$

The laboratory energy of the outgoing particle is found from Eqs. (II C2.5) and (II C2.6) to be

$$E' = \left[\frac{1}{m+M}\left\{m\mu + \sqrt{M^2 - m^2\left(1-\mu^2\right)}\ \right\}\right]^2 E \quad , \qquad \text{(II C2 b.3)}$$

with $\mu = \cos\theta$.

The relationships between the COM and lab angles, Eqs. (II C2.7) and (II C2.8), become

$$\nu = -\frac{m}{M}\left(1-\mu^2\right) + \mu\sqrt{1-\left(\frac{m}{M}\right)^2\left(1-\mu^2\right)} \qquad \text{(II C2 b.4)}$$

and

$$\mu = \frac{M\nu + m}{\sqrt{M^2 + m^2 + 2mM\nu}} \quad , \qquad \text{(II C2 b.5)}$$

where $\nu = \cos\beta$ and β is the COM angle. The derivative of ν with respect to μ, Eq. (II C2.9), is

$$\frac{d\nu}{d\mu} = \frac{\left(\mu m + \sqrt{M^2 - m^2\left(1-\mu^2\right)}\right)^2}{\sqrt{M^2 - m^2\left(1-\mu^2\right)}} \quad . \qquad \text{(II C2 b.6)}$$

II.C.3. Evaluation of Hard-Sphere Phase Shift

Formulae for the hard-sphere phase shift (otherwise known as the potential-scattering phase shift) are given in Table II A.1 for non-Coulomb interactions. What is actually needed in SAMMY is not, however, the phase shifts φ themselves but rather $\cos(2\varphi)$ and $\sin(2\varphi)$. Since evaluation of φ requires the inverse tangent function, results for $\cos(2\varphi)$ and $\sin(2\varphi)$ are more readily generated with fewer computer round-off errors by using trigonometric relationships to generate formulae for $\cos(2\varphi)$ and $\sin(2\varphi)$ directly.

For all l, it is clear from Table II A.1 that φ may be written in the form

$$\varphi = \rho - X \quad , \tag{II C3.1}$$

where

$$X = \tan^{-1} f \tag{II C3.2}$$

and f is a different function of ρ for each value of l. From Eq. (II C3.1), using elementary trigonometric relationships, we find

$$\cos\varphi \;=\; \cos\rho\;\cos X \;+\; \sin\rho\;\sin X \tag{II C3.3}$$

and

$$\sin\varphi \;= -\cos\rho\;\sin X \;+\; \sin\rho\;\cos X \quad . \tag{II C3.4}$$

Thus, $\cos(2\varphi)$ becomes

$$\begin{aligned}\cos(2\varphi) \;&=\; 2\cos^2\varphi - 1 = 2\cos^2\rho\;\;\cos^2 X\;\left(1+\tan\rho\;\tan X\right)^2 - 1 \\ &= 2\,\frac{\cos^2\rho}{1+f^2}\,\left(1+f\,\tan\rho\right)^2 - 1 \quad .\end{aligned} \tag{II C3.5}$$

Similarly, $\sin(2\varphi)$ can be written

$$\begin{aligned}\sin(2\varphi) \;&=\; 2\cos\varphi\sin\varphi \;=\; 2\cos^2\rho\;\;\cos^2 X\,\left(1+\tan\rho\tan X\right)\left(-\tan X+\tan\rho\right) \\ &=\; 2\,\frac{\cos^2\rho}{1+f^2}\left(1+f\,\tan\rho\right)\left(-f+\tan\rho\right) \quad .\end{aligned} \tag{II C3.6}$$

Equations (II C3.5) and (II C3.6) are the form used in SAMMY to evaluate the hard-sphere phase shift terms for non-Coulomb situations.

II.C.4. Modifications for Charged Particles

The penetrabilities P_l, shift factors S_l, and potential-scattering phase shifts φ_l defined in Table II A.1 apply only to non-Coulomb interactions such as those involving incident neutrons. Often, however, the two particles in a channel will both have a positive charge; examples are the exit channels for (n,α) or (n,p) interactions, and the incident channels in the inverse (reciprocal) measurements (α,n) and (p,n). In this case the expressions for penetrabilities, shift factors, and phase shifts must be modified to include the long-range interaction; see, for example, the discussion of Lane and Thomas [AL58].

An extension for SAMMY to include Coulomb penetrabilities, shift factors, and phase shifts was developed by R. O. Sayer [RS00] (and modified by the SAMMY author) and used first for analysis of ^{16}O data [LL98, RS00]. FORTRAN routines used for this purpose are a modified version of the routine COULFG of Barnett [AB82].

Additional changes were required to calculate the cross sections for incident charged particles; details are given in Section II.C.4.a. Because the Coulomb interaction is long range, only the angle-differential cross sections are calculable; the angle-integrated cross sections are infinite.

Expressions for P_l, S_l, and φ_l for particle pair α involve the parameter η_α, which is defined as

$$\eta_\alpha = \frac{z_\alpha Z_\alpha e^2 \mu_\alpha}{\hbar^2 k_\alpha} \quad , \tag{II C4.1}$$

where z and Z are the charge numbers for the two particles in the particle pair. The reduced mass μ_α is defined in the usual manner as

$$\mu_\alpha = \frac{m_\alpha M_\alpha}{m_\alpha + M_\alpha} \quad , \tag{II C4.2}$$

where m_α and M_α are the masses of the two particles in channel α. The center-of-mass (COM) momentum $\hbar k_\alpha$ is defined in the same manner as in Eq. (II C2 a.8), as

$$\hbar^2 k_\alpha^2 = \frac{2 m_\alpha M_\alpha}{\left(m_\alpha + M_\alpha\right)} \frac{M}{\left(m + M\right)} \left(E - \Xi\right) \quad . \tag{II C4.3}$$

In Eq. (II C4.3), the masses of particles in the incident channel are denoted without subscripts; these masses may be different from the masses in particle pair α. If the excitation energy is given in the COM system, this expression takes the form

$$\hbar^2 k_\alpha^2 = \frac{2 m_\alpha M_\alpha}{\left(m_\alpha + M_\alpha\right)} \frac{M}{\left(m + M\right)} \left(E - \left[\frac{m + M}{M} \right] \Xi_{\mathrm{com}} \right) \quad . \tag{II C4.4}$$

In the SAMMY input, the user can specify the value of the excitation energy either in the laboratory system [as in Eq. (II C4.3)] or in the COM system; SAMMY will make the appropriate conversions. The default is laboratory. Users who wish to provide COM values should include the phrase "CM COULOMB EXCITATION ENERGIES" as needed.

The reaction Q-value is the negative of variable Ξ_{COM} = ECHAN (in the COM system) in card set 10.1 or 10.2 of Table VI A.1. When using the particle-pair input, card set 4 or 4a of Table VIA.1, it is possible to give the Q-value directly; this is the recommended input format.

Recall that a channel is defined by the particle pair (with mass, spin, and charge for each of the two particles, plus the Q-value) plus the spin quantum numbers *l*, *s*, and *J*. Quantities defined above in Eqs. (II C4.1) through (II C4.4) depend only on the particle pair α and not on the spin quantum numbers. Other quantities (below) depend also on the value of *l*.

If a_c is the channel radius for this channel, we again define ρ as

$$\rho = k_\alpha a_c \tag{II C4.5}$$

The penetrabilities $P_l(\eta,\rho)$, shift factors $S_l(\eta,\rho)$, and phase shifts $\varphi_l(\eta,\rho)$ are then calculated as functions of $F_l(\eta,\rho)$ and $G_l(\eta,\rho)$, the regular and irregular Coulomb wave functions, respectively. The equations are as follows:

$$P_l = \frac{\rho}{A_l^2}, \qquad S_l = \frac{\rho}{A_l}\frac{\partial A_l}{\partial \rho}, \qquad \text{and} \quad \cos\varphi_l = \frac{G_l}{A_l} \quad , \tag{II C4.6}$$

where

$$A_l^2 = F_l^{\,2} + G_l^2 \quad . \tag{II C4.7}$$

In Eqs. (II A.1) and (II A.5), the Coulomb phase-shift difference w_c is required for charged-particle interactions. From Lane and Thomas [AL58], this quantity has the value

$$w_c = \begin{cases} 0 & l = 0 \\ \displaystyle\sum_{n=1}^{l} \tan^{-1}\left(\frac{\eta_\alpha}{n}\right) & l \neq 0 \end{cases} \quad . \tag{II C4.8}$$

Finally, we note that an alternative version of the Coulomb functions is available in SAMMY. This alternative, modified from files provided by Hale [GH02], requires longer run time but appears to be more accurate at low values of ρ (and corresponding high values of η). SAMMY will automatically switch to the more accurate version when it discerns the need. To invoke this alternative for all calculations, include the phrase "USE ALTERNATIVE COULomb functions" in the INPut file.

II.C.4.a. Charged-particle initial states

To derive the equations for the angle-differential cross sections for charged-particle incident channels, we begin with the Lane and Thomas [AL58] expression [page 292, Eq. (2.6)]. When this expression is corrected (for a missing complex conjugate, a missing minus sign, and missing delta functions), summed over the exit channel spins s', and averaged over the incident channel spins s, the resulting equation for the angle-differential cross section is

$$\begin{aligned}\frac{d\sigma_{\alpha\alpha'}}{d\Omega_{CM}} &= \sum_L B_{L\alpha\alpha'}(E)\,P_L(\cos\beta) \;+\; \frac{\pi}{k_\alpha^2}\left|C_\alpha(\beta)\right|^2\delta_{\alpha\alpha'} \\ &+ \frac{\sqrt{4\pi}}{k_\alpha^2}\sum_{Jsl} g_J\,\mathrm{Re}\left[-i\left(\frac{e^{2iw_{l\alpha}}-U_{cc}}{2}\right)C_\alpha^*\,P_l(\cos\beta)\right]\delta_{\alpha\alpha'} \quad .\end{aligned} \tag{II C4 a.1}$$

Here we have again used the convention that $c=\{\alpha,l,s,J\}$. For the charged-particle case, the definition of $B_{L\alpha\alpha'}(E)$ is modified slightly from the non-Coulomb case [Eq. (II B1 b.2)] to give

$$\begin{aligned}B_{L\alpha\alpha'}(E) &= \frac{1}{4k_\alpha^2}\sum_{J_1}\sum_{J_2}\sum_{l_1 s_1}\sum_{l'_1 s'_1}\sum_{l_2 s_2}\sum_{l'_2 s'_2} \\ &\times\; G_{\{l_1 s_1 l'_1 s'_1 J_1\}\{l_2 s_2 l'_2 s'_2 J_2\}L}\;\frac{1}{(2i+1)(2I+1)} \\ &\times\; \mathrm{Re}\left[(e^{2iw_{l\alpha}}\delta_{c_1c'_1}-U_{c_1c'_1})\,(e^{-2iw_{l\alpha}}\delta_{c_2c'_2}-U^*_{c_2c'_2})\right] \quad .\end{aligned} \tag{II C4 a.2}$$

In the final line of Eq. (II C4 a.2), the quantity c_1 is substituted for the expression $\{\alpha,l_1,s_1,J_1\}$, c_2 for $\{\alpha,l_2,s_2,J_2\}$, c'_1 for $\{\alpha',l'_1,s'_1,J_1\}$, and c'_2 for $\{\alpha',l'_2,s'_2,J_2\}$. The geometric term G in Eq. (II C4 a.2) is the same as for the non-Coulomb case and is defined in Eqs. (II B1 b.3) to (II B1 b.10). Notation for summation indices is the same as in the non-Coulomb case.

What is different here is the presence of the exponential involving the Coulomb phase-shift difference $w_{l\alpha}$, defined in Eq. (II C4.7). Also, the scattering matrix contains the $w_{l\alpha}$ in the definition of Ω; the Sommerfeld parameter η_α in Eq. (II C4.1) is defined as

$$\eta_\alpha = \frac{z\,Z\,e^2\mu_\alpha}{\hbar^2 k_\alpha} \quad . \tag{II C4 a.3}$$

The additional terms in Eq. (II C4 a.1) involve the function C_α, which is defined as

$$C_\alpha = \frac{1}{\sqrt{4\pi}} \eta_\alpha \ \mathrm{cosec}^2\left(\frac{\beta}{2}\right) e^{-2i\eta_\alpha \ \ln\left[\sin\left(\frac{\beta}{2}\right)\right]} \quad . \qquad \text{(II C4 a.4)}$$

It is this term which is infinite at $\beta = 0$ (forward scattering) and which causes the (angle-integrated) elastic-scattering cross section to be infinite.

Center-of-mass vs Laboratory

Angular distribution cross sections are sometimes reported as if measured in the center-of-mass system rather than in the laboratory system; hence, SAMMY can calculate either version. To specify which is wanted, insert one of the phrases

```
USE CENTER OF MASS Cross sections
USE LABORATORY CROSS sections
```

into your INPut file (see Tables VI A.1 and VI A1.2). Center-of-mass is the default.

Acknowledgements

The author is grateful to SAMMY users Jeff Blackmon and Olivier Bouland for uncovering bugs in early implementations of charged-particle elastic scattering, and to Eric Berthoumieux (author of the ANARKI R-matrix code) for providing calculations to assist in debugging this portion of SAMMY.

II.C.5. Inverse Reactions (Reciprocity)

Occasionally a user may wish to include data from an inverse reaction in the same evaluation as the forward reaction. For example, for an evaluation of the ^{16}O resonance parameters, Sayer [RS00] wanted to include $^{16}O(n,\alpha)^{13}C$ data. No such data existed, but $^{13}C(\alpha,n)^{16}O$ data were available.

Unfortunately SAMMY does not have the capability of including reciprocal data in the same evaluation (using the same resonance parameters). SAMMY was designed with the intent of treating one incident particle (originally a neutron) and many different types of nuclides within the target. Other codes (e.g., EDA [GH75]) were designed with a different philosophy: to simultaneously treat all interactions leading to the same compound nucleus. Eventually the SAMMY author hopes to add similar capabilities to the SAMMY code.

Meanwhile, two alternatives are available: (1) The SAMMY user can convert the data using reciprocal relationships, and include the converted data within his or her evaluation. (2) If there is no need for simultaneous* fitting, resonance parameter values can be converted to those appropriate for the reciprocal reaction. Either of these two can be accomplished by application of the principle of detailed balance.

To convert the cross section from the $A'(a',a)A$ reaction to the $A(a,a')A'$ reaction, we first consider the center-of-mass (COM) system, in which the energies are easily related by

$$E_{COM} = E'_{COM} - Q \quad . \tag{II C5.1}$$

Elementary kinematics (as illustrated in Figure II C5.1) gives the conversion to the laboratory values E and E',

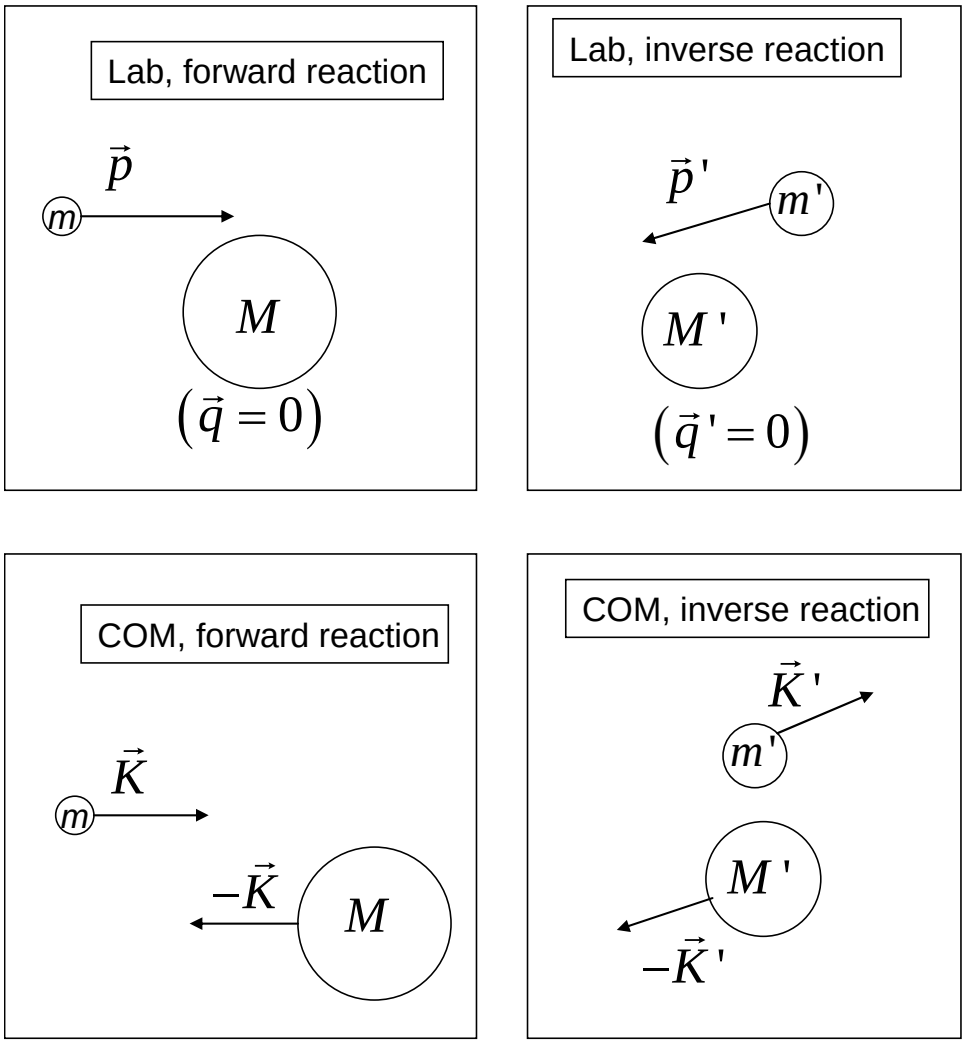
$$E_{COM} = \frac{M}{m+M} E \quad , \qquad E'_{COM} = \frac{M'}{m'+M'} E' \quad , \qquad Q = -\frac{M}{m+M} \Xi_{lab} \quad , \tag{II C5.2}$$

and algebra then gives

$$E' = \left(E - \Xi_{lab}\right) \frac{M}{m+M} \frac{m'+M'}{M'} \quad . \tag{II C5.3}$$

* By "simultaneous" is meant either (1) truly simultaneous or (2) "sequential using the covariance matrix from one SAMMY run fitting one data set as input to another run fitting another data set." See Section IV of this manual for details of both possibilities.

Figure II C5.1. Schematic of kinematics for inverse reactions.



The R-matrix for the $A'(a',a)A$ system must have the same value (at comparable energies) as the R-matrix for the $A(a,a')A'$ system. Hence

$$
\begin{aligned}
R'_{cc''} &= \sum_{\lambda} \frac{\gamma'_{\lambda c}\gamma'_{\lambda c''}}{E'_{\lambda} - E' - i\Gamma'_{\lambda\gamma}/2} \\
&= \sum_{\lambda} \frac{\gamma'_{\lambda c}\gamma'_{\lambda c''}}{E'_{\lambda} - \left[\left(E - \Xi_{lab}\right)\dfrac{M}{m+M}\dfrac{m'+M'}{M'}\right] - i\Gamma'_{\lambda\gamma}/2} = \sum_{\lambda} \frac{\gamma_{\lambda c}\gamma_{\lambda c''}}{E_{\lambda} - E - i\Gamma_{\lambda\gamma}/2} = R_{cc''} \quad .
\end{aligned}
\tag{II C5.4}
$$

In order for the equality on the bottom line of Eq. (II C5.4) to hold, the unprimed resonance parameters must be defined as follows:

$$E_\lambda = E'_\lambda\, q + \Xi_{lab} \quad , \qquad \Gamma_{\lambda c} = \Gamma'_{\lambda c}\, q \quad , \qquad \gamma_{\lambda c} = \gamma'_{\lambda c}\sqrt{q} \quad , \tag{II C5.5}$$

where

$$q = \left[\frac{m+M}{M}\right]\left[\frac{M'}{m'+M'}\right] \tag{II C5.6}$$

(for c = any channel, for example neutron, fission, or capture). These equations may be used to convert the resonance parameters.

To convert the experimental data, recall that there is a multiplicative kinematic factor of $1/K^2$, where K is the momentum of the incident particle in the COM frame. For $A'(a',a)A$, this term is

$$\frac{1}{K'^2} = \frac{(m'+M')^2}{2m'(M')^2 E'} \quad , \tag{II C5.7}$$

and for $A(a,a')A'$, the term is

$$\frac{1}{K^2} = \frac{(m+M)^2}{2mM^2 E} \quad . \tag{II C5.8}$$

The experimental cross sections must be multiplied by the ratio of these two values, and appropriate energy substitutions made.

Another multiplicative factor that must be adjusted is the spin statistical factor, which also reflects the parameters of the incident channel. Since the compound nuclear spin J is the same in either system, the correct multiplier is the ratio of the two:

$$\frac{g_{J:A(aa')A'}}{g_{J:A'(a'a)A}} = \frac{(2i'+1)(2I'+1)}{(2i+1)(2I+1)} \quad . \tag{II C5.9}$$

With these changes, the cross section for the $A(a,a')A'$ reaction may be written in terms of the cross section for the $A'(a',a)A$ reaction as

$$\sigma_{A(aa')A'}(E) = \frac{(2i'+1)(2I+1)}{(2i+1)(2I+1)}\frac{m'M'^2}{mM^2}\frac{(m+M)^2}{(m'+M')^2}\frac{E'}{E}\sigma_{A'(a'a)A}(E') \quad . \tag{II C5.10}$$

II.D. DERIVATIVES

In order to make use of sophisticated fitting procedures such as Bayes' equations (Section IV of this manual), it is necessary to know the partial derivatives of the theory with respect to the parameters to be fitted (the "varied parameters"). The easiest method for calculating derivatives of cross sections with respect to resonance parameters is to use a numerical difference approximation, of the form

$$\frac{\partial\sigma}{\partial P} \approx \frac{\sigma\left(P+\Delta P\right)-\sigma\left(P\right)}{\Delta P} \quad , \tag{II D.1}$$

or, to avoid problems from the asymmetry of that approximation,

$$\frac{\partial\sigma}{\partial P} \approx \frac{\sigma\left(P+\Delta P\right)-\sigma\left(P-\Delta P\right)}{2\Delta P} \quad . \tag{II D.2}$$

Numerical methods, however, are neither as accurate nor as efficient or rapid as analytic derivatives. For that reason, SAMMY uses analytic derivatives wherever possible. In particular, derivatives of cross sections with respect to resonance parameters are all calculated analytically.

To reiterate: SAMMY does NOT use numerical derivatives of the form (II D.1). When a numerical derivative is absolutely necessary, the form (II D.2) is used. <u>For R-matrix parameters, analytic derivatives are always used</u>. (The only exception to this rule is for charged-particle shift factors and penetrabilities, for which calculations of both the functions and the derivatives require numerical techniques.)

The R-matrix equations are expressed in terms of the reduced-width amplitude γ rather than the partial width Γ. In the SAMMY code, the amplitudes are the parameters to be varied. In general, SAMMY distinguishes between "*u*-parameters" and "*p*-parameters": The *u*-parameter is the variable whose value is sought by the fitting procedure. The *p*-parameter is the parameter whose value is given in the SAMMY input and output files. There is a well-defined relationship between the two, but the relationship is not necessarily one to one. For example, the value for the neutron width specified in the input PARameter file (see Table VI B.2 in Section VI.B) is related to three parameters, any or all of which might be varied:

$$\Gamma_{\lambda n} = 2P_l(\rho)\gamma_{\lambda n}^2 \quad ,$$

$$\rho_\lambda = k_\lambda a_n \quad , \tag{II D.3}$$

and

$$\hbar k_\lambda = \frac{M}{m+M}\sqrt{2mE_\lambda} \quad .$$

Here γ_λ, a_n, and E_λ all may be varied parameters. In the SAMMY input, varied parameters are indicated by a flag, whose value (0, 1, or 3) indicates how that parameter is to be treated. The

convention is that a flag on Γ denotes the status of the γ parameter, because the other two (the radius and the energy) are separately flagged.

Throughout this document, when the varied *u*-parameter is different from the flagged *p*-parameter, the equations relating the two are given explicitly. For the R-matrix (in all its various guises), the *u*-parameter associated with the resonance energy is

$$u\left(E_\lambda\right) = \pm\sqrt{\left|E_\lambda\right|} \quad , \tag{II D.4}$$

where the negative sign is chosen if E_λ is negative, and the *u*-parameter associated with the width is

$$u\left(\Gamma_{\lambda c}\right) = \gamma_{\lambda c} \quad . \tag{II D.5}$$

In the following sections, equations are given for the derivatives of the cross section with respect to the R-matrix parameters for the Reich-Moore approximation (Section II.D.1) and for the Breit-Wigner approximations (Section II.D.2). Additional details are in Section II.D.3.

II.D.1. Derivatives for Reich-Moore Approximation

The derivative of the cross section with respect to a resonance parameter is found by making use of the chain rule:

$$\frac{\partial \sigma}{\partial u_i} = \sum_{\substack{\mu \le \nu \\ \omega \le \tau}} \frac{\partial R_{\mu\nu}}{\partial u_i} \frac{\partial W_{\omega\tau}}{\partial R_{\mu\nu}} \frac{\partial U_{\omega\tau}}{\partial W_{\omega\tau}} \frac{\partial \sigma}{\partial U_{\omega\tau}} \quad , \qquad \text{(II D1.1)}$$

where the index J has been suppressed, since it is fixed for a given parameter u. Each term in this expression is evaluated separately.

Derivatives of cross sections with respect to the scattering matrix U, derivatives of U with respect to W, and derivatives of W with respect to R are found in Section II.D.1.a. Derivatives of R with respect to resonance parameters are given in Section II.D.1.b.

Derivatives of the cross sections with respect to the channel radius require additional terms beyond those in Eq. (II D1.1), because the radius is also used to determine the hard-sphere phase shift. These derivatives are discussed in Section II.D.1.c.

Derivatives of R with respect to the variables of the logarithmic parameterization of the external R-function (defined in Section II.B.1.d) are given in Section II.D.1.d.

II.D.1.a. Derivatives with respect to R-matrix

For resonance and R^{ext} parameters, the derivative of the cross section may be written as

$$\frac{\partial \sigma}{\partial u_i} = \sum_{\substack{c \le d \\ e \le f}} \frac{\partial R_{cd}}{\partial u_i} \frac{\partial W_{ef}}{\partial R_{cd}} \frac{\partial U_{ef}}{\partial W_{ef}} \frac{\partial \sigma}{\partial U_{ef}} \quad , \qquad \text{(II D1 a.1)}$$

where the index J has been suppressed, since it is fixed for a given parameter u. Indices c, d, e, and f denote channels. The restriction $c \le d$ indicates that the sum includes, for example, only terms with indices $c_1 c_2$ and not terms with indices $c_2 c_1$ (for $c_1 \ne c_2$); this restriction results from the symmetry of R and W (or X) with respect to interchange of indices.

Each term in the expression (II D1 a.1) will be evaluated separately, starting with the right-most term. All except $\partial R / \partial u$ are evaluated in this section; $\partial R / \partial u$ is discussed in subsequent sections.

The derivatives of cross section with respect to the real part of U can be expressed as

$$\frac{\partial \sigma}{\partial U^r} = \frac{\partial \sigma}{\partial U}\frac{\partial U}{\partial U^r} + \frac{\partial \sigma}{\partial U^*}\frac{\partial U^*}{\partial U^r} = \frac{\partial \sigma}{\partial U} + \frac{\partial \sigma}{\partial U^*} = 2\,\mathrm{Re}\left[\frac{\partial \sigma}{\partial U}\right] \quad , \qquad \text{(II D1 a.2)}$$

where the asterisk implies complex conjugate, and U and U^* are treated as independent entities. Similarly the derivative with respect to the imaginary part of U is given by

$$\frac{\partial \sigma}{\partial U^i} = \frac{\partial \sigma}{\partial U}\frac{\partial U}{\partial U^i} + \frac{\partial \sigma}{\partial U^*}\frac{\partial U^*}{\partial U^i} = i\frac{\partial \sigma}{\partial U} - i\frac{\partial \sigma}{\partial U^*} = -2\,\mathrm{Im}\left[\frac{\partial \sigma}{\partial U}\right] \quad . \qquad \text{(II D1 a.3)}$$

It follows that the derivative of the cross section with respect to U can be written as

$$\frac{\partial \sigma}{\partial U} = \mathrm{Re}\left[\frac{\partial \sigma}{\partial U}\right] + i\,\mathrm{Im}\left[\frac{\partial \sigma}{\partial U}\right] = \frac{1}{2}\left(\frac{\partial \sigma}{\partial U^r} - i\frac{\partial \sigma}{\partial U^i}\right) \quad . \qquad \text{(II D1 a.4)}$$

Using Eq. (II D1 a.4), values for the partial derivative of σ with respect to U are found from Eqs. (II A.8) to (II A.11), which give

$$\frac{\partial \sigma^{total}}{\partial U_{ef}} = -\frac{\pi g}{k^2}\delta_{ef} \quad , \qquad \text{(II D1 a.5)}$$

$$\frac{\partial \sigma_{\alpha\alpha}}{\partial U_{ef}} = -\frac{\pi g}{k^2}\left(\delta_{ef} - U^*_{ef}\right) \quad , \qquad \text{(II D1 a.6)}$$

$$\frac{\partial \sigma_{\alpha\alpha'}}{\partial U_{ef}} = \frac{\pi g}{k^2} U^*_{ef} \qquad \text{for } \alpha' \neq \alpha, \tag{II D1 a.7}$$

and

$$\frac{\partial \sigma^{capture}}{\partial U_{ef}} = -\frac{\pi g}{k^2} U^*_{ef} \quad . \tag{II D1 a.8}$$

Derivatives of a complex variable (such as U) with respect to another complex variable (such as W) may be generated directly, without separately considering the real and imaginary parts of each variable; this is demonstrated explicitly in Section II.D.3. Here, we make use of this result to evaluate $\partial U / \partial W$ and $\partial W / \partial R$.

Derivatives of U_{ef} with respect to W_{ef} are formed directly from Eq. (II A.4), which may be expressed as

$$U_{ef} = \Omega_e W_{ef} \Omega_f \quad , \tag{II D1 a.9}$$

so that

$$\frac{\partial U_{ef}}{\partial W_{ef}} = \Omega_e \Omega_f \quad . \tag{II D1 a.10}$$

Derivatives of W with respect to R are formed from Eqs. (II B1.3) and (II B1.4), which we rewrite as

$$\begin{aligned} W = I + 2iX &= I + 2i\left(\sqrt{P} L^{-1}\left(L^{-1} - R\right)^{-1} R\sqrt{P}\right) \\ &= I + 2i\sqrt{P} L^{-1}\left(L^{-1} - R\right)^{-1}\left[R - L^{-1} + L^{-1}\right]\sqrt{P} \\ &= I + 2i\sqrt{P} L^{-1}\left(L^{-1} - R\right)^{-1}\left[R - L^{-1}\right]\sqrt{P} + 2i\sqrt{P} L^{-1}\left(L^{-1} - R\right)^{-1}\left[L^{-1}\right]\sqrt{P} \\ &= I - 2i\sqrt{P} L^{-1}\sqrt{P} + 2i\sqrt{P} L^{-1}\left(L^{-1} - R\right)^{-1} L^{-1}\sqrt{P} \quad . \end{aligned} \tag{II D1 a.11}$$

Explicitly displaying the indices, Eq. (II D1 a.11) takes the form

$$W_{ef} = I - 2i\delta_{ef} P_e L_f^{-1} + 2i\sqrt{P_e}\, L_e^{-1} Y_{ef}\, L_f^{-1} \sqrt{P_f} \quad , \tag{II D1 a.12}$$

where we have set

$$Y_{ef} = \left[\left(L^{-1} - R\right)^{-1}\right]_{ef} \quad . \tag{II D1 a.13}$$

In [NL80, Appendix A] and also in Section II.D.3 of this manual, we show that the derivative of Y with respect to R is given by

$$\frac{\partial Y_{ef}}{\partial R_{cd}} = Y_{ec} Y_{df} + Y_{ed} Y_{cf} \left(1 - \delta_{cd}\right) \quad . \qquad \text{(II D1 a.14)}$$

Substitution of this expression into the derivative of Eq. (II D1 a.12) gives

$$\frac{\partial W_{ef}}{\partial R_{cd}} = 2i \sqrt{P_e}\, L_e^{-1} \left[Y_{ec} Y_{df} + Y_{ed} Y_{cf} \left(1 - \delta_{cd}\right) \right] L_f^{-1} \sqrt{P_f} \quad . \qquad \text{(II D1 a.15)}$$

Alternatively, we may write

$$\frac{\partial X_{ef}}{\partial R_{cd}} = \sqrt{P_e}\, L_e^{-1} \left[Y_{ec} Y_{df} + Y_{ed} Y_{cf} \left(1 - \delta_{cd}\right) \right] L_f^{-1} \sqrt{P_f} \quad , \qquad \text{(II D1 a.16)}$$

which is the more practically useful form in SAMMY.

Derivatives of R with respect to u depend upon which particular u-parameter is being considered. Parameters of the external R-matrix, resonance parameters, and channel radii are described in the next subsections.

II.D.1.b. Derivatives with respect to resonance parameters

From Eq. (II B1.1), the derivatives of the real and imaginary part of R with respect to the resonance u-parameter associated with the resonance energy are

$$\frac{\partial \operatorname{Re}\left[R_{\mu\nu}\right]}{\partial\sqrt{E_\lambda}} = \left[2\,\gamma_{\lambda\mu}\,\gamma_{\lambda\nu}\sqrt{E_\lambda}\right]\left[\left\{-\left(E_\lambda - E\right)^2 + \left(\overline{\gamma}_{\lambda\gamma}^2\right)^2\right\}/\,d_\lambda^2\right] \qquad \text{(II D1 b.1)}$$

and

$$\frac{\partial \operatorname{Im}\left[R_{\mu\nu}\right]}{\partial\sqrt{E_\lambda}} = \left[-4\,\gamma_{\lambda\mu}\,\gamma_{\lambda\nu}\sqrt{E_\lambda}\right]\left[\left\{\left(E_\lambda - E\right)\overline{\gamma}_{\lambda\gamma}^2\right\}/\,d_\lambda^2\right] \quad . \qquad \text{(II D1 b.2)}$$

The derivatives of R with respect to the u-parameter associated with the eliminated capture width can be written as

$$\frac{\partial \operatorname{Re}\left[R_{\mu\nu}\right]}{\partial\overline{\gamma}_{\lambda\gamma}} = \left[-4\,\gamma_{\lambda\mu}\,\gamma_{\lambda\nu}\,\overline{\gamma}_{\lambda\gamma}\right]\left[\left\{\left(E_\lambda - E\right)\overline{\gamma}_{\lambda\gamma}^2\right\}/\,d_\lambda^2\right] \qquad \text{(II D1 b.3)}$$

and

$$\frac{\partial \operatorname{Im}\left[R_{\mu\nu}\right]}{\partial\overline{\gamma}_{\lambda\gamma}} = \left[2\,\gamma_{\lambda\mu}\,\gamma_{\lambda\nu}\,\overline{\gamma}_{\lambda\gamma}\right]\left[\left\{\left(E_\lambda - E\right)^2 - \left(\overline{\gamma}_{\lambda\gamma}^2\right)^2\right\}/\,d_\lambda^2\right] \quad . \qquad \text{(II D1 b.4)}$$

The derivatives for the particle widths are

$$\frac{\partial \operatorname{Re}\left[R_{\mu\nu}\right]}{\partial\gamma_{\lambda\mu}} = \left[\gamma_{\lambda\nu}\left(1+\delta_{\mu\nu}\right)\right]\left[\left(E_\lambda - E\right)/\,d_\lambda\right] \qquad \text{(II D1 b.5)}$$

and

$$\frac{\partial \operatorname{Im}\left[R_{\mu\nu}\right]}{\partial\gamma_{\lambda\mu}} = \left[\gamma_{\lambda\nu}\left(1+\delta_{\mu\nu}\right)\right]\left[\overline{\gamma}_{\lambda\gamma}^2/\,d_\lambda\right] \quad . \qquad \text{(II D1 b.6)}$$

In the expressions above, the denominator term d is defined as

$$d_\lambda = \left(E_\lambda - E\right)^2 + \overline{\gamma}_{\lambda\gamma}^{\,4} \quad . \qquad \text{(II D1 b.7)}$$

In each of these equations, the first square bracket contains an energy-independent factor; in the code SAMMY, this factor (times 2) is evaluated outside the energy loop in subroutine BABB and is stored as BR($\mu\nu$,i) for the derivative of the real part of $R_{\mu\nu}$ with respect to the ith parameter, and BI($\mu\nu$,i) for the derivative of the imaginary part of $R_{\mu\nu}$. The quantity in the second square bracket is energy dependent but channel independent. Therefore, it must be generated for each energy and is temporarily stored as UPR(i) and UPI(i) in subroutine ABPART.

To avoid problems arising from the computer's limited precision, and to minimize computing time, partial derivatives for non-*s*-wave ($l > 0$) resonances are truncated to zero far away from the resonance. The working definition of "far away" is 20 times the sum of the partial widths for that resonance, plus 3 times the sum of the Doppler- and resolution-broadening widths, that is, far beyond the region where a resonance can produce any noticeable effect. Specifically, the derivative of the cross section at energy E is set to zero for resonance level λ, if

$$\left|E - E_\lambda\right| > 20\left[\sum_c \Gamma_{\lambda c} + \bar{\Gamma}_{\lambda\gamma}\right] + 3\left(D + r\right) \qquad \text{(II D1 b.8)}$$

for resonances with $l > 0$, where D represents the Doppler and r the resolution width. Moreover, the contribution to the imaginary part of R is set to zero whenever the distance from level λ is greater than 100 times that specified in Eq. (II D1 b.8). (The contribution to the *real* part of R is never assumed to be negligible.)

For s-wave resonances ($l = 0$), the user has the option of setting derivatives equal to zero beyond a certain distance, where the distance is twice that specified for non-*s*-waves. To invoke this option, include the command USE S-WAVE CUTOFF in the INPut file.

CAUTION: Though the cross-section segment in SAMMY may run slightly faster with the cutoff option invoked, results will not be as accurate. Use of this option is not encouraged.

II.D.1.c. Derivatives with respect to channel radius

Derivatives with respect to channel radius a require modification of the procedure outlined in Section II.D.1.b, since phase shifts φ and penetrabilities P also depend on channel radius (sometimes called "matching radius"). All dependence on a is via ρ, where

$$\rho = k\,a \quad , \tag{II D1 c.1}$$

and momentum $\hbar k$ in the center-of-mass reference frame is described in Section II.C.2; k is the wave number in units of inverse length. The derivative of the cross section with respect to the radius can be written

$$\frac{\partial\sigma}{\partial a} = \frac{\partial\sigma}{\partial\rho}\frac{\partial\rho}{\partial a} = k\frac{\partial\sigma}{\partial\rho} \quad . \tag{II D1 c.2}$$

Our problem therefore reduces to finding $\partial\sigma/\partial\rho$.

The derivative of the cross section with respect to ρ may be formed from Eq. (II A.1):

$$\begin{aligned}\frac{\partial\sigma_{cc'}}{\partial\rho} &= \frac{\pi}{k_c^2}g_c\left[\left(\delta_{cc'}-U_{cc'}\right)\frac{\partial U^*_{cc'}}{\partial\rho} + \left(\delta_{cc'}-U^{J*}_{cc'}\right)\frac{\partial U_{cc'}}{\partial\rho}\right] \\ &= \frac{2\pi}{k_c^2}g_c\left[\delta_{cc'}\frac{\partial\,\mathrm{Re}\left(U_{cc'}\right)}{\partial\rho} - \mathrm{Re}\left(U^{J*}_{cc'}\frac{\partial U_{cc'}}{\partial\rho}\right)\right] \quad .\end{aligned} \tag{II D1 c.3}$$

From the definitions of Ω and φ, Eqs. (II A.4) and (II A.5), the partial of U with respect to ρ may be written as

$$\frac{\partial U_{cc'}}{\partial\rho} = -i\frac{\partial\varphi_c}{\partial\rho}U_{cc'} + \Omega_c\frac{\partial W_{cc'}}{\partial\rho}\Omega_{c'} - i\,U_{cc'}\frac{\partial\varphi_{c'}}{\partial\rho} \quad . \tag{II D1 c.4}$$

Equation (II D1 c.3) can therefore be written as

$$\begin{aligned}\frac{\partial\sigma_{cc'}}{\partial\rho} = \frac{2\pi}{k_c^2}g_c\Bigg\{&\delta_{cc'}\,\mathrm{Re}\left(-2i\frac{\partial\varphi_c}{\partial\rho}U_{cc}+\Omega_c^2\frac{\partial W_{cc}}{\partial\rho}\right) \\ &-\mathrm{Re}\left(U^*_{cc'}\left[-i\left(\frac{\partial\varphi_c}{\partial\rho}+\frac{\partial\varphi_{c'}}{\partial\rho}\right)U^J_{cc'}+\Omega_c\frac{W_{cc'}}{\partial\rho}\Omega_{c'}\right]\right)\Bigg\} \quad ,\end{aligned} \tag{II D1 c.5}$$

or

$$\frac{\partial \sigma_{cc'}}{\partial \rho} = \frac{2\pi}{k_c^2} g_c \left\{ \delta_{cc'} \operatorname{Re}\left(-2i \frac{\partial \varphi_c}{\partial \rho} U_{cc}^J + \Omega_c^2 \frac{\partial W_{cc}}{\partial \rho} \right) \right.$$
$$\left. - \operatorname{Re}\left(\Omega_c^* W_{cc'}^* \Omega_{c'}^* \left[-i \left(\frac{\partial \varphi_c}{\partial \rho} + \frac{\partial \varphi_{c'}}{\partial \rho} \right) \Omega_c W_{cc'} \Omega_{c'} + \Omega_c \frac{W_{cc'}}{\partial \rho} \Omega_{c'} \right] \right) \right\} \quad . \tag{IID1c.6}$$

Because $\Omega_c \, \Omega^*_c = 1$, this simplifies to the form

$$\frac{\partial \sigma_{cc'}}{\partial \rho} = \frac{2\pi}{k_c^2} g_c \operatorname{Re}\left\{ \delta_{cc'} \Omega_c^2 \left(-2i \frac{\partial \varphi_c}{\partial \rho} W_{cc} + \frac{\partial W_{cc}}{\partial \rho} \right) \right.$$
$$\left. - \left(W_{cc'}^* \left[-i \left(\frac{\partial \varphi_c}{\partial \rho} + \frac{\partial \varphi_{c'}}{\partial \rho} \right) W_{cc'} + \frac{\partial W_{cc'}}{\partial \rho} \right] \right) \right\} \quad . \tag{II D1 c.7}$$

Derivatives of hard-sphere phase shifts φ are formed by direct differentiation of the formulae in Table II A.1 for non-Coulomb and of the equations in Section II.C.4 for Coulomb.

The derivatives of W are found in similar fashion to the derivatives with respect to resonance parameters, beginning with Eq. (II D1 a.11):

$$\begin{aligned}
\frac{\partial W_{cc'}}{\partial \rho} = & -2i\,\delta_{cc'}\, L_c^{-1} \frac{\partial P_c}{\partial \rho} + 2i\delta_{cc'}\, P_c\, L_c^{-2} \left(\frac{\partial S_c}{\partial \rho} + i \frac{\partial P_c}{\partial \rho} \right) \\
& + 2i \frac{\partial P_c}{\partial \rho} \frac{1}{2\sqrt{P_c}} L_c^{-1} \left[\left(L^{-1} - R \right)^{-1} \right]_{cc'} L_{c'}^{-1} \sqrt{P_{c'}} \\
& + 2i \sqrt{P_c} \left(-L_c^{-2} \right) \left(\frac{\partial S_c}{\partial \rho} + i \frac{\partial P_c}{\partial \rho} \right) \left[\left(L^{-1} - R \right)^{-1} \right]_{cc'} L_{c'}^{-1} \sqrt{P_{c'}} \\
& + 2i \sqrt{P_c}\, L_c^{-1} \left[\left(L^{-1} - R \right)^{-1} \right]_{cc'} \left(\frac{\partial S_{c'}}{\partial \rho} + i \frac{\partial P_{c'}}{\partial \rho} \right) \left(L_{c'}^{-2} \right) \sqrt{P_{c'}} \\
& + 2i \sqrt{P_c} L_c^{-1} \left[\left(L^{-1} - R \right)^{-1} \right]_{cc'} L_{c'}^{-1} \frac{\partial P_{c'}}{\partial \rho} \frac{1}{2\sqrt{P_{c'}}} \\
& + 2i \sum_{c''} \sqrt{P_c} L_c^{-1} \left[\left(L^{-1} - R \right)^{-1} \right]_{cc''} L_{c''}^{-1} \left(\frac{\partial S_{c''}}{\partial \rho} + i \frac{\partial P_{c''}}{\partial \rho} \right) \\
& \qquad \times L_{c''}^{-1} \left[\left(L^{-1} - R \right)^{-1} \right]_{c''c'} L_{c'}^{-1} \sqrt{P_{c'}} \quad .
\end{aligned} \tag{II D1 c.8}$$

This expression can be greatly simplified by setting

$$\vartheta_{cc'} = \sqrt{P_c}\, L_c^{-1} \left[\left(L^{-1} - R \right)^{-1} \right]_{cc'} L_{c'}^{-1} \sqrt{P_{c'}} - P_c L_c^{-1} \delta_{cc'} \quad , \qquad \text{(II D1 c.9)}$$

which gives

$$\begin{aligned} \frac{\partial W_{cc'}^{J}}{\partial \rho} \; = \; + \; i \; \frac{\partial P_c}{\partial \rho} \; \frac{1}{P_c} \vartheta_{cc'} \; + \; i \; \vartheta_{cc'} \; \frac{1}{P_{c'}} \; \frac{\partial P_{c'}}{\partial \rho} \\ + \; 2 i \sum_{c''} \vartheta_{cc''} P_{c''}^{-1} \left(\frac{\partial S_{c''}}{\partial \rho} + i \frac{\partial P_{c''}}{\partial \rho} \right) \vartheta_{c''c'} \quad . \end{aligned} \qquad \text{(II D1 c.10)}$$

Derivatives of penetrabilities P_c and shift factors S_c are found by direct differentiation of the formulae in Table II A.1 for non-Coulomb and Section II.C.4 for Coulomb. Derivatives of the cross sections with respect to ρ are then found by substituting results from Eq. (II D1 c.10) into Eq. (II D1 c.7).

II.D.1.d. Derivatives of logarithmic external R-function

Derivatives of R^{ext} with respect to the u-parameters are found from Eqs. (II B1 d.1) and (II B1 d.2) to be of the form

$$\frac{\partial R_c^{ext}}{\partial E_c^{up}} = -\frac{s_{con,c} + s_{lin,c}\, E_c^{up}}{E_c^{up} - E} \quad , \qquad \text{(II D1 d.1)}$$

$$\frac{\partial R_c^{ext}}{\partial E_c^{down}} = -\frac{s_{con,c} + s_{lin,c}\, E_c^{down}}{E - E_c^{down}} \quad , \qquad \text{(II D1 d.2)}$$

$$\frac{\partial R_c^{ext}}{\partial \bar{R}_{con,c}} = 1 \quad , \qquad \text{(II D1 d.3)}$$

$$\frac{\partial R_c^{ext}}{\partial \bar{R}_{lin,c}} = E \quad , \qquad \text{(II D1 d.4)}$$

$$\frac{\partial R_c^{ext}}{\partial \bar{R}_{q,c}} = E^2 \quad , \qquad \text{(II D1 d.5)}$$

$$\frac{\partial R_c^{ext}}{\partial \sqrt{s_{con,c}}} = -2\sqrt{s_{con,c}}\, \ln\left[\frac{E_c^{up} - E}{E - E_c^{down}}\right] \quad , \qquad \text{(II D1 d.6)}$$

and

$$\frac{\partial R_c^{ext}}{\partial s_{lin,c}} = -\left(E_c^{up} - E_c^{down}\right) - E\, \ln\left[\frac{E_c^{up} - E}{E - E_c^{down}}\right] \quad . \qquad \text{(II D1 d.7)}$$

II.D.1.e. Derivatives with respect to *p*-parameters

As described in Section II.B.1, internally SAMMY operates in terms of the *u*-parameters, these being the parameters whose values are to be fitted via Bayes' equations (see Section IV). The *u*-parameters are related, but not necessarily equal, to the parameters whose values are given in the INPut and/or PARameter files, which are denoted as *p*-parameter.

When only the SAMMY code is used for calculations, there is no confusion arising from switching between *u*- and *p*-parameters. The transformation from *u*- to *p*-parameters also poses no difficulties in communicating parameter *values* between SAMMY and other codes (e.g., via ENDF files). However, in communicating uncertainty, covariance, or sensitivity (partial derivative) information, care must be taken to ensure that transformations are properly made.

In particular, the transformations involving the resonance energy and the partial widths must be calculated carefully.* The *p*-parameter for a particle width Γ, for example, is related to the corresponding *u*-parameter γ via the transformation [see Eq. (II B1.7)]

$$u_{\Gamma_{\lambda c}} = \gamma_{\lambda c} = \pm \sqrt{\frac{\Gamma_{\lambda c}}{2P_l\left(\left|E_\lambda - \Xi_c\right|\right)}} \quad , \qquad \text{(II D1 e.1)}$$

where P in this equation is the penetrability (with the appropriate angular momentum l for this channel) evaluated at E_λ, the energy of the resonance.

From Eqs. (II A.8) and (II A.9), P has the form

$$P_l = P_l(\rho) \quad \text{with} \quad \rho = \beta\, a_c \sqrt{\left(\left|E_\lambda - \Xi\right|\right)} \quad , \qquad \text{(II D1 e.2)}$$

in which β is a mass factor given explicitly in Eq. (II A.9), a_c is the channel radius, and Ξ represents the threshold energy. The ± sign in Eq. (II D1 e.1) is as given in the PARameter file (Table VI B.2). E_λ is another *p*-parameter, for which the corresponding *u*-parameter is

$$u_{E_\lambda} = \begin{cases} \sqrt{E_\lambda} & \text{for } E_\lambda > 0 \\ -\sqrt{-E_\lambda} & \text{for } E_\lambda < 0 \end{cases} \quad , \qquad \text{(II D1 e.3)}$$

from Eq. (II B1.6).

In the following discussion, most subscripts are omitted, for simplicity's sake. Equations for negative-energy resonances are indicated within square brackets.

---

* In early versions of SAMMY, these transformations were done incorrectly. These mistakes have been corrected in release R7 of this manual and in sammy-7.0.0 and subsequent releases of the code.

Consider a function f of the two u-parameters γ and u (which we take to be the u-parameter associated with the resonance energy). This function might be the cross section, or some other function such as transmission or average cross section. The equations of transformation to the two p-parameters Γ and E_λ are given above. The derivatives of f with respect to the p-parameters are therefore

$$\frac{\partial f}{\partial \Gamma} = \frac{\partial \gamma}{\partial \Gamma}\frac{\partial f}{\partial \gamma} + \frac{\partial u}{\partial \Gamma}\frac{\partial f}{\partial u} \qquad \text{(II D1 e.4)}$$

and

$$\frac{\partial f}{\partial E_\lambda} = \frac{\partial \gamma}{\partial E_\lambda}\frac{\partial f}{\partial \gamma} + \frac{\partial u}{\partial E_\lambda}\frac{\partial f}{\partial u} \quad . \qquad \text{(II D1 e.5)}$$

The partial derivatives of the u-parameters with respect to the p-parameter Γ can readily be found from Eqs. (II D1 e.1) and (II D1 e.3) as

$$\frac{\partial \gamma}{\partial \Gamma} = \pm \frac{1}{\sqrt{2P}}\frac{1}{2}\Gamma^{-1/2} = \pm \frac{1}{2}\sqrt{\frac{\Gamma}{2P}}\frac{1}{\Gamma} = \frac{\gamma}{2\Gamma} \quad , \qquad \text{(II D1 e.6)}$$

and

$$\frac{\partial u}{\partial \Gamma} = 0 \quad . \qquad \text{(II D1 e.7)}$$

The derivative of u with respect to E_λ is relatively straight forward:

$$\frac{\partial u}{\partial E_\lambda} = \frac{1}{2}E_\lambda^{-1/2} = \frac{1}{2u} = \frac{u}{2E_\lambda}$$
$$\left[\frac{\partial u}{\partial E_\lambda} = \frac{1}{2}\left(-E_\lambda\right)^{-1/2} = -\frac{1}{2u} = \frac{u}{2E_\lambda} \quad \text{if } E_\lambda < 0\right]. \qquad \text{(II D1 e.8)}$$

The derivative of γ with respect to E_λ is somewhat more complicated, having the form

$$\frac{\partial \gamma}{\partial E_\lambda} = \pm\sqrt{\frac{\Gamma}{2}}\left(-\frac{1}{2}\right)P^{-3/2}\frac{dP}{d\rho}\frac{\partial \rho}{\partial E_\lambda} = \mp\frac{1}{2}\sqrt{\frac{\Gamma}{2P}}\frac{P'}{P}\frac{\partial \rho}{\partial E_\lambda} = -\frac{\gamma P'}{2P}\frac{\partial \rho}{\partial E_\lambda} \quad , \text{(II D1 e.9)}$$

in which we have defined P' to be $dP/d\rho$. From Eq. (II D1 e.2), for $E_\lambda > \Xi$, it follows that

$$\frac{\partial \gamma}{\partial E_\lambda} = -\frac{\gamma P'}{2P}\frac{\beta a}{2\sqrt{\left(E_\lambda - \Xi\right)}} = -\frac{\gamma P'}{4P}\frac{\rho}{\left(E_\lambda - \Xi\right)} \quad . \qquad \text{(II D1 e.10)}$$

Similarly, for $E_\lambda < \Xi$, we find

$$\frac{\partial \gamma}{\partial E_\lambda} = -\frac{\gamma P'}{2P}\frac{\partial}{\partial E_\lambda}\beta a\sqrt{-\left(E_\lambda - \Xi\right)} = -\frac{\gamma P'}{2P}\frac{\beta a(-1)}{2\sqrt{-\left(E_\lambda - \Xi\right)}}$$
$$= +\frac{\gamma P'}{4P}\frac{\beta a\sqrt{-\left(E_\lambda - \Xi\right)}}{-\left(E_\lambda - \Xi\right)} = -\frac{\gamma P'}{4P}\frac{\rho}{\left(E_\lambda - \Xi\right)} \quad . \qquad \text{(II D1 e.11)}$$

Equations (II D1 e.4) and (II D1 e.5) can therefore be rewritten as

$$\frac{\partial f}{\partial \Gamma} = \frac{\gamma}{2\Gamma}\frac{\partial f}{\partial \gamma} + 0 \qquad \text{(II D1 e.12)}$$

and

$$\frac{\partial f}{\partial E_\lambda} = -\frac{\gamma P'}{4P}\frac{\rho}{\left(E_\lambda - \Xi\right)}\frac{\partial f}{\partial \gamma} + \frac{u}{2E_\lambda}\frac{\partial f}{\partial u} \quad . \qquad \text{(II D1 e.13)}$$

Similarly, if the function *f* is defined in terms of *p*-parameters, the derivatives of *f* with respect to the *u*-parameters are given by

$$\frac{\partial f}{\partial \gamma} = \frac{\partial \Gamma}{\partial \gamma}\frac{\partial f}{\partial \Gamma} + \frac{\partial E_\lambda}{\partial \gamma}\frac{\partial f}{\partial E_\lambda} \qquad \text{(II D1 e.14)}$$

and

$$\frac{\partial f}{\partial u} = \frac{\partial \Gamma}{\partial u}\frac{\partial f}{\partial \Gamma} + \frac{\partial E_\lambda}{\partial u}\frac{\partial f}{\partial E_\lambda} \quad . \qquad \text{(II D1 e.15)}$$

That is, the inverse transformation (from *p*-space to *u*-space) requires the use of the partial derivatives of *p*-parameters with respect to the *u*-parameters. These derivatives have the form

$$\frac{\partial \Gamma}{\partial \gamma} = \pm 2P\ 2\gamma = \pm 4P\gamma = \frac{2\Gamma}{\gamma} \quad , \qquad \text{(II D1 e.16)}$$

$$\frac{\partial E_\lambda}{\partial \gamma} = 0 \quad , \qquad \text{(II D1 e.17)}$$

and

$$\frac{\partial E_\lambda}{\partial u} = 2u = \frac{2E_\lambda}{u} \qquad \left[\frac{\partial E_\lambda}{\partial u} = -2u = \frac{2E_\lambda}{u} \text{ if } E_\lambda < 0\right] \quad . \qquad \text{(II D1 e.18)}$$

The partial derivative of Γ with respect to u requires special care to evaluate correctly. For $u^2 = E_\lambda > \Xi$, this derivative has the form

$$\begin{aligned}\frac{\partial\Gamma}{\partial u} &= 2\frac{\partial P}{\partial u}\gamma^2 = \frac{2P\gamma^2}{P}\frac{dP}{d\rho}\frac{\partial\rho}{\partial u} = \Gamma\frac{P'}{P}\frac{\partial}{\partial u}\left(\beta a\sqrt{\left(u^2-\Xi\right)}\right) \\ &= \Gamma\frac{P'}{P}\frac{\beta a 2u}{2\sqrt{\left(u^2-\Xi\right)}} = \Gamma\frac{P'}{P}\frac{\beta a\sqrt{\left(u^2-\Xi\right)}\,u}{\left(E_\lambda-\Xi\right)} = \Gamma\frac{P'}{P}\frac{\rho}{\left(E_\lambda-\Xi\right)}\frac{E_\lambda}{u} \ .\end{aligned} \tag{II D1 e.19}$$

If $0 < E_\lambda = u^2 < \Xi$, this partial derivative takes the form

$$\begin{aligned}\frac{\partial\Gamma}{\partial u} &= 2\frac{\partial P}{\partial u}\gamma^2 = \frac{2P\gamma^2}{P}\frac{dP}{d\rho}\frac{\partial\rho}{\partial u} = \Gamma\frac{P'}{P}\frac{\partial}{\partial u}\left(\beta a\sqrt{-\left(u^2-\Xi\right)}\right) \\ &= \Gamma\frac{P'}{P}\frac{\beta a\left(-2u\right)}{2\sqrt{-\left(u^2-\Xi\right)}} = \Gamma\frac{P'}{P}\frac{\beta a\sqrt{-\left(u^2-\Xi\right)}\left(-u\right)}{-\left(u^2-\Xi\right)} \\ &= \Gamma\frac{P'}{P}\frac{\rho}{\left(E_\lambda-\Xi\right)}\frac{E_\lambda}{u} \ .\end{aligned} \tag{II D1 e.20}$$

[Finally, if $0 > E_\lambda = -u^2$, then

$$\begin{aligned}\frac{\partial\Gamma}{\partial u} &= 2\frac{\partial P}{\partial u}\gamma^2 = \frac{2P\gamma^2}{P}\frac{dP}{d\rho}\frac{\partial\rho}{\partial u} = \Gamma\frac{P'}{P}\frac{\partial}{\partial u}\left(\beta a\sqrt{-\left(-u^2-\Xi\right)}\right) \\ &= \Gamma\frac{P'}{P}\frac{\beta a\left(2u\right)}{2\sqrt{\left(u^2+\Xi\right)}} = \Gamma\frac{P'}{P}\frac{\beta a\,u\sqrt{\left(u^2+\Xi\right)}}{\left(-\right)\left(-u^2-\Xi\right)} \\ &= \Gamma\frac{P'}{P}\frac{\rho}{\left(E_\lambda-\Xi\right)}\frac{E_\lambda}{u} \ ,\end{aligned} \tag{II D1 e.21}$$

in a form which is compatible with the other versions.]

Substituting Eqs. (II D1 e.16) through (II D1 e.19) into Eqs. (II D1 e.14) and (II D1 e.15) gives

$$\frac{\partial f}{\partial\gamma} = \frac{2\Gamma}{\gamma}\frac{\partial f}{\partial\Gamma} + 0 \tag{II D1 e.22}$$

and

$$\frac{\partial f}{\partial u} = \Gamma\frac{P'}{P}\frac{\rho}{\left(E_\lambda-\Xi\right)}\frac{E_\lambda}{u}\frac{\partial f}{\partial\Gamma} + \frac{2E_\lambda}{u}\frac{\partial f}{\partial E_\lambda} \ . \tag{II D1 e.23}$$

Using the formulae in Eqs. (II D1 e.22) and (II D1 e.23), it is possible to demonstrate that the second transformation is the inverse of the first. That is, if one substitutes the expressions for $\partial f / \partial \Gamma$ and $\partial f / \partial E_\lambda$ from Eqs. (II D1 e.22) and (II D1 e.23) into Eqs. (II D1 e.12) and (II D1 e.13), or vice-versa, the resulting equations are identities.

Consider, now, the definition of the covariance matrix associated with a particular set of values. The covariance matrix associated with the *u*-parameters is denoted (as in Section IV) as matrix *M*, where

$$M_{ij} = \left\langle \delta u_i \, \delta u_j \right\rangle \quad , \qquad \text{(II D1 e.24)}$$

in which δu_i represents a small increment in the value of parameter u_i , and the angle brackets represent the "expectation value." Diagonal elements of this matrix are the square of the uncertainties on the parameter values; off-diagonal elements describe the connectedness between different parameters.

To communicate SAMMY results to ENDF files, it is necessary to generate the covariance matrix associated with the *p*-parameters (here this matrix is denoted by *Q*). This matrix is generated by making use of the relationship between a small increment in a *p*-parameter and a small increment in each of the *u*-parameters:

$$\delta p_k = \sum_i \frac{\partial p_k}{\partial u_i} \delta u_i \quad , \qquad \text{(II D1 e.25)}$$

so that Q becomes

$$Q_{kl} = \left\langle \delta p_k \, \delta p_l \right\rangle = \sum_{i,j} \frac{\partial p_k}{\partial u_i} \left\langle \delta u_i \, \delta u_j \right\rangle \frac{\partial p_l}{\partial u_j} \quad . \qquad \text{(II D1 e.26)}$$

The expansion of this covariance matrix for the two-parameter example discussed above will not be given here, but is proposed as an exercise for the student.

Reminder: It is the *p*-parameters (not the *u*-parameters) that are listed in the SAMMY PARameter files (input and output) and in the SAMMY output file (SAMMY.LPT). Likewise, it is the *p*-parameters* which are listed in ENDF File 2.** Therefore, the covariance matrix elements given in ENDF File 32 must correspond to the *Q* matrix defined above; that is, the covariance matrix listed in ENDF File 32 must be the appropriate covariance matrix for the resonance parameters.

---

* For the LRF=7 format, an option exists to list the reduced width amplitudes γ rather than the partial widths Γ. In this case, no transformation from *u*- to *p*-parameter space is necessary for the partial widths, but only for the resonance energies.

** Caveat: When a reduced-width amplitude is negative, it is not Γ but $G = -\Gamma$ that is listed in the ENDF file. ENDF covariance matrices are expressed in terms of *G*, not Γ.

When the cross section is calculated as a function of the *u*-parameters, a small increment in the calculated cross section is given by

$$\delta\sigma = \sum_n \frac{\partial\sigma}{\partial u_n}\delta u_n \quad . \tag{II D1 e.27}$$

Therefore the covariance matrix $\boldsymbol{C_{ij}}$ for the cross section is found from

$$C_{ij} = \left\langle \delta\sigma_i\,\delta\sigma_j \right\rangle = \left\langle \sum_n \left(\frac{\partial\sigma_i}{\partial u_n}\delta u_n \right) \sum_m \left(\frac{\partial\sigma_j}{\partial u_m}\delta u_m \right) \right\rangle$$

$$= \sum_{n,m} \frac{\partial\sigma_i}{\partial u_n} \left\langle \delta u_n\,\delta u_m \right\rangle \frac{\partial\sigma_j}{\partial u_m} \tag{II D1 e.28}$$

$$= \sum_{n,m} \frac{\partial\sigma_i}{\partial u_n} M_{nm} \frac{\partial\sigma_j}{\partial u_m} \quad ,$$

in which *M* is again defined as the covariance matrix for the *u*-parameters. In order to print the covariance matrix resonance parameters for the *p*-parameters into the ENDF formats, it is necessary to transform the parameter covariance matrix from *M* to *Q*. That transformation is made by inserting the formulae

$$\frac{\partial\sigma_i}{\partial u_n} = \sum_k \frac{\partial p_k}{\partial u_n} \frac{\partial\sigma_i}{\partial p_k} \tag{II D1 e.29}$$

and

$$\frac{\partial\sigma_j}{\partial u_m} = \sum_l \frac{\partial p_l}{\partial u_m} \frac{\partial\sigma_j}{\partial p_l} \tag{II D1 e.30}$$

into the previous expression, Eq. (II D1 e.28), yielding

$$C_{ij} = \sum_{n,m,k,l} \frac{\partial\sigma_i}{\partial p_k} \frac{\partial p_k}{\partial u_n} M_{nm} \frac{\partial p_l}{\partial u_m} \frac{\partial\sigma_j}{\partial p_l} \tag{II D1 e.31}$$

or

$$C_{ij} = \sum_{k,l} \frac{\partial\sigma_i}{\partial p_k} Q_{kl} \frac{\partial\sigma_j}{\partial p_l} \quad , \tag{II D1 e.32}$$

where *Q* is given by

$$Q_{kl} = \sum_{n,m} \frac{\partial p_k}{\partial u_n} M_{nm} \frac{\partial p_l}{\partial u_m} \quad . \tag{II D1 e.33}$$

For the case in which only one elastic width contains an energy-dependent penetrability, the *p*-parameter covariance matrix must be modified for all elements involving a width having energy-dependent penetrability.

II.D.2. Derivatives for MLBW and SLBW Approximations

From the form of the cross sections in Eqs. (II B3 a.1), (II B3 a.5), and (II B3 a.6), we note that there are only four expressions in which the resonance energies or widths occur. These expressions are denoted as follows:

$$A_{1c\lambda} = \Gamma_{\lambda c}\left(E - E_\lambda\right)/d_\lambda \quad , \tag{II D2.1}$$

$$A_{2c\lambda} = \Gamma_{\lambda c}\overline{\Gamma}_{\lambda\gamma}/d_\lambda \quad , \tag{II D2.2}$$

$$A_{3cc'\lambda} = \Gamma_{\lambda c}\Gamma_{\lambda c'}/d_\lambda \quad , \tag{II D2.3}$$

and

$$A_{4c\lambda} = \Gamma_{\lambda c}\Gamma_{\lambda}/d_\lambda \quad , \tag{II D2.4}$$

where d is given by Eq. (II B3 a.4) as

$$d_\lambda = \left(E - E_\lambda\right)^2 + \left(\Gamma_\lambda/2\right)^2 \quad . \tag{II D2.5}$$

Equation (II D2.4) is actually redundant, since

$$A_{4c\lambda} = \sum_{c'} A_{3cc'\lambda} + A_{2c\lambda} \quad . \tag{II D2.6}$$

As discussed in Section II.D, the assumption in the SAMMY code is that the *u*-parameters are independent and the *p*-parameters are derived quantities. Thus we need only evaluate partial derivatives of $A_{1c\lambda}$, $A_{2c\lambda}$, and $A_{3c\lambda}$ with respect to the *u*-parameters (i.e., with respect to the partial-width amplitudes and to the square root of the resonance energy). These derivatives may be written as follows:

$$\frac{\partial A_{1c\lambda}}{\partial\sqrt{E_\lambda}} = 2\sqrt{E_\lambda}\Gamma_{\lambda c}\left\{-1 + 2\left(E - E_\lambda\right)^2/d_\lambda\right\}/d_\lambda \quad , \tag{II D2.7}$$

$$\frac{\partial A_{2c\lambda}}{\partial\sqrt{E_\lambda}} = 4\sqrt{E_\lambda}\Gamma_{\lambda c}\overline{\Gamma}_{\lambda\gamma}\left(E - E_\lambda\right)/d_\lambda^2 \quad , \tag{II D2.8}$$

$$\frac{\partial A_{3cc'\lambda}}{\partial\sqrt{E_\lambda}} = 4\sqrt{E_\lambda}\,\Gamma_{\lambda c}\Gamma_{\lambda c'}\left(E - E_\lambda\right)/d_\lambda^2 \quad , \tag{II D2.9}$$

$$\frac{\partial A_{1c\lambda}}{\partial \overline{\gamma}_{\lambda\gamma}} = -2\overline{\gamma}_{\lambda\gamma}\Gamma_{\lambda c}\left(E - E_{\lambda}\right)\Gamma_{\lambda} / d_{\lambda}^{2} \quad , \tag{II D2.10}$$

$$\frac{\partial A_{2c\lambda}}{\partial \overline{\gamma}_{\lambda\gamma}} = 2\,\overline{\gamma}_{\lambda\gamma}\,\Gamma_{\lambda c}\left\{\,2 - \overline{\Gamma}_{\lambda\gamma}\,\Gamma_{\lambda} / d_{\lambda}\right\} / d_{\lambda} \quad , \tag{II D2.11}$$

$$\frac{\partial A_{3cc'\lambda}}{\partial \overline{\gamma}_{\lambda\gamma}} = -2\,\overline{\gamma}_{\lambda\gamma}\,\Gamma_{\lambda c}\,\Gamma_{\lambda c'}\,\Gamma_{\lambda} / d_{\lambda}^{2} \quad , \tag{II D2.12}$$

$$\frac{\partial A_{1c\lambda}}{\partial \gamma_{\lambda c''}} = 2\Gamma_{\lambda c}\left(E - E_{\lambda}\right)\left\{\delta_{cc''} - \Gamma_{\lambda c}\,\Gamma_{\lambda c''} / \left(2d_{\lambda}\right)\right\} / \left\{\gamma_{\lambda c''}\,d_{\lambda}\right\} \quad , \tag{II D2.13}$$

$$\frac{\partial A_{2c\lambda}}{\partial \gamma_{\lambda c''}} = 2\Gamma_{\lambda c}\,\overline{\Gamma}_{\lambda\gamma}\left\{\,\delta_{cc''} - \Gamma_{\lambda c}\,\Gamma_{\lambda c''} / \left(2d_{\lambda}\right)\right\} / \left\{\gamma_{\lambda c''}\,d_{\lambda}\right\} \quad , \tag{II D2.14}$$

and

$$\frac{\partial A_{3cc''\lambda}}{\partial \gamma_{\lambda c''}} = 2\Gamma_{\lambda c}\,\Gamma_{\lambda c'}\left\{\delta_{cc''} + \delta_{c'c''} - \Gamma_{\lambda}\,\Gamma_{\lambda c''} / \left(2d_{\lambda}\right)\right\} / \left\{\gamma_{\lambda c''}\,d_{\lambda}\right\} \quad , \tag{II D2.15}$$

All other derivatives are zero.

II.D.3. Details Involving Derivatives

In this section are presented some of the algebraic details relating to the partial derivatives. We first consider the derivative of one complex variable with respect to another, and then the derivative of the inverse of a matrix quantity. Both are needed in Section II.D.1.a.

Derivative of one complex variable with respect to another

Given any two complex variables $A = A^r + iA^i$ and $B = B^r + iB^i$, where A is an analytical function of B, the derivative of the components of A with respect to the components of B may be expressed as follows:

$$\frac{\partial A^r}{\partial B^r} = \mathrm{Re}\frac{\partial A}{\partial B^r} = \mathrm{Re}\frac{\partial A}{\partial B}\frac{\partial B}{\partial B^r} = \mathrm{Re}\frac{\partial A}{\partial B} \quad , \tag{II D3.1}$$

$$\frac{\partial A^r}{\partial B^i} = \mathrm{Re}\frac{\partial A}{\partial B^i} = \mathrm{Re}\frac{\partial A}{\partial B}\frac{\partial B}{\partial B^i} = \mathrm{Re}\frac{\partial A}{\partial B}(i) = -\mathrm{Im}\frac{\partial A}{\partial B} \quad , \tag{II D3.2}$$

$$\frac{\partial A^i}{\partial B^r} = \mathrm{Im}\frac{\partial A}{\partial B^r} = \mathrm{Im}\frac{\partial A}{\partial B}\frac{\partial B}{\partial B^r} = \mathrm{Im}\frac{\partial A}{\partial B} \quad , \tag{II D3.3}$$

and

$$\frac{\partial A^i}{\partial B^i} = \mathrm{Im}\frac{\partial A}{\partial B^i} = \mathrm{Im}\frac{\partial A}{\partial B}\frac{\partial B}{\partial B^i} = \mathrm{Im}\frac{\partial A}{\partial B}(i) = \mathrm{Re}\frac{\partial A}{\partial B} \quad . \tag{II D3.4}$$

Also, the usual chain rule applies:

$$\begin{aligned}\frac{\partial A^r}{\partial C^r} &= \frac{\partial A^r}{\partial B^r}\frac{\partial B^r}{\partial C^r} + \frac{\partial A^r}{\partial B^i}\frac{\partial B^i}{\partial C^r} \\ &= \left[\mathrm{Re}\left(\frac{\partial A}{\partial B}\right)\right]\left[\mathrm{Re}\left(\frac{\partial B}{\partial C}\right)\right] + \left[-\mathrm{Im}\left(\frac{\partial A}{\partial B}\right)\right]\left[\mathrm{Im}\left(\frac{\partial B}{\partial C}\right)\right] = \mathrm{Re}\left[\frac{\partial A}{\partial B}\frac{\partial B}{\partial C}\right] \quad ,\end{aligned} \tag{II D3.5}$$

$$\begin{aligned}\frac{\partial A^r}{\partial C^i} &= \frac{\partial A^r}{\partial B^r}\frac{\partial B^r}{\partial C^i} + \frac{\partial A^r}{\partial B^i}\frac{\partial B^i}{\partial C^i} \\ &= \left[\mathrm{Re}\left(\frac{\partial A}{\partial B}\right)\right]\left[-\mathrm{Im}\left(\frac{\partial B}{\partial C}\right)\right] + \left[-\mathrm{Im}\left(\frac{\partial A}{\partial B}\right)\right]\left[\mathrm{Re}\left(\frac{\partial B}{\partial C}\right)\right] = -\mathrm{Im}\left[\frac{\partial A}{\partial B}\frac{\partial B}{\partial C}\right] \quad ,\end{aligned} \tag{II D3.6}$$

$$\frac{\partial A^i}{\partial C^r} = \frac{\partial A^i}{\partial B^r}\frac{\partial B^r}{\partial C^r} + \frac{\partial A^i}{\partial B^i}\frac{\partial B^i}{\partial C^r}$$
$$= \left[\mathrm{Im}\left(\frac{\partial A}{\partial B}\right)\right]\left[\mathrm{Re}\left(\frac{\partial B}{\partial C}\right)\right] + \left[\mathrm{Re}\left(\frac{\partial A}{\partial B}\right)\right]\left[\mathrm{Im}\left(\frac{\partial B}{\partial C}\right)\right] = \mathrm{Im}\left[\frac{\partial A}{\partial B}\frac{\partial B}{\partial C}\right] \quad , \tag{II D3.7}$$

and

$$\frac{\partial A^i}{\partial C^i} = \frac{\partial A^i}{\partial B^r}\frac{\partial B^r}{\partial C^i} + \frac{\partial A^i}{\partial B^i}\frac{\partial B^i}{\partial C^i}$$
$$= \left[\mathrm{Im}\left(\frac{\partial A}{\partial B}\right)\right]\left[-\mathrm{Im}\left(\frac{\partial B}{\partial C}\right)\right] + \left[\mathrm{Re}\left(\frac{\partial A}{\partial B}\right)\right]\left[\mathrm{Re}\left(\frac{\partial B}{\partial C}\right)\right] = \mathrm{Re}\left[\frac{\partial A}{\partial B}\frac{\partial B}{\partial C}\right] \quad . \tag{II D3.8}$$

Derivative of the inverse of a matrix

In Eq. (II D1 a.13), the quantity Y is defined as

$$Y_{ef} = \left[\left(L^{-1} - R\right)^{-1}\right]_{ef} \quad . \tag{II D3.9}$$

To find the derivative of Y with respect to R, we first note that

$$\sum_a Y_{ea} Y^{-1}_{ab} = \delta_{eb} \quad , \tag{II D3.10}$$

so that the derivative is zero; that is,

$$0 = \frac{\partial}{\partial R_{cd}}\left[\sum_a Y_{ea} Y^{-1}_{ab}\right] = \sum_a \frac{\partial Y_{ea}}{\partial R_{cd}} Y^{-1}_{ab} + \sum_a Y_{ea}\frac{\partial Y^{-1}_{ab}}{\partial R_{cd}}$$
$$= \sum_a \frac{\partial Y_{ea}}{\partial R_{cd}} Y^{-1}_{ab} + \sum_a Y_{ea}\left\{-\delta_{ac}\delta_{bd} - \delta_{ad}\delta_{bc}\left(1-\delta_{cd}\right)\right\} \quad . \tag{II D3.11}$$

The quantity in curly brackets comes from the symmetry of the R-matrix and from the stipulation that only unique matrix elements are to be considered [$c \le d$, $e \le f$ in Eq. (II D1.1) and Eq. (II D1 a.1)]. Multiplying both terms by Y_{bf}, summing over b, and rearranging give

$$\sum_a \frac{\partial Y_{ea}}{\partial R_{cd}} \sum_b Y_{ab}^{-1} Y_{bf} = \sum_{a,b} Y_{ea} \left\{ \delta_{ac}\delta_{bd} + \delta_{ad}\delta_{bc}\left(1-\delta_{cd}\right) \right\} Y_{bf} \quad ,$$

$$\sum_a \frac{\partial Y_{ea}}{\partial R_{cd}} \delta_{af} = Y_{ec}Y_{df} + Y_{ed}Y_{cf}\left(1-\delta_{cd}\right) \quad , \qquad \text{(II D3.12)}$$

or, finally,

$$\frac{\partial Y_{ef}}{\partial R_{cd}} = Y_{ec}Y_{df} + Y_{ed}Y_{cf}\left(1-\delta_{cd}\right) \quad . \qquad \text{(II D3.13)}$$

This is the derivative used in Eq. (II D1 a.14).

III. CORRECTIONS FOR EXPERIMENTAL CONDITIONS

In general it is not possible to directly compare the cross sections extracted from experiments to those generated via R-matrix theory (or via any other theory). This is because "perfect" experimental conditions do not exist: (1) individual nuclei within the sample are not at rest; (2) finite time intervals are required both for the neutron beam and for the detecting apparatus; (3) the flight-path length traversed by a neutron depends on its position of origin within the neutron-producing target, on its position of interaction within the sample, and on the position at which it is detected; (4) the finite size of the sample causes interactions beyond those described by the cross section for individual nuclei. The first of these conditions leads to the effect known as Doppler broadening, the second and third lead to resolution broadening, and the fourth to multiple-scattering and self-shielding effects. There are other effects as well, not included in this enumeration. To compare theory to experiment, either the theory must include these effects or corrections must be applied to the experimental data. Often the former is easier, or the latter is impossible. SAMMY therefore includes options to simulate a great many of these effects, and modify the theoretical calculations appropriately.

To simulate Doppler or resolution broadening (i.e., to "broaden the theory"), it is necessary to first have a mathematical description of the broadening (generally, as an integral of the unbroadened cross section times a broadening function), and then to evaluate those integrals analytically if possible or numerically if necessary.

In Section III.A, the scheme used in SAMMY for most of the numerical integrations is described in some detail. It is important to note that it is the *user*, not the code author, who is responsible for ensuring that the numerical integrations are performed sufficiently well; this is discussed in Section III.A.1, which should be read and carefully considered before analysis results are published.

SAMMY contains four distinct procedures for Doppler broadening, which are described in Section III.B. The various available methodologies for resolution broadening are discussed in Section III.C. Section III.D is devoted to multiple-scattering effects, and other phenomena are treated in Section III.E.

III. A. THEORETICAL FOUNDATION FOR NUMERICAL BROADENING

The primary method used in SAMMY for evaluating the integrals required in Doppler and resolution broadening involves several operations for which details are given in the subsequent subsections. The method was borrowed originally from the MULTI code [GA74] and subsequently modified as the need arose. Note that in SAMMY, broadening is applied both to the cross sections and to the partial derivatives, while in MULTI, it was applied only to the cross sections. A summary of the operations is given here.

1. Choose an appropriate "auxiliary energy grid" at which to evaluate the integrands. The auxiliary grid consists of (a) the original energy grid (i.e., the energies at which experimental data are given), (b) points below the minimum energy of the experimental data and above the maximum energy, and (c) additional points sufficient to describe the structure of any "narrow" resonance. See Section III.A.2 for more details regarding the choice of auxiliary grid and Section III.A.3 for details regarding the integration scheme. (Different criteria are required for Leal-Hwang Doppler broadening; see Section III.B.2.)

2. A discussion of pitfalls that can arise when insufficient care is devoted to the choice of auxiliary grid is given in Section III.A.1. While Sections III.A.2 and III.A.3 may safely be regarded as "black boxes" by some analysts, all SAMMY users are encouraged to pay careful attention to issues raised in Section III.A.1.

3. For each energy in the auxiliary grid, evaluate the theoretical cross sections and derivatives thereof, as described in Section II.

4. Determine Doppler-broadened cross section and derivatives wherever possible (i.e., for all but the highest and the lowest energies in the auxiliary grid). Generate derivatives with respect to Doppler temperature. See Section III.B for details.

5. Transform from cross section to transmission as needed; apply transformation to derivatives also. See Section III.E.1. Generate derivative with respect to sample thickness.

6. Apply self-shielding and multiple-scattering corrections as needed, both to cross sections and to derivatives. See Section III.D for details.

7. For each energy in the original (experimental) grid, determine the resolution-broadened cross section (or transmission) and derivatives thereof. Also generate derivatives with respect to resolution-broadening parameters. See Section III.C.

8. If needed, transform from transmission back to cross section; transform derivatives also.

9. Multiply by normalization and add backgrounds, as needed. Generate derivatives with respect to normalization and background. See Section III.E.3.a.

III.A.1. Analyst's Responsibility for Auxiliary Energy Grid

In SAMMY, the user/analyst (*not* the author) is responsible for being sure that the numerical integrations are performed properly. That is to say, the auxiliary energy grid (discussed in detail in Section III.A.2) must be sufficiently dense so that the numerical integration scheme produces the correct results.

Why must the grid be dense? Unbroadened cross sections would not be well defined on a sparse grid. Hence, the integrations would not be accurate. This is illustrated in Figures III A1.1 – 4, which are greatly exaggerated for demonstration purposes. In the first figure, red dots indicate the default grid points on which the unbroadened cross section might be calculated. The dashed curve represents the actual unbroadened cross section, while the solid curve represents the approximate cross section found by interpolating between grid points. With this sparse grid, agreement between the two curves in poor.

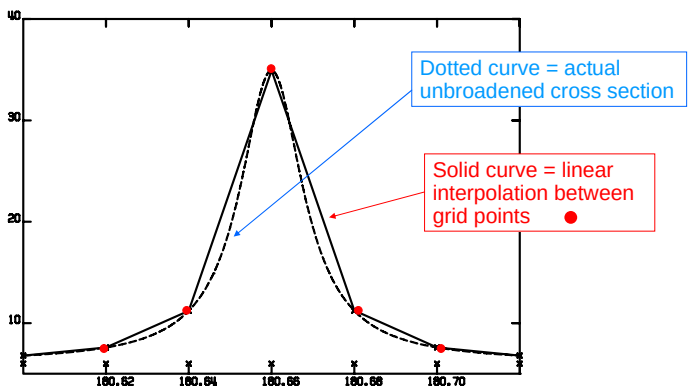


Figure III A1.1. Unbroadened cross section calculated using too few points in the auxiliary grid.

Figure III A1.2 shows the Doppler-broadened cross section (solid curve) that would result from using the auxiliary grid of Figure III A1.1 to perform the numerical integration. The calculated Doppler-broadened cross section is significantly larger than the actual Doppler-broadened cross section.

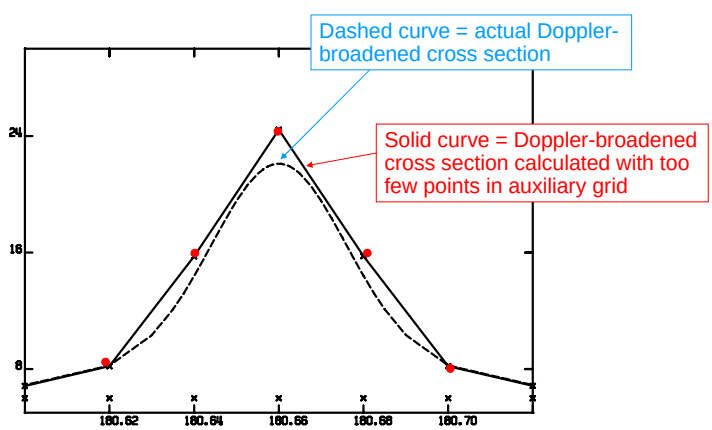


Figure III A1.2. Incorrect Doppler-broadened cross section calculated with too few points in the auxiliary grid.

In contrast, Figure III A1.3 shows a denser auxiliary grid, one which adequately describes the unbroadened cross section. The Doppler-broadened cross section calculated with this grid is shown in Figure III A1.4, in which the actual and the calculated Doppler-broadened cross sections are indistinguishable. (Note that the "experimental" grid is the same in Figures III A1.2 and III A1.4.)

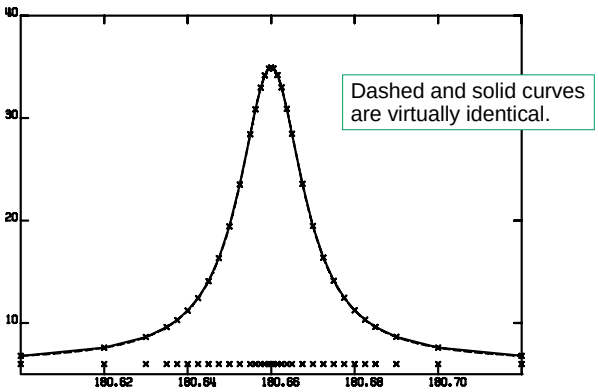


Figure III A1.3. Unbroadened cross section calculated using an adequate number of points in the auxiliary grid.

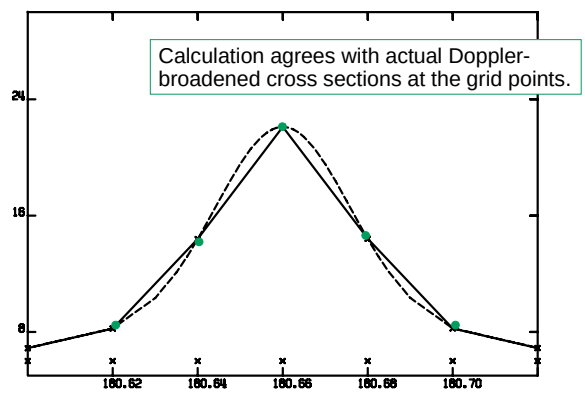


Figure III A1.4. Doppler-broadened cross section calculated with an adequate number of points in the auxiliary grid.

The reader may ask why SAMMY does not automatically check to be certain that the auxiliary grid is adequate, especially since this is done by other codes (e.g., processor codes such as AMPX [MD02] or NJOY [RM82]) which calculate Doppler-broadened cross sections. Significant amounts of computation time are required for such checks. With processor codes, the Doppler-broadened cross section is generally calculated only once, and then used many times, so accuracy is far more important than speed of computation. With analysis codes such as SAMMY, the Doppler-broadened cross section is recalculated whenever new resonance parameters are used, so speed of computation can be an issue. During initial stages of an analysis, the user may wish to sacrifice accuracy to gain speed. During later stages of the analysis, the user will want to test whether there is sufficient accuracy.

Options for increasing the density of points in the auxiliary grid are given in line 2 of the INPut file, Table VI A.1. These should be used to make comparisons between Doppler- and resolution-broadened results from dense vs. sparse grids. (For example, if the number of points is doubled by setting NXTRA = 1, and broadened cross sections are nearly the same as with NXTRA = 0, then the sparser grid is adequate.) Early in the analysis, it is probably sufficient to use the sparsest grid that gives reasonable results. Near the end of the project, a denser grid might be used to ensure greater accuracy.

III.A.2. Choose Auxiliary Energy Grid

We wish to evaluate integrals of the form

$$f\left(E_i\right)=\int_{E_{\min}}^{E_{\max}} \overline{f}\left(E'\right)B\left(E_i,E'\right)dE' \quad , \qquad \text{(III A2.1)}$$

where $\overline{f}(E')$ represents the unbroadened theoretical cross section (or transmission) and $f\left(E_i\right)$ the broadened. B represents the appropriate broadening function as described in Section III.B or III.C. The set of points E_i are the original grid, for which data are available and at which theoretical values are required.

Standard practice for evaluating integrals such as those in Eq (III A2.1) is to choose a set of points E'_j and associated weights W_j in such a way that

$$\int_a^b \overline{f}\left(E'\right)B\left(E_i,E'\right)dE' \cong \sum_j \overline{f}\left(E'_j\right)B\left(E_i,E'_j\right)W_j \quad , \qquad \text{(III A2.2)}$$

where the approximation is exact if the product $\overline{f}\left(E'_j\right)B\left(E_i,E'_j\right)$ is a polynomial of some specified degree, say n. Use of these points and weights to evaluate the integral over a non-polynomial function [such as $\overline{f}\left(E'\right)B\left(E_i,E'\right)$ in Eq. (III A2.1)] will give a result that is accurate to the extent that the function can be approximated by a polynomial of degree n. In practice, if one divides the integration region [E_{min}, E_{max}] into sufficiently small subregions [a, b], the polynomial approximation will be quite accurate within each subregion.

The choice of points $\left\{E'_j\right\}$ is, to some extent, arbitrary. (Once $\left\{E'_j\right\}$ is fixed, weights $\left\{W_j\right\}$ are determined from Eq. (III A2.2).) Because it is necessary to integrate Eq. (III A2.1) many times (i.e., once for each E_i), it is expedient to have the set $\left\{E'_j\right\}$ be the same for each E_i in order to minimize the total number of evaluations of $\overline{f}\left(E'_j\right)$. These points $\left\{E'_j\right\}$ will hereafter be designated collectively as the "auxiliary grid," and the points $\left\{E_i\right\}$ for which data are given will be designated as the "original grid."

Several types of points contribute to the auxiliary grid:

a. All points in the original grid are included in the auxiliary grid.

b. "Extra" points are added between each point in the original grid. The number "NXTRA" of such points is specified by the user in the INPut file (see card set 2 of Table VIA.1). (See Section III.A.1 for a discussion of why this may be necessary.)

c. Points are added at the extremities of the data region, to be used in broadening the cross sections at the end points. The relative spacing of these points is similar to that of points inside the energy region being analyzed. The grid is chosen in one of two ways:

   1. Points from the data set, but outside the energy region being analyzed, are added to the auxiliary grid.

   2. If (1) is not possible because the data set contains no such points, then the spacing Δ between data points E_1 and E_2 is used to locate other points equally spaced at $E_1-\Delta$, $E_1-2\Delta$, $E_1-3\Delta$, ... ; a sufficient number of points are chosen to cover the integration region for E_1.

d. Equation (III A2.2) is a good approximation only if the integrand closely resembles a low-order polynomial. Therefore, it may be necessary to add points over the width of narrow resonances so that the structure of the integrand will be properly represented. Also, the auxiliary grid must vary smoothly to avoid numerical difficulties in evaluating the integrals. This problem can be broken into several pieces:

   1. Decide which resonances require additional points. IPTDOP is the number of points required across a resonance; the default value for IPTDOP is 9, but the user may increase this as desired (see Table VI A.1, card set 2). If there are fewer than IPTDOP points between (E_λ - D) and (E_λ + D), where D is the sum of the absolute values of the gamma and particle widths, then more points must be added near this resonance.

   2. For each narrow resonance, add auxiliary points at E_λ and at positions $E_\lambda \pm 2D_j/(\text{IPTDOP}-1)$, where j ranges from 1 to IPTDOP.

   3. Add points at $E_\lambda \pm 1.5D$ and $E_\lambda \pm 2D$.

   4. If IPTWID is positive (but smaller than 7), add additional points at positions $E_\lambda \pm 3D$, $E_\lambda \pm 4D$, and $E_\lambda \pm D(\text{IPTWID}+1)$, where the input quantity IPTWID is specified in Table VI A.1, card set 2.

   5. If IPTWID is negative, add points as in #4, and also at $E_\lambda \pm 10D$ and at $E_\lambda \pm 20D$.

   6. Test the resulting auxiliary grid to see that no two neighboring points are either very close together (relative to neighboring spacing) or very far apart. Drop or add points as needed.

Caveat: If the original (MULTI-style) Doppler broadening is used, and energy points in the auxiliary grid fall at negative energy, SAMMY will issue a warning and abort execution. For subsequent runs, the analyst has several options: either choose a higher E_{min}, specify "NO LOW-ENERGY BROADEning is to be used" in the INPut file (see Tables VI A.1 and VI A.2 for details), specify "USE LEAL,HWANG DOPPLer broadening" for the low-energy region (see Section III.B.2), or specify "USE FREE GAS MODEL Of doppler broadening." The final option (i.e., the free-gas model) is the default and is the author's recommendation for most calculations; see Section III.B.1.

III.A.3. Perform Numerical Integration

The numerical integration scheme used in SAMMY to evaluate the integrals shown in Eqs. (III A2.1) and (III A2.2) is borrowed from MULTI [GA74] and is based on the four-point progressive interpolation method of Mintz and Jordan [MM64]. For the value of an integral from x_2 to x_3 of some function $y(x)$, where the value of y is known only at the four values of x $(x = x_1, x_2, x_3, \text{or } x_4)$, this method uses the approximation

$$\int_{x_2}^{x_3} y(x)\,dx \cong \sum_{i=1}^{4} y(x_i)\,w_i \quad , \tag{III A3.1}$$

in which the weights w_i are given by

$$\begin{aligned}
w_1 &= \frac{(x_2 - x_3)^3}{12(x_1 - x_2)(x_1 - x_3)} \quad , \\
w_2 &= \frac{(x_2 - x_3)}{12}\left[\frac{(x_1 - x_3)}{(x_2 - x_1)} + \frac{(x_4 - x_3)}{(x_2 - x_4)} - 4\right] \quad , \\
w_3 &= \frac{(x_3 - x_2)}{12}\left[4 - \frac{(x_1 - x_2)}{(x_3 - x_1)} + \frac{(x_4 - x_2)}{(x_3 - x_4)}\right] \quad , \\
w_4 &= \frac{(x_2 - x_3)^3}{12(x_4 - x_2)(x_4 - x_3)} \quad .
\end{aligned} \tag{III A3.2}$$

These equations give the exact result if $y(x)$ is a polynomial of degree 2 or less [i.e., if $y(x)$ is a quadratic, linear, or constant function of x].

What is required for the broadening integrals is, however, a function of the form

$$\int_{E_{min}}^{E_{max}} y(E')\,dE' \cong \sum_{j=j_{min}}^{j_{max}-1} \int_{E'_j}^{E'_{j+1}} y(E')\,dE' \quad , \tag{III A3.3}$$

in which j_{min} and j_{max} are chosen such that $E'_{j_{min}} \le E_{min} \le E'_{j_{min}+1}$ and $E'_{j_{max}-1} \le E_{max} \le E'_{j_{max}}$. Each integral on the right-hand side of Eq. (III A3.3) may be evaluated using Eq. (III A3.1), with

$$x_1 = E_{j-1}, \quad x_2 = E_j, \quad x_3 = E_{j+1}, \text{ and } x_4 = E_{j+2} \quad . \tag{III A3.4}$$

Define w_{ij} as "w_i from Eq. (III A3.2) with the x_i given by Eq. (III A3.4)," or more precisely,

$$x_{i\,j} = E'_{j+i-2} \quad . \tag{III A3.5}$$

Equation (III A3.3) can then be put into the form

$$\int_{E_{min}}^{E_{max}} y\left(E'\right)\, dE' \;\cong\; \sum_{j=j_{min}}^{j_{max}} \;\sum_{i=1}^{4} w_{i\,j}\; y\left(E'_{j+i-2}\right) \quad . \tag{III A3.6}$$

Performing the summation over i gives

$$\int_{E_{min}}^{E_{max}} y\left(E'\right)\, dE' \;\cong\; \sum_{j=j_{min}}^{j_{max}} W_j \;\; y\left(E'_j\right) \quad , \tag{III A3.7}$$

where the weight W_j is given by

$$W_j = \sum_{i=1}^{4} w_{i\,(j+2-i)} \quad . \tag{III A3.8}$$

The summation in Eq. (III A3.8) may be evaluated explicitly using Eq. (III A3.1) with Eq. (III A3.4), yielding

$$\begin{aligned} W_j &= \left(E'_{j+1} - E'_{j-1}\right)/3 + \left(E'_{j+2} - E'_{j-2}\right)/12 \\ &\quad + \frac{1}{12}\left[\frac{\left(E'_j - E'_{j-1}\right)^2 - \left(E'_{j+2} - E'_{j+1}\right)^2}{\left(E'_{j+1} - E'_j\right)} + \frac{\left(E'_{j+1} - E'_j\right)^2 - \left(E'_{j-1} - E'_{j-2}\right)^2}{\left(E'_j - E'_{j-1}\right)}\right] \quad . \end{aligned} \tag{III A3.9}$$

SAMMY uses the values given by Eq. (III A3.9) even for $j = j_{min}$ and $j = j_{max}$, even though they implicitly require the use of $E'_{j_{min}-1}$ and $E'_{j_{max}+1}$, which technically are outside the range of integration $\left(E_{min}\text{ to }E_{max}\right)$; this is legitimate because the range of integration is chosen so that the integrand $y\left(E'\right)$ is effectively zero outside that range. Thus, the values of $y\left(E'_{j_{min}-1}\right)$ and $y\left(E'_{j_{max}+1}\right)$ are zero and are implicitly included in the above formulation. In contrast, the code MULTI performed extra calculations to end exactly at $\left(E'_{j_{min}}\text{ to }E'_{j_{max}}\right)$; our studies have found this an unneeded complication.

The scheme described above is used in SAMMY only if there are more than twelve points between $E'_{j_{min}}$ and $E'_{j_{max}}$, inclusive. If there are fewer than twelve but more than five points, Simpson's rule is used. For five or fewer points, it is assumed that the broadened value is equal to the unbroadened value, and no integration is performed.

It should be noted that there are situations in which it is imperative to end the integration precisely at the specified limits. At least two examples occur in the SAMMY code: (1) Multiple-scattering corrections for capture or fission experiments (Section III.D) involve integration over the scattering angle, from 0 to 180 degrees. When “integration over angle” is converted to “integration over energy of the scattered neutron,” one might be tempted to extend the energy integral to the nearest grid point. However, to obtain accurate results, the integration clearly must not extend beyond the energies corresponding to back-angle scattering or forward-angle scattering. (2) Absolute limits are also required for the calculation of average cross sections (Section V.C).

In situations in which the integrand does not smoothly approach zero outside the limits of the integration, Eq. (III A3.9) is modified to give the appropriate weights to define an absolute integration limit.

III. B. DOPPLER BROADENING

Four options are available within SAMMY to accomplish Doppler broadening; three are based on the free-gas model (FGM), and the fourth is a solid-state model.

SAMMY's free-gas model is described in Section III.B.1. This model was introduced into SAMMY in order to overcome shortcomings of the two earlier versions (Sections III.B.2 and III.B.3), and is now the default method. This is the option that should be used for most calculations. For additional details, see [NL98].

A second method, described in Section III.B.2, is an elegant and rigorous adaptation of the FGM based on work by Leal and Hwang [LL85]. This method works best with smooth cross sections, and thus has limitations for use in the resonance region.

SAMMY's original method, a high-energy Gaussian approximation (HEGA) to the FGM, is based on an adaptation of the method used by George Auchampaugh in his code MULTI [GA74]. This method is described in Section III.B.3. Because this is a high-energy approximation, it cannot be used for very low-energy computations.

A fourth option is available for use in those situations in which the FGM is inadequate. The crystal-lattice model (CLM) of Doppler broadening, added to SAMMY for Release M6 of the code, is described in Section III.B.4. SAMMY's implementation is based on the DOPUSH model of Naberejnev [DN99, DN99a].

III.B.1. Free-Gas Model of Doppler Broadening

A detailed discussion of the "exact" free-gas model (FGM) of Doppler broadening is given in [NL98]; results are summarized in this section. The formula for the FGM of Doppler broadening (see, for example, [FF80, Eq. 102]) takes the form

$$\sigma_D\left(E\right)=\frac{1}{\Delta_D\sqrt{\pi}}\int_0^\infty\left[e^{-4\left(E-\sqrt{EE'}\right)^2/\Delta_D^2}-e^{-4\left(E+\sqrt{EE'}\right)^2/\Delta_D^2}\right]\sigma\left(E'\right)\sqrt{E'/E}\;dE \quad . \qquad \text{(III B1.1)}$$

In this expression, σ_D is the Doppler-broadened cross section and σ is the unbroadened cross section. (Any type of cross section could be represented here: elastic, total, capture, fission, or other reaction, either angle-integrated or angle-differential cross sections.) The Doppler width Δ_D is given by

$$\Delta_D=\sqrt{\frac{4\,m\,E\,k\,T}{M}} \quad . \qquad \text{(III B1.2)}$$

Here, as elsewhere in this section, *m* represents the neutron mass, *M* the target (sample) mass, *k* is Boltzman's constant, and *T* is the effective temperature. (This Doppler width is reported in the SAMMY.LPT file; see Section VII.A.) Alternatively, this equation may be written in terms of "velocity" *v*, where *v* is the square root of energy *E* ($v=\sqrt{E}$), as

$$v\,\sigma_D\left(v^2\right)=\frac{1}{u\sqrt{\pi}}\int_0^\infty\left[e^{-\left(v-v'\right)^2/u^2}-e^{-\left(v+v'\right)^2/u^2}\right]v'\,\sigma\left(v'^2\right)\frac{v'}{v}\;d\,v' \quad , \qquad \text{(III B1.3)}$$

in which we have substituted *v*' for the square root of *E* ' and defined *u* as

$$u=\sqrt{m\,k\,T/M} \quad . \qquad \text{(III B1.4)}$$

To evaluate this integral, replace *v*' by -*w* in the second term; this gives

$$\begin{aligned} v\,\sigma_D\left(v^2\right) \;=\; & \frac{1}{u\sqrt{\pi}}\int_0^\infty e^{-\left(v-v'\right)^2/u^2}v'\,\sigma\left(v'^2\right)\frac{v'}{v}\;d\,v' \\ & -\;\frac{1}{u\sqrt{\pi}}\int_0^{-\infty} e^{-\left(v-w\right)^2/u^2}\left(-w\right)\sigma\left(\left(-w\right)^2\right)\frac{\left(-w\right)}{v}\;d\left(-w\right) \quad . \end{aligned} \qquad \text{(III B1.5)}$$

Replacing v' by w in the first term of Eq. (III B1.5), rearranging the second term, and defining

$$s(w) = \begin{cases} \sigma\left(w^2\right) & \text{for } w > 0 \\ 0 & \text{for } w = 0 \\ -\sigma\left(w^2\right) & \text{for } w < 0 \end{cases} \qquad \text{(III B1.6)}$$

puts this equation into the form

$$v\,\sigma_D\left(v^2\right) = \frac{1}{u\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-(v-w)^2/u^2}\; w\,s(w)\frac{w}{v}\; d\,w \quad . \qquad \text{(III B1.7)}$$

In the form of Eq. (III B1.7) with definition (III B1.6), the Doppler-broadening integration can be accomplished readily within SAMMY using the same numerical techniques used for other integrations, without having to give special consideration to “the second term” of Eq. (III B1.1). The integration scheme of Section III A.3 is used directly. The auxiliary energy grid is chosen as described in Section III.A.2, with the exception that the additional low-energy points are equally spaced in *velocity* rather than in energy. Negative velocities are included as needed, in order to properly evaluate the integral at low values of *E*.

III.B.1.a. Derivatives with respect to effective temperature *T*

In SAMMY, the Doppler temperature *T* may be treated as a *u*-parameter (see Section IV) and varied via Bayes' equations. Thus, it is necessary to determine derivatives of the broadened cross section (or transmission) with respect to *T*.

The Doppler-broadening integral of Eq. (III B1.7) depends on effective temperature *T* only through the Doppler width Δ_D of Eq. (III B1.2). Using the chain rule we find

$$\frac{\partial \sigma_D}{\partial T} = \frac{\partial \Delta_D}{\partial T} \frac{\partial \sigma_D}{\partial \Delta_D} \quad , \qquad \text{(III B1 a.1)}$$

where the first of these partial derivatives is found from Eq. (III B1.2) to be

$$\frac{\partial \Delta_D}{\partial T} = \frac{\Delta_D}{2T} \quad . \qquad \text{(III B1 a.2)}$$

The partial derivative of the cross section with respect to the Doppler width is evaluated numerically in SAMMY, via

$$\frac{\partial \sigma_D}{\partial \Delta_D} = \frac{\sigma_D\left(\Delta_D + d\right) - \sigma_D\left(\Delta_D - d\right)}{2d} \quad . \qquad \text{(III B1 a.3)}$$

The value of *d* to use in this expression is somewhat arbitrary, subject to the restrictions that (1) *d* be small enough that $\sigma\left(\Delta\right)$ is approximately a linear function of Δ in the region $\Delta_D - d \le \Delta \le \Delta_D + d$ and (2) *d* be big enough that sufficient significant digits are retained by the computer in generating the numerical difference in $\sigma_D\left(\Delta_D + d\right) - \sigma_D\left(\Delta_D - d\right)$. Through trial and error, it was determined that setting *d* equal to $\Delta_D q$, with $q = 0.02$, gives reasonable results for those cases tested. Since the value of this parameter *q* is not subject to direct user control, anyone experiencing difficulty when varying the effective temperature should contact the author.

III.B.2. Leal-Hwang Doppler Broadening

The assumption of a free gas model (FGM) for the sample atoms leads to a relatively simple relationship between the cross-section values at different temperatures. Leal and Hwang [LL85] have used this idea to write the Doppler-broadened cross section in the form

$$\sigma_D(E) = F(v)/E \quad , \tag{III B2.1}$$

where "velocity" v is the square root of energy E,

$$v = \sqrt{E} \quad , \tag{III B2.2}$$

and $F(v)$ obeys a partial differential equation having the same form as a one-dimensional time-dependent heat equation. That is, $F(v)$ obeys

$$\left(\frac{\partial^2}{\partial v^2} - \frac{\partial}{\partial \Theta}\right) F(v) = 0 \quad , \tag{III B2.3}$$

in which Θ is given by

$$\Theta = \frac{k\,T}{2\,M} \quad , \tag{III B2.4}$$

where again T is the effective temperature of the sample, k is Boltzmann's constant, and M is the mass of the sample (target) nucleus. This is equivalent to the integral equation in Eq. (III B1.1).

The numerical solution of Eq. (III B2.3) may be readily accomplished by difference techniques. Leal and Hwang have shown that if the step sizes Δv and $\Delta\Theta$ are constant for both velocity v and "temperature" Θ, and if

$$(\Delta v)^2 = 6\,\Delta\Theta \quad , \tag{III B2.5}$$

then the error in the numerical solution is of the order of $(\Delta v)^4$ or $(\Delta\Theta)^2$.

The solution of Eq. (III B2.3) can be written in the form

$$F_i^j = \frac{1}{6} F_{i-1}^{j-1} + \frac{2}{3} F_i^{j-1} + \frac{1}{6} F_{i+1}^{j-1} \quad , \tag{III B2.6}$$

in which the superscript j denotes the value of F evaluated at $\Theta = \Theta_j$, and subscript i denotes the value of F evaluated at $v = v_i$.

By combining Eq. (III B2.6) with the analogous equations for F_i^m, with $m = 1$ to $j - 1$, we find that the $F_i^{\,j}$ may be written as

$$F_i^{\,j} = \sum_{k=-j}^{j} a_k^j \, F_{i+k}^0 \quad , \tag{III B2.7}$$

where F_n^0 are the "initial" values of F (i.e., at zero temperature), and where the $a_k^{\,j}$, for negative k, are found from the relationship

$$a_{-k}^{j} = a_k^{j} \quad . \tag{III B2.8}$$

For positive k, the values of a_k^j are found from the recursion relationships

$$\begin{aligned} &a_1^1 = 1/6 \qquad a_0^1 = 2/3 \\ &a_2^2 = (1/6)^2 \qquad a_1^2 = 2(1/6)(2/3) \qquad a_0^2 = 2(1/6)^2 + (2/3)^2 \quad , \end{aligned} \tag{III B2.9}$$

and, in general,

$$\begin{aligned} a_n^n &= (1/6)^n \\ a_{n-1}^n &= (1/6)\,a_{n-2}^{n-1} + (2/3)\,a_{n-1}^{n-1} \\ a_{n-2}^n &= (1/6)\,a_{n-3}^{n-1} + (2/3)\,a_{n-2}^{n-1} + (1/6)\,a_{n-1}^{n-1} \\ &\ldots \\ a_k^n &= (1/6)\,a_{k-1}^{n-1} + (2/3)\,a_k^{n-1} + (1/6)\,a_{k+1}^{n-1} \qquad \text{for } 0 < k < n-1 \\ &\ldots \\ a_0^n &= (1/6)\,a_1^{n-1} + (2/3)\,a_0^{n-1} + (1/6)\,a_1^{n-1} = 2(1/6)\,a_1^{n-1} + (2/3)\,a_0^{n-1} \quad . \end{aligned} \tag{III B2.10}$$

The procedure employed in SAMMY is as follows.

(1) Somewhat arbitrarily, choose ΔT = 5 degrees; this number is a user input, so it may be changed if desired. (See Table VI A.1, card set 5, variable DELTTT.) Figure the number of steps required to reach from zero temperature to the effective temperature T, and adjust ΔT so that T can be reached in exactly J steps. Determine the corresponding $\Delta\Theta$ and Δv.

(2) Generate the coefficients a_k^J for k = 0 to J. These coefficients will be large for small k and effectively zero for large k. Choose M such that $a_k^J > 0$ for all $k > M$.

(3) Generate the auxiliary energy grid ENERGB, which is uniform in velocity space. M points will be included on each side of the energy region [Emin − Wmin, Emax + Wmax], where Emin and Emax are the experimental energy limits, and Wmin and Wmax are resolution limits at Emin and Emax, respectively.

(4) Generate theoretical cross sections $\sigma(E)$ for all ENERGB points.

(5) Evaluate F_i^J for all points i in the auxiliary grid, using Eq. (III B2.8), and convert to cross section using Eq. (III B2.1). If needed, the partial derivative of the cross section with respect to the temperature may be generated from

$$\left.\frac{\partial\sigma}{\partial\Theta}\right|_{\Theta=\Theta_J,\, v=v_i} = \frac{1}{\Delta\Theta}\left(F_i^{\,J+1} - F_i^{\,J}\right) \quad . \qquad \text{(III B2.11)}$$

Using the chain rule with Eq. (III B2.4), combined with Eqs. (III B2.6) and (III B2.11), gives

$$\left.\frac{\partial\sigma}{\partial T}\right|_{\Theta=\Theta_J,\, v=v_i} = \frac{T}{E}\,\frac{\Theta}{\Delta\Theta}\left[\frac{1}{6}F_{i-1}^{J} - \frac{1}{3}F_i^{J} + \frac{1}{6}F_{i+1}^{J}\right] \qquad \text{(III B2.12)}$$

for the derivatives of the cross section with respect to the temperature.

(6) From here on, follow the prescription given in Section III.A, beginning at step 4.

Finally, we recall from the discussion of the free-gas model (Section III.B.1) that the integral equation for Doppler broadening [Eq. (III B1.1) or (III B1.7)] is symmetric with respect to the transformation $v' \rightarrow -v'$, provided $\sigma\left(-|v'|\right)$ is defined as $-\sigma\left(|v'|\right)$ as in Eq. (III B1.6). In a similar manner, the Leal-Hwang option permits the direct evaluation of the broadened cross section even for points near $E = 0$.

[In earlier versions of SAMMY (prior to the 2006 release, sammy-7.0.0), studies suggested that results obtained for *very* low energies (well below thermal) were not completely accurate; specifically, Doppler-broadened $1/v$ cross sections did not retain the $1/v$ shape at these very low energies, and the step size ΔT was critically important. This was found to be due to a mistake in the coding, which was corrected for the sammy-7.0.0 release.]

To minimize the number of points required for use in the auxiliary grid, SAMMY users are encouraged to rely on the FGM (see Section III.B.1) for most calculations. The Leal-Hwang model is useful for double-checking results at low energies, and in other situations that call for accurate calculation of Doppler broadening of smooth cross sections.

To use the Leal-Hwang Doppler broadening, include in your INPut file a line which reads

USE LEAL,HWANG DOPPLER BROADENING

and specify the step size ΔT on card set 5 of the INPut file, Table VIA.1.

III.B.3. High-Energy Gaussian Approximation to Doppler Broadening

The high-energy Gaussian approximation (HEGA) to the free-gas model (FGM) for Doppler broadening has been used successfully for many years [WV12, AF71, FF80], and is the original option available within SAMMY. Its use, however, is now discouraged [NL98]: It is unusable at low energies, inaccurate at all energies, and requires the same amount of computer time and memory as does the FGM. Nevertheless, it is still included in the code for comparison purposes.

The Doppler-broadened cross section may be approximated by convoluting the unbroadened cross section with a Gaussian function of energy as

$$\sigma_D(E) = \frac{1}{\Delta_D\sqrt{\pi}} \int_{Emin}^{Emax} \exp\left\{\frac{(E-E')^2}{\Delta_D^2}\right\} \sigma(E')\,dE' \quad , \qquad \text{(III B3.1)}$$

where the Doppler width Δ_D is again given by

$$\Delta_D = \sqrt{\frac{4mE\ kT}{M}} \quad . \qquad \text{(III B3.2)}$$

In this equation, m represents the mass of the neutron, M is the target mass, k is Boltzmann's constant, and T is the effective temperature of the sample material. SAMMY evaluates the Doppler width directly from this formula (i.e., without using heavy-mass approximations). The integration limits in Eq. (III B3.1) are actually infinite but are approximated by $Emax = E + 5\Delta_D$ and $Emin = E - 5\Delta_D$.

For Doppler broadening via the high-energy Gaussian approximation, the only input quantity that the user must provide to SAMMY is the effective temperature T. See Table VI A.1, card set 5, variable TEMP, or Table VI B.2, card set 4, variable TEMP.

Caveat: For very low energies, the integration limits may fall below zero. In this case, SAMMY will issue a warning and switch to the FGM. To circumvent this problem, either use the FGM directly (see Section III.B.1), use the Leal-Hwang Doppler broadening (Section III.B.2), or invoke the option "NO LOW-ENERGY BROADEning is to be used" in the INPut file (see Table VI A1.2).

Again, the *recommended* method of Doppler broadening is the FGM, described in Section III.B.1. Use of the high-energy Gaussian approximation described in this section is not encouraged.

III.B.4. Crystal-Lattice Model of Doppler Broadening

The crystal-lattice model (CLM) of Doppler broadening used in SAMMY is based on the DOPUSH model of Naberejnev [DN99, DN99a], which in turn is based on the LEAPR model of NJOY [RM82]. Only the continuous and the discrete modes were developed further in DOPUSH.

(Readers are encouraged to consult the references for a description of the physics; a later revision of the SAMMY manual will include more detail. Alternative descriptions can be found in works by Meister [AM94].)

The algorithm used in SAMMY is virtually identical to the algorithm used in the DOPUSH code, where "identical" implicitly implies "for the examples that were available." No attempt has yet been made by this author to extend the validity of the model beyond ensuring agreement between DOPUSH and SAMMY when run with the same input.

Prior to implementing the DOPUSH CLM into SAMMY, this author created a modified version of DOPUSH (denoted DOPUSHx) which uses the same input and runs in the same manner as DOPUSH but whose coding is streamlined and more readily portable than the original DOPUSH code. Below is an itemization of the changes made for DOPUSHx (and also incorporated into SAMMY).

1. Values of physical and mathematical constants conform to ENDF standards. See Section IX.A of this document.

2. One or two "trivial" errors were corrected [notably, mass-factor self-consistency is ensured by using $(M+m)/M$ not $(M+1)/M$ with M and m in units of amu].

3. Redundant calculations were moved outside the energy loops; many of the intermediate computations required for convolving the phonon distributions are energy independent and do not need to be repeated for each energy. This change resulted in a significant decrease in computer processor unit (cpu) time.

4. More efficient sorting algorithms are employed; in general, FORTRAN operations have been made more efficient.

Changes made from DOPUSHx to SAMMY include the following.

1. Nomenclature has been modified to conform to SAMMY conventions.

2. Savings in cpu time from DOPUSHx to SAMMY are primarily the result of SAMMY's organizational scheme, in which the unbroadened cross sections are first calculated on an energy grid designed to describe the curvature of the cross section with reasonable accuracy, assuming a quadratic interpolation scheme. When the unbroadened cross section is required at a different energy, interpolation is used. In contrast, DOPUSH and DOPUSHx re-

calculate the unbroadened cross section whenever it is needed, using algorithms similar to those employed in NJOY. (The cost which SAMMY users must pay for this increased speed is that the accuracy of integrations cannot be tested during the integration process, as it is in NJOY. SAMMY users are reminded to make such tests themselves in order to have full confidence in their results.)

The examples of input for DOPUSH which were provided by Naberejnev have been organized into SAMMY test case tr124. For those examples that run on all three programs (DOPUSH, SAMMY, & DOPUSHx), the three codes give virtually the same results. The time required for the computations is significantly shorter with the newer codes (details available from the author upon request). This is true even when the number of points in SAMMY's auxiliary grid was increased dramatically (NXTRA was changed from 0 to 99), as a double-check on the accuracy of SAMMY's calculation. Accuracy was not significantly affected by the additional energy points, indicating that SAMMY's original grid is sufficiently dense.

For this release of SAMMY, no attempts have been made to improve or expand upon the model as provided by Naberejnev. One improvement that will likely be made for a subsequent release is the ability to treat the temperature as a search parameter in the fitting procedure.

For a description of the input to SAMMY's CLM, see Section VI.F.5.

III.C. RESOLUTION BROADENING

Unlike Doppler broadening, for resolution broadening there is no "standard" or "best" function that is appropriate everywhere. Instead, each analysis code has its own version of resolution broadening, with specific formulations for specific experimental sites or setups. For this reason, many distinct types of resolution broadening are available in SAMMY.

Readers interested in a detailed study of resolution broadening, with emphasis on the 200-m flight path at the Oak Ridge Electron Linear Accelerator (ORELA), are referred to the paper by Larson, Larson, and Harvey [DL84].

The original resolution-broadening function in SAMMY is a combination of Gaussian plus exponential. This formulation is based upon the method used in the MULTI code [GA74] and is described in Section III.C.1.

A second option is a more realistic function — the ORR or "Oak Ridge Resolution function," which uses mathematical descriptions of the components in the experimental broadening as determined from careful studies of ORELA experiments. Section III.C.2 gives specifics about this resolution function.

Another option is a realistic function designed to describe the experimental situation for the linac at Rensselaer Polytechnic Institute; this "RPI resolution function" is described in Section III.C.3. This option has been expanded to include features which may make it also useful for data from the Geel Electron Linear Accelerator (GELINA) at the Institute for Reference Materials and Measurements (IRMM) in Belgium or for data from the neutron time-of-flight (nTOF) facility at the European Council for Nuclear Research (CERN) in Switzerland.

A straight-line energy average resolution function is available, primarily for use with charged-particle or angular distribution data. See Section III.C.4.

A numerical user-defined resolution (UDR) function is described in Section III.C.5.

It is possible to include more than one of the above resolution functions for a single SAMMY run. To use this feature, include the command

```
TWO RESOLUTION FUNCTions together
```

in your INPut file. With this command, you are permitted to use the following combinations of resolution functions:

1. one occurrence of the Gaussian plus exponential function; and/or
2. one straight-line energy average resolution function; and/or
3. at most one of the ORR, RPI, or UDR resolution functions.

III. C. 1. Gaussian plus Exponential Resolution Broadening

To understand how a resolution broadening may be described mathematically, we first consider the formula that describes how the neutron's energy is extracted from measured quantities:

$$E = \frac{1}{2}mv^2 = \frac{1}{2}m\left(\frac{L}{t}\right)^2 \quad , \qquad \text{(III C1.1)}$$

where m is the neutron mass and v its velocity. The velocity is equal to the flight-path length L divided by travel time t. From this definition, it is clear that two types of resolution broadening are possible — one due to distributions in time and the other due to distributions in length.

Several factors may contribute to each of the two types of resolution broadening. In this version of SAMMY's resolution function, the following components of the resolution function are treated explicitly (but approximately): (1) a square distribution in flight-path length (due, for example, to the neutron moderator and/or detector), (2) a square distribution in time (channel width), and (3) a Gaussian distribution in time (burst width). Together these are expressed as an approximate Gaussian distribution in energy (see Section III.C.1.a). An exponential distribution may also be included (see Section III.C.1.b).

Table III C 1.1 shows relationships between input parameters and the resolution width associated with various types of resolution distribution functions. This table is included here as an aid in determining appropriate values to use as input to SAMMY. Note that "equivalent," as used in the following pages, indicates only that the first and second moments of the distributions are identical, not that the distributions have the same shapes.

For a detailed discussion of resolution broadening with emphasis on flight path 1 at ORELA, see [DL84].

Table III C1.1. Resolution-broadening input parameters

SAMMY input variable	"Equivalent" quantity	Description
ΔL or DELTAL (Section III.C.1.a)		ΔL is the full width of a square distribution in flight-path length
	$\sqrt{12}\ \sigma_L$	σ_L is the standard deviation of a Gaussian distribution in flight-path length
	$F_L / \sqrt{(\ln 2) 2/3}$	F_L is the full width at half maximum of a Gaussian distribution in flight-path length
	$S_L \sqrt{3}\ L/E$	S_L is the standard deviation of a Gaussian distribution in energy E, where L is the flight-path length
	$\Delta_L \sqrt{3/2}\ L/E$	Δ_L is the full width at half maximum of a Gaussian distribution in energy E, where L is the flight-path length
Δt_c or DELTAB $\times$ Cf_i (see Section III.C.1.a)		Δt_c is the full width of a square distribution in time (channel width); this is the equivalent of the quantity b in [DL84], page 30
	$\sqrt{12}\ \sigma_c$	σ_c is standard deviation of Gaussian in time
	$\sqrt{3/2 \ln 2}\ F_c$	F_c is full width at half max of Gaussian in time
	$\frac{\sqrt{3}\ t}{E} S_c = \sqrt{\frac{3m}{2}} \frac{L}{E^{3/2}} S_c$	S_c is the standard deviation of a Gaussian distribution in energy
Δt_G or DELTAG (Section III.C.1.a)		Δt_G is the full width at half max of a Gaussian distribution in neutron transit time
	$\sqrt{8 \ln 2}\, \sigma_G$	σ_G is the standard deviation of a Gaussian distribution in time
	$\sqrt{2 \ln 2/3}\ f$	f is the full width of square distribution in time
Δt_E or DELTAE (see Section III.C.1.b)		Δt_E is the exponential folding width in microseconds of an exponential distribution in time; note that this is an asymmetric function
	$\frac{L(m/2)^{1/2} \Delta_E}{2E^{3/2}}$	Δ_E is the exponential folding width of the exponential distribution in energy

III.C.1.a. Resolution broadening: Gaussian

Broadening in L is due to the "spread" or "distribution of locations" at which the flight path begins or ends (for details, see ref. [DL84]). This distribution may include contributions from both the source and the detector, and may be described by a square function in length L; that is,

$$dE''\rho_L\left(E',E''\right)=\begin{cases}\dfrac{dL''}{\Delta L} & \text{for } L'-\Delta L/2 \le L'' \le L'+\Delta L/2 \\ 0 & \text{otherwise} \quad .\end{cases} \qquad \text{(III C1 a.1)}$$

Note that ΔL is equal to $\sqrt{12}$ times the standard deviation of an "equivalent" Gaussian distribution in length. Note also that the input quantity ΔL may be expressed either as a constant (see variable DELTAL in card set 5 of the INPut file, Table VI A.1, or card set 4 of the PARameter file, Table VI B.2), or as an energy-dependent function of the form

$$\Delta L = E\,\Delta L_1 + \Delta L_0 \quad . \qquad \text{(III C1 a.2)}$$

(See card set 11, line number 2, of the PARameter file, Table VI B.2).

For convenience in later calculations, this square function in length will be converted to a Gaussian function in energy; that is,

$$dE''\rho_L\left(E',E''\right)\cong\frac{dE''}{\Delta_L\sqrt{\pi}}\exp\left\{-\left|\frac{E''-\bar{E}}{\Delta_L}\right|^2\right\} \quad , \qquad \text{(III C1 a.3)}$$

where $\bar{E}$ and Δ_L are found by equating means and variances of the two expressions in Eqs. (III C1 a.1) and (III C1 a.3).

The mean energy for the distribution described in Eq. (III C1 a.1) is given by

$$\begin{aligned}\int_{L'-\Delta L/2}^{L'+\Delta L/2} E''\frac{dL''}{\Delta L} &= \frac{m}{2t^2}\frac{1}{\Delta L}\int_{L'-\Delta L/2}^{L'+\Delta L/2}\left(L''\right)^2 dL'' \\ &= \frac{m}{2t^2}\frac{1}{\Delta L}\left(L'^2\,\Delta L+\left(\Delta L\right)^3/12\right)=E'\left[1+\frac{\Delta^2 L}{12\,L'^2}\right] \quad .\end{aligned} \qquad \text{(III C1 a.4)}$$

Similarly, the second moment of that distribution is given to first order in $\left(\Delta L/L'\right)^2$ by

$$\int_{L'-\Delta L/2}^{L'+\Delta L/2} E''^2\,\frac{dL''}{\Delta L}\cong E'^2\left[1+\frac{\Delta^2 L}{2L'^2}\right] \qquad \text{(III C1 a.5)}$$

so that the variance of the square distribution is given by

$$E'^2\left[1+\left(\Delta L/L'\right)^2/2\right]-E'^2\left[1+\left(\Delta L/L'\right)^2/12\right]^2 \cong E'^2\left[1+\left(\Delta L/L'\right)^2/3\right] \quad . \text{(III C1 a.6)}$$

Since the mean of the Gaussian distribution in Eq. (III C1 a.3) is $\bar{E}$ and the variance is $\Delta_L^2/2$, the parameters of the Gaussian are given (to lowest order) by

$$\bar{E} = E' \qquad \text{(III C1 a.7)}$$

and

$$\Delta_L = \sqrt{2/3}\,E'\left(\Delta L/L'\right) \quad . \qquad \text{(III C1 a.8)}$$

Finite channel width is one contributor to broadening in time (for details, see [DL84]). The channel width is represented by a square function in time with width Δt_c as

$$dE'\rho_c\left(E,E'\right) = \begin{cases} \dfrac{d\,t'}{\Delta t_c} & \text{for } t-\Delta t_c/2 \le t' \le t+\Delta t_c/2 \\ 0 & \text{otherwise} \quad . \end{cases} \qquad \text{(III C1 a.9)}$$

Generally the channel width is constant for a certain energy range, but changes from one range to the next. SAMMY input accommodates this characteristic: values for Δt_c are given as a constant DELTAB times a "crunch factor" CF_i for energies between Bc_{i-1} and Bc_i. Details are given in Table VI A.1, card set 6.

This component of the resolution function also will be converted to an equivalent Gaussian function in the energy variable. Arguments similar to those given above for Eqs. (III C1 a.3) through (III C1 a.8) show that this Gaussian has the form

$$dE'\rho_c\left(E,E'\right) = \frac{dE'}{W_c\sqrt{\pi}}\exp\left\{-\frac{\left(E'-E\right)^2}{W_c^2}\right\} \qquad \text{(III C1 a.10)}$$

where

$$W_c = \sqrt{2/3}\;E\,\Delta t_c/t \quad . \qquad \text{(III C1 a.11)}$$

Combining approximations (III C1 a.3) and (III C1 a.10) using (III C1 a.7), (III C1 a.8), and (III C1 a.11) gives, for the resolution-broadened cross section (or transmission),

$$f_{Lc}\left(E\right) = \frac{1}{W_c\sqrt{\pi}}\int_{-\infty}^{+\infty} dE'\exp\left\{-\frac{\left(E'-E\right)^2}{W_c^2}\right\}\;\frac{1}{\Delta_L\sqrt{\pi}}\int_{-\infty}^{+\infty} dE''\exp\left\{-\frac{\left(E''-E'\right)^2}{\Delta_L^2}\right\} \quad . \quad \text{(III C1 a.12)}$$

This form may be greatly simplified by recalling that the convolution of two Gaussians is also a Guassian, with variance equal to the sum of the two variances. This is strictly true only if the width Δ_L of the second Gaussian is independent of the variable of integration E' of the first Gaussian. Nevertheless, we may approximate E' and L' in our expression for Δ_L, Eq. (III C1 a.8), by E and L since the integrand of Eq. (III C1 a.12) is large only near $E' \cong E$ (i.e., $L' \cong L$). Then Eq. (III C1 a.12) may be written

$$f_{Lc}(E) = \frac{1}{\Delta_{Lc}\sqrt{\pi}} \int_{-\infty}^{+\infty} dE'' \exp\left\{ -\frac{(E''-E)^2}{\Delta_{Lc}^2} \right\} f(E'') \quad , \qquad \text{(III C1 a.13)}$$

where

$$\Delta_{Lc}^2 = \frac{2}{3} E^2 \left[(\Delta t_c / t)^2 + (\Delta L / L)^2 \right] \quad . \qquad \text{(III C1 a.14)}$$

Neutron burst width is another contributor to the resolution broadening. This effect may be approximated by a Gaussian (or convolution of Gaussian plus exponential; see Sections III.C.1.b and III C1.c) with full width at half max Δt_G. (See variable DELTAG in Table VIA.1, card set 5, or Table VI B.2, card set 4.) That is, the Gaussian distribution function in time is given by

$$dE' \rho_G(E, E') = \frac{dt'}{w_G \sqrt{\pi}} \exp\left\{ -\frac{(t-t')^2}{w_G^2} \right\} \quad , \qquad \text{(III C1 a.15)}$$

which translates into

$$dE' \rho_G(E, E') = \frac{dE'}{W_G \sqrt{\pi}} \exp\left\{ -\frac{(E-E')^2}{W_G^2} \right\} \quad , \qquad \text{(III C1 a.16)}$$

in which the quantities w_G and W_G are defined in terms of the full width at half max via

$$w_G = \Delta t_G / \sqrt{\ln 2} \qquad \text{(III C1 a.17)}$$

and

$$W_G = \sqrt{\frac{E^3}{(m/2)\ln 2}} \left(\frac{\Delta t_G}{L} \right) \quad . \qquad \text{(III C1 a.18)}$$

[The derivation of Eq. (III C1 a.16) requires the approximation that $\sqrt{E'} \approx \sqrt{E}$ to zeroth order.]

This function may then be combined with the other components of the resolution function of Eq. (III C1 a.12). Again, because the convolution of two Gaussians is itself a Gaussian, the result may be written directly as

$$f_G(E) = \frac{1}{\Delta_G \sqrt{\pi}} \int_{-\infty}^{+\infty} dE' \exp\left\{ -\frac{(E'-E)^2}{\Delta_G^2} \right\} f(E') \quad , \qquad \text{(III C1 a.19)}$$

where the width is given by

$$\Delta_G^2 = \frac{2}{3} E^2 \left[\left(\frac{\Delta t_c}{t} \right)^2 + \left(\frac{\Delta L}{L} \right)^2 \right] + \frac{E^3}{\frac{m}{2} \ln 2} \left(\frac{\Delta t_G}{L} \right)^2 \quad . \qquad \text{(III C1 a.20)}$$

Replacing t in Eq. (III C1 a.20) by its equivalent in terms of E and L and rearranging give

$$\Delta_G^2 = \frac{2}{m} E^3 \left[\frac{1}{\ln 2} \left(\frac{\Delta t_G}{L} \right)^2 + \frac{2}{3} \left(\frac{\Delta t_c}{L} \right)^2 \right] + \frac{2}{3} E^2 \left(\frac{\Delta L}{L} \right)^2 \quad , \qquad \text{(III C1 a.21)}$$

which may be rewritten in the form

$$\Delta_G = E\left[aE + b \right]^{1/2} \quad . \qquad \text{(III C1 a.22)}$$

If E is given in units of eV, Δt_G in μsec, and L in meters, then the neutron mass m may be expressed as

$$m \cong 2(72.3)^2 \quad . \qquad \text{(III C1 a.23)}$$

This follows directly from $m = 1.67482 \times 10^{-24}\, g$ and $1\,\text{erg} = g\ \text{cm}^2/\text{s}^2 = 6.2418 \times 10^{11}\,\text{eV}$. With this value for the mass, the parameters a and b in Eq. (III C1 a.22) become

$$\begin{aligned} a &= \left(\frac{1}{\frac{m}{2} \ln 2} \frac{\Delta t_G}{L} \right)^2 + \left(\left(\frac{2}{3} \frac{2}{m} \right)^{1/2} \frac{\Delta t_c}{L} \right)^2 \\ &\cong \left(0.01661 \frac{\Delta t_G}{L} \right)^2 + \left(0.011293 \frac{\Delta t_c}{L} \right)^2 \end{aligned} \qquad \text{(III C1 a.24)}$$

and

$$b = \left(\sqrt{2/3}\ \Delta L / L \right)^2 \cong \left(0.81650\, \Delta L / L \right)^2 \quad . \qquad \text{(III C1 a.25)}$$

Partial derivatives

From Eq. (III C1 a.19), the partial derivative of cross section (or transmission) f_G with respect to Δt_G and ΔL may be written as

$$\frac{\partial f_G}{\partial \Delta t_G} = \frac{\partial \Delta_G}{\partial \Delta t_G} \frac{\partial f_G}{\partial \Delta_G} \qquad \text{(III C1 a.26)}$$

and

$$\frac{\partial f_G}{\partial \Delta L} = \frac{\partial \Delta_G}{\partial \Delta L} \frac{\partial f_G}{\partial \Delta_G} \quad . \qquad \text{(III C1 a.27)}$$

Partial derivatives of Δ_G are, from Eqs. (III C1 a.20) and (III C1 a.21),

$$\frac{\partial \Delta_G}{\partial t_G} = \frac{E^3 a}{\Delta_G \, \Delta t_G} \qquad \text{(III C1 a.28)}$$

and

$$\frac{\partial \Delta_G}{\Delta L} = \frac{E^2 b}{\Delta_G \, \Delta L} \quad . \qquad \text{(III C1 a.29)}$$

The partial derivative with respect to Δ_G is found numerically via

$$\frac{\partial f_G}{\partial \Delta_G} \cong \frac{f_G\left(\Delta_G + d\right) - f_G\left(\Delta_G - d\right)}{2d} \quad , \qquad \text{(III C1 a.30)}$$

where d is set equal to $\Delta_G \, q$ with $q = 0.02$.

III.C.1.b. Resolution broadening: exponential

An exponential form for the resolution broadening is also provided in SAMMY (and MULTI). Physically this may correspond to an asymmetry in the burst width or moderator or detector resolution function. When only the exponential function is to be used, the broadened cross section (or transmission) is given by the integral

$$f_{\exp}(E) = \frac{1}{\Delta t_E} \int_t^{\infty} \exp\left\{ -\frac{(t-t')}{\Delta t_E} \right\} f(E')\, d\,t' \quad , \qquad \text{(III C1 b.1)}$$

where $f(E')$ represents the unbroadened cross section. This expression may be rewritten in terms of E' rather than t' using the relationship in Eq. (III C1.1), and assuming $\sqrt{E'} \cong \sqrt{E}$ as needed. Eq. (III C1 b.1) becomes

$$f_{\exp}(E) = \frac{1}{\Delta_E} \int_E^{\infty} \exp\left\{ -\frac{(E-E')}{\Delta_E} \right\} f(E')\, d\,E' \quad , \qquad \text{(III C1 b.2)}$$

in which the width is given by

$$\Delta_E = \frac{2E^{3/2}}{L(m/2)^{1/2}} \Delta t_E \quad . \qquad \text{(III C1 b.3)}$$

Setting $m/2 = (72.3)^2$ as in the previous section gives the result used in SAMMY,

$$\Delta_E = cE^{3/2} \quad , \qquad \text{(III C1 b.4)}$$

in which c is defined as

$$c \;=\; 2\sqrt{m/2}\;\Delta t_E / L \;\cong\; 0.02766\,\Delta t_E / L \quad ; \qquad \text{(III C1 b.5)}$$

exact values used for the constants are discussed in Section IX.A.

The width Δt_E is the "exponential folding width in microseconds" and is the required input quantity DELTAE (see Table VI A.1, card set 5, or Table VI B.2, card set 4). Two options are available for energy-dependent width: The first assumes the form

$$\Delta t_E = \frac{\Delta t_x}{\sqrt{E/E_x}} \quad . \qquad \text{(III C1 b.6)}$$

In this case the input quantity is Δt_x and E_x is fixed at 100 eV. The line "EXPONENTIAL FOLDING width is energy dependent" must be included in the INPut file; see Table VI A1.2. The second option assumes energy dependence of the form

$$\Delta t_E = D_1 E + D_0 + D_2 \ln(E) \quad ; \qquad \text{(III C1 b.7)}$$

parameters D_i are specified in card set 11, line 10, of the PARameter file.

Partial derivatives

The partial derivative of $f_{\exp}$ with respect to Δt_E is given by

$$\frac{\partial f_{\exp}}{\partial \Delta t_E} = \frac{\partial \Delta_E}{\partial \Delta t_E} \frac{\partial f_{\exp}}{\partial \Delta_E} \quad , \qquad \text{(III C1 b.8)}$$

where the first partial derivative is found from Eq. (IIIC1b.3) to be

$$\frac{\partial \Delta_E}{\partial \Delta t_E} = \frac{\Delta_E}{\Delta t_E} \quad . \qquad \text{(III C1 b.9)}$$

The second partial derivative in Eq. (III C1 b.8) is evaluated numerically via

$$\frac{\partial f_{\exp}}{\partial \Delta_E} = \frac{f_{\exp}\left(\Delta_E + d\right) - f_{\exp}\left(\Delta_E - d\right)}{2d} \quad , \qquad \text{(III C1 b.10)}$$

where d is set to $q\Delta_E$ with q = 0.02.

III.C.1.c. Resolution broadening: convolution of Gaussian and exponential

Gaussian and exponential resolution broadening may be invoked simultaneously, giving the broadened cross section (or transmission) as

$$f_{GE}\left(E\right)=\frac{1}{\Delta_E\Delta_G\pi}\int_{E-\Delta E_S}^{\infty}dE''\exp\left\{-\frac{\left(E''-\left(E-\Delta E_S\right)\right)}{\Delta_E}\right\}$$
$$\times\int_{-\infty}^{+\infty}dE'\exp\left\{-\frac{\left(E'-E''\right)^2}{\Delta_G^2}\right\}f\left(E'\right)\quad, \qquad \text{(III C1 c.1)}$$

where the shift ΔE_S is introduced in order that the maximum of the broadening function be located at $E=E'$.

Rearrangement of the integrands in Eq. (III C1 c.1) and explicit integration over the E^0 variable yield

$$f_{GE}\left(E\right)=\frac{1}{2\Delta_E}\exp\left\{\frac{\Delta_G^2}{4\Delta_E^2}\right\}\int_{-\infty}^{+\infty}dE'\,f\left(E'\right)\exp\left\{-\frac{\left(E'-E+\Delta E_S\right)}{\Delta_E}\right\}$$
$$\times\operatorname{erfc}\left(\frac{\Delta_G}{2\Delta_E}-\frac{\left(E'-E+\Delta E_S\right)}{\Delta_G}\right)\quad. \qquad \text{(III C1 c.2)}$$

Historical Note: this is not the form which is given in the MULTI manual [GA74] but is the (correct) form that is used in both the MULTI and the SAMMY codes.

The energy shift ΔE_S is found by setting $g\left(E'\right)=\exp\left(.\right)\operatorname{erfc}\left(.\right)$ from the integrand of Eq. (III C1 c.2) and locating the value of $E'_{\max}$ for which $g\left(E'_{\max}\right)$ is a maximum by setting $dg/dE'=0$ at that value. This value $E'_{\max}$ is then set equal to *E*, and the resulting equation solved for ΔE_S. Newton's method is used to find the solution.

Alternatively, one can assume that the energy shift is zero. This requires the inclusion of a line in the INPut file reading

```
DO NOT SHIFT ENERGY for exponential tail on resolution broadening
```

The lower and upper integration limits in Eq. (III C1 c.2) are truncated to $E-5\Delta_G$ and $\max\left(E+6.25\Delta_E\,,\,E+5\Delta_G\right)$, respectively.

Partial derivatives

Derivatives of the broadened cross section (or transmission) f_{GE} with respect to Δt_G, ΔL, or Δt_E are found exactly as in the previous two subsections, with f_G and $f_{\exp}$ replaced by f_{GE}.

III.C.2. Oak Ridge Resolution Function (ORR)

For ORELA data, the resolution-broadening functions described in Section III.C.1 are not especially accurate approximations. We have therefore developed a more realistic mathematical description of the experimental situation at ORELA, based on concepts described by D. C. Larson et al. [DL84] and initially derived by F. G. Perey [FP89].

The resolution function has four components: the electron burst, the ORELA moderator, the neutron detector, and the time-of-flight channel width. Experimentally, the resolution-broadened cross section $\bar{\sigma}(E)$ is formed when each contributing feature provides its own broadening; the combined effect of the several components is all that is actually noticed. Mathematically, this may be viewed as follows: Each component is modeled separately as a function of flight time (rather than energy), and then each is convoluted in turn with the unbroadened (or partially broadened) cross section; the convolution process is performed analytically where possible and numerically where necessary. That is, the resolution-broadened cross section $\bar{\sigma}(t)$ may be expressed as

$$\bar{\sigma}(t) = \int I_1(t-t_1)\,dt_1 \int I_2(t_1-t_2)\,dt_2 \int I_3(t_2-t_3)\,dt_3 \int I_4(t_3-t_4)\,dt_4\ \sigma(t_4) \quad , \qquad \text{(III C2.1)}$$

where I_i is our mathematical model for the ith component. This expression may then be rearranged into the form

$$\bar{\sigma}(t) = \int I(t-t')\sigma(t')\,dt' \quad , \qquad \text{(III C2.2)}$$

where the resolution function $I(t-t')$ is defined as

$$I(t-t') = \int I_1(t-t_1)\,dt_1 \int I_2(t_1-t_2)\,dt_2 \int I_3(t_2-t_3)\,dt_3\ \ I_4(t_3-t') \quad . \qquad \text{(III C2.3)}$$

Because SAMMY deals with cross sections as functions of energy, rather than time, the relationship

$$E = \frac{1}{2}mv^2 = \frac{1}{2}m\frac{L^2}{t^2} \qquad \text{(III C2.4)}$$

is used to convert from energy to time (or time to energy) in Eq. (III C2.2), yielding

$$\bar{\sigma}(E) = \int I'(t(E)-t')\sigma(E'(t'))\,dt' \quad . \qquad \text{(III C2.5)}$$

In the following sections we describe the components I_i and the convolution procedure. Input for using this resolution function is described in card set 9, Table VI B.2. See also Section X.H, which describes program SAMORT, used for plotting the individual pieces and the complete ORR function at a specified energy.

III.C.2.a. Individual components of the ORR resolution function

1. Electron burst

The electron burst from ORELA is closely approximated by a square function in time:

$$I_1(t) = \begin{cases} 1/p & \text{for } 0 < t < p \\ 0 & \text{otherwise} \end{cases} , \qquad \text{(III C2 a.1)}$$

where p is the burst width in nanoseconds. The value $1/p$ for this function gives a normalization of unity.

2. Neutron sources

Experiments at ORELA can utilize neutrons from a tantalum target, or collimate on the water moderator surrounding the tantalum target. The two are modeled separately; experiments are assumed to use predominantly one or the other, rather than a mixture of both. (The implications to this representation if neutrons are emitted from both the tantalum target and the water moderator will be studied as time and funding permit.)

ORELA water moderator

The distribution of flight-path lengths of neutrons in the ORELA water moderator that has the most physical basis [SC92] is the chi-square distribution with $2(m+1)$ degrees of freedom, where m is an integer. (Originally m = 4 or 5, but any integer from 1 to 10 will now work; the default value is m = 4.)

$$I'_{2a}(l) = \frac{l^m}{m!\Lambda^{m+1}} \exp\left(-\frac{l}{\Lambda}\right) , \qquad \text{(III C2 a.2)}$$

where l is the flight-path-length variable and where the moderation distance Λ is a mean free path. The value of Λ varies with energy as $\Lambda = \Lambda_0 + \Lambda_1 \ln(E) + \Lambda_2 (\ln(E))^2$ [CC83]. Default values for the Λ_i are chosen to give agreement with [SC92].

Tantalum target

The distribution of flight-path lengths for the tantalum target is somewhat more complicated: Monte Carlo calculations of F. G. Perey [FP92] have shown that this distribution function has the form

$$I'_{2b}(l) = \begin{cases} 0 & \text{for} \quad l < x'_1 \\ u'(l) + v'(l) & \text{for } x'_1 < l < x'_2 \\ u'(l) + w'(l) & \text{for } x'_2 < l < x'_3 \\ w'(l) & \text{for } x'_3 < l \quad , \end{cases} \qquad \text{(III C2 a.3)}$$

where the functions $u'(l)$, $v'(l)$, and $w'(l)$ are defined as

$$u'(l) = N' \exp\left\{-\varepsilon'^2 \left(l - x'_0\right)^2\right\} \quad \text{for} \quad x'_1 < l < x'_3 \quad , \qquad \text{(III C2 a.4)}$$

$$v'(l) = \frac{N'\alpha' l}{x'_2} \exp\left\{-\beta\left(l - x'_2\right)\right\} \quad \text{for} \quad x'_1 < l < x'_2 \quad , \qquad \text{(III C2 a.5)}$$

and

$$w'(l) = N'\alpha' \exp\left\{-\beta'\left(l - x'_2\right)\right\} \quad \text{for} \quad x'_2 < l \quad . \qquad \text{(III C2 a.6)}$$

The factor N' is a normalization, and α' determines the relative strengths of the pieces of the function I'_{2b}. The relative values of the x's are given by

$$x'_1 \le x'_0 \le x'_2 \le x'_3 \quad . \qquad \text{(III C2 a.7)}$$

3. Time-of-flight channel width

Like the electron burst, the time-of-flight channel width may be modeled as a rectangular distribution of width c. This functional form ignores "electronic" time jitter, which is a reasonable approximation. The time distribution due to the finite channel width is therefore assumed to be

$$I_3(t) = \begin{cases} 1/c & \text{for} \quad 0 < t < c \\ 0 & \text{otherwise} \quad , \end{cases} \qquad \text{(III C2 a.8)}$$

where the channel width c may be different for different energy regions.

4. Detectors

Two types of neutron detectors are commonly used for transmission measurements at ORELA: the NE110 (a recoil proton detector) and the lithium glass (for which moderation of neutrons in the detector plays an important role).

NE110 detector

If δ is the thickness of the NE110 detector, then the resolution function appropriate for that detector is

$$I'_{4a}(l) = \begin{cases} \Delta \exp(-\lambda\sigma l) & \text{for } 0 < l < \delta \\ 0 & \text{otherwise} \end{cases} . \qquad \text{(III C2 a.9)}$$

where λ is the number of molecules per volume (molecules per millimeter barn) of the detector (0.0047 for NE110), and $\sigma(E)$ is the total cross section of the detector material ($CH_{1.104}$ for NE110). The normalization factor Δ is found by setting the integral over all space of I'_{4a} equal to 1.

Lithium glass detector

For the lithium glass detector, the resolution function is assumed to have the form

$$I_{4b}(l) = \begin{cases} Dg & \text{for } 0 < t < d \\ D\exp(-f(t-d)) & \text{for } d < t \end{cases} , \qquad \text{(III C2 a.10)}$$

where g, f, and d are constants, and D is chosen to give an integral of unity.

III.C.2.b. Converting length to time dependence

The relationship between energy E, flight time t, and flight-path length l may be used to convert from a function of l to a function of t (assuming E is fixed):

$$E = \frac{m}{2}\frac{l^2}{t^2} \quad , \qquad \text{(III C2 b.1)}$$

which may be rearranged to give

$$l = \sqrt{\frac{2E}{m}}\, t = b\,t \quad , \qquad \text{(III C2 b.2)}$$

in which we have defined b as the square root of $2E/m$. A distribution function in l may then be converted to a distribution function in t by (a) replacing l by bt everywhere and (b) replacing dl by $b\,dt$. In particular, the distances x'_i (tantalum target) translate to the time dimension via

$$x_i = x'_i / b \quad , \qquad \text{(III C2 b.3)}$$

and, similarly, δ (NE110 detector) translates via

$$d = \delta / b \quad . \qquad \text{(III C2 b.4)}$$

For the NE110 detector, we also define f via

$$f = \lambda \sigma b \quad . \qquad \text{(III C2 b.5)}$$

III.C.2.c. Convolution of the components of the ORR resolution function

Mathematical details of the process of convoluting the four components of the resolution function is non-trivial; only a summary is presented here.

The convolution of the electron-burst resolution function with the resolution function representing the channel width is straightforward and yields a trapezoidal function whose exact shape depends upon the relative magnitudes of the parameters *p* and *c*. Combining that result with the detector resolution function (either NE110 or lithium glass) gives a continuous function of the form

$$I_{134}(t) = \frac{D}{pcf^2}\left\{ A_{ei}\, e^{-f\,t} + A_{2i}\, f^2 t^2 + A_{1i}\, f\,t + A_{0i} \right\} \quad , \qquad \text{(III C2 c.1)}$$

which is valid in the region defined by $t_{i-1} < t < t_i$. Here t_i is the *i*th member of the ordered set of times $\{0, p, c, d, p+c, c+d, p+c+d\}$ with t_0 defined as 0. Algebraic expressions for the A_{ji} $(j = e, 2, 1, 0)$ in terms of the model parameters depend very strongly on the relative sizes of the parameter values; the specific formulae are too numerous and too complicated to list here, but are implemented within the code. Note that while the function is continuous, it is not smooth; the first derivative of this function is piecewise continuous, with discontinuities at the t_i.

Combining the above result with the resolution function for either the water moderator or the tantalum target gives a result which is a combination of polynomials and exponentials in $(t - t_i)$. The final resolution function is continuous but again not smooth; the first derivative has discontinuities at each of the t_i; for the tantalum target, the derivative has additional discontinuities at x_1, x_2, x_3, and at $t_i + x_j$. Nevertheless, the resolution function generally *appears* smooth.

III.C.3. RPI (and GELINA and nTOF) Resolution Broadening

Researchers at Rensselaer Polytechnic Institute (RPI) have carefully measured the resolution function associated with the "bounce target" and the transmission detector (lithium glass) for the LINAC at RPI [BM96]. This resolution function may be described by the sum of a chi-squared function (with six degrees of freedom) plus two exponential terms. The total resolution function appropriate for data measured on that machine is then the convolution of the target-detector resolution function, with a Gaussian function representing the electron burst and a square function representing the channel width.

An extension to the RPI resolution function has been shown by Gunsing [FG05] to provide a reasonable description for the resolution functions for two other time-of-flight facilities: the Geel Electron Linear Accelerator (GELINA) at IRMM in Belgium and the neutron time of flight (nTOF) facility at CERN in Switzerland. This extension (discussed in the next section) has been implemented in SAMMY.

Within SAMMY, the RPI resolution function is formed in much the same manner as described for the realistic resolution function of Section III.C.2, that is, the resolution-broadened cross section $\bar{\sigma}(t)$ may be expressed as

$$\bar{\sigma}(t) = \int I_1(t-t_1)\,dt_1 \int I_2(t_1-t_2)\,dt_2 \int I_3(t_2-t_3)\,dt_3\ \sigma(t_3) \quad , \qquad \text{(III C3.1)}$$

where I_i is our mathematical model for the ith component. This expression may then be rearranged into the form

$$\bar{\sigma}(t) = \int I(t-t')\,\sigma(t')\,dt' \quad , \qquad \text{(III C3.2)}$$

where the resolution function $I(t-t')$ is defined as

$$I(t-t') = \int I_1(t-t_1)\,dt_1 \int I_2(t_1-t_2)\,dt_2\ I_3(t_2-t'). \qquad \text{(III C3.3)}$$

Because SAMMY deals with cross sections as functions of energy, rather than time, the relationship

$$E = \frac{1}{2} m v^2 = \frac{1}{2} m \frac{L^2}{t^2} \qquad \text{(III C3.4)}$$

is used to convert from energy to time and vice versa in Eq. (IIIC3.2), yielding

$$\bar{\sigma}(E) = \int I'\big(t(E)-t'\big)\ \sigma\big(E'(t')\big)\,dt' \quad . \qquad \text{(III C3.5)}$$

In the following section (Section III.C.3.a), the component functions I_i are described, along with the parameters for those components.

Test cases tr053, tr054, tr094, and tr095 show several examples using the RPI resolution function, with parameter values suitable for RPI data and candidate parameters for use with GELINA data. More recently, the RPI resolution function has been extended to give a more suitable energy-dependent form for use with both GELINA and nTOF data; this form was suggested by Gunsing [FG05], who also provided preliminary parameter values. Testing for the extension is given in test cases tr104 and tr107; Gunsing's parameter values are used in tr108.

To make plots of this resolution function and the individual components, see Section X.K. Also see test case tr107 for examples of another method of plotting the RPI resolution function, using the Dirac delta function option for pseudo cross section with uniform energy grid (Section V.E).

Section III.C.3.b discusses the various input options for the RPI/GELINA/nTOF resolution function.

III.C.3.a. Components of the RPI / GELINA / nTOF resolution function

1. Electron burst

The electron burst from the RPI linac may be described by a Gaussian function in time, of the form:

$$I_1(t) = \frac{w}{\sqrt{\pi}} e^{-w^2 t^2} \quad , \qquad \text{(III C3 a.1)}$$

where $2\sqrt{\ln 2}/w = p$ is the full width at half max of the burst. Normalization is unity for this function.

2. Target plus detector

The RPI transmission resolution function, which represents the combined components for the "bounce target" and transmission detector, has been found by RPI researchers [BM96] to be best described by the sum of a chi-squared function with six degrees of freedom plus two exponential terms. A similar function (with different values for the parameters) describes the bounce target plus capture detector.

The original RPI function had constant values for A_3 and A_5. The GELINA and nTOF resolution functions proposed by Gunsing [FG05] use energy dependent values of the A_3 and A_5 parameters.

Specifically, the RPI resolution function has the form

$$I_2(t) = A_0 \left\{ \frac{(t+\tau)^2}{2!\Lambda^3} e^{-(t+\tau)/\Lambda} + A_1 \left[A_2 e^{-A_3(t+t_0)} + A_4 e^{-A_5(t+t_0)} \right] X(t) + \sum_{i=1}^{5} B_{2i-1} e^{-B_{2i}(t+t_0)} \right\} \quad , \qquad \text{(III C3 a.2)}$$

in which the function $X(t)$ is zero if the quantity within the square brackets (the sum of the exponential terms) is negative, and unity otherwise. Likewise the χ^2 function is assumed to have zero value when the exponent is positive (i.e., when $t+\tau<0$). The value of A_0 is chosen to give an overall normalization of unity for this function. Parameters Λ, τ, A_1, A_3, and A_5 are functions of energy, the specific forms being, respectively,

$$\Lambda(E) = \Lambda_0 + \Lambda_1 \ln(E) + \Lambda_2 \left[\ln(E)\right]^2 + \Lambda_3 E^{\Lambda_4} \quad , \qquad \text{(III C3 a.3)}$$

$$\tau\left(E\right)=\tau_1 e^{-\tau_2 E}+\tau_3 e^{-\tau_4 E}+\tau_5+\tau_6 E^{\tau_7} \quad , \qquad \text{(III C3 a.4)}$$

and

$$A_i\left(E\right)=\left\{\, a_{i1}e^{-a_{i2}E}+a_{i2}e^{-a_{i4}E}+a_{i5}+a_{i6}E^{a_{i7}} \,\right\}\alpha_i \quad , \qquad \text{(III C3 a.5)}$$

where i represents 1, 3, or 5, and α_i is 1 for i = 1 but may be either unity or $\sqrt{E}$ for i = 3 or 5. All other quantities in Eq.(III C3 a.2) are independent of energy.

As many as five exponential terms may be included in the sum over i; it is implicitly assumed that the coefficients of the exponentials (B_{2i-1}) and the coefficients of time within the exponentials (B_{2i}) are positive numbers. These terms were added in an early attempt to provide a useful form for the GELINA and nTOF resolution function; they have been retained in order to permit additional flexibility for the analyst.

3. Time-of-flight channel width

The time-of-flight channel width may be modeled as a rectangular distribution of width c. The time distribution due to the finite channel width is therefore assumed to be

$$I_3\left(t\right)=\begin{cases} 1/c & \text{for } -c/2<t<c/2 \\ 0 & \text{otherwise} \end{cases} \quad . \qquad \text{(III C3 a.6)}$$

The channel width c may be energy dependent. For constant values of c within an energy range, the input is described in Table VI.B, card set 14, line 20. This is appropriate, for example, for data having "crunch boundaries." (In Europe, the French word "accordeon" is often used to denote the system of crunch boundaries.)

When the channel width varies continuously with energy, for example, for data from the nTOF facility, then the channel width (or bin width) is expressed as "n bins per decade." That is, in an energy decade from 10^k to $10^{(k+1)}$ for integer k, there are n bins equally spaced on a logarithmic scale. The energy limits for the ith bin in this decade are given by

$$E_{k,i}=10^{k+\frac{i-1}{n}} \;\le\; E=10^{k+\frac{i-1+\varepsilon}{n}} \;\le\; E_{k,i+1}=10^{k+\frac{i}{n}} \quad , \qquad \text{(III C3 a.7)}$$

where i = 1 to n, and ε is a positive number between 0 and 1. Converting to time limits, using $t=\tau/\sqrt{E}$ where τ is a constant whose value is unimportant for this discussion, we find

$$t_{k,i+1} = \frac{\tau}{\sqrt{10^{k+\frac{i}{n}}}} \le t = \frac{\tau}{\sqrt{10^{k+\frac{i-1+\varepsilon}{n}}}} \le t_{k,i} = \frac{\tau}{\sqrt{10^{k+\frac{i-1}{n}}}} \quad , \qquad \text{(III C3 a.8)}$$

so that the channel width c may be found from

$$c = t_{k,i} - t_{k,i+1} = t\left\{\frac{1}{\sqrt{10^{\frac{\varepsilon}{n}}}} - \frac{1}{\sqrt{10^{\frac{1-\varepsilon}{n}}}}\right\} = t\left\{10^{-\frac{\varepsilon}{2n}} - 10^{\frac{-1+\varepsilon}{2n}}\right\} \quad . \qquad \text{(III C3 a.9)}$$

To calculate this quantity in SAMMY, we consider the value at $\varepsilon = 0$,

$$c_0 \;\cong\; t\;\left\{1 - 10^{-1/(2n)}\right\} \quad , \qquad \text{(III C3 a.10)}$$

and at $\varepsilon = 1$,

$$c_1 \;\cong\; t\;\left\{10^{1/(2n)} - 1\right\} \quad . \qquad \text{(III C3 a.11)}$$

In either case, for large n these expressions may be expanded to first order in $1/n$ to give

$$c_0 \;=\; t\;\left\{1 - 10^{-1/(2n)}\right\} \;\cong t\left\{1 - \left[1 - \left(\frac{1}{2n}\ln(10)\right)\right]\right\} = \frac{t}{2n}\ln(10) \qquad \text{(III C3 a.12)}$$

and

$$c_1 \;=\; t\;\left\{10^{1/(2n)} - 1\right\} \;\cong t\left\{1 + \left(\frac{1}{2n}\ln(10)\right) - 1\right\} = \frac{t}{2n}\ln(10) \quad . \qquad \text{(III C3 a.13)}$$

Because these two values agree to first order in $1/n$, and n is large (~5000), it is therefore sufficient to use the approximation

$$c \cong t\ln(10)/(2n) \qquad \text{(III C3 a.14)}$$

rather than to spend the not-insignificant amount of computer time to generate exact values of k and i (and therefore of c) for each value of E.

Input for the continuously varying definition of channel width c is given in Table VI.B, card set 14, line 19.

III.C.3.b. Input for the RPI/GELINA/nTOF resolution function

Input formats for all parameters of the RPI/GELINA/NTOF resolution function are given in Table VI B.2, card set 14. Note that zero values are assumed to actually be zero and are not replaced by default values. The first line of this card set contains one of the following phrases (which are treated as equivalent):

RPI Resolution function
GELINa resolution function
NTOF resolution function

As usual, only those characters in capital letters are required; those in lower case letters are optional.

In Table III C3 b.1, default values for the constants from Eqs. (III C3 a.2) through (III C3 a.5) are defined for transmission and capture measurements. To invoke these defaults (without the option to flag them for varying), the user must specify the appropriate phrase

RPI Transmission resolution function *or*
RPI Capture resolution function

on the first line of card set 14.

Table III C3 b.2, provided courtesy of Frank Gunsing of Saclay [FG05], gives parameter values that may be suitable for use with data from the Geel Electron Linear Accelerator (GELINA) at IRMM and with data from the neutron time-of-flight facility (nTOF) at CERN. Note that these values are *preliminary*; they are reasonable starting values which should be fine-tuned on measurements of well-known resonances (i.e., on resonances that have been measured many times at different installations). To invoke these values automatically (without the option to flag them for varying), use one of the following phrases for the first line of card set 14:

GEEL DEFAUlt values for resolution parameters
GELINa DEFAUlt values
NTOF DEFAUlt values

With the RPI/GELINA/nTOF resolution function, it is necessary to specify whether the resolution function should be used exactly as given in the input or whether, instead, it should be shifted so that it is centered on the current energy. To center the function, include one of the phrases

SHIFT RPI RESOLUTION function to center
SHIFT GEEL RESOLUTIOn function to center
SHIFT GELINA RESOLUtion function to center
SHIFT NTOF RESOLUTIOn function to center

in the command section of the INPut file. To use the function exactly as given in the input, include one of the phrases

DO NOT SHIFT RPI RESolution function to center
DO NOT SHIFT GEEL Resolution function to center
DO NOT SHIFT GELINA resolution function to center
DO NOT SHIFT NTOF Resolution function to center

Many test cases provide examples of input for the RPI resolution function; see, for example, tr053, tr054, tr090, tr094, tr095, tr115, or tr136. For examples using the GELINA and nTOF resolution function, see test cases tr104, tr107, and (especially) tr108.

Table III C3 b.1. Default values for parameters for RPI resolution function

	Parameter name	Value for transmission "RPI Transmission"	Value for capture [a] "RPI Capture"	Units
1	$p = 2\sqrt{\ln 2} / w$			Ns
2	τ_1	326.	381.	Ns
3	τ_2	0.0241	0.0058	per eV
4	τ_3	323.	323.	Ns
5	τ_4	0.029	0.094	per eV
6	τ_5	240.	105.	Ns
7	τ_6	0.	0.	Ns
8	τ_7	0.	0.	[dimensionless]
9	Λ_0	686.5	686.5	Ns
10	Λ_1	-224.9	-224.9	Ns
11	Λ_2	21.04	21.04	ns
12	Λ_3	0.	0.	ns
13	Λ_4	0.	0.	[dimensionless]
14	a_1	-0.000985	-0.001106	per ns
15	a_2	0.0241	0.0058	per eV
16	a_3	-0.000626	0.04752	per ns
17	a_4	3.531	65.083	per eV
18	a_5	0.001029	0.001264	per ns
19	a_6	0.	0.	per ns
20	a_7	0.	0.	[dimensionless]
21	t_0	940.	940.	ns
22	A_2	-65.638	-65.638	[dimensionless]
23	A_3	0.005	0.005	per ns
24	A_4	0.39383	0.39383	[dimensionless]
25	A_5	0.0008	0.0008	per ns
next	B_i	0.0	0.0	
last	c			ns

[a] Values listed in this column are *not* necessarily those that are appropriate for the RPI capture resolution function, which has not yet been fully defined; these values are for illustrative purposes only.

Table III C3 b.2. Parameters suitable for use with experimental data from GELINA at IRMM and from nTOF at CERN. Values are from preliminary work of F. Gunsing [FG05]. Parameters not listed in this table have value zero. Test case tr108 contains these values

Parameter name	Value for GELINA 90-degree flight path[a]	Values for nTOF	Units
τ_5	-0.7722	-3.7004	ns
τ_6	1363.85	-684.39	ns
τ_7	-0.5322	-0.5189	[dimensionless]
Λ_0	1.4460	3.8457	ns
Λ_3	454.9720	502.9930	ns
Λ_4	-0.5077	-0.4155	[dimensionless]
a_1	0.0	-0.0381	per ns
a_2	0.0	9.974×10^{-6}	per eV
a_3	0.04152	-0.01172	per ns
a_4	-5.847×10^{-6}	0.0001019	per eV
a_5	-0.0415	0.05009	per ns
a_6	9.247×10^{-6}	0.0	per ns
a_7	0.5961	0.0	[dimensionless]
A_2	1.0	1.0	[dimensionless]
A_4	-1.0	-1.0	[dimensionless]
A3SQE (A_3): a_{35}	0.0003047	-0.0001689	per [ns $\times$(eV)$^{1/2}$]
A3SQE (A_3): a_{36}	7.818×10^{-5}	0.0004254	per [ns $\times$(eV)$^{1/2}$]
A3SQE (A_3): a_{37}	-2.011	-0.06043	[dimensionless]
A3SQE (A_5): a_{55}	0.007331	0.0002766	per [ns $\times$(eV)$^{1/2}$]

[a]The GELINA resolution function refers to the beam only and does not include a contribution from a detection system.

III.C.4. Straight-Line Energy Average

This relatively simple resolution function takes the form

$$I_1(E') = \begin{cases} 1/D & \text{for } E - D < E' \\ 0 & \text{otherwise} \end{cases} , \qquad \text{(III C4.1)}$$

so that the broadened cross section is given by

$$\bar{\sigma}(E) = \frac{1}{D} \int_{E-D}^{E} \sigma(E')\, dE' \quad . \qquad \text{(III C4.2)}$$

Note that the apparent position of a resonance is altered (shifted to a higher energy) by the use of this resolution function.

It is also possible to use this resolution function without shifting the apparent position of the resonances. To invoke this option, include the phrase

```
CENTER THE CONSTANT ENERGY RESOLUTION FUNCTION
```

in the INPut file. In this case, the resolution function of Eq. (III C4.1) is replaced by

$$I_1(E') = \begin{cases} 1/D & \text{for } E - D/2 < E' < E + D/2 \\ 0 & \text{otherwise} \end{cases} , \qquad \text{(III C4.3)}$$

and the broadened cross section is given by

$$\bar{\sigma}(E) = \frac{1}{D} \int_{E-D/2}^{E+D/2} \sigma(E')\, dE' \quad . \qquad \text{(III C4.4)}$$

Input for the value of *D* is variable DDDEEE in card set 5 of the INPut file. See test case tr105 for examples. Note that this parameter cannot be fitted (i.e., it cannot be treated as a search parameter in the fitting procedure).

CAUTION: Difficulties have been experienced in using this resolution function in the neighborhood of extremely narrow resonances (probably due to the discontinuous nature of the function). When results look very odd (abrupt changes in value of cross section as a function of energy, for example), try increasing the number of mesh points in the auxiliary grid (see Sections III.A.1 and III.A.2). If problems persist, contact the SAMMY author.

III.C.5. User-Defined Numerical Resolution Function

The user-defined resolution (UDR) function is another "realistic" resolution function, a convolution of several numericalcomponents, designed for use when other forms are not adequate. The components are

- electron burst width (Gaussian function of time)
- time-of-flight channel width (square function of time; accordeon = crunch boundaries)
- user-defined numerical function of time at specified energies, with linear interpolation both in time and in energy
- other user-defined numerical function(s) as required

The "complete" resolution function is then the numerical convolution of the individual pieces:

$$I(t) = \int I_1(t - t_1)\,dt_1 \int I_2(t_1 - t_2)\,dt_2 \cdots \int I_{n-1}(t_{n-2} - t_{n-1})\,dt_{n-1} I_n(t_{n-1}) \quad . \qquad \text{(III C5.1)}$$

To use the UDR resolution function, include card set 16 of Table VI B.2 in the PARameter file, or card set P16 of Table VIA.1 in the INPut file. Create file with UDR function, formatted as described in Table III C5.1. See test case tr114 for examples.

NOTE: What is gained in flexibility is lost in accuracy and computation speed. This resolution function should be used with extreme caution.

Table III C5.1. Format for numerical UDR function file.

Line number	Column	What	Meaning
1,2,...	any		Descriptive information, as many lines as needed
3	1–5	----- (at least five hyphens)	end of descriptive information
4	1–?	Energy (eV)	energy at which resolution function will be given
5,6,...	1–?	Time (ns), Function	value of resolution function at the specified time
7	(end with a blank line)		
Repeat lines 4–7 as many times as needed, being sure to have same number of (time, function) values for each energy.			

III.D. SELF-SHIELDING AND MULTIPLE-SCATTERING CORRECTIONS TO CAPTURE OR FISSION YIELDS

The theoretical capture or fission cross section may be calculated directly from the equations in Section II using the Reich-Moore (or other) approximation to the multilevel R-matrix. However, in order to compare with experiment, corrections must be made for the finite (non-infinitesimal) size of the sample. Both "self-shielding" and "multiple-scattering" effects must be included in the calculation. (Note: for the rest of this section, "capture" will be taken to mean "capture or fission" to avoid arduous repetition; the corrections described here apply to both.)

Derivation of the appropriate expressions for self-shielding and multiple-scattering corrections, including details of the methods of calculation, is non-trivial and will not be presented here. Results of comparison tests with Monte Carlo calculations indicate good agreement between Monte Carlo results and results obtained via SAMMY, as reported in [NL02]. See Section X.M for a description of the Monte Carlo code used for such comparisons.

The capture yield $Y(E)$ can be written as the sum of four components, each of which is described separately below; that is,

$$Y(E) = Y_0(E) + Y_1(E) + Y_2(E) + Y_{ns}(E) \quad . \qquad \text{(III D.1)}$$

Self-shielding

Self-shielding is the reduction in the observed capture cross section due to interactions of incident neutrons with other nuclei in front of the current position. The probability that capture will occur at depth *z* (within *dz*) can be written as

$$\frac{n}{D} e^{-n\sigma_t z/D} \sigma_c \, dz \quad , \qquad \text{(III D.2)}$$

where *n* is the sample thickness in atoms/barn and *D* is the sample thickness in the same units as *z*. Subscripts *t* and *c* denote total and capture cross sections, respectively. Integrating over *z* (from 0 to *D*) gives the self-shielded capture yield

$$Y_0 = \left\{ 1 - e^{-n\sigma_t} \right\} \left(\frac{\sigma_c}{\sigma_t} \right) \quad . \qquad \text{(III D.3)}$$

(See the end of this section for a discussion of the normalization options for capture yields.)

Single scattering

The scattering correction is the increase in the observed capture cross section due to capture of neutrons that have been scattered out of the original beam path. Calculation of the scattering effect is more complicated than the self-shielding because it involves the product of (1) the

probability of reaching a position (x,y,z) inside the sample, (2) the probability of scattering from that position into solid angle Ω within $d\Omega$, (3) the probability of those scattered nuclei reaching position q within dq along that direction, and (4) the probability of being captured at that location. This product is then integrated over the position q, over solid angle, and over the sample volume, giving the *single*-scattering result. If the z axis is defined by the beam line, this expression can be reduced to the form

$$Y_1(E) = \frac{1}{S}\int dx \int dy \frac{n}{D}\int dz \exp\left(-\frac{n}{D}\sigma_t z\right)\int d\Omega \frac{d\sigma}{d\Omega}\sigma'_c \frac{n}{D}\int dq \exp\left(-\frac{n}{D}\sigma'_t q\right) \quad , \text{(III D.4)}$$

in which primes indicate evaluation at the scattered energy, rather than at the incident energy of the neutron. The scattered energy is given by

$$E' = E\left[\frac{\cos\theta}{1+r} + \sqrt{\frac{1}{(1+1/r)^2} - \frac{\sin^2\theta}{(1+r)^2}}\right]^2 = E\varepsilon(\theta) \quad , \qquad \text{(III D.5)}$$

where r is the ratio of the mass of the target nuclide to the mass of the neutron. [See Section II.C.2 and especially Eq. (II C2 b.3) for a derivation of this equation.]

Explicit evaluation of the expression in Eq. (III D.4) requires detailed knowledge of the geometry of the sample and its positioning relative to the neutron beam, as shown in the sketch in Figure III D.1. In the case where the sample is a round disk, with a flat surface perpendicular to the beam, the expression can be reduced to

$$Y_1(E) = Y_{1\infty f} + Y_{1\infty b} + Y_{1cf} + Y_{1cb} \quad , \qquad \text{(III D.6)}$$

where the subscripts "f" and "b" refer to forward and backward scattering, respectively. The subscript "∞" indicates that this term assumes the sample extends to infinity in the dimensions perpendicular to the beam; subscript "c" indicates that this term is the correction for finite size. (NOTE: Corrections for a rectangular shape, rather than a round disk, will be available in future releases of the code.)

The "infinite" terms in Eq. (III D.6) are one-dimensional integrals,

$$Y_{1\infty f}(E) = \frac{1}{2}\int_0^1 d\mu \frac{d\sigma}{d\Omega}\frac{\sigma'_{cap}}{\sigma'_{tot}}\left(\frac{1-e^{-n\sigma_{tot}}}{\sigma_{tot}} + \frac{e^{-n\sigma_{tot}} - e^{-n\sigma'_{tot}/\mu}}{\sigma_{tot} - \sigma'_{tot}/\mu}\right) \qquad \text{(III D.7)}$$

and

$$Y_{1\infty b}(E) = \frac{1}{2}\int_{-1}^0 d\mu \frac{d\sigma}{d\Omega}\frac{\sigma'_{cap}}{\sigma'_{tot}}\left(\frac{1-e^{-n\sigma_{tot}}}{\sigma_{tot}} + \frac{e^{-n\sigma_{tot}} - e^{-n\sigma'_{tot}/\mu}}{\sigma_{tot} - \sigma'_{tot}/\mu}\right) \quad , \qquad \text{(III D.8)}$$

in which $\mu = \cos(\theta)$. The "finite" corrections involve four-dimensional integrals of the form

$$Y_{1cf}(E) = \frac{1}{2}\int_0^1 d\mu \frac{d\sigma}{d\Omega}\frac{\sigma'_{cap}}{\sigma'_{tot}} Q_f\left(\mu, \sigma_{tot}, \sigma'_{tot}\right) \qquad \text{(III D.9)}$$

and

$$Y_{1cb}(E) = \frac{1}{2}\int_{-1}^0 d\mu \frac{d\sigma}{d\Omega}\frac{\sigma'_{cap}}{\sigma'_{tot}} Q_b\left(\mu, \sigma_{tot}, \sigma'_{tot}\right) \quad . \qquad \text{(III D.10)}$$

Here the three-dimensional integral Q_f is given by

$$Q_f\left(\mu, \sigma, \sigma'\right) = \int dz\, e^{-n\sigma' D/z} \int d^2S \left(e^{-n\sigma(D-z)/(D\mu)} - e^{-n\sigma L/D}\right) \qquad \text{(III D.11)}$$

and Q_b by

$$Q_b\left(\mu, \sigma, \sigma'\right) = \int dz\, e^{-n\sigma'(D-z)/z} \int d^2S \left(e^{-n\sigma(D-z)/(D\mu)} - e^{-n\sigma L/D}\right) \quad , \qquad \text{(III D.12)}$$

where L is the actual path length, within the sample, available for travel by the scattered neutron; note that L is geometry dependent. The integration over d^2S in this expression for Q is over the beam cross section; the integration over z is over the thickness of the sample. SAMMY evaluates Q on a separate grid and interpolates to produce the required values for Eqs. (III D.9) and (III D.10).

Values for Q are generated in advance (in segment SAMPAR) and stored in a file named SAMMY.SSM. This file may be renamed and reused for subsequent runs, as long as the geometry remains the same.

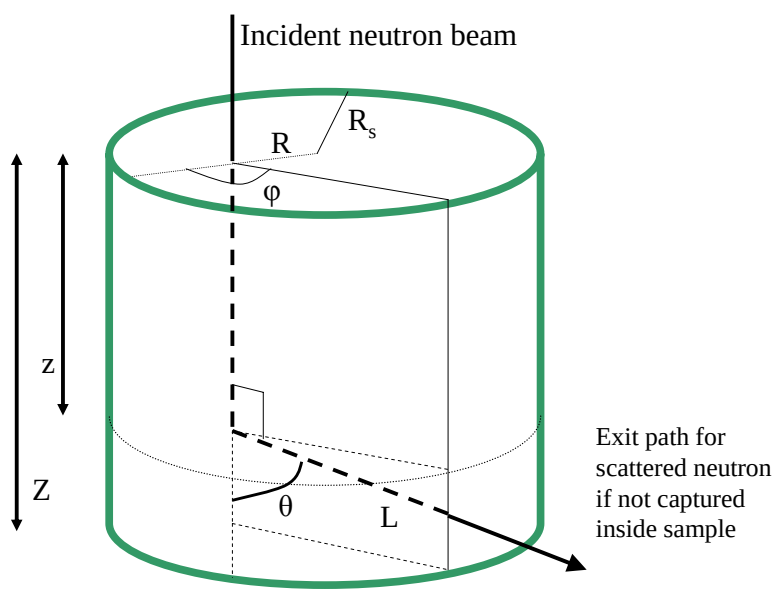


Figure III D.1. Geometry for the single-scattering correction to capture or fission yield, for a neutron incident on the flat surface of a cylindrical sample.

Two or more scatters

Derivation of the effect of two or more scatters followed by capture is accomplished in a similar manner to the derivation of the single-scattering effect. The exact expression for k scatters involves $(3k+3)$ embedded integrations; it is therefore necessary to make severe approximations in order to derive an expression that can be calculated in a finite amount of time. The approximation currently employed by SAMMY is borrowed from Moxon [MM89], based on a derivation by Case et al. [KC53]; an independent derivation was developed in preparation for implementation into the SAMMY code. The approximation assumes that after two scatterings, neutrons are uniformly distributed both in direction of motion and in position within the sample. This approximation has the effect of decoupling $2k$ of the embedded integrals, so that they can be performed separately from the others. Quantization of this approximation is achieved by assuming that the escape probability for a neutron after k scatterings (i.e., at energy $E^{(k)}$) depends only on the energy; specifically, the escape probability is given by the formula

$$p_{escape}\left(E^{(k)}\right) = \frac{1}{n\sigma^{(k)}}\left[\frac{1}{2}-\int_1^\infty u^{-3}e^{-n\sigma^{(k)}u}du\right]\frac{1+2n\sigma_{tot}^{(k)}}{1+\dfrac{2n\sigma_{tot}^{(k)}}{1+Z/R}} \quad , \qquad \text{(III D.13)}$$

where R is the radius of the sample. With this approximation, one can recursively define a function y via

$$y_{j-1} = \int d\Omega_j \frac{d\sigma^{(j-1)}}{d\Omega_j}\left(\sigma_c^{(j)}+y_j\right)\left(1-p_{escape}\left(E^{(j)}\right)\right) \quad , \qquad \text{(III D.14)}$$

in which the superscript denotes the energy at which the cross section is to be calculated. The initial estimate for a neutron scattered k times is

$$y_{k-1} \approx 2\pi\int d\mu_k \frac{d\sigma^{(k-1)}}{d\Omega_k}\sigma_c^{(k)}\left(1-p_{escape}\left(E^{(k)}\right)\right) \quad . \qquad \text{(III D.15)}$$

This function y can then be used to estimate the capture yield for two or more scatterings,

$$Y_2(E) = \frac{1}{S}\int dx\int dy\frac{n}{E}\int dz\, e^{-\frac{n}{D}\sigma_{tot}z}\int d\Omega\frac{d\sigma}{d\Omega}y_l\frac{n}{D}\int dq\, e^{-\frac{n}{D}\sigma'_{tot}q} \quad . \qquad \text{(III D.16)}$$

In this form the multiple-scattering capture yield has the same mathematical properties as the single-scattering capture yield of Eq. (III D.4). Similar computational techniques can therefore be used to evaluate both quantities.

Neutron sensitivity

In capture experiments, not only gamma rays but also scattered neutrons reach the detector. The detector is not always able to distinguish between the two; hence, corrections must be made for the neutron sensitivity of the detector. Following Borella [AB05] with only notational changes, this correction term has the form

$$Y_{ns}\left(E\right) = A\left\{1-e^{-\sigma_{tot}}\right\}\frac{\sigma_n}{\sigma_{tot}}\frac{\varepsilon_n}{\varepsilon_c} \quad , \qquad \text{(III D.17)}$$

in which ε_n represents the neutron sensitivity of the detector and ε_c the capture sensitivity. The ratio of these sensitivities as a function of energy was provided by Peter Schillebeeckx [PS06], and log-log interpolation gives the value at a particular energy. The multiplier *A* is an input parameter whose value is the binding energy of the target nuclide. Nevertheless, *A* may be flagged as a variable or as a PUP when the user wishes to include an estimate of the uncertainty on the neutron sensitivity. See line 12 of card set 11 of Table VI B.2 for input details for this feature.

Normalization and input options

Capture yield data may be normalized in a variety of ways; therefore, SAMMY allows the user to choose which normalization is to be taken. The normalization generally referred to as capture "yield" is the one shown in the equations in this section; this choice has the property that values are in the range from 0 to 1. Another commonly used normalization requires dividing by thickness *n*; in this case, the value approaches the capture cross section in the limit of zero thickness. Finally, the data may be normalized as $\left(1-e^{-n\sigma_{tot}}\right)\sigma_{tot}$, that is, by multiplying the yield by the total cross section. To use these options, the user must include the appropriate phrase in the alphanumeric section of the INPut file:

```
NORMALIZE AS CROSS Section rather than yield
NORMALIZE AS YIELD Rather than cross section
NORMALIZE AS (1-E)SIgma
```

No default is assumed for normalization; instead, SAMMY requires that one of the above options be specified by the user.

The default mode in SAMMY is to <u>not</u> include self-shielding and multiple-scattering corrections; therefore, to invoke these corrections, users will need to include one or more of the following phrases in their INPut file:

For self-shielding but no multiple-scattering correction:

```
USE SELF SHIELDING Only, no scattering,
SELF SHIELD
```
or

For self-shielding, single-scattering (with edge-effects), and no double-scattering correction:

```
USE SINGLE SCATTERINg plus self shielding, or
SINGLE
```

For self-shielding, single-scattering (infinite slab approximation), and no double-scattering corrections:

```
SINGLE
INFINITE SLAB
```

For self-shielding, single-scattering (with edge-effects correction), and multiple-scattering corrections:

```
USE DOUBLE SCATTERINg plus single scattering, or
DOUBLE
```

For self-shielding, single-scattering (infinite-slab approximation), and multiple-scattering corrections:

```
DOUBLE
INFINITE SLAB
```

When finite-size corrections (for single scattering) are wanted, additional input is needed to express the geometric properties of the beam and of the sample. These include the dimensions of the sample, the cross-sectional dimensions of the beam if smaller than the sample, and integers that determine the accuracy to which the function *Q* will be calculated. Details are given in Table VI A.1, card set 11.

Examples using multiple-scattering corrections can be found in test cases tr039, tr052, tr064, tr099, and others.

III.E. OTHER EXPERIMENTAL CORRECTIONS

This section contains information about a variety of other corrections for experimental conditions not covered in earlier portions of Section III. Included here are the following:

1. Modifications needed for analyzing transmission measurements are covered in Section III.E.1.

2. The means by which one may analyze samples containing multiple nuclides (multiple isotopes, chemical compounds, contaminants) is discussed in Section III.E.2.

3. Two methods of including data-reduction parameters (such as normalizations or backgrounds) within the SAMMY analysis are described in Section III.E.3.

4. Paramagnetic cross sections are discussed in Section III.E.4

5. A treatment of *l*-dependent detector efficiencies is outlined in Section III.E.5.

6. Self-indication measurements are discussed in Section III.E.6.

7. Attenuation and angle-averaging for angular-distribution data are described in Section III.E.7.

III.E.1. Transmission Experiments

The analysis of transmission (or total cross section) data requires an extension to the description given in Section III.A, since what is actually measured (and thus what is to be "fitted") is not cross section σ but transmission *T*, where

$$T = e^{-n\sigma} \quad . \tag{III E1.1}$$

Here *n* is the sample thickness, measured independently and expressed in units of atoms/barn.

Theoretical values of *T* and $\partial T / \partial u$ are generated in SAMMY according to the following procedure:

1. Generate total cross section σ and partial derivatives $\partial\sigma / \partial u$ as described in Section II.

2. Doppler broaden the cross section and derivatives as described in Section III.B.

3. Convert to transmission using Eq. (III E1.1) for the cross section and

$$\frac{\partial T}{\partial u} = -n\, e^{-n\sigma} \frac{\partial \sigma}{\partial u} \tag{III E1.2}$$

   for the derivatives.

4. If thickness *n* is a varied parameter, generate $\partial T / \partial n$ from

$$\frac{\partial T}{\partial n} = -\sigma e^{-n\sigma} = -\sigma T \quad . \tag{III E1.3}$$

5. Resolution broaden the transmission and derivatives, as described in Section III.C.

6. If total cross sections are to be fitted, rather than transmissions, convert the broadened transmissions and derivatives thereof back to cross section. **NOTE: Experience has shown that fewer numerical difficulties are encountered if transmissions, rather than cross sections, are used for the fitting procedure.**

The total cross section determined using the above procedure corresponds to the actual unbroadened total cross section. It may differ considerably from the "cross section" extracted directly from the measured transmission using the relationship

$$"\sigma" = -\frac{1}{n} \ln\left(T_{\text{measured}}\right) \quad . \tag{III E1.4}$$

In the study of transmission data, the distinction is made between "effective cross section" σ_{eff} and "true cross section" σ_{true}. The effective cross section is defined by first resolution broadening the transmission:

$$\mathrm{Tr}(E) = \int e^{-n\,\sigma_D(E')} R(E - E')\, d\,E' \quad , \qquad \text{(III E1.5)}$$

where $\sigma_D(E')$ is the Doppler-broadened total cross section and $R(E - E')$ is the resolution function, and then converting to cross section,

$$\sigma_{\mathrm{eff}}(E) \;=\; -\frac{1}{n}\ln\left(\mathrm{Tr}(E)\right) \quad . \qquad \text{(III E1.6)}$$

The so-called true cross section, on the other hand, is defined by resolution-broadening the Doppler-broadened total cross section directly (i.e., by omitting the conversion to and from transmission):

$$\sigma_{\mathrm{true}}(E) = \int \sigma_D(E')\, R(E - E')\, d\,E' \quad . \qquad \text{(III E1.7)}$$

The difference between σ_{eff} and σ_{true} corresponds to the "self-shielding effect" in transmission measurements.

In SAMMY, the "true cross section" can be generated (i.e., the conversion to and from transmission can be omitted from the calculations) by including the command

```
USE TRUE TOTAL CROSS section for resolution broadening
```

in the INPut file. With this command invoked, the treatment of transmission and total cross section (as outlined on the previous page) is replaced with the following:

1. Generate total cross section σ and partial derivatives $\partial\sigma/\partial u$ as described in Section II.
2. Doppler broaden the cross section and derivatives, as described in Section III.B.
3. Resolution broaden the cross section and derivatives, as described in Section III.C.

Fitting to experimental data is inappropriate with this command, since Eq. (III E1.7) does not correspond to data measured by any practical experiment.

III.E.2. Combining Several Nuclides in a Single Sample

Because the samples used in neutron experiments are often made from natural materials rather than isotopically pure materials and may contain chemical combinations of elements and/or impurities, the SAMMY INPut and PARameter files may need to describe resonances corresponding to several different nuclides. A number of features of SAMMY have evolved to deal with this consideration; these features are described below. In addition, users are referred to test case tr060, which treats multiple isotopes of barium as well as oxygen and carbon. The user must provide abundances for each nuclide; however, if the exact composition of a diluent is unknown, abundances may be flagged (varied) so that SAMMY can determine the optimal values to fit the experimental data.

The SAMMY features relevant to multiple nuclides in a single sample are as follows:

1. Spin groups may be specified in one of two ways, either of which may contain information about abundances of isotopes or elements. See Section VI.A, Table VI A.1, card sets 10.1 and 10.2, for details. The nuclear spin (as well as mass and isotopic abundance) can be specified for each nuclide separately.

2. When using a multi-nuclide PARameter file, flags on the appropriate spin groups in the INPut file will eliminate the use of those spin groups in performing the calculation of cross sections; thus, the same PARameter file may be used both for the analysis of data from an isotopically pure sample and for the analysis of data from a "natural" sample, or for data from a specific nuclide and for a chemical combination. Input details are again given in Table VIA.1.

3. Channel radii (see Section II.A.1) for the different nuclei (and for different spin groups) may be specified separately. In addition, the channel radius (PAREFF) used in evaluation of the potential-scattering phase shift φ_l may differ from the channel radius (PARTRU) used in evaluation of penetration factor P_l and level shift factor S_l,; this is included for compatibility with ENDF [ENDF-102]. Input details are given in card set 7a of Table VI B.2; alternatively, one may use the older and more cumbersome card set 7. Any or all of these radii may be varied in a SAMMY run.

4. To specify a single abundance and the correct mass for all spin groups corresponding to a given nucleus, use card set 10 of the PARameter file (see Section VI.B.). Abundances, but not masses, may be varied.

SAMMY will confirm that the sets of spin groups corresponding to a given nuclide are defined consistently between the INPut and the PARameter files.

SAMMY is no longer restricted to a small number of spin groups. Previously, there were two limitations:

1. Only two digits are permitted for the spin group number in the format for the resonance parameters (card set 1 of Table VI B.2). Furthermore, spin group numbers greater than 50 (or negative) are used to designate resonances to be omitted from the calculation. When more than 50 spin groups are needed, an alternative (4-digit) format can now be used; see Table VI B.2 for details. (The maximum permitted number of spin groups is now 500, because the format in the INPut file permits only 3 digits.)

2. The second limitation relates to the itemization of spin groups associated with channel radii or with nuclide abundance in the PARameter file. Originally, this itemization used a two-digit format and required that all spin groups be listed on one line. It is now possible to use a five-digit format (when there are more than 99 spin groups) and to continue the itemization on other lines if needed. Details are given in Table VI B.2. (A better method of input for channel radii is available in card set 7a of the PARameter file, which uses key-word-based input without fixed format.)

III.E.3. Data-Reduction Parameters

Analysis of experimental data requires, first of all, a reduction of raw data to cross section (or transmission). Values of the parameters for the data-reduction process may not be perfectly known, and the effects of these uncertainties should be incorporated into the data analysis. Within SAMMY there are several methods of doing this:

1. The uncertainties can be carefully propagated through the data-reduction process, so that the full off-diagonal covariance matrix of the reduced data is generated. This covariance matrix is then explicitly input to SAMMY; see Section VI.C.2 for input details.

2. The user-supplied implicit data covariance (IDC) matrix may be used. See Section IV.D.3 for a description of the IDC method and Section VI.C.3.b for input for this option.

3. Another method of incorporating data-reduction parameters into the SAMMY analysis is to perform the background subtraction and/or normalization process explicitly, analytically, within SAMMY. In this case the operations are applied to the theoretical calculations, not to the experimental data. Section III.E.3.a discusses this option in detail.

4. The PUP (Propagated Uncertainty Parameter) method is perhaps the easiest method for the analyst to use for incorporating measurement-related uncertainties into the analysis process. See Sections IV.D.1 for derivation of the PUP method, Section IV.D.2 for a summary and description of its use in SAMMY, and Section VI.C.3.a for input information. The PUP method is applicable only for parameters for which SAMMY has derivatives internally available; therefore, it is more restrictive than # 1 or # 2 (but more general than # 3).

5. Partial derivatives of the (reduced) data with respect to the data-reduction parameters can be generated externally, and these derivatives read into SAMMY, which will then generate the explicit data covariance matrix. Details are given in Section III.E.3.b. (The code ALEX [NL84] can be used to generate the needed partial derivatives.) While this method requires similar input to # 2 above (though in different format), it is an older formulation and has not been extensively tested. Probably this option will be eliminated in the near future.

The computer code ALEX was designed to generate the data covariance matrix for ORELA data and can therefore be used to prepare input for options # 1, 2, or 5. For a description of ALEX and a detailed discussion on the role of uncertainties in the data-reduction process, see [DL83] and [NL84]. An update of this code, to be more directly applicable for option # 2, is planned.

See test case tr140 for equivalent examples of many of these options.

III.E.3.a. Explicit normalization and/or background functions

A constant overall normalization and a variety of different analytical models for backgrounds may be applied to the theoretical values (cross sections, transmissions, etc.) generated within SAMMY. These corrections are applied to the theory, not to the data. Normalization is applied first, followed by background corrections, so that the backgrounds are not multiplied by the normalization.

Let T_u represent the uncorrected theoretical value (for cross section, transmission, etc.); then the corrected value is given by

$$T(E) = aT_u(E) + b(E) \quad , \qquad \text{(III E3 a.1)}$$

in which energy dependences have been explicitly displayed.

Input for the normalization a and four specific backgrounds is specified in card set 6 of the PARameter file. The four backgrounds are

$$\begin{aligned} b_1(E) &= B_a \quad , \\ b_2(E) &= B_b / \sqrt{E} \quad , \\ b_3(E) &= B_c \sqrt{E} \quad , \\ \text{and} \qquad b_4(E) &= B_d \exp\left\{-B_f / \sqrt{E}\right\} \quad . \end{aligned} \qquad \text{(III E3 a.2)}$$

With this format, the user provides one value (which may be zero) for each of the five background parameters B_a through B_f. It is not possible, however, to give more than one value for any of the backgrounds; hence, one cannot, with this format, specify two exponential decay rates for the background.

A second, more general, format for background functions is given in card set 13 of the PARameter file. Here there are eight different types of background functions; however, unlike those given above, any number of each type may be included, so that the actual background is the sum of all such functions. The functional forms for the first four of these backgrounds are, respectively, constant, exponential, power, and exponential of a logarithmic function. An energy range (Emin to Emax) may be specified for each of these functions. Explicitly, these functions are

$$\begin{aligned} b_1 &= A \quad , \\ b_2(E(t)) &= Ae^{-Bt} \quad , \\ b_3(E(t)) &= At^B \quad , \\ \text{and} \qquad b_4(E(t)) &= \exp\left\{A + Bt + C / \ln(t)\right\} \quad , \end{aligned} \qquad \text{(III E3 a.3)}$$

in which the flight time t is derived from the energy in the usual manner,

$$t = \sqrt{\frac{mL^2}{2E}} \quad , \qquad \text{(III E3 a.4)}$$

where L is the flight-path length. If the value for L is already given (e.g., for transmission data), that value can be used here. Otherwise, L can be specified along with the other parameters for these functions.

The fifth type of background function is a point-wise linear function in time. This function has the form

$$b_5\left(E\left(t\right)\right) = A_i \frac{t_{i+1} - t}{t_{i+1} - t_i} + A_{i+1} \frac{t - t_{i+1}}{t_{i+1} - t_i} \quad , \qquad \text{(III E3 a.5)}$$

in which the value of $b_5\left(E\left(t_i\right)\right) = A_i$ is specified at two or more particular times t_i. Equation (III E3 a.5) is valid for $t_i \le t \le t_{i+1}$. For time t outside the range of times given for this background type, the value of $b_5\left(E\left(t\right)\right)$ is set to zero. As with the other types of background function, the flight-path length L may be given with the input for this function if it is not already specified.

The sixth type of background is a point-wise linear function in energy. Specifically,

$$b_6\left(E\right) = A_i \frac{E_{i+1} - E}{E_{i+1} - E_i} + A_{i+1} \frac{E - E_{i+1}}{E_{i+1} - E_i} \quad , \qquad \text{(III E3 a.6)}$$

in which the value of $b_6\left(E_i\right) = A_i$ is specified at two or more particular energies E_i. Equation (III E3 a.6) is valid for $E_i \le E \le E_{i+1}$. For energy E outside the range of energies given for this background type, the value of $b_6\left(E\right)$ is set to zero.

The seventh type of background is again a point-wise linear function in time, with essentially the same form as type 5 except for a multiplicative factor B:

$$b_7\left(E\left(t\right)\right) = B\left[A_i \frac{t_{i+1} - t}{t_{i+1} - t_i} + A_{i+1} \frac{t - t_{i+1}}{t_{i+1} - t_i}\right] \quad . \qquad \text{(III E3 a.7)}$$

Likewise, the eighth type of background is a point-wise linear function in energy, with essentially the same form as type 6 except for a multiplicative factor B:

$$b_8\left(E\right) = B\left[A_i \frac{E_{i+1} - E}{E_{i+1} - E_i} + A_{i+1} \frac{E - E_{i+1}}{E_{i+1} - E_i}\right] \quad . \qquad \text{(III E3 a.8)}$$

For both type 7 and type 8, the point-wise values are listed in a separate file and cannot be varied. The multiplicative factor can, however, be varied. Details are given in Table VI B.2.

Because most of these parameters [excluding Emin, Emax, t_i, E_i, and L, and the A_i of Eqs. (III E3 a.7) and (III E3 a.8)] can be varied, partial derivatives of the theoretical values T are required. These derivatives are found directly from Eqs. (III E3 a.1) through (III E3 a.4) and are not listed explicitly here. Derivatives generated prior to these corrections (e.g., derivatives with respect to resonance parameters or broadening parameters) are also corrected by the normalization factor, as needed.

For examples of the use of normalization and/or background functions, the reader is referred to the test cases that are distributed with the SAMMY code. Test cases tr032 and tr045 (among others) include normalization and constant background in card set 6 of the PARameter file. Test case tr056 specifically addresses the use of more general background functions provided in card set 13 of the PARameter file.

III.E.3.b. User-supplied data-reduction parameters

When uncertainties inherent in the parameters of the data-reduction process are carefully propagated through that process, the covariance matrix associated with the reduced data is off-diagonal. While SAMMY can handle off-diagonal data covariance matrices, it is often more convenient as well as more informative to treat the data covariance matrix as diagonal and incorporate the uncertainty information directly into the solution of Bayes' equations.

To understand how this is done, let d represent the raw (unreduced) data and D the reduced data. The relationship between D and d is

$$D_i = f_i\left(\{d\},\{q\}\right) \quad , \qquad \text{(III E3 b.1)}$$

where f_i is some function of $\{d\}$ (which represents the entire set of raw data) and of $\{q\}$ (which represents the set of data-reduction parameters). A small increment in D may then be written as

$$\delta D_i = \sum_j \frac{\partial f_i}{\partial d_j}\delta d_j + \sum_k \frac{\partial f_i}{\partial q_k}\delta q_k \quad . \qquad \text{(III E3 b.2)}$$

Squaring this expression, taking expectation values, and noting that the d_j and q_k are mutually independent give

$$\left\langle \delta D_i \; \delta D_{i'} \right\rangle = \sum_j \frac{\partial f_i}{\partial d_j}\Delta^2 d_j \frac{\partial f_{i'}}{\partial d_j} + \sum_{k,k'} \frac{\partial f_i}{\partial q_k}\left\langle \delta q_k \; \delta q_{k'} \right\rangle \frac{\partial f_{i'}}{\partial q_{k'}} \qquad \text{(III E3 b.3)}$$

for the covariance between D_i and $D_{i'}$. In Eq. (III E3 b.3), use has been made of the uncorrelated nature of the raw data:

$$\left\langle \delta d_j \; \delta d_{j'} \right\rangle = \Delta^2 d_j \; \delta_{j j'} \quad . \qquad \text{(III E3 b.4)}$$

The first term in Eq. (III E3 b.3) represents the statistical uncertainty on D_i. Generally, it is diagonal with respect to i and i', since f_i will usually depend only on d_i and not on other $d_{i'}$, but we have included off-diagonal terms for the sake of completeness. The second term contains information from the data-reduction process. Generally, this term is off-diagonal with respect to i and i'; that is, the reduced data D_i all depend upon the same parameters q_k, and thus are correlated. Thus the data covariance matrix $V_{i\,i'}$ to be used in Bayes' equations involves off-diagonal terms.

It is possible for the full covariance matrix to be calculated from Eq. (III E3 b.3) and read directly into SAMMY (see Section VI.C.2). However, all data points that are connected by off-diagonal terms need to be included in the same analysis. Because typical time-of-flight experiments may involve thousands of data points, this process is often impractical computationally.

An alternative method of handling uncertainties on data-reduction parameters is to treat those parameters as variables whose value is to be determined by the analysis process, that is, to treat them in the same fashion as the resonance parameters.

In the development of Bayes' equations (Section IV), the conditional probability $p(D|PX)$ was needed. Since the data-reduction parameters $\{q\}$ are now considered to be a part of the set $\{P\}$, Eq. (IV A1.3) requires the probability of D being true <u>given that $\{q\}$ are exactly the correct values</u>. That is, we use the data covariance matrix V formed from only the first term in Eq. (III E3 b.3), the second term giving zero if the values for$\{q\}$ are exact.

Since data D, as well as theory T, now depend on parameters P, Eq. (II A1.4) must be expanded to include

$$T(P) - D(q) = \bar{T} - \bar{D} + G\left(P - \bar{P}\right) - g\left(q - \bar{q}\right) \quad , \qquad \text{(III E3 b.5)}$$

in which we have set the partial derivative of D_i with respect to q_k equal to g_{ik}; that is,

$$\frac{\partial D_i}{\partial q_k} = g_{ik} \quad . \qquad \text{(III E3 b.6)}$$

Therefore, by expanding the set of parameters $\{P\}$ to include the data-reduction parameters $\{q\}$, and by redefining G_{ik}, the partial derivative of the theory T_i with respect to the parameter P_k, to be the partial derivative of $(T_i - D_i)$ with respect to P_k, the equations take on the exact form discussed in Section IV.A.

To use this method in SAMMY, the analyst must generate the partial derivatives g_{ik} prior to the SAMMY runs, and provide the values to SAMMY. (The code ALEX [DL83 and NL84] may be used for this purpose.) Input details are given in Section VI.C of this report.

Caveat: This option has been available in SAMMY almost from the beginning, but it has (to the author's knowledge) never been used extensively and hence never been thoroughly tested. Moreover, the techniques used are not optimal. Unless there is demand for this option, it will probably be discontinued with the next release of the code.

III.E.4. Paramagnetic Cross Section

The total cross section of nuclides like erbium, holmium, and thulium at low neutron energies may include both nuclear and paramagnetic cross sections. The paramagnetic cross section may be written in the following form [YD98]:

$$\sigma_{PM} = C\left(\frac{\left(A\tan^{-1}\left(BE^{P}\right)\right)}{BE^{P}\left(1+\left(BE^{P}\right)^{2}\right)^{4}}\right)^{2} \quad . \qquad \text{(III E4.1)}$$

Here E is the energy in eV, and A, B, P, and C are parameters (variables) whose default values are given in Table III E4.1; these may be treated either as constants or as varied parameters whose values are to be determined by the Bayes (generalized least-squares) fitting procedure.

As presently implemented within SAMMY, the paramagnetic cross section may be invoked only in calculations for data types "total cross section" or "transmission." In particular, paramagnetic cross sections cannot be included in angular distributions nor in generating self-shielding or multiple-scattering corrections for capture or fission yields.

Table III E4.1. Default parameter values for paramagnetic cross sections

	A	*B*	*P*	*C*
Tm	6.1691	1.1308	0.3367	1.0
Er	7.9012	1.1278	0.3263	1.0
Ho	8.7597	1.1435	0.3225	1.0

Input for using PM cross section (for total cross sections only) is given in Table VI B.2, card set 12. See test case tr055 for examples of this input.

Although SAMMY can search on any or all of these parameters, the user should be aware that variables A and C are mathematically redundant; it is only the product CA^2 that is unique. When values for both parameters are permitted to vary, the correlation coefficient will always be -1.

Derivatives of σ_{PM} are as follows: Let x represent the quantity BE^{P}. The derivatives with respect to each of the four parameters are then

$$\frac{\partial\sigma}{\partial A} = \frac{2\sigma}{A} \quad , \qquad \text{(III E4.2)}$$

$$\frac{\partial \sigma}{\partial B} = C\,A^2\,2\,f\,\frac{d\,f}{d\,x}\,\frac{x}{B} \quad , \tag{III E4.3}$$

$$\frac{\partial \sigma}{\partial P} = C\,A^2\,f\,\frac{d\,f}{d\,x}\,x\ln\left(E\right) \quad , \tag{III E4.4}$$

and

$$\frac{\partial \sigma}{\partial C} = \frac{\sigma}{C} \quad . \tag{III E4.5}$$

In these equations we have made the substitution

$$f = \frac{\tan^{-1} x}{x\left(1+x^2\right)^4} \quad , \tag{III E4.6}$$

so that

$$\frac{d\,f}{d\,x} = \frac{1}{x\left(1+x^2\right)^5}\left[1-\frac{1-9x^2}{x}\tan^{-1} x\right] \quad . \tag{III E4.7}$$

III.E.5. Detector Efficiency

For measurements of capture or fission yields, the detectors may have different efficiencies for different *l*-values. SAMMY is equipped with a spin-group-dependent detector efficiency (multiplicative factor), which can be used to model this effect. The user may specify as many different efficiencies as needed, and delineate the spin groups to which those efficiencies apply. (See Table VI B.2, card set 15, for input details.) SAMMY will multiply the calculated capture or fission partial cross sections by the efficiencies prior to applying self-shielding and multiple-scattering corrections; these efficiencies can also be used with self-indication data. Note that the total and elastic cross sections (used in the calculation of self-shielding and multiple-scattering effects) are *not* multiplied by the efficiencies.

Test case tr078 contains examples of the use of spin-group-dependent detector efficiencies.

III.E.6. Self-Indication Measurements

Self-indication experiments involve a combination of both capture and transmission measurements. Two samples are used: the one closer to the source is used for transmission and the other is used for capture. Both samples contain the nuclide of interest. Such an experiment preferentially removes neutrons near the peak of the resonances for this nuclide, thus focusing on the shoulders or wings of a resonance.

Analysis of a self-indication experiment requires both calculation of transmission through the first sample and calculation of capture yield with self-shielding and multiple-scattering corrections for the second sample. Transmission is calculated as described in Section III.E.1, using parameters appropriate for that sample (for thickness, nuclide abundances, contaminants, temperature, etc.). Essentially, transmission T is given by

$$T(E) = e^{-n_T \sigma_t} \quad , \qquad \text{(III E6.1)}$$

in which n_T represents the sample thickness and σ_t the total cross section (appropriately Doppler broadened). Subscript T indicates that the thickness is that of the transmission sample; subscript t refers to the total cross section. The capture yield $Y(E)$ is calculated as described in Section III.D, using parameters appropriate for the capture sample; note that any of the three normalizations (as cross section, as yield, or as yield times total cross section) described in that section may be applied to the capture "yield" calculation here. The self-indication result is the product of the transmission and the capture yield,

$$SI(E) = T(E)Y(E) \quad , \qquad \text{(III E6.2)}$$

followed by resolution broadening.

Parameters such as "isotopic" (nuclide) abundances, effective temperature, and thickness, which are input in the usual fashion into SAMMY, are assumed to be those of the capture sample. Input of parameters appropriate for the transmission sample is via card set 11, line 7 of the PARameter file (see Table VI B.2). The phrase "self-indication" must occur in the INPut file (card set 8).

Test case tr057 has examples, using artificial data, for self-indication experiments.

[Note that the option to calculate the self-indication *ratio* is not yet implemented into SAMMY. This quantity is defined as the resolution-broadened $SI(E)$ divided by the resolution-broadened capture yield $Y(E)$; implementation of this feature is one of many "on the drawing board" for future work.]

III.E.7. Corrections for Angular Distributions

Angular distribution measurements may require additional treatments for experimental conditions beyond those required by angle-integrated measurements. Two kinds of treatment are currently available in SAMMY; as experiments improve and the need arises for more sophisticated treatments, others will be added to the code.

Attenuation

One type of correction for finite sample size in angular distributions is handled in much the same manner as in the code RFUNC, which was developed by F. G. Perey [FP89a] for calculating elastic angular distributions using the R-function approximation for spin-zero samples. Two effects are included, which are denoted "incident neutron attenuation" and "scattered neutron attenuation," respectively.

Incident neutron attenuation is accomplished by multiplying the cross section by the factor

$$\exp\left\{-n_{in}\left(\theta\right)\sigma_{tot,D}\left(E\right)\right\} \quad , \qquad \text{(III E7.1)}$$

where the "thickness" or attenuation $n_{in}\left(\theta\right)$ may be specified independently for each angle and may be treated as a search parameter. The cross section appearing in Eq. (III E7.1) is the Doppler-broadened total cross section.

The so-called "scattered neutron attenuation" is used to approximately describe three distinct effects: (1) Neutrons initially scattered in the direction of the detector may be re-scattered (or captured, or involved in some other reaction). (2) Neutrons not initially scattered toward the detector may, after two or more scatterings, ultimately reach the detector. (3) Both the sample and the detectors have large angular spreads.

To describe these effects, the cross section is multiplied by the attenuation factor

$$\exp\left\{-n_{out}\left(\theta\right)\sigma_{tot,x}\left(E'\right)\right\} \quad . \qquad \text{(III E7.2)}$$

Here the attenuation $n_{out}\left(\theta\right)$ again may be different for each angle and may be treated as a search parameter. The cross section in this equation is evaluated at the scattered energy for the particular angle and has been broadened (using a triangular resolution function) to approximate the effects of the angular spread of the detector and sample.

See Table VI B.2, card set 11, line 4, for details of the input for these attenuation factors.

Angle Average

Another available correction for the finite sample size is a straight-line average over solid angle, of the form

$$\left\langle \frac{d\sigma}{d\Omega} \right\rangle = \int_{\cos(\theta+D\theta)}^{\cos(\theta-D\theta)} \frac{d\sigma}{d\Omega} d\mu \Bigg/ \int_{\cos(\theta+D\theta)}^{\cos(\theta-D\theta)} d\mu \quad , \qquad \text{(III E7.3)}$$

in which the differential elastic cross section is assumed to be a function of cos(θ) but a constant with respect to the azimuthal angle φ.

The actual calculation in SAMMY is carried out in a relatively crude approximation which implicitly assumes that the angular spread is not large. The cross section is calculated at three angles: $\theta + D\theta$, θ, and $\theta - D\theta$. Quadratic interpolation in cos(θ) is used so that the cross section at other angles is assumed to be given by

$$\sigma(\mu) \;=\; A\frac{(\mu-b)(\mu-c)}{(a-b)(a-c)} + B\frac{(\mu-a)(\mu-c)}{(b-a)(b-c)} + C\frac{(\mu-a)(\mu-b)}{(c-a)(c-b)} \quad , \qquad \text{(III E7.4)}$$

in which we have set

$$a = \cos(\theta + D\theta) \qquad b = \cos(\theta - D\theta) \qquad c = \cos(\theta) \qquad \text{(III E7.5)}$$

and

$$A = \frac{d\sigma(a)}{d\Omega} \qquad B = \frac{d\sigma(b)}{d\Omega} \qquad C = \frac{d\sigma(c)}{d\Omega} \quad . \qquad \text{(III E7.6)}$$

Substituting Eq. (III E7.4) into Eq. (III E7.3) and integrating gives the resulting average cross section

$$\left\langle \frac{d\sigma}{d\Omega} \right\rangle = \frac{1}{6}\left[A\frac{3c-b-2a}{c-a} + B\frac{-3c+2b+a}{b-a} + C\frac{(b-a)^2}{(c-a)(b-c)} \right] \quad . \qquad \text{(III E7.7)}$$

To invoke this option, include the phrase

```
ANGLE-AVERAGE FOR DIfferential cross sections
```

in the command section of the INPut file. The angles θ and angular spreads $D\theta$ are given in card set 8 of that file (see Table VI A.1).

III.E.8. Energy-Scale Dependence on t_0 and L

When analyzing two or more independent data sets, the problem of displacement between energy scales often arises. Proper alignment of energy scales has traditionally been a task for the analyst; however, help is available from SAMMY. Two methods are described here.

First method:

In time-of-flight measurements, the energy of the incident neutron is determined from the flight-path length L, the flight time t, and the initial time t_0 as

$$E = \frac{m}{2}\frac{L^2}{\left(t - t_0\right)^2} \quad . \tag{III E8.1}$$

By treating L and t_0 as variables (parameters) and searching for those values of L and t_0 which provide the best fit of experimental measurement to the calculated cross section, it is possible to adjust the energy scales to provide agreement between different data sets. See card set 11, line 6, of the PARameter file, Section VI, for input details.

Derivatives of the cross section with respect to flight-path length L and initial time t_0 are given in terms of the derivative with respect to energy as

$$\frac{\partial\sigma}{\partial t_0} = \frac{\partial E}{\partial t_0}\frac{\partial\sigma}{\partial E} = \frac{2E}{\left(t - t_0\right)}\frac{\partial\sigma}{\partial E} \tag{III E8.2}$$

and

$$\frac{\partial\sigma}{\partial L} = \frac{\partial E}{\partial L}\frac{\partial\sigma}{\partial E} = \frac{2E}{L}\frac{\partial\sigma}{\partial E} \quad . \tag{III E8.3}$$

Recall that the cross section σ is given in terms of the scattering matrix U. The energy-dependence of σ is therefore that of U (via ρ) and of the $\left(1/k^2\right)$ multiplicative factor. That is, this derivative is given by

$$\frac{\partial\sigma}{\partial E} = \frac{\partial\sigma}{\partial\rho}\frac{\partial\rho}{\partial k}\frac{\partial k}{\partial E} - \frac{2}{k}\sigma\frac{\partial k}{\partial E} \quad , \tag{III E8.4}$$

which can be rewritten as

$$\frac{\partial\sigma}{\partial E} = \left(\frac{\partial\sigma}{\partial\rho}a - \frac{2}{k}\sigma\right)\frac{k}{2E} \quad . \tag{III E8.5}$$

Combining this equation with Eqs.(III E8.2) and (III E8.3) gives

$$\frac{\partial\sigma}{\partial t_0} = \frac{\rho}{\left(t-t_0\right)}\frac{\partial\sigma}{\partial\rho} - \frac{2}{\left(t-t_0\right)}\sigma \qquad \text{(III E8.6)}$$

and

$$\frac{\partial\sigma}{\partial L} = \frac{\rho}{L}\frac{\partial\sigma}{\partial\rho} - \frac{2}{L}\sigma \quad . \qquad \text{(III E8.7)}$$

The derivative of the cross section with respect to ρ is again, as in Section II.D.1.c, found by substituting Eq. (II D1 c.9) into Eq. (II D1 c.6).

Note that relativistic corrections are often added to the expression in Eq. (III E8.1); such corrections are ignored in SAMMY's treatment of the t_0 dependence.

Within SAMMY the value of L is not varied directly; rather, L is set equal to the product of the "initial" value L_i times a dimensionless quantity L_0. This dimensionless multiplier is generally given an initial value of 1.0, and the value is varied in the SAMMY run.

In preliminary studies, what has been found practical is to use this option somewhat apart from the mainstream of SAMMY analyses. The procedure that worked best in our trials was to first obtain a reasonably good fit to the "best" data set (the data set which, in the analyst's judgment, has the "most correct" energy scale), with particular emphasis on obtaining accurate resonance energies. Next, modify the parameter file to vary only L_0 and t_0 (i.e., do not vary resonance energies or other resonance parameters) and make a SAMMY run to determine the best values for L_0 and t_0 for the data set in which the energy scale is "wrong." Once those values have been determined, generate a modified data set which has the corrected energy scale and use the modified set in subsequent work. The code SAMFTZ, described in Section X.G of this manual, can be used to generate the modified data set.

Second method:

Begin by fitting each data set separately from the others, establishing in particular appropriate energies for the largest resonances. Choose one data set (probably the transmission measurement with the longest flight path) as the standard. For each other data set, compare energies for individual resonances to those in the standard data set. By considering the relative energy difference as a function of resonance energy, a fit can be made to the functional form

$$\frac{E'-E}{E} = \frac{\Delta E}{E} = a + b\sqrt{E} \quad , \qquad \text{(III E8.8)}$$

in which E is the energy of the resonance in the standard data set, and E' the energy in the other data set. Equation (III E8.8) is the appropriate functional form, as can be seen by taking increments of Eq. (III E8.1),

$$\Delta E = \frac{\partial E}{\partial L}\Delta L + \frac{\partial E}{\partial t_0}\Delta t_0 = \frac{2E}{L}\Delta L + \frac{2E}{\left(t - t_0\right)}\Delta t_0 \quad , \qquad \text{(III E8.9)}$$

or

$$\frac{\Delta E}{E} = \frac{2\Delta L}{L} + \frac{2\sqrt{2E/m}}{L}\Delta t_0 = \frac{2\ \Delta L}{L} + \left(\frac{2\Delta t_0\sqrt{2/m}}{L}\right)\sqrt{E} \quad . \qquad \text{(III E8.10)}$$

Once appropriate values are determined for a and b, all energies in the non-standard data set can be modified by replacing the original (incorrect) energy E' by E'', where

$$E' = E'' + \left(a + b\sqrt{E''}\right)E'' \quad . \qquad \text{(III E8.11)}$$

Solution of this equation for E'' can be done iteratively, with $E'' \approx E'$ as starting value.

IV. THE FITTING PROCEDURE

In order to determine the parameter values that give the "best fit" of theoretical values to experimental measurements, a fitting procedure is needed. The procedure must properly incorporate all uncertainties in the measured data, including both statistical and systematic uncertainties, and should provide appropriate uncertainties and correlations for the resulting set of parameter values.* The fitting procedure must be able to deal with nonlinear systems.

The procedure used in SAMMY is Bayes' method, sometimes denoted "generalized least squares." See Section XI.C for a philosophical discussion of the implications of the use of Bayes' method.

(In the limit of infinite prior uncertainty, under the customary assumptions of normality, Bayes' method reduces to the more familiar least-squares method. SAMMY contains provisions for using the least-squares method rather than the more powerful generalized least squares; see Section IV.E.3 for details.)

Section IV.A is devoted to a formal description of the relevant equations for Bayes' method. Starting from Bayes' theorem [HJ61] and three basic assumptions, formulae are derived for updating parameter values and parameter covariance matrix elements based on information contained in the data currently being analyzed. These formulae, in their several guises, are hereafter referred to as Bayes' equations. The three versions used in the SAMMY code are derived in Section IV.A.1, and the iterative versions thereof (for use with nonlinear systems) in Section IV.A.3. Formulae for chi squared are developed and discussed in Section IV.A.2.

Implementation of each of the three versions of Bayes' equations in SAMMY is described in Section IV.B.

Most input parameters may be fitted in the SAMMY code, though the actual fitted parameter is not always the variable given in the input. For example, though values for the resonance energies are given in the PARameter file, the variable used in the fitting procedure is the square root of the resonance energy. In Section IV.C, parameters that may be varied are listed.

Section IV.D contains a discussion of the Data Covariance Matrix (DCM), its role in Bayes' equations, and SAMMY's various treatments of the DCM. SAMMY has the ability to read, store, and invert a full off-diagonal DCM; however, the reader should be aware that this is a highly inefficient method for treating experimental uncertainties. Instead, when components of the DCM are generated external to SAMMY, those components (rather than the DCM itself) should be used as input to the code via the User-Supplied Implicit DCM option (Section VI.C.3.b has input details for this option). To include the contribution from uncertainties on SAMMY input parameters, the

---

* Often, however, the uncertainties determined by SAMMY are deemed to be too small. This may be true even when the best of experimental-data uncertainty information is provided, for a variety of reasons, some of which are discussed in Section IV.E.6. Therefore, options are provided for modifying the SAMMY-generated parameter covariance matrix, as described in Section IV.E.6.

Propagated Uncertainty Parameter (PUP) option is available; see the discussion in Section IV.D.2 and the input details in Section VI.C.3.a. In both cases, the full DCM is not calculated; instead, the treatment is via SAMMY's Implicit Data Covariance (IDC) method, described in Section IV.D.3.

Section IV.E contains information about a variety of topics related to covariances. For a discussion of simultaneous (rather than sequential) fitting of several data sets, see Section IV.E.1. In Section IV.E.2, information is found on SAMMY's retroactive covariance method, whereby a parameter covariance matrix can be generated that is approximately correct for a given parameter set. To use an infinite prior parameter covariance matrix (i.e., to use the least-squares equations), see Section IV.E.3. Generating the covariance matrix associated with the theoretical cross section is described in Section IV.E.4. Section IV.E.5 describes SAMMY's method for calculating average values and uncertainties for certain classes of resonance parameters (e.g., the average capture or neutron width for all resonances in a particular spin group). Finally, in Section IV.E.6, available methods are described for altering (increasing) the SAMMY-produced resonance-parameter covariance matrix, in preparation for reporting to ENDF and/or publishing results.

IV.A. DERIVATION OF BAYES' EQUATIONS

A derivation of Bayes' equations is given in this section. It should be noted that this is not the only possible derivation; alternatives can be found in [JM80] and [AG73].

In Section IV.A.1, results obtained in this section are used as the starting point for defining the three forms of Bayes' equations used in SAMMY. A discussion of the chi-squared values is given in Section IV.A.2, and the iteration scheme that compensates for non-linearity is presented in Section IV.A.3.

Our derivation begins with Bayes' theorem, which may be written in the form

$$p\left(P \mid DX\right) = p\left(P \mid X\right) p\left(D \mid PX\right) \qquad \text{(IV A.1)}$$

where

- P represents the parameters of the (extended) R-matrix theory, and D represents the experimental data to be analyzed.
- X represents "background" or "prior" information such as the data from which prior knowledge of the parameters P was derived. X is assumed to be independent of D.
- $p(P|DX)$ is the probability for the value of the parameters, conditional upon the new data D, and is what we seek. It is conventional to call $p(P|DX)$ the posterior probability. Since P represents several parameters, $p(P|DX)$ is a joint probability density function (joint pdf). The expectation values of P times $p(P|DX)$ are taken as the new estimates for the parameters; the associated covariance matrix gives us a measure of how well the parameters are determined and of the interdependencies of those determinations.
- $p(D|PX)$ is the probability density function for observing the data D given that the parameters P are correct. It is a function of the parameters P of the model and is proportional to the likelihood function of the data D.
- $p(P|X)$ is the joint pdf for the values of the parameters P of the model, prior to consideration of the new data D; it is known as the prior joint pdf. The expectation values of P times $p(P|X)$ are the prior estimates for the values of the parameters; the associated covariance matrix gives a measure of how well the parameters are known before consideration of the new data.

Let $P = \{P_k\}$ for $k = 1$ to K be the set of all parameters of the theoretical model to be considered. The joint pdf $p(P|X)$ is assumed to be a joint normal pdf having as expectation value the vector $\overline{P}$ and the covariance matrix M. Under this assumption, the pdf may be written

$$p\left(P \mid X\right) \propto \exp\left[-\frac{1}{2}\left(P-\overline{P}\right)^t M^{-1}\left(P-\overline{P}\right)\right] \quad , \qquad \text{(IV A.2)}$$

where superscript t denotes the transpose.

The experimental data are represented by a data vector D whose components D_i are the L data points. The experimental conditions are assumed to be such that the data D (i.e., the D_i's) have a joint normal distribution with mean $\langle D \rangle = T = T(P)$ and covariance matrix V. The likelihood function is then

$$p(D \mid PX) \sim \exp\left[-\frac{1}{2}(D-T)^t V^{-1}(D-T) \right] \quad . \tag{IV A.3}$$

Here T represents theory (i.e., calculated values of cross section or transmission plus corrections), and the covariance matrix V represents not only the experimental "errors" of the data but also any theoretical "errors" resulting from approximations used in calculating T. Obviously V need not be diagonal.

Combining Eqs. (IV A.1), (IV A.2), and (IV A.3) gives an expression for the pdf of P after consideration of new data D [i.e., for $p(P|DX)$], expressed in terms of the "true" value T. What is needed, however, is an expressions for $p(P|DX)$ expressed in terms of the parameters P. This is obtained formally by considering T a function of P, performing a Taylor expansion about $\overline{P}$ [the expectation value of $p(P|X)$], and keeping only the linear terms:

$$T(P) = \overline{T} + G\left(P - \overline{P}\right) + \ldots \quad , \tag{IV A.4}$$

where $\overline{T} = T\left(\overline{P}\right)$. The elements of G, often denoted the "sensitivity matrix," are the partial derivatives of T_n with respect to the parameters P_k, evaluated at $P = \overline{P}$:

$$G_{nk} = \left.\frac{\partial T_n}{\partial P_k}\right|_{P=\overline{P}} \quad \text{for} \begin{cases} n = 1 \text{ to } L \\ k = 1 \text{ to } K \end{cases} \quad . \tag{IV A.5}$$

Because T is a vector of dimension L (equal to the number of data points), and P is a vector of dimension K (equal to the number of parameters), the sensitivity matrix G has dimension $L \times K$.

Substituting Eq. (IV A.4) into Eq. (IV A.3) and using Eq. (IV A.2), we obtain for the posterior joint pdf [Eq. (IV A.1)]

$$\begin{aligned} p(P \mid DX) \sim \exp\Big[& -\frac{1}{2}\left(P - \overline{P}\right)^t M^{-1}\left(P - \overline{P}\right) + \\ & \left(D - \overline{T} - G\left(P - \overline{P}\right)\right)^t V^{-1}\left(D - \overline{T} - G\left(P - \overline{P}\right)\right) \Big] \quad . \end{aligned} \tag{IV A.6}$$

Because of the three basic assumptions we have made, that is,

i. the prior joint pdf is a joint normal, Eq. (IV A.2),
ii. the likelihood function is a joint normal, Eq. (IV A.3), and
iii. the true value is a linear function of the parameters, Eq. (IV A.4) with (IV A.5),

it follows that the posterior joint pdf is also a joint normal. Denoting its expectation value by $\bar{P}'$ and its covariance matrix by M', we may write

$$p\left(P \mid DX\right) \sim \exp\left[-\frac{1}{2}\left\{\left(P-\bar{P}'\right)^t \left(M'\right)^{-1}\left(P-\bar{P}'\right)\right\}\right] \quad . \tag{IV A.7}$$

Substituting Eqs. (IV A.2), (IV A.3), and (IV A.7) into (IV A.1) gives

$$\begin{aligned}\exp\left[-\frac{1}{2}\left\{\left(P-\bar{P}'\right)^t \left(M'\right)^{-1}\left(P-\bar{P}'\right)\right\}\right] \sim \exp\left[-\frac{1}{2}\left(P-\bar{P}\right)^t M^{-1}\left(P-\bar{P}\right)\right] \\ \times\ \exp\left[-\frac{1}{2}\left(D-T\right)^t V^{-1}\left(D-T\right)\right] \quad ,\end{aligned} \tag{IV A.8}$$

which is valid up to a normalization constant. To simplify this expression, we substitute Eq. (IV A.4) for *T*, obtaining

$$\begin{aligned}\exp\left[-\frac{1}{2}\left\{\left(P-\bar{P}'\right)^t \left(M'\right)^{-1}\left(P-\bar{P}'\right)\right\}\right] \sim \exp\left[-\frac{1}{2}\left(P-\bar{P}\right)^t M^{-1}\left(P-\bar{P}\right)\right] \\ \times\ \exp\left[-\frac{1}{2}\left(D-\bar{T}-G\left(P-\bar{P}\right)\right)^t V^{-1}\left(D-\bar{T}-G\left(P-\bar{P}\right)\right)\right] \quad .\end{aligned} \tag{IV A.9}$$

In this form, the theoretical function *T* is treated as strictly linear with respect to the parameters. (In Section.IV.A.3, this formula will be generalized for nonlinear *T*.) Rearranging the exponents gives

$$\begin{aligned}\exp\Bigg[-\frac{1}{2}\Big\{&\left(P-\bar{P}'\right)^t \left(M'\right)^{-1}\left(P-\bar{P}'\right) \\ &-\left(P-\bar{P}\right)^t \left(M^{-1}+G^t V^{-1} G\right)\left(P-\bar{P}\right) \\ &+\left(P-\bar{P}\right)^t G^t V^{-1}\left(D-\bar{T}\right)+\left(D-\bar{T}\right)^t V^{-1} G\left(P-\bar{P}\right) \\ &-\left(D-\bar{T}\right)^t V^{-1}\left(D-\bar{T}\right)\Big\}\Bigg] \qquad = \quad \text{constant},\end{aligned} \tag{IV A.10}$$

where the value of the constant depends upon the unspecified normalizations. After setting

$$P-\bar{P}' = P-\bar{P}+\bar{P}-\bar{P}' \tag{IV A.11}$$

and rearranging, Eq. (IV A.10) becomes

$$
\begin{aligned}
\exp\Bigg[-\frac{1}{2}\Big\{&\left(P-\bar{P}\right)^t\left(M'\right)^{-1}\left(P-\bar{P}\right)+\left(\bar{P}-\bar{P}'\right)^t\left(M'\right)^{-1}\left(P-\bar{P}\right)\\
&+\left(P-\bar{P}\right)^t\left(M'\right)^{-1}\left(\bar{P}-\bar{P}'\right)+\left(\bar{P}-\bar{P}'\right)^t\left(M'\right)^{-1}\left(\bar{P}-\bar{P}'\right)\\
&-\left(P-\bar{P}\right)^t\left(M^{-1}+G^tV^{-1}G\right)\left(P-\bar{P}\right)\\
&+\left(P-\bar{P}\right)^tG^tV^{-1}\left(D-\bar{T}\right)+\left(D-\bar{T}\right)^tV^{-1}G\left(P-\bar{P}\right)\\
&-\left(D-\bar{T}\right)^tV^{-1}\left(D-\bar{T}\right)\Big\}\Bigg] \qquad = \quad \text{constant,}
\end{aligned}
\tag{IV A.12}
$$

or

$$
\begin{aligned}
\exp\Bigg[-\frac{1}{2}\Big\{&\left(P-\bar{P}\right)^t\left[\left(M'\right)^{-1}-\left(M^{-1}+G^tV^{-1}G\right)\right]\left(P-\bar{P}\right)\\
&+\left(P-\bar{P}\right)^t\left[\left(M'\right)^{-1}\left(\bar{P}-\bar{P}'\right)+G^tV^{-1}\left(D-\bar{T}\right)\right]\\
&+\left[\left(\bar{P}-\bar{P}'\right)^t\left(M'\right)^{-1}+\left(D-\bar{T}\right)^tV^{-1}G\right]\left(P-\bar{P}\right)\\
&+\left(\bar{P}-\bar{P}'\right)^t\left(M'\right)^{-1}\left(\bar{P}-\bar{P}'\right)-\left(D-\bar{T}\right)^tV^{-1}\left(D-\bar{T}\right)\Big\}\Bigg] = \text{constant.}
\end{aligned}
\tag{IV A.13}
$$

In order for Eq. (IV A.13) to be valid for all P, the exponent must be constant. For this to happen, the terms linear and quadratic in $\left(P-\bar{P}\right)$ must separately be equal to zero. This gives us two equations relating the primed (posterior) values to the unprimed (prior) values:

$$\left(M'\right)^{-1}-\left(M^{-1}+G^tV^{-1}G\right)=0 \tag{IV A.14}$$

and

$$\left(M'\right)^{-1}\left(\bar{P}-\bar{P}'\right)+G^tV^{-1}\left(D-\bar{T}\right)=0 \quad , \tag{IV A.15}$$

which can be rewritten in the form

$$\left(M'\right)^{-1}=M^{-1}+G^tV^{-1}G \tag{IV A.16}$$

and

$$\bar{P}'=\bar{P}+M'G^tV^{-1}\left(D-\bar{T}\right) \quad . \tag{IV A.17}$$

Equations (IV A.16) and (IV A.17) are denoted “Bayes’ Equations,” sometimes called “generalized least squares” for reasons which shall be discussed later. Three distinct but equivalent versions of these equations are used within the SAMMY code, as described in the next section of this manual (Section IV.A.1).

IV.A.1. Derivation of SAMMY's Solution Schemes

Three distinct versions of Bayes' equations are used in the SAMMY computer code. More specifically, it is the equation for M' that differs in the three versions. Each has computational advantages and disadvantages for particular situations; these are described in Section IV.B. In this section, the three versions are derived from the forms found in Eqs. (IV A.16) and (IV A.17), which are repeated here:

$$\left(M'\right)^{-1} = M^{-1} + G^t V^{-1} G \qquad \text{(IV A1.1)}$$

and

$$P' = P + M' G^t V^{-1} \left(D - T\right) \quad . \qquad \text{(IV A1.2)}$$

Here the bars have been dropped for simplicity of notation.

For readers who may be unfamiliar with matrix notation, the final equations are given at the end of this section with indices and summations explicitly displayed.

M+W Version

The version of Bayes' Equations which uses Eqs. (IV A1.1) and (IV A1.2) directly is denoted the "M+W" version,

$$\begin{aligned} M' &= \left(M^{-1} + W\right)^{-1} & P' &= P + M'Y \\ W &= \quad G^t V^{-1} G & Y &= G^t V^{-1}\left(D - T\right) \quad , \end{aligned} \qquad \text{(IV A1.3)}$$

in which the matrix quantities Y and W have been introduced to simplify later discussion. (See especially Section IV.E.1.)

In this form, the relationship of Bayes' equations to the more common least-squares equations is transparent: If the prior parameter covariance matrix M is infinite on the diagonal $\left(M^{-1} = 0\right)$, then the equations in Eq. (IV A1.3) become the least-squares equations; the only difference is in the first equation. Hence the least-squares equations may be considered to be a special case of Bayes' equations; alternatively, Bayes' Equations may be viewed as generalized least squares.

I+Q Version

Multiplying Eq. (IV A1.1) on the right by M and on the left by M' gives

$$\begin{aligned}(M')^{-1} M &= M^{-1}M + G^t V^{-1} G M = I + G^t V^{-1} G M \\ M'(M')^{-1} M &= M = M'\left(I + G^t V^{-1} G M\right) \quad .\end{aligned} \tag{IV A1.4}$$

Defining Q via

$$Q = G^t V^{-1} G M \tag{IV A1.5}$$

puts Eq. (IV A1.4) into the form

$$M' = M\left(I + Q\right)^{-1} \quad . \tag{IV A1.6}$$

Substituting Eq. (IV A1.6) into Eq. (IV A1.2) gives

$$P' = P + M\left(I + Q\right)^{-1} G^t V^{-1}\left(D - T\right) \quad , \tag{IV A1.7}$$

which is Bayes' equation for P' in the I+Q version.

N+V Version

To obtain the N+V version of Bayes' equations, use the identity

$$X^{-1} = Z\left(XZ\right)^{-1} \tag{IV A1.8}$$

$$\text{with} \quad X = I + Q \quad \text{and} \quad Z = G^t\left(G M G^t + V\right)^{-1} G \quad . \tag{IV A1.9}$$

Combining Eqs. (IV A1.6) with Eqs. (IV A1.8) and (IV A1.9) gives

$$M' = M G^t\left(G M G^t + V\right)^{-1} G\left\{\left(I + Q\right) G^t\left(G M G^t + V\right)^{-1} G\right\}^{-1} \quad , \tag{IV A1.10}$$

which can be simplified by defining

$$N = G M G^t \tag{IV A1.11}$$

to give

$$\begin{aligned} M' &= M G^t\left(N + V\right)^{-1} G\left\{\left(I + G^t V^{-1} G M\right) G^t\left(N + V\right)^{-1} G\right\}^{-1} \\ &= M G^t\left(N + V\right)^{-1} G\left\{G^t\left(N + V\right)^{-1} G + G^t V^{-1} G M G^t\left(N + V\right)^{-1} G\right\}^{-1} \\ &= M G^t\left(N + V\right)^{-1} G\left\{G^t\left(N + V\right)^{-1} G + G^t V^{-1} N\left(N + V\right)^{-1} G\right\}^{-1} \quad . \end{aligned} \tag{IV A1.12}$$

Rearranging gives

$$
\begin{aligned}
M' &= M\,G^t\left(N+V\right)^{-1}G\left\{G^t\left(\left(N+V\right)^{-1}+V^{-1}N\left(N+V\right)^{-1}\right)G\right\}^{-1} \\
&= M\,G^t\left(N+V\right)^{-1}G\left\{G^t\left(\left(N+V\right)^{-1}+V^{-1}\left(N+V-V\right)\left(N+V\right)^{-1}\right)G\right\}^{-1} \\
&= M\,G^t\left(N+V\right)^{-1}G\left\{G^t\left(\left(N+V\right)^{-1}+V^{-1}-\left(N+V\right)^{-1}\right)G\right\}^{-1} \\
&= M\,G^t\left(N+V\right)^{-1}G\left\{G^tV^{-1}G\right\}^{-1} \\
&= M\,G^t\left(N+V\right)^{-1}V\,V^{-1}G\left\{G^tV^{-1}G\right\}^{-1} \\
&= M\,G^t\left(N+V\right)^{-1}\left(N+V-N\right)V^{-1}G\left\{G^tV^{-1}G\right\}^{-1} \\
&= M\,G^t\left(\left[I-\left(N+V\right)^{-1}N\right]V^{-1}G\right)\left\{G^tV^{-1}G\right\}^{-1} \\
&= M\,G^t\left(V^{-1}G-\left(N+V\right)^{-1}G\,M\,G^t\,V^{-1}G\right)\left\{G^tV^{-1}G\right\}^{-1} \\
&= M\left(G^t\,V^{-1}G-G^t\left(N+V\right)^{-1}G\,M\,G^t\,V^{-1}G\right)\left\{G^tV^{-1}G\right\}^{-1} \\
&= M-M\,G^t\left(N+V\right)^{-1}G\,M \quad . \qquad \text{(IV A1.13)}
\end{aligned}
$$

This is the N+V version of Bayes' Equation for M':

$$
M' = M - M\,G^t\left(N+V\right)^{-1}G\,M \quad . \qquad \text{(IV A1.14)}
$$

The N+V version of Bayes' equation for P' is found by inserting Eq. (IV A1.14) into Eq. (IV A1.2) and rearranging:

$$
\begin{aligned}
P' &= P+\left[M-M\,G^t\left(N+V\right)^{-1}G\,M\right]G^t\,V^{-1}\left(D-T\right) \\
&= P+\left[M\,G^t-M\,G^t\left(N+V\right)^{-1}G\,MG^t\right]V^{-1}\left(D-T\right) \\
&= P+M\,G^t\left[I-\left(N+V\right)^{-1}N\right]V^{-1}\left(D-T\right) \\
&= P+M\,G^t\left[I-\left(N+V\right)^{-1}\left[N+V-V\right]\right]V^{-1}\left(D-T\right) \qquad \text{(IV A1.15)} \\
&= P+M\,G^t\left[I-\left(N+V\right)^{-1}\left(N+V\right)+\left(N+V\right)^{-1}V\right]V^{-1}\left(D-T\right) \\
&= P+M\,G^t\left[I-I+\left(N+V\right)^{-1}V\right]V^{-1}\left(D-T\right) \\
&= P+M\,G^t\left(N+V\right)^{-1}\left(D-T\right) \quad .
\end{aligned}
$$

Equations with indices and summations explicitly displayed:

<u>*M+W Version*</u>, Eq. (IV A1.3):

$$M'_{ij} = \left(M^{-1} + W\right)^{-1}_{ij} \qquad P_i' = P_i + \sum_j M_{ij}' Y_j$$
$$W_{ij} = \sum_{km} G_{ki} V^{-1}_{km} G_{mj} \qquad Y_j = \sum_{km} G_{kj} V^{-1}_{km} \left(D_m - T_m\right) \tag{IV A1.16}$$

<u>*I+Q Version*</u>, Eqs.(IV A1.5), (IV A1.6), and (IV A1.7):

$$Q_{ij} = \sum_{kmn} G_{ki} V^{-1}_{km} G_{mn} M_{nj}$$
$$M'_{ij} = \sum_k M_{ik} \left(I + Q\right)^{-1}_{kj} \tag{IV A1.17}$$
$$P_i' = P_i + \sum_{jkm} M'_{ij} G_{kj} V^{-1}_{km} \left(D_m - T_m\right)$$

<u>*N+V Version*</u>, Eqs. (IV A1.11), (IV A1.14), and (IV A1.15):

$$N_{km} = \sum_{ij} G_{ki} M_{ij} G_{mj}$$
$$M'_{ij} = M_{ij} - \sum_{nklm} M_{in} G_{kn} \left(N + V\right)^{-1}_{kl} G_{lm} M_{mj} \tag{IV A1.18}$$
$$P'_i = P_i + \sum_{nkl} M_{in} G^t{}_{kn} \left(N + V\right)^{-1}_{kl} \left(D_l - T_l\right)$$

IV.A.2. Chi-Squared and Weighted Residuals

The negative of the constant term (the *P*-independent term) in the exponent of Eq. (IVA.13), which we shall label as χ^2_{Bayes} and denote the "Bayesian chi squared," is of the form

$$\chi^2_{\text{Bayes}} = -\left(\bar{P}-\bar{P}'\right)^t \left(M'\right)^{-1}\left(\bar{P}-\bar{P}'\right)+\left(D-\bar{T}\right)^t V^{-1}\left(D-\bar{T}\right) \quad . \qquad \text{(IV A2.1)}$$

The second term in this expression is exactly the usual χ^2 value, defined as

$$\chi^2_{\text{LS}} = \left(D-\bar{T}\right)^t V^{-1}\left(D-\bar{T}\right) \quad . \qquad \text{(IV A2.2)}$$

The least-squares χ^2 is always larger than the Bayesian χ^2 because the difference [the first term in the right-hand side of Eq.(IV A2.1)] is the negative of a squared quantity. What is observed during a successful Bayes fit is that the value of the least-squares χ^2_{LS} decreases with each iteration, while the value of the Bayesian χ^2_{Bayes} changes very little. In fact, the value of χ^2_{LS} becomes very close to the value of χ^2_{Bayes} as the iterations proceed. (See Section IV.A.3 for a discussion of iteration as compensation for nonlinearity.)

Hence, the Bayesian χ^2 is, in some sense, a measure of the "best fit" that can be found between this theoretical formulation and these experimental data. When a very small χ^2_{LS} value is considered to be a goal of the analysis process, but the value of χ^2_{Bayes} is relatively large, the analyst may find it prudent to look for problems with either the theory or the data before attempting to find a good fit. For example, spin assignments might be incorrect (Section II.C.1), background might not have been properly included (Section III.E.3.a), or multiple-scattering corrections might be needed (Section III.D).

The expression for χ^2_{Bayes} can be written in terms of known quantities as follows: Replacing $\left(\bar{P}-\bar{P}'\right)$ by its value as given in the expression in Eq. (IV.A.16) gives

$$\begin{aligned}
\chi^2_{\text{Bayes}} &= -\left(\bar{P}-\bar{P}'\right)^t \left(M'\right)^{-1}\left(\bar{P}-\bar{P}'\right) \;+\; \left(D-\bar{T}\right)^t V^{-1}\left(D-\bar{T}\right) \\
&= -\left(\left(D-T\right)^t V^{-1} G M'\right)\left(M'\right)^{-1}\left(M' G^t V^{-1}\left(D-T\right)\right) \;+\; \left(D-\bar{T}\right)^t V^{-1}\left(D-\bar{T}\right) \\
&= -\left(D-T\right)^t V^{-1} G M' G^t V^{-1}\left(D-T\right) \;+\; \left(D-\bar{T}\right)^t V^{-1}\left(D-\bar{T}\right) \\
&= \left(D-\bar{T}\right)^t \left\{-V^{-1} G M' G^t V^{-1} + V^{-1}\right\}\left(D-\bar{T}\right) \quad .
\end{aligned} \qquad \text{(IV A2.3)}$$

In the M+W version for M', χ^2_{Bayes} therefore becomes

$$\chi^2_{\text{Bayes}} = \left(D-\bar{T}\right)^t \left\{-V^{-1}G\left(M^{-1}+W\right)^{-1} G^t V^{-1} + V^{-1}\right\}\left(D-\bar{T}\right) \quad , \qquad \text{(IV A2.4)}$$

where W is again defined as $G^t V^{-1} G$.

In the I+Q version, χ^2_{Bayes} takes the form

$$\chi^2_{\text{Bayes}} = \left(D-\bar{T}\right)^t \left\{-V^{-1}G\,M\left(I+Q\right)^{-1} G^t V^{-1} + V^{-1}\right\}\left(D-\bar{T}\right) \quad , \qquad \text{(IV A2.5)}$$

where Q is $G^t V^{-1} G M$.

Finally, in the N+V version,

$$\chi^2_{\text{Bayes}} = \left(D-\bar{T}\right)^t \left\{-V^{-1}G\left[M - M\,G^t\left(N+V\right)^{-1} G\,M\right]G^t V^{-1} + V^{-1}\right\}\left(D-\bar{T}\right), \qquad \text{(IV A2.6)}$$

in which N is equal to $G\,M\,G^t$. The expression in the curly brackets in Eq. (IV A2.6) can be simplified significantly as

$$\begin{aligned}
\{\ \} &= -V^{-1}G\left[M - M\,G^t\left(N+V\right)^{-1} G\,M\right]G^t V^{-1} + V^{-1} \\
&= -V^{-1}G\,M\,G^t V^{-1} + V^{-1}G\,M\,G^t\left(N+V\right)^{-1} G\,M\,G^t V^{-1} + V^{-1} \\
&= -V^{-1}N\,V^{-1} + V^{-1}N\left(N+V\right)^{-1} N\,V^{-1} + V^{-1} \\
&= V^{-1}\left[-N + N\left(N+V\right)^{-1} N + V\right]V^{-1} \\
&= V^{-1}\left[-N + \left(N+V-V\right)\left(N+V\right)^{-1} N + V\right]V^{-1} \qquad \text{(IV A2.7)} \\
&= V^{-1}\left[-N + N - V\left(N+V\right)^{-1} N + V\right]V^{-1} \\
&= V^{-1}\left[-V\left(N+V\right)^{-1}\left(N+V-V\right) + V\right]V^{-1} \\
&= V^{-1}\left[-V + V\left(N+V\right)^{-1} V + V\right]V^{-1} \\
&= V^{-1}\left[V\left(N+V\right)^{-1} V\right]V^{-1} \quad = \quad \left(N+V\right)^{-1} \quad .
\end{aligned}$$

Making this substitution into Eq. (IV A2.6) gives

$$\chi^2_{\text{Bayes}} = \left(D-\bar{T}\right)^t \left(N+V\right)^{-1}\left(D-\bar{T}\right) \qquad \text{(IV A2.8)}$$

for the N+V version of χ^2_{Bayes}.

Values for χ^2 (of both types) are reported in the SAMMY output file SAMMY.LPT (see Section VII.A). It should be noted, however, that SAMMY does not report $\chi^2/\ dof$ (where *dof* = degrees of freedom = NDAT − NPAR, with NDAT being the number of data points and NPAR the number of varied parameters), since with Bayes' method *dof* can be zero or negative. Instead SAMMY will report χ^2 and χ^2/NDAT.

Caveat: In the past (prior to the release of sammy-7.0.0 in 2006), the value of χ^2_{LS}, as reported in the SAMMY.LPT file, was calculated under the implicit assumption that the data covariance matrix *V* was diagonal. This is no longer true; χ^2_{LS} is now calculated using the actual data covariance matrix, including off-diagonal elements if they are present.

Another quantity that the analyst will often find useful to examine is the so-called weighted residual, which is the difference between measured value and theoretical value weighted (divided) by the uncertainty on the measured value. Specifically, the weighted residual at point *i* is defined as

$$R_i^{\mathrm{LS}} = \left(D_i - T_i\right) \Big/ \sqrt{V_{ii}} \quad , \qquad \text{(IV A2.9)}$$

a formula that implicitly assumes that the data covariance matrix is diagonal, since off-diagonal elements are ignored. To ask for this array to be printed, the user should specify "PRINT WEIGHTED RESIDuals" in the command section of the INPut file; see Table VI A1.2. The array will be printed, however, only if the data covariance matrix is diagonal.

SAMMY recognizes another array related to the weight residuals and denotes it as the "Bayesian weighted residual,"

$$R_i^{\mathrm{B}} = \sum_j \left(N + V\right)^{-1}_{ij} \left(D_j - T_j\right) \quad . \qquad \text{(IV A2.10)}$$

No particular physical interpretation is applied to this quantity. To calculate and print this array, insert the command "PRINT BAYES WEIGHTED residuals" into the INPut file. If the command "PRINT WEIGHTED RESIDuals" is given, and this array is generated in the normal course of solving Bayes' equations, then it will be printed even though it was not explicitly called for.

IV.A.3. Iteration Scheme

The linearity hypothesis, that is, the assumption that the Taylor expansion of the theoretical values around the prior expectation value truncates after the linear term, is in general only approximately true. Therefore, the parameter values $\bar{P}'$ resulting from application of Bayes' equations are also only approximately correct. To obtain more accurate values, the Taylor expansion, Eq. (IV A.4), may be performed not around $\bar{P}$ but around the new (intermediate) values $\bar{P}^{(n)}$, where n represents the nth iteration and $\bar{P}^{(0)} = \bar{P}$. That is, we assume

$$\begin{aligned} T &\cong \bar{T}^{(n)} + G^{(n)}\left(P - \bar{P}^{(n)}\right) = \bar{T}^{(n)} + G^{(n)}\left(P - \bar{P}^{(0)} + \bar{P}^{(0)} - \bar{P}^{(n)}\right) \\ &= \bar{T}^{(n)} + G^{(n)}\left(\bar{P}^{(0)} - \bar{P}^{(n)}\right) + G^{(n)}\left(P - \bar{P}^{(0)}\right) \end{aligned} \qquad \text{(IV A3.1)}$$

Here the sensitivity matrix $G^{(n)}$ and the theoretical values $\bar{T}^{(n)}$ are evaluated at $P = \bar{P}^{(n)}$. With Eq. (IV A3.1) for T, the formula analogous to Eq. (IV A.13) is

$$\begin{aligned} &\exp\Bigg[-\frac{1}{2}\Bigg\{\left(P - \bar{P}^{(0)}\right)^t \left[\left(M^{(n+1)}\right)^{-1} - \left(M^{-1} + G^{(n)t} V^{-1} G^{(n)}\right)\right]\left(P - \bar{P}^{(0)}\right) \\ &\quad + \left(P - \bar{P}^{(0)}\right)^t \Bigg[\left(M^{(n+1)}\right)^{-1}\left(\bar{P}^{(n)} - \bar{P}^{(n+1)}\right) \\ &\qquad\qquad - G^{(n)t} V^{-1}\left(D - \bar{T}^{(n)} - G^{(n)}\left(\bar{P}^{(n)} - \bar{P}^{(n+1)}\right)\right)\Bigg] \\ &\quad + \Bigg[\left(\bar{P}^{(0)} - \bar{P}^{(n+1)}\right)^t \left(M^{(n+1)}\right)^{-1} \\ &\qquad - \left(D - \bar{T}^{(n)} - G^{(n)}\left(\bar{P}^{(n)} - \bar{P}^{(n+1)}\right)\right)^t V^{-1} G^{(n)}\Bigg]\left(P - \bar{P}^{(0)}\right) \\ &\quad + \left(\bar{P}^{0} - \bar{P}^{(n+1)}\right)^t \left(M^{(n+1)}\right)^{-1}\left(\bar{P}^{(0)} - \bar{P}^{(n+1)}\right) \\ &\quad - \left(D - \bar{T}^{(n)} - G^{(n)}\left(\bar{P}^{(n)} - \bar{P}^{(n+1)}\right)\right)^t V^{-1}\left(D - \bar{T}^{(n)} - G^{(n)}\left(\bar{P}^{(n)} - \bar{P}^{(n+1)}\right)\right)\Bigg\}\Bigg] \\ &= \text{constant} \quad . \end{aligned} \qquad \text{(IV A3.2)}$$

The iterative forms of Bayes' equations follow immediately, by replacing G by $G^{(n)}$ and T by $T^{(n)} - G^{(n)}\left(P^{(n)} - P^{(n+1)}\right)$ in the equations of Section IV A.1. Note that again we have dropped the bars to simplify the notation.

Explicitly, the equations are as follows: For the M+W version, Eq. (IV A1.3) becomes

$$\begin{aligned} M^{(n+1)} &= \left(M^{-1} + W^{(n)}\right)^{-1} & P^{(n+1)} &= P^{(0)} + M^{(n+1)} Y^{(n)} \\ W^{(n)} &= \quad G^{(n)t} V^{-1} G^{(n)} & Y^{(n)} &= G^{(n)t} V^{-1} \left(D - T - G^{(n)} \left(P^{(0)} - P^{(n)}\right)\right) \quad . \end{aligned} \qquad \text{(IV A3.3)}$$

For the I+Q version, the covariance equations, Eqs. (IV A1.5) and (IV A1.6), take the form

$$Q^{(n)} = G^{(n)t} V^{-1} G^{(n)} M \qquad \text{and} \qquad M^{(n+1)} = M \left(I + Q^{(n)}\right)^{-1} \quad , \qquad \text{(IV A3.4)}$$

and for the N+V version, Eqs. (IV A1.10) and (IV A1.13) become

$$M^{(n+1)} = M - M\, G^{(n)t} \left(N^{(n)} + V\right)^{-1} G^{(n)} M \quad \text{with} \quad N = G^{(n)} M\, G^{(n)t} \quad . \qquad \text{(IV A3.5)}$$

For all versions, the parameter equation is

$$P^{(n+1)} = P^{(0)} + M^{(n+1)} G^{(n)\,t} V^{-1} \left(D - T - G^{(n)} \left(P^{(0)} - P^{(n)}\right)\right) \quad . \qquad \text{(IV A3.6)}$$

To control the number of iterations

When running SAMMY, the default number of iterations is 2; that is, SAMMY stops after calculating $P^{(2)}$ and $M^{(2)}$. This value was chosen based on early experience which suggested that, for many practical applications, little was gained from additional iterations: After two iterations, the value of a parameter would generally be accurate to within the uncertainty on that parameter. To illustrate, suppose the "true" value of a parameter was 1.23456789 ± 0.03456789. After two iterations, the value was found to be approximately 1.23500000 ± 0.03500000, so no useful new information is gained by continuing the computations.

Nevertheless, especially during early stages of an analysis, the user will often find it helpful to iterate more times. To increase the number of iterations, specify ITMAX in columns 46–50 of line 2 (i.e., card set 2) of the INPut file, Table VIA.1.

Caveat: Setting ITMAX = 0 in the INPut file will cause the default value ITMAX = 2 to be used. In order to obtain zero iterations (i.e., to evaluate the cross section but not update the parameter values), the user must specify "DO NOT SOLVE BAYES Equations" in the command section of the INPut file.

Caveat: Some older compilers interpret "1" (one) in column 49 as "10" (ten). To avoid undue difficulties caused by having misplaced a number by one column, SAMMY assumes that

a value of ITMAX greater than 9 was an input error. If more than 9 iterations are wanted, the user must insert the negative of the correct value into the INPut file.

At present there are no criteria in SAMMY for stopping the iterations when convergence is reached. These may be added in the future.

IV.B. IMPLEMENTATION OF BAYES' EQUATIONS

Each of the three forms of Bayes' equations has its own strengths and weaknesses.

In the original version of SAMMY (circa 1978), only the N+V method was available. This method requires inversion of a symmetric square matrix whose size is the number of experimental data points – a prohibitive requirement, in the case where off-diagonal data covariance matrix elements exist. The I+Q method requires inversion of a non-symmetric square matrix whose size is the number of varied parameters; in its original form, however, I+Q also required that the data covariance matrix be diagonal. The M+W method also requires inversion of a matrix whose size is the number of varied parameters; in this case, the matrix is symmetric.

SAMMY's method of solution of Bayes' equations for N+V inversion scheme is described in Section IV.B.1, and the solution for the I+Q scheme in Section IV.B.2. The M+W solution method is discussed in Section IV.B.3.

By default, analyses in the resolved resonance region (RRR) use either the N+V or the I+Q method, and SAMMY will choose the method requiring the least amount of computer memory. In general, this means that analyses involving a large number of parameters and/or an off-diagonal data covariance matrix will use N+V, and analyses involving relatively few parameters and a diagonal data covariance matrix will use I+Q.

Under certain circumstances, it is possible for the user to override SAMMY's default choice of which method to use. (This is accomplished by inserting the command "NPV" or "IPQ" in the INPut file; see Table VI A1.2.) When both N+V and I+Q are possible, they give the same results but consume different amounts of computer resources (memory and time).

Analyses in the unresolved resonance region use only the M+W method.

For truly simultaneous fitting of a number of data sets in the RRR, the M+W is used and can be made to behave as a least-squares process. The retroactive covariance matrix generation scheme also uses M+W. See Section IV.E for discussions of these topics.

Certain types of off-diagonal data covariance matrices can be accommodated by any of the three forms of Bayes' equations. See Section IV.D for a discussion of the implicit data covariance (IDC) techniques and propagated uncertainty parameters (PUPs).

IV.B.1. Solving Bayes' Equations: N+V Inversion Scheme

SAMMY uses coding similar to that in the code BAYES [NL82] to solve Bayes' equations in the N+V inversion scheme. In matrix notation, the noniterative form of Bayes' equations can be written

$$P' - P = M\,G^t\left(N+V\right)^{-1}\left(D-T\right) \qquad \text{(IV B1.1)}$$

and

$$M' = M - M\,G^t\left(N+V\right)^{-1}G\,M \quad , \qquad \text{(IV B1.2)}$$

where N is given by

$$N = G\,M\,G^t \quad . \qquad \text{(IV B1.3)}$$

Solving these equations is equivalent to solving

$$AX = Y \qquad \text{(IV B1.4)}$$

K + 1 times (where K is the number of parameters for the problem), with A the $L \times L$ symmetric matrix $N + V$ (where L is the number of data points), and Y a column matrix equal to $\left(D-T\right)$ in Eq. (IV B1.1) or equal to each of the K columns of the rectangular matrix GM in Eq. (IV B1.2).

The inverse of matrix A is not evaluated directly. Rather, A is first factorized as

$$A = U\,B\,U^t \qquad \text{(IV B1.5)}$$

where B is a block-diagonal matrix and U is the product of elementary unit triangular and permutation matrices, so that inverses of U and B are immediately available. The solution X to Eq.(IV B1.4) is then found from

$$X = \left(U^{-1}\right)^t B^{-1}\,U^{-1}Y \quad . \qquad \text{(IV B1.6)}$$

In SAMMY, the factorization of Eq. (IV B1.5) is performed by the LINPACK [JD79] subroutine SSPCO, and the (K + 1) solutions are obtained by LINPACK subroutine SSPSL (with the SAMMY author's updates for double precision). Subroutine NEWPAR oversees these operations.

As explained earlier, it is necessary to modify this procedure slightly to account for the approximations built into Bayes' equations. Details are given in Section IV.A.3.

IV.B.2. Solving Bayes' Equations: I+Q Inversion Scheme

In matrix notation, the noniterative form of Bayes' equations for the I+Q inversion scheme can be written

$$P' - P = M\left(I+Q\right)^{-1} G^t V^{-1}\left(D-T\right) \qquad \text{(IV B2.1)}$$

and

$$M' = M\left(I+Q\right)^{-1} \quad , \qquad \text{(IV B2.2)}$$

where Q is given by

$$Q = G^t V^{-1} G M \quad . \qquad \text{(IV B2.3)}$$

Although Q (and thus $I + Q$) is not symmetric, nevertheless M' is symmetric. This can be shown by noting that

$$M' = M\left(I+Q\right)^{-1} = M\left(M + M G^t V^{-1} G M\right)^{-1} M \qquad \text{(IV B2.4)}$$

provided that M^{-1} exists. In the form of Eq.(IV B2.4), M' is clearly symmetric.

The inversion of $\left(I+Q\right)$ is found by using NAG [NAG] routine F01AAF. When M' is needed (i.e., for the final iteration), Eq. (IV B2.2) is solved first and the array M' used in Eq. (IV B2.1) to find P'. When M' is not needed, the quantity $\left(I+Q\right)^{-1} G^t V^{-1}\left(D-T\right)$ is first generated and then the multiplication by M is performed. Fewer computer operations and thus faster run time result from performing the multiplications in this order.

As with the N+V inversion scheme, two iterations is the default in SAMMY.

The user has the option to choose which inversion scheme to use (as defined in a command line in the INPut file). If the user makes no choice, SAMMY will choose I+Q or N+V based on which method requires the smaller array size. However, if the data covariance matrix V is neither diagonal nor separable (see Section IV.D.3), then the N+V inversion scheme **must** be used.

IV.B.3. Solving Bayes' Equations: M+W Inversion Scheme

The noniterative form of Bayes' equations for the M+W inversion scheme can be written

$$P' - P = M'Y \quad , \tag{IV B3.1}$$

with Y defined as

$$Y = G^t V^{-1} \left(D - T \right) \quad , \tag{IV B3.2}$$

and

$$M' = \left(M^{-1} + W \right)^{-1} \tag{IV B3.3}$$

where W is given by

$$W = G^t V^{-1} G \quad . \tag{IV B3.4}$$

The inverse of M is relatively easy to obtain. Initially M is generally diagonal, so the inverse is trivial. After the initial step, M is no longer diagonal but the inverse is already known from Eq.(IV B3.3) at the previous step.

The solution of Eqs. (IV B3.1) through (IV B3.4) is found from LINPACK [JD79] routines, in the same manner as the solution is found for the N+V inversion scheme.

For calculations in the unresolved resonance region (URR), M+W is the method used.

In the resolved resonance region (RRR), the M+W inversion scheme is not yet as fully integrated into SAMMY as are the I+Q and N+V methods. In the RRR, the M+W scheme currently may be used in a limited fashion, requiring several distinct SAMMY runs to complete the process. The M+W scheme was first employed as a means of retroactively producing an approximate covariance matrix for an existing set of resonance parameters, but now has other uses as well. See Section IV.E for a discussion of retroactive parameter covariance matrices, and for other topics related to covariance matrices.

IV.C. CONSTRUCTING THE PARAMETER SET

Several distinct types of parameters may be varied (i.e., "fitted" or "searched on" in least-squares jargon) in SAMMY. Alternatively, these parameters may be treated as PUPs (propagated uncertainty parameters, as described in Section IV.D.2). Input values for all varied parameters are given in the PARameter file, Table VI B.2; input values for PUPs may generally be given in either the PARameter file or the INPut file. The different types of parameters are listed below; the list is not necessarily all-inclusive.

- Resonance energies and widths: that is, the Reich-Moore R-matrix parameters as described in Section II.B.1 (or the Breit-Wigner parameters as discussed in Section II.B.3). Values for energies and widths are provided via card set 1 of Table VI B.2.

- The matching radii (or channel radii) for the different spin groups and/or potential scattering vs. penetrabilities and shift factors. Values for the matching radii are given in card set 7 or card set 7a of Table VI B.2.

- The seven parameters of the external R-function. These are described in Section II.B.1.d; values are input to the code as shown in card set 3 of Table VI B.2.

- Effective temperature for Doppler broadening, as described in Section III.B. Input is in card set 4 of Table VI B.2.

- Resolution-broadening parameters. For the original formulation (Gaussian and/or exponential) of resolution broadening, Section III.C.1, input is in card set 4 of Table VI B.2. For the Oak Ridge Resolution Function of Section III.C.2, input is in card set 9. For the RPI/GELINA/nTOF Resolution Function of Section III.C.3, input is in card set 14.

  [The parameter for the straight-line energy average resolution function, Section III.C.4, is not variable. Until the author is able to do more extensive testing, it is recommended that parameters of the user-defined resolution function, Section III.C.5, also not be considered variable.]

- Normalization and background functions. See Section III.E.3.a for description and card sets 6 and 13 for input details.

- Abundances for the various nuclides. See card set 10 of Table VI B.2.

- Sample thickness *n*. See card set 4 of Table VI B.2.

- Any of the miscellaneous parameters in card set 11 of Table VI B.2.

- Detector efficiencies, card set 15 of Table VI B.2.

For each parameter of each type, the user sets a flag that specifies whether that particular parameter is to be treated as a constant number (flag = 0), varied (flag = 1), or PUP'd (flag = 3).

SAMMY counts the number NFPALL of flagged (varied + PUP'd) parameters and sets up an array *U* of dimension NFPALL. The initial values *P* needed in Bayes' equations [see, for example, Eq. (IV A1.2)] are stored in *U*. These values are not necessarily the same as those input in the PARameter file, but bear some functional relationship to the input form. For example, *U* will equal the reduced width amplitude $\gamma_{\lambda c}$ rather than the channel width $\Gamma_{\lambda c}$ [see Eq. (II A1.3)]. Details concerning conversion to the "*u*-parameters" are given in the sections relevant to the particular parameter.

Input uncertainties and correlations are likewise converted to represent the uncertainties and correlations on the *u*-parameters. Let p_i represent a physical parameter as input in the PARameter file, and let u_i be the related *u*-parameter. Since $u_i = u_i\left(p_i\right)$ is a precisely specified functional relationship, we also know $\partial u_i / \partial p_i$. Therefore, assuming u_i is unrelated to other parameters, a small increment in u_i is related to an increment in p_i via $\delta u_i = \left(\partial u_i / \partial p_i\right) \delta p_i$. This relationship may then be used to convert from the covariance matrix for *p* to the covariance matrix for *u*; that is,

$$M_{ij} = \left\langle \delta u_i \, \delta u_j \right\rangle = \frac{\partial u_i}{\partial p_i} \left\langle \delta p_i \, \delta p_j \right\rangle \frac{\partial u_j}{\partial p_j} \quad , \qquad \text{(IV C.1)}$$

where *M* is the covariance matrix needed for Bayes' equations, and $\left\langle \delta p_i \delta p_j \right\rangle$ represents the "input" or initial covariance matrix.

In some cases, a *u*-parameter may be related to more than one of the *p*-parameters. This is true, for example, when both the resonance energy and the neutron width are flagged; see Section II.D.1.e for a discussion of the modifications that must be made in this case. The appropriate version of Eq. (IV C.1) for this situation is

$$M_{ij} = \left\langle \delta u_i \delta u_j \right\rangle = \sum_{k,l} \frac{\partial u_i}{\partial p_k} \left\langle \delta p_k \delta p_l \right\rangle \frac{\partial u_j}{\partial p_l} \quad . \qquad \text{(IV C.2)}$$

IV.D. TREATMENT OF DATA COVARIANCE MATRICES

If we accept the assumption that the use of Bayes' equations (or least squares) is an appropriate choice for the data-fitting procedure, then there are two possible methods for propagating the uncertainty on a data-reduction parameter (e.g., normalization) through the analysis process. The first is to treat the parameter as a variable to be fitted, having a prior uncertainty associated with the initial value of that parameter. The second is to treat the value of the parameter as fixed, but include the uncertainty in the data covariance matrix (DCM).

The expectation is that if both methods are correct, then the two methods should yield identical results (at least in the absence of complicating features such as nonlinearities). If results are not identical, then one or the other of the methods must be flawed in some fashion.

In this section, we present a description of the DCM that works equally well for fitting raw data and for fitting reduced data, giving consistent and reliable results. Prior uncertainties are reflected in the final results, both for varied parameters and for those fixed parameters that are used to determine the DCM.

A derivation of this description of the DCM is outlined here; details are shown in Section IV.D.1. See also [NL04a], [NL04b], and the SAMMY workshop notes.

We begin with the assumption that correct results are obtained by treating a data-reduction parameter as a variable to be fitted. This is a reasonable assumption because this treatment uses a diagonal DCM, and there is little or no argument regarding appropriate treatment for diagonal DCMs. The data being analyzed are the "raw" measurements (e.g., measurements of a quantity related to the cross section) plus other measurements related to the value of the data-reduction parameter.

Simple algebra is then used to re-express the equations in terms of "reduced" data (e.g., data that have been converted from raw counts to cross section by dividing by the normalization parameter). Comparison of the resulting equations to the usual version of Bayes' equations for fitting to reduced data indicates the need for modification of the usual version, with regard to the definition of the DCM. In particular, it is necessary to define the DCM in terms of the theoretical values, not in terms of the measured values, for the quantity to be fitted (e.g., the cross section).

The resulting formulae for Bayes' equations can be written as follows for the M+W method:

$$\begin{aligned} P' - P &= M'Y & M' &= \left(W + M^{-1} \right)^{-1} \\ Y &= G^t V^{-1} (D - T) & W &= G^t V^{-1} G \end{aligned} \quad , \qquad \text{(IV D.1)}$$

in which V is shown to have the form

$$V = v + g\, m\, g^t \quad . \qquad \text{(IV D.2)}$$

In these equations, the data D may be either raw or reduced, and the DCM V is calculated at the true (i.e., theoretical) value of the cross sections. The quantity v represents the portion of V that derives from the statistics of the data-taking process, and $g\,m\,g^t$ represents the "common" or "systematic" portion that derives from corrections made to the raw data (e.g., division by an overall normalization factor). In this formulation, the systematic portion must be calculated from theory rather than measurement.

The only difference between this approach and the "usual" approach is in the definition of the partial derivatives (sometimes denoted "sensitivities") g: in the usual approach, these are evaluated at the experimental value. Here, these are evaluated at the theoretical value. (For example, the derivative associated with division by an overall normalization factor would be the cross section divided by the normalization. In the usual approach, the experimental cross section would be used for this derivative; in this approach, the theoretical cross section would be used.)

Not only does this approach allow us to obtain the same results (to first order) as would be obtained by fitting raw data, but we are also able to avoid numerical problems, logical inconsistencies, and some of the issues related to discrepant data.

A simple example may serve to illustrate the difference between the usual DCM and the version advocated here. Suppose two measurements were taken of the same quantity, one yielding 10000 ± 100 counts and the other 12100 ± 110. The covariance matrix associated with the raw data is therefore

$$\begin{bmatrix} (100)^2 & 0 \\ 0 & (121)^2 \end{bmatrix} . \qquad \text{(IV D.3)}$$

After being normalized by a factor of 100, the reduced data are $d_1 = 100$ and $d_2 = 121$. Generating the covariance matrix for the reduced data in the usual fashion requires the following steps: First, write the reduced data in terms of the raw data, and then take small increments of both sides of the equation, giving

$$\begin{aligned} d_i &= r_i / n \\ \delta d_i &= \delta r_i / n - (\delta n / n)(r_i / n) \quad . \end{aligned} \qquad \text{(IV D.4)}$$

Squaring and taking expectation values then gives

$$\begin{aligned} V_{ij} &= \langle \delta d_i \delta d_j \rangle \\ &= \langle \delta r_i \delta r_j \rangle / n^2 + (\langle \delta n \delta n \rangle / n^2)(r_i / n)(r_j / n) \\ &\qquad + \langle \delta r_i \delta n \rangle / n^2 (r_i / n) + \langle \delta n \delta r_j \rangle / n^2 (r_j / n) \\ &= \langle \delta r_i \delta r_j \rangle / n^2 + (\langle \delta n \delta n \rangle / n^2)(r_i / n)(r_j / n) \\ &= \delta_{ij} \; \Delta^2 r_i / n^2 + (\Delta^2 n / n^2) d_i d_j \quad . \end{aligned} \qquad \text{(IV D.5)}$$

(This derivation assumes that $\langle \delta r_i \delta n \rangle = \langle \delta n \, \delta r_j \rangle = 0$, that is, that r and n are uncorrelated, a reasonable assumption.) If $\Delta n = 0.5$, then the usual DCM for the reduced data has the form

$$
\begin{aligned}
V &= \begin{bmatrix} \Delta^2 r_1 / n^2 + \left(\Delta^2 n / n^2\right) d_1^2 & \left(\Delta^2 n / n^2\right) d_1 d_2 \\ \left(\Delta^2 n / n^2\right) d_1 d_2 & \Delta^2 r_2 / n^2 + \left(\Delta^2 n / n^2\right) d_2^2 \end{bmatrix} \\
&= \begin{bmatrix} (1)^2 + (0.005)^2 (100)^2 & (0.005)^2 (100)(121) \\ (0.005)^2 (100)(121) & (1.21)^2 + (0.005)^2 (121)^2 \end{bmatrix} = \begin{bmatrix} 1.25 & 0.325 \\ 0.325 & 1.5125 \end{bmatrix} .
\end{aligned}
\tag{IV D.6}
$$

For this simple example, Bayes' equations can be used to calculate the average of these two values; simply set $t = P$ (theory equal to parameter) so that $G^t = [1 \quad 1]$. The solution is $t = 109.20 \pm 0.92$.

In contrast, the DCM using the more rigorous approach advocated here would have the form

$$
\begin{aligned}
V &= \begin{bmatrix} \Delta^2 r_1 / n^2 + \left(\Delta^2 n / n^2\right) t^2 & \left(\Delta^2 n / n^2\right) t^2 \\ \left(\Delta^2 n / n^2\right) t^2 & \Delta^2 r_2 / n^2 + \left(\Delta^2 n / n^2\right) t^2 \end{bmatrix} \\
&= \begin{bmatrix} (1)^2 + (0.005)^2 t^2 & (0.005)^2 t^2 \\ (0.005)^2 t^2 & (1.21)^2 + (0.005)^2 t^2 \end{bmatrix} ,
\end{aligned}
\tag{IV D.7}
$$

in which t is the as-yet-unknown theoretical value for the quantity being measured. Clearly, in this form the solution of Bayes' equations is somewhat more complicated, but not unduly so. The solution is $t = 108.52 \pm 0.94$, which in this example is only slightly different from the "usual" solution. In cases where the data are markedly discrepant, the differences can be significant.

In SAMMY, any parameter for which derivatives are available (i.e., any parameter that is capable of being fitted) can be treated as a contributor to the DCM. Such parameters are denoted "propagated uncertainty parameters," or PUPs. In Section IV.D.2, application of the PUP method within SAMMY is described. A list is given of those parameters that may be treated as PUPs.

Section IV.D.3 deals with methods of generating and inverting the DCM. In particular, the "implicit data covariance" (IDC) method is introduced, which has many advantages over explicitly generating, storing, and inverting the full DCM.

Even though the method is known to be flawed,* it is nevertheless possible to generate the DCM externally in the usual fashion [e.g., as described in Eqs. (IV D.4) and (IV D.5) for normalization] and provide this as input to SAMMY. Providing the DCM in this fashion is far preferable to another common practice, totally ignoring the off-diagonal elements of the DCM.

Many SAMMY test cases give examples of the various treatments of DCM. See Section XII.B for a list of test cases.

* These flaws include inconsistency with the fit-to-raw-data method; excessive computer time and memory requirements for explicitly creating, storing, and inverting the full DCM; potential problems with discrepant data; and possible loss of accuracy and associated numerical difficulties if using ASCII formats to communicate values for the matrix elements.

IV.D.1. Derivation of Data Covariance Matrix Equation

In this section, we derive the equation for the data covariance matrix (DCM) in terms of the data-reduction parameters and derivatives with respect to those parameters, as discussed in Section IV.D. See also references [NL04a] and [NL04b]. Readers uninterested in details of the derivation may safely bypass these pages.

Matrix notation is used in this derivation, with indices omitted. We begin with definitions of terms:

- P = theory parameters
  - R-matrix widths & energies, channel radii
  - may also include some measurement-related parameters (Doppler widths, etc.) if not included in p
- p = data-reduction parameter
  - normalization or backgrounds
  - resolution or Doppler widths
  - others
- d = experimental measurement (raw data)
  - related to cross section, but exactly as measured by the experiment
- M = initial covariance matrix for parameters P
  - can be diagonal or off-diagonal
  - can be very large (suggesting little a priori information) or quite small (suggesting the parameters are well known)
- m = initial (measured) covariance matrix for p
  - can be diagonal or off-diagonal
  - are determined during the measurement or data-reduction process
- v = covariance matrix for raw data d
  - no assumption regarding diagonality is made yet, though generally the covariance matrix for measured data is diagonal
- $\tilde{t}$ = theoretical cross section
  - a function of R-matrix parameters in P
  - the quantities whose values are to be determined by this experiment and analysis
- t = theory corresponding to the measured data
  - a function of $\tilde{t}$ and p
- g = partial derivative of theory t with respect to data-reduction parameters p
- G = partial derivative of theory t with respect to theory parameters P

The theory t is a complicated function of the cross section. This function incorporates such effects as beam intensity, duration of the experiment, cosmic and room backgrounds, Doppler- and resolution-broadening, detector dead time, finite-size corrections, and others. The ultimate goal of the measurement and analysis is to learn what that cross section is as a function of energy. In general, one can write

$$t = f\,(\tilde{t}, p) \quad , \tag{IV D1.1}$$

where $\tilde{t}$ represents the cross section and p represents any parameters involved in the transformation.

Again we consider Bayes' equations (M+W version), using slightly different notation,

$$\begin{aligned} \mathcal{P}' &= \mathcal{P} + \mathcal{M}'\mathcal{Y} & \mathcal{M}' &= \left(\mathcal{M}^{-1} + \mathcal{W}\right)^{-1} \\ \mathcal{Y} &= \mathcal{G}^t \mathcal{V}^{-1}\left(\mathcal{D} - \mathcal{T}\right) & \mathcal{W} &= \mathcal{G}^t \mathcal{V}^{-1} \mathcal{G} \quad , \end{aligned} \tag{IV D1.2}$$

where $\mathcal{P}$ represents **all** parameters, $\mathcal{M}$ the full covariance matrix for **all** parameters, $\mathcal{D}$ the measured data, $\mathcal{T}$ the corresponding theoretical calculation, $\mathcal{G}$ the partial derivative of $\mathcal{T}$ with respect to $\mathcal{P}$, and $\mathcal{V}$ the DCM. Primes represent updated values for $\mathcal{P}$ and $\mathcal{M}$. Superscript t, as usual, indicates transpose.

In Eq. (IV D1.2), substitute $\mathcal{D} = d$ and $\mathcal{T} = t$, and $\mathcal{V} = v$; in addition, substitute the matrix identities

$$\mathcal{P} = \begin{bmatrix} P \\ p \end{bmatrix}, \qquad \mathcal{M} = \begin{bmatrix} M & 0 \\ 0 & m \end{bmatrix}, \qquad \mathcal{G} = \begin{bmatrix} G & g \end{bmatrix} \quad . \tag{IV D1.3}$$

The inverse of $\mathcal{M}$ is then

$$\mathcal{M}^{-1} = \begin{bmatrix} M^{-1} & 0 \\ 0 & m^{-1} \end{bmatrix} \quad . \tag{IV D1.4}$$

$\mathcal{W} = \mathcal{G}^t \mathcal{V}^{-1} \mathcal{G}$ is therefore found from

$$\mathcal{G}^t \mathcal{V}^{-1} = \begin{bmatrix} G^t v^{-1} \\ g^t v^{-1} \end{bmatrix} \quad \text{and} \quad \mathcal{G}^t \mathcal{V}^{-1} \mathcal{G} = \begin{bmatrix} G^t v^{-1} G & G^t v^{-1} g \\ g^t v^{-1} G & g^t v^{-1} g \end{bmatrix} \quad , \tag{IV D1.5}$$

so that $\left(\mathcal{M}'\right)^{-1}$ becomes

$$\left(\mathcal{M}'\right)^{-1} = \mathcal{G}^t \mathcal{V}^{-1} \mathcal{G} + \mathcal{M}^{-1} = \begin{bmatrix} G^t v^{-1} G + M^{-1} & G^t v^{-1} g \\ g^t v^{-1} G & g^t v^{-1} g + m^{-1} \end{bmatrix} \quad . \tag{IV D1.6}$$

$\mathcal{M}'$ is found by inverting that equation. For matrix X of the form

$$X = \begin{bmatrix} A & C^t \\ C & B \end{bmatrix} \quad , \tag{IV D1.7}$$

the inverse of X can be shown to be

$$X^{-1} = \begin{bmatrix} \left(A - C^t B^{-1} C\right)^{-1} & -\left(A - C^t B^{-1} C\right)^{-1} C^t B^{-1} \\ -\left(B - C A^{-1} C^t\right)^{-1} C A^{-1} & \left(B - C A^{-1} C^t\right)^{-1} \end{bmatrix} \quad , \qquad \text{(IV D1.8)}$$

in which the off-diagonal terms are the transpose of each other:

$$\begin{aligned} \left[\left(B - C A^{-1} C^t\right)^{-1} C A^{-1}\right]^t &= A^{-1} C^t \left(B - C A^{-1} C^t\right)^{-1} \\ &= \left(A - C^t B^{-1} C\right)^{-1} \left(A - C^t B^{-1} C\right) A^{-1} C^t \left(B - C A^{-1} C^t\right)^{-1} \\ &= \left(A - C^t B^{-1} C\right)^{-1} \left[C^t - C^t B^{-1} C A^{-1} C^t\right] \left(B - C A^{-1} C^t\right)^{-1} \\ &= \left(A - C^t B^{-1} C\right)^{-1} C^t B^{-1} \left[B - C A^{-1} C^t\right] \left(B - C A^{-1} C^t\right)^{-1} \\ &= \left(A - C^t B^{-1} C\right)^{-1} C^t B^{-1} \quad . \end{aligned} \qquad \text{(IV D1.9)}$$

That Eq. (IV D1.8) is a correct form for the inverse can readily be verified by calculating $X X^{-1} = X^{-1} X = I$ = the identity matrix, using Eq. (IV D1.9) as necessary.

Substituting the pieces of Eq. (IV D1.6) for $\mathcal{M}'$ into Eq. (IV D1.8) and (IV D1.9) gives

$$\begin{aligned} A - C^t B^{-1} C &= G^t v^{-1} G + M^{-1} - G^t v^{-1} g \left(g^t v^{-1} g + m^{-1}\right)^{-1} g^t v^{-1} G \\ &= G^t \left\{ v^{-1} - v^{-1} g \left(g^t v^{-1} g + m^{-1}\right)^{-1} g^t v^{-1} \right\} G + M^{-1} \\ &= G^t \left(v + g\, m\, g^t \right)^{-1} G + M^{-1} \quad . \end{aligned} \qquad \text{(IV D1.10)}$$

If we then define H as

$$H = v + g\, m\, g^t \quad , \qquad \text{(IV D1.11)}$$

then Eq. (IV D1.10) takes the form

$$A - C^t B^{-1} C = G^t H^{-1} G + M^{-1} \quad . \qquad \text{(IV D1.12)}$$

Analogously, define h as

$$h = v + G\, M\, G^t \quad , \qquad \text{(IV D1.13)}$$

so that

$$B - C A^{-1} C^t = g^t \left(v + G\, M\, G^t \right)^{-1} g + m^{-1} = g^t h^{-1} g + m^{-1} \quad . \qquad \text{(IV D1.14)}$$

Also, since

$$A = G^t v^{-1} G + M^{-1} \quad \text{and} \quad B = g^t v^{-1} g + m^{-1} \quad , \qquad \text{(IV D1.15)}$$

it follows that

$$A^{-1} = M - M\,G^{t}h^{-1}\,G\,M \quad \text{and} \quad B^{-1} = m - m\,g^{t}H^{-1}\,g\,m \quad . \qquad \text{(IV D1.16)}$$

Making those substitutions into Eq.(IV D1.8) for X^{-1} gives the following for $\mathcal{M}'$:

$$\mathcal{M}' = \begin{bmatrix} \left\{ G^{t}H^{-1}G + M^{-1} \right\}^{-1} & -\left\{ G^{t}H^{-1}G + M^{-1} \right\}^{-1} G^{t}v^{-1}g \times \left(m - m\,g^{t}H^{-1}gm \right) \\ -\left\{ g^{t}h^{-1}g^{-1} + m^{-1} \right\}^{-1} g^{t}v^{-1}G \times \left(M - MG^{t}h^{-1}GM \right) & \left\{ g^{t}h^{-1}g + m^{-1} \right\}^{-1} \end{bmatrix} . \qquad \text{(IV D1.17)}$$

Similarly, for $\mathcal{Y}$ from Eq. (IV D1.2) we find

$$\mathcal{Y} = \begin{bmatrix} G^{t}v^{-1}(d-t) \\ g^{t}v^{-1}(d-t) \end{bmatrix} , \qquad \text{(IV D1.18)}$$

which leads to

$$\begin{bmatrix} P' - P \\ p' - p \end{bmatrix} = \begin{bmatrix} \left\{ G^{t}H^{-1}G + M^{-1} \right\}^{-1} G^{t}v^{-1}(d-t) \ldots \\ \quad -\left\{ G^{t}H^{-1}G + M^{-1} \right\}^{-1} G^{t}v^{-1}g \left(m - m\,g^{t}H^{-1}g\,m \right) g^{t}v^{-1}(d-t) \\ -\left\{ g^{t}h^{-1}g + m^{-1} \right\}^{-1} g^{t}v^{-1}G \left(M - MG^{t}h^{-1}GM \right) G^{t}v^{-1}(d-t) \ldots \\ \quad +\left\{ g^{t}h^{-1}g + m^{-1} \right\}^{-1} g^{t}v^{-1}(d-t) \end{bmatrix} . \qquad \text{(IV D1.19)}$$

Rearranging, this becomes

$$\begin{bmatrix} P' - P \\ p' - p \end{bmatrix} = \begin{bmatrix} \left\{ G^{t}H^{-1}G + M^{-1} \right\}^{-1} G^{t}v^{-1} \left\{ 1 - g\left(m - m\,g^{t}H^{-1}g\,m \right) g^{t}v^{-1} \right\} (d-t) \\ \left\{ g^{t}h^{-1}g + m^{-1} \right\}^{-1} g^{t}v^{-1} \left\{ -G\left(M - M\,G^{t}h^{-1}GM \right) G^{t}v^{-1} + 1 \right\} (d-t) \end{bmatrix}$$

$$= \begin{bmatrix} \left\{ G^{t}H^{-1}G + M^{-1} \right\}^{-1} G^{t}v^{-1} \left\{ 1 - g\,m\,g^{t}v^{-1} + g\,m\,g^{t}H^{-1}g\,m\,g^{t}v^{-1} \right\} (d-t) \\ \left\{ g^{t}h^{-1}g + m^{-1} \right\}^{-1} g^{t}v^{-1} \left\{ -GMG^{t}v^{-1} + GMG^{t}h^{-1}GMG^{t}v^{-1} + 1 \right\} (d-t) \end{bmatrix} \qquad \text{(IV D1.20)}$$

$$= \begin{bmatrix} \left\{ G^{t}H^{-1}G + M^{-1} \right\}^{-1} G^{t}v^{-1} \left\{ vH^{-1} \right\} (d-t) \\ \left\{ g^{t}h^{-1}g + m^{-1} \right\}^{-1} g^{t}v^{-1} \left\{ vh^{-1} \right\} (d-t) \end{bmatrix} ,$$

or
$$\begin{bmatrix} P'-P \\ p'-p \end{bmatrix} = \begin{bmatrix} \left\{ G^t H^{-1} G + M^{-1} \right\}^{-1} G^t H^{-1} (d-t) \\ \left\{ g^t h^{-1} g + m^{-1} \right\}^{-1} g^t h^{-1} (d-t) \end{bmatrix} \quad . \qquad \text{(IV D1.21)}$$

Now, consider only the theory parameters P. The formulae for these parameters, considered separately from the equations for the data-reduction parameters p, take the same form as Bayes' equations, provided that the DCM V is replaced by $v + g\,m\,g^t$. Specifically, from Eqs. (IV D1.17) and (IV D1.21), these equations have the form

$$\begin{aligned} &P'-P = M'Y && M' = \left(W + M^{-1} \right)^{-1} \\ &Y = G^t H^{-1} (d-t) && W = G^t H^{-1} G \\ &H = v + g\,m\,g^t && . \end{aligned} \qquad \text{(IV D1.22)}$$

The equations in (IV D1.22) are almost what is needed, except that they are written in terms of the raw data rather than the reduced data (e.g., counts per time channel rather than cross section per energy). Because most analyses are performed in terms of reduced data, it is necessary to convert these equations. If a tilde is used to represent the reduced data, the transformation can be written as

$$\tilde{d} = \tilde{u}\left(d, p\right) \quad . \qquad \text{(IV D1.23)}$$

In Eq. (IV D1.1), we defined f as the transformation from "theoretical cross section $\tilde{t}$" to "theory corresponding to measurement t". The transformation defined in (IV D1.23) is the inverse of that transformation; that is,

$$\tilde{d} = \tilde{u}\left(d, p\right) = f^{-1}\left(d, p\right) \quad . \qquad \text{(IV D1.24)}$$

Making this transformation everywhere in Bayes' equations for the theory parameters [Eq.(IV D1.22)] will give the equivalent equations in terms of the reduced data rather than the raw data.

This is easily seen in the simple case of a two-parameter data reduction, where parameter a is a normalization and b a constant background. In this case

$$t = f\,(\tilde{t}, p) = a\,\tilde{t} + b \qquad \text{(IV D1.25)}$$

and

$$\tilde{d} = f^{-1}\,(d, p) = (d-b)/a \quad . \qquad \text{(IV D1.26)}$$

The derivative G can therefore be written as

$$G = \frac{\partial t}{\partial P} = a\,\frac{\partial \tilde{t}}{\partial P} = a\,\tilde{G} \quad ; \qquad \text{(IV D1.27)}$$

this equation defines $\tilde{G}$. Likewise, we may define $\tilde{v}$ and $\tilde{g}$ as

$$\tilde{v} = a^{-1} v a^{-1} \quad \text{and} \quad \tilde{g} = a^{-1} g \quad , \tag{IV D1.28}$$

and therefore rewrite H in the form

$$H = v + g\ m\ g^t \ = \ a^{-1}\ \tilde{v}\, a^{-1} + a^{-1}\ \tilde{g}\ m\ \tilde{g}^t a^{-1} \ = a^{-1}\ \tilde{H}\, a^{-1} \quad . \tag{IV D1.29}$$

Substituting into Eq. (IV D1.22) for Y and W gives

$$\begin{aligned} Y &= G^t H^{-1}\left(d - t\right) = \left(\tilde{G}^t a\right)\left(a^{-1}\tilde{H}^{-1} a^{-1}\right)\left(a\,\tilde{d} + b - a\,\tilde{t} - b\right) \\ &= \tilde{G}^t \tilde{H}^{-1}\left(\tilde{d} - \tilde{t}\right) \end{aligned} \tag{IV D1.30}$$

and

$$W = G^t H^{-1} G = \left(\tilde{G}^t a\right)\left(a^{-1}\tilde{H}^{-1} a^{-1}\right)\left(a\,\tilde{G}\right) = \tilde{G}^t \tilde{H}^{-1} \tilde{G} \quad . \tag{IV D1.31}$$

The form of the equation is the same, with or without tildes.

In the general case, equations analogous to (IV D1.25) and (IV D1.26) are

$$\begin{aligned} \tilde{t} &= \tilde{u}\left(x, p\right) \quad \text{at} \quad x = t \\ \text{or} \quad t &= f\left(\tilde{x}, p\right) \quad \text{at} \quad \tilde{x} = \tilde{t} \end{aligned} \tag{IV D1.32}$$

and

$$\begin{aligned} \tilde{d} &= \tilde{u}\left(x, p\right) \quad \text{at} \quad x = d \\ \text{or} \quad d &= f\left(\tilde{x}, p\right) \quad \text{at} \quad \tilde{x} = \tilde{d} \quad . \end{aligned} \tag{IV D1.33}$$

The function $\tilde{u}$ is the inverse of the function f:

$$\begin{aligned} x &= f\left(\tilde{x}, p\right) = f\left(\tilde{u}\left(x, p\right), p\right) \\ \text{or} \quad \tilde{x} &= \tilde{u}\left(x, p\right) = \tilde{u}\left(f\left(\tilde{x}, p\right), p\right) \quad . \end{aligned} \tag{IV D1.34}$$

Relationships between various partial derivatives can be established by using the chain rule,

$$1 = \frac{\partial x}{\partial x} = \frac{\partial f\left(\tilde{u}\left(x, p\right), p\right)}{\partial x} = \frac{\partial f\left(\tilde{x}, p\right)}{\partial \tilde{x}} \frac{\partial \tilde{u}\left(x, p\right)}{\partial x} \tag{IV D1.35}$$

or

$$\frac{\partial \tilde{u}\left(x, p\right)}{\partial x} = \left[\frac{\partial f\left(\tilde{x}, p\right)}{\partial \tilde{x}}\right]^{-1} \quad . \tag{IV D1.36}$$

Note that both $\tilde{t}$ and d are independent of the data-reduction parameters p: $\tilde{t}$ is calculated directly from the theory parameters P, and d is measured directly with no corrections. Therefore, the following relationships hold:

$$0 = \frac{\partial d}{\partial p} = \left.\frac{\partial f}{\partial p}\right|_{\tilde{x}=\tilde{d}} + \left.\frac{\partial f}{\partial \tilde{x}}\right|_{\tilde{x}=\tilde{d}} \left.\frac{\partial \tilde{u}}{\partial p}\right|_{x=d} \qquad \text{(IV D1.37)}$$

and

$$0 = \frac{\partial \tilde{t}}{\partial p} = \left.\frac{\partial \tilde{u}}{\partial p}\right|_{x=t} + \left.\frac{\partial \tilde{u}}{\partial x}\right|_{x=t} \left.\frac{\partial f}{\partial p}\right|_{\tilde{x}=\tilde{t}} \quad . \qquad \text{(IV D1.38)}$$

The last term, however, is exactly equal to our definition of g at the beginning of this section.

We now consider a Taylor expansion of $d = f(x,p)\big|_{x=\tilde{d}}$ in the neighborhood of $\tilde{t}$, for fixed p:

$$d = f\left(\tilde{d}, p\right) \approx f\left(\tilde{t}, p\right) + \left.\frac{\partial f}{\partial \tilde{x}}\right|_{\tilde{x}=\tilde{t}} \left\{\tilde{d} - \tilde{t}\right\} \approx t + \left.\frac{\partial f}{\partial \tilde{x}}\right|_{\tilde{x}=\tilde{t}} \left\{\tilde{d} - \tilde{t}\right\} \quad . \qquad \text{(IV D1.39)}$$

For simplicity, define F as

$$F = \left.\frac{\partial f}{\partial \tilde{x}}\right|_{\tilde{x}=\tilde{t}} \quad ; \qquad \text{(IV D1.40)}$$

it follows that

$$d - t = t + F\left\{\tilde{d} - \tilde{t}\right\} - t = F\left\{\tilde{d} - \tilde{t}\right\} \quad . \qquad \text{(IV D1.41)}$$

In similar fashion, the derivative with respect to the R-matrix parameters can be written as

$$G = \frac{\partial t}{\partial P} = \frac{\partial t}{\partial \tilde{t}} \frac{\partial \tilde{t}}{\partial P} = F\,\tilde{G} \quad . \qquad \text{(IV D1.42)}$$

Substituting those expressions into Eq. (IV D1.22) for Y and W gives

$$Y = G^{t} H^{-1} (d - t) = \left(\tilde{G}^{t} F^{t}\right) H^{-1} F \left\{\tilde{d} - \tilde{t}\right\} = \tilde{G}^{t} F^{t} H^{-1} F \left\{\tilde{d} - \tilde{t}\right\} \qquad \text{(IV D1.43)}$$

and

$$W = G^{t} H^{-1} G = \left(\tilde{G}^{t} F^{t}\right) H^{-1} \left(F\,\tilde{G}\right) = \tilde{G}^{t} F^{t} H^{-1} F\,\tilde{G} \quad . \qquad \text{(IV D1.44)}$$

Inserting the definition of H from Eq. (IV D1.11) gives

$$
\begin{aligned}
F^t H^{-1} F &= \left(F^{-1} H \left(F^t\right)^{-1}\right)^{-1} = \left(F^{-1}\left\{v + g\, m\, g^t\right\}\left(F^t\right)^{-1}\right)^{-1} \\
&= \left(F^{-1} v \left(F^t\right)^{-1} + F^{-1} g\, m\, g^t \left(F^t\right)^{-1}\right)^{-1} \qquad \text{(IV D1.45)} \\
&= \left(F^{-1} v \left(F^t\right)^{-1} + \left(F^{-1} g\right) m \left(F^{-1} g\right)^t\right)^{-1} \quad ,
\end{aligned}
$$

so that Y and W can be written in the desired form,

$$Y = \tilde{G}^t\ \tilde{H}^{-1}\ \left\{\tilde{d} - \tilde{t}\right\} \qquad \text{(IV D1.46)}$$

and

$$W = \tilde{G}^t\ \tilde{H}^{-1}\ \tilde{G} \quad , \qquad \text{(IV D1.47)}$$

provided $\tilde{H}$ is defined as

$$\tilde{H} = F^{-1} H \left(F^t\right)^{-1} = F^{-1} v \left(F^t\right)^{-1} + \left(F^{-1} g\right) m \left(F^{-1} g\right)^t \quad . \qquad \text{(IV D1.48)}$$

If we then invoke Eqs. (IV D1.36), (IV D1.38), and (IV D1.40), the expression for $F^{-1} g$ in Eq. (IV D1.48) can be written as

$$F^{-1} g = \left.\frac{\partial \tilde{u}}{\partial x}\right|_{x=t} \left.\frac{\partial f}{\partial p}\right|_{\tilde{x}=\tilde{t}} = -\left.\frac{\partial \tilde{u}}{\partial p}\right|_{x=t} \quad , \qquad \text{(IV D1.49)}$$

which yields

$$
\begin{aligned}
\tilde{H} &= F^{-1}\ v \left(F^t\right)^{-1} + \left(F^{-1} g\right)\ m\ \left(F^{-1} g\right)^t \\
&= \left.\frac{\partial \tilde{u}}{\partial x}\right|_{x=t} v \left.\frac{\partial \tilde{u}}{\partial x}\right|_{x=t} + \left(-\left.\frac{\partial \tilde{u}}{\partial p}\right|_{x=t}\right) m \left(-\left.\frac{\partial \tilde{u}}{\partial p}\right|_{x=t}\right)^t \qquad \text{(IV D1.50)}
\end{aligned}
$$

or

$$\tilde{H} = \left.\frac{\partial u}{\partial x}\right|_{x=t} v \left.\frac{\partial \tilde{u}}{\partial x}\right|_{x=t} + \left.\frac{\partial \tilde{u}}{\partial p}\right|_{x=t} m \left(\left.\frac{\partial \tilde{u}}{\partial p}\right|_{x=t}\right)^t \quad . \qquad \text{(IV D1.51)}$$

Bayes' equations can therefore be written in the form

$$
\begin{aligned}
&P' - P = M'Y && M' = \left(W + M^{-1} \right)^{-1} \\
&Y = \tilde{G}^{t} \tilde{H}^{-1} \left(\tilde{d} - \tilde{t} \right) && W = \tilde{G}^{t} \tilde{H}^{-1} \tilde{G} \\
&\tilde{H} = \tilde{v} + \tilde{g}\, m\, \tilde{g}^{t} \quad ,
\end{aligned}
\qquad \text{(IV D1.52)}
$$

in which we have defined $\tilde{v}$ and $\tilde{g}$ as

$$
\tilde{v} = \left. \frac{\partial u}{\partial x} \right|_{x=t} v \left. \frac{\partial \tilde{u}}{\partial x} \right|_{x=t} \quad \text{and} \quad \tilde{g} = \left. \frac{\partial \tilde{u}}{\partial p} \right|_{x=t} \quad . \qquad \text{(IV D1.53)}
$$

We now consider how $\tilde{H}$ is related to the covariance matrix for the reduced data (i.e., for $\tilde{d}$). The covariance matrix for the reduced data is customarily found from

$$
\begin{aligned}
\tilde{V} &= \left\langle \delta\tilde{d}\, \delta\tilde{d} \right\rangle = \left. \frac{\partial \tilde{u}}{\partial x} \right|_{x=d} \left\langle \delta d\, \delta d \right\rangle \left. \frac{\partial \tilde{u}}{\partial x} \right|_{x=d} + \left. \frac{\partial \tilde{u}}{\partial p} \right|_{x=d} \left\langle \delta p\, \delta p \right\rangle \left. \frac{\partial \tilde{u}}{\partial p} \right|_{x=d} \\
&= \left. \frac{\partial \tilde{u}}{\partial x} \right|_{x=d} v \left. \frac{\partial \tilde{u}}{\partial x} \right|_{x=d} + \left. \frac{\partial \tilde{u}}{\partial p} \right|_{x=d} m \left. \frac{\partial \tilde{u}}{\partial p} \right|_{x=d} \quad .
\end{aligned}
\qquad \text{(IV D1.54)}
$$

In this form, $\tilde{V}$ in Eq. (IV D1.54) is very similar to $\tilde{H}$ of Eq. (IV D1.51). The only difference between the two is the value at which the derivatives are evaluated, that is, at $x = t$ for $\tilde{H}$ and $x = d$ for the usual $\tilde{V}$. It therefore follows that the only modification needed in the "usual" definition of data covariance matrix is to evaluate the various terms at the theoretical values, not the experimental values.

Conclusion

Exact agreement between the fit-to-raw-data method and the fit-to-reduced-data method is obtained by evaluating partial derivatives at the "true" cross section values (theoretical cross section values) rather than at the measured (experimental) values.

The agreement is exact only for first-order fitting, without iteration for nonlinearities.

IV.D.2. Propagated Uncertainty Parameters

In the previous section, it was demonstrated that writing the data covariance matrix (DCM) in terms of the theoretical cross sections (rather than in terms of the measured data) leads to equivalent results when fitting to reduced data as are obtained when fitting to raw data. This is particularly important if there are discrepancies in the measured data, a situation for which the usual definition of DCM can lead to strange results. See, for example, Peelle's Pertinent Puzzle [RP87] and the many attempts to reconcile this puzzle [ZZ92, SC94, NL04a, NL04b].

To reiterate, the benefits of this definition of DCM are numerous: Consistent and reasonable results are obtained when fitting raw data and when fitting reduced data. (By "results" is meant both parameter values and the corresponding parameter covariance matrix.) All prior uncertainties are reflected in the final results, for varied parameters (as usual) and also for unvaried parameters when the associated uncertainty is properly incorporated in the DCM.

The parameters that are unvaried but whose uncertainties are incorporated into the DCM are hereafter denoted as Propagated Uncertainty Parameters, or PUPs.* In SAMMY, any parameter for which derivatives are available (i.e., any parameter that is capable of being varied) can instead be PUP'd, at the user's discretion. Any of the experiment-related parameters can be treated as PUPs. In addition, although the derivation of Section IV.D.1 discussed only data-reduction parameters, there is nothing to prevent a non-varied theory parameter from being treated as a PUP in an individual run. However, a theory parameter will not currently be treated properly if it is PUP'd in two successive runs because there is then a neglected component of the DCM connecting the two data sets. The SAMMY user should be aware that results will not be correct for that situation.

Specifically, the SAMMY parameter types that can be PUP'd are the shown in Table IV D2.1, along with relevant test cases (see Section XII.B for a discussion of test cases).

Table IV D2.1. Types of parameters that may be PUP'd

Test case for PUPs	Related test case without PUPs	Type of parameter
tr044	tr009	resonance parameters (res)
tr059	tr093	R-matrix radii (rad)
tr040	tr011	R-external (ext)
tr038	tr007	broadening etc (brd)
tr041	tr012	normalization and background (nbk)
tr097	tr056	background functions (bgf)
tr068	tr021	Oak Ridge resolution function (orr)
tr096	tr054	RPI resolution function (rpi)
tr062	tr029	nuclide abundance (iso)
tr066	many	miscellaneous parameters (msc)
tr055	tr055	paramagnetic cross section (pmc)

* Thanks to Royce Sayer for suggesting this nomenclature.

Extensive testing has been done for each type of parameter, to ensure that the PUP theory and implementation are indeed correct. The tests consisted primarily of running the code with as many different options as possible for treating the parameter uncertainty, and comparing the resulting values and covariance matrices for the varied parameters. The available options are

1. varying the parameter,
2. treating the parameter as a PUP,
3. giving an explicit DCM,
4. providing user-supplied implicit DCM (see Section VI.C.3.b for details), and
5. treating via SAMMY's original IDC parameter method (Section VI.C.3.c), available for normalization and background parameters.

In the tests, options #1 and #2 gave identical results for the first iteration. When available, options #2 and #5 gave exactly identical results for all iterations. Options #3 and #4 gave almost identical results, sd long as each element of the explicit DCM was specified with a sufficient number of significant digits. When the data are not discrepant (so that a "fixed" DCM is a good approximation), all methods gave similar results.

To designate that a parameter is a PUP, the SAMMY user must simply set the flag for that parameter equal to "3" rather than "0" (to hold constant) or "1" (to vary). Uncertainties are provided in the same manner as for varied parameters; details are given in Table VI B.2.

In the SAMMY.LPT output file, the ordinal numbers for PUPs are given in angle brackets, for example, <38>, while numbers for varied parameters are given in parentheses, for example (38).

Card sets for most types of parameters may be put into the INPut file (Table VI A.1) rather than the PARameter file (Table VI B.2), provided none of that type of parameter is flagged for varying. Varied parameters must always be in the PARameter file. PUP'd parameters, on the other hand, may be in either the PARameter file or the INPut file. (A card set, however, can occur in at most one of the two files.) A flag = 1 in the INPut file will be ignored; a flag = 3 in either the INPut or the PARameter file will signify that the parameter is to be PUP'd. Values (and corresponding uncertainties) for most PUP'd data-related parameters may be different from one run to the next in a series for which the covariance matrix is carried along.

The exception to the above paragraph is any R-matrix parameter, all of which must be in the PARameter file. Values and uncertainties for PUP'd R-matrix parameters may NOT be changed from one run to the next in a sequential series. Furthermore, the current implementation neglects the DCM component (caused by PUP'ing the theory parameter) relating one data set to another. Hence, even though the option to PUP the R-matrix parameters is available, its use is not encouraged.

Uncertainties for PUP'd parameters may be input to SAMMY in the same fashion as uncertainties on the varied parameters. The user should be aware, however, that the "EXPLIcit" option (card set "Last B" of the PARameter file) is not appropriate for PUPs because it cannot be

used when a COVariance file exists (card set “Last A”) for the varied parameters. (Therefore, for example, the final no-Bayes computation would not understand the EXPLIcit uncertainty for PUP’d parameter.) Instead, the uncertainty for the parameter should be input in the card set containing the parameter value itself. For the 2006 revision of the code (sammy-7.0.0), options to include the uncertainties have been added to several of the card sets (e.g., card set 4, the BROADening parameters).

When off-diagonal elements of the PUP covariance matrix exist, input of the covariance matrix for some or all of the PUP’d parameters can be accomplished by means of a separate file. This file can be created by the analyst using available information, or it can be created by preliminary SAMMY runs. Details are given in Section VI.C.3.a.

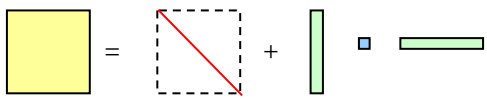
IV.D.3. Implicit Data Covariance Matrix

As seen in previous sections, Bayes' Equations for updating parameter and covariance matrices require the inversion of the data covariance matrix (DCM) V. Because the dimension of V can be very large (~1000's), performing this inversion explicitly can consume significant computer resources (CPU time and memory). Results can also be inaccurate, due to the round-off errors that occur when dealing with such a large quantity of numbers. Fortunately, there is an alternative method that is far more efficient than explicit calculation and inversion of V. This alternative method is denoted the Implicit Data Covariance (IDC) method.

As demonstrated in Section IV.D.1, the DCM can be written as a sum of two terms. The first, v, is a diagonal portion that contains statistical errors due to the measurement itself. The second term, $g\,m\,g^t$, characterizes the uncertainties in the data-reduction process; these are called systematic or common errors, since they apply systematically to all data points. This term is, in general, fully off-diagonal.

In matrix notation, the formula for the DCM is

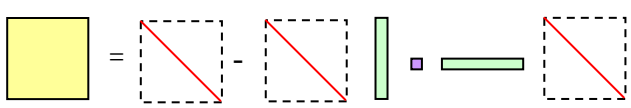
$$V = v + g\ m\ g^t \qquad \text{(IV D3.1)}$$



Here the boxes* are intended to represent the size of the matrices and are best viewed logarithmically. The dimensions of V may be quite large (~ tens or hundreds of thousands), and the dimensions of m are generally quite small (~ tens). Solid boxes represent full (non-diagonal) matrices; a dashed box indicates a diagonal matrix.

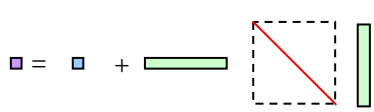
Because V has the form shown above, the inverse may be calculated symbolically as

$$\begin{aligned} V^{-1} &= \left(v + g\,m\,g^t\right)^{-1} \\ &= v^{-1} - v^{-1} g \left(m^{-1} + g\,v^{-1} g\right)^{-1} g\,v^{-1} \qquad \text{(IV D3.2)} \\ &= v^{-1} - v^{-1}\ g\ Z^{-1}\ g\ v^{-1}\ , \end{aligned}$$



in which Z is given by

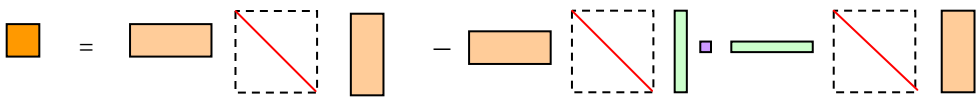
$$Z = m^{-1} + g^t\ v^{-1}\ g\ . \qquad \text{(IV D3.3)}$$



* Thanks to Helmut Leeb for suggesting this method of visualization.

Equations (IV D3.2) and (IV D3.3) provide an easy way to generate the inverse of the DCM. However, further simplification is possible. It is not V^{-1} that is needed, but the product of V^{-1} with other quantities. In particular, for the M+W version of Bayes' equations, matrices W and Y are needed. The expression for W may be written as follows:

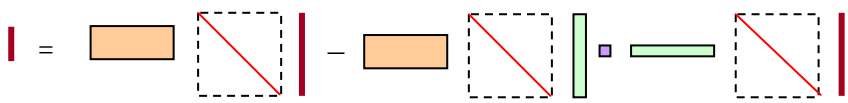
$$\begin{aligned} W &= G^t \; V^{-1} \; G \\ &= G^t \; v^{-1} \; G \; - \; G^t \; v^{-1} \; g \; Z^{-1} \; g^t \; v^{-1} \; G \; . \end{aligned} \qquad \text{(IV D3.4)}$$



In this expression, a third dimension has been added, this being the number of varied parameters (~ hundreds or thousands). Typically, this is intermediate between the number of data points and the number of data-reduction parameters.

The expression for Y is

$$\begin{aligned} Y &= G^t \; V^{-1}\left(D-T\right) \\ &= G^t \; v^{-1}\left(D-T\right) \; - \; G^t \; v^{-1} \; g \; Z^{-1} \; g^t \; v^{-1}\left(D-T\right) \end{aligned} \qquad \text{(IV D3.5)}$$



The new dimension introduced in this expression is 1, since $D - T$ and Y are simple vectors.

On first inspection, the expressions in the second lines of Eqs. (IV D3.4) and (IV D3.5) appear to be more complicated than the original expressions in the first lines. Indeed, they are somewhat more complicated to program. However, there are significant advantages to using the second expressions: The only large matrix, v^{-1}, is diagonal and therefore trivial to compute. The other two matrices that must be inverted, m and Z, are both very small (and m is often diagonal). Thus computation time is reduced because no large dense matrix is ever inverted. The required computer memory is reduced because no large matrix is ever stored. Finally, numerical accuracy and stability are improved because there are fewer opportunities to encounter round-off problems.

See papers [NL04a] and [NL04b] for computational verification of the claims made in the preceding paragraph. For the example cited in those papers, computation time for solving Bayes' equations was reduced by a factor of ~300 and array size by a factor of ~6 when using the IDC method. Accuracy was also improved, as great care is needed to ensure that sufficient significant digits are provided when using an explicit DCM.

Several options are available in SAMMY for using the IDC method. The earliest available form was restricted to normalization and background corrections. See Section III.E.3 for a discussion of these corrections and Section VI.C.3.c for a description of the original IDC-relevant input. For the release of sammy-7.0.0 in 2006, two additional options were made available: The first is the PUP option, discussed in Sections IV.D.1 and IV.D.2. The second is for the user to provide externally generated values for g and m. Input details are provided in Section VI.C.3.b.

IV.E. MISCELLANEOUS TOPICS RELATED TO COVARIANCES

Section IV.E.1 provides information regarding simultaneous fitting of several data sets.

SAMMY's so-called "retroactive covariance method" is a particular application of the simultaneous fitting procedure of Section IV.E.1. This retroactive method is a means of generating a parameter covariance matrix that is approximately correct for a given (pre-determined) parameter set. See Section IV.E.2 for details.

For a means to set the prior parameter covariance matrix to infinity, thereby reducing Bayes' equations to the usual least-squares equations, see Section IV.E.3. Other topics (such as fitting to multiple data sets while including iteration for nonlinearities) are also covered here.

Generating the covariance matrix associated with the theoretical cross section is described in Section IV.E.4.

For each spin group and channel, the average resonance width and associated uncertainty are calculated and printed in the SAMMY.LPT file. In Section IV.E.5, the algorithm used to generate those values is described.

Section IV.E.6 describes the rationale and methodology for modifying the SAMMY output resonance parameter covariance matrix prior to reporting the values or using for post-processing (e.g., for calculating multigroup averages).

IV.E.1. Simultaneous Fitting to Several Data Sets

The M+W scheme can be used for truly simultaneous fitting to several independent data sets in the resolved-resonance region. Any number of data sets of any type (capture, fission, integral, transmission, etc.) may be included. The procedure requires a series of separate SAMMY runs, first to generate the information separately for each data set and then to solve Bayes' Equations once for the entire system. The procedure is as follows:

Step a. Create a single PARameter file containing only R-matrix parameters and no measurement-specific information. Flag all variables of interest; PUP no parameters. This parameter file will be used as the prior parameter set for all runs in steps b through d below.

Step b. For each independent data set, create an INPut file as usual. Put all measurement-related information into the INPut file (see the end of Table VI A.1); PUP parameters as needed (Section IV.D.2). Include the command

`GENERATE Y AND W MATrices` *or* `YW`

in the INPut file. Run SAMMY with this INPut file, the PARameter file from step a, and the appropriate DATa file, SAMMY will produce sub-matrices Y_i and W_i, which are this data set's contribution to Y and W needed in Bayes' Equations (Section IV.B.3). Arrays Y_i and W_i are defined as

$$Y_i = G_i^{\,t} V_i^{-1} \left(D - T_i \right) \qquad \text{and} \qquad W_i = G_i^{\,t} V_i^{-1} G_i \quad , \qquad \text{(IV E1.1)}$$

in which the subscript i denotes the specific data set. These values are stored in file SAMMY.YWY, which the user should rename and keep for use in step d.

Step c. Repeat step b as many times as needed, once for each data set.

Step d. Once Y_i and W_i are known for each set of experimental data, they can be summed over the data sets i, giving

$$Y = \sum_i Y_i \qquad \text{and} \qquad W = \sum_i W_i \quad . \qquad \text{(IV E1.2)}$$

These matrices will be used in Bayes' equations, Eq. (IV B3.2) and Eq. (IV B3.4), respectively, to solve for updated parameter values and covariance matrix. This step is accomplished by an additional SAMMY run in which the INPut file includes the phrase

`READ Y AND W MATRICEs` *or* `WY`

The PARameter file from step a is used, and a dummy name may be given for the data set. Names of the files containing the sub-matrices Y_i and W_i are specified, one per line, immediately following the dummy data-file name in the input stream.

This run produces the SAMMY.PAR and SAMMY.COV files. Be sure to rename these to use in later steps.

If iteration for nonlinearities is to be used, an additional command is required in the INPut file in step d:

```
REMEMBER ORIGINAL PArameter values
```

This command causes a file REMORI.PAR to be created; this file contains values for $P^{(0)}$ and M^{-1}, as needed in the iterative form of Bayes' equations for M+W [Eq. (IV A3.3)].

Step e. To iterate for nonlinearities, create a second INPut file for each data set identical to the INPut file created in step b but containing one additional command:

```
USE REMEMBERED ORIGInal parameter values
```

This command does not tell SAMMY to calculate theoretical cross sections at the original parameter values but rather to use $P^{(0)}$, as specified in the REMORI.PAR file, for generating Y via the iterative form of Bayes' equations [Eq. (IV A3.3)]. That file (with that name) must be available in the subdirectory in which these runs are made.

Run SAMMY with this INPut file and the appropriate data file, using the PARameter file and COVariance matrix created in step d. This will cause SAMMY to generate a new Y_i and W_i using the parameter values determined in Step b.

Step f. Repeat step e as many times as needed, once for each data set.

Step g. Fit the data sets using the M+W scheme using the commands

```
USE REMEMBERED ORIGInal parameter values
READ Y AND W MATRICES, or WY
```

The "use remembered…" command will cause SAMMY to use the $P^{(0)}$ and M^{-1} from REMORI.PAR when solving for updated parameter values and covariance matrix, as in Eq. (IV A3.3).

Step h. Repeat steps e, f, and g as many times as desired, or until convergence (i.e., until there are no more changes in the χ^2 values for any of the data sets).

Step i. To obtain plot files with the final fits to the data, it is necessary to make another set of runs, one for each data set. In these runs, the INPut files should include the command

```
GENERATE PLOT FILE Automatically
```

Test cases tr082, tr089, tr131, and tr149 give examples of steps a through d of this procedure. A slight variation of this procedure is used for least-squares runs in test case tr163; see Section IV.E.3 for details.

IV.E.2. Retroactive Parameter Covariance Matrix Method

Occasionally it is necessary to produce an approximate covariance matrix associated with a pre-existing set of resonance parameters.

For example, most current evaluated nuclear data files (ENDF) contain resonance parameters, but not uncertainties / covariances for those parameters. The ideal cure for this situation would be to re-analyze the experimental data, including all appropriate uncertainties (both measurement and theory related), thus producing a new set of resonance parameters and the corresponding covariance matrix. However, it is not possible to immediately produce complete new evaluations for all nuclides in the ENDF. Therefore, a method is needed to generate an approximate covariance matrix appropriate for the current ENDF resonance parameters.

This may be accomplished using a scheme called the "retroactive parameter covariance matrix method": First, create representative data sets covering the energy range of the R-matrix evaluation. This may be done by running SAMMY in the no-Bayes mode with suitable energy grids, and using the calculated cross sections as the "experimental data" in later runs. Make reasonable choices for the covariance matrix for this set of data. Do a simultaneous fit to all those data sets, taking the ENDF File 2 parameter set for initial values and varying all resonance parameters. Check whether the output parameter values are not very different from the input values. If that is the case (as it should be, with the artificial experimental data in use here), then the output parameter covariance matrix (PCM) may safely be assumed to be a reasonable approximation for the covariance matrix associated with the input parameter values.

Test case tr149 gives an example of the procedure for retroactively producing an approximate covariance matrix.

After the retroactive covariance matrix has been produced, it is possible to use that covariance matrix with the original parameter values in another SAMMY run. To do this, include one of the following (equivalent) commands

```
RETROACTIVE OLD PARAmeter file new covariance or
RETROACTIVE or
U COVARIANCE MATRIX is correct, p is not
```

in the INPut file. In addition, make a new file, identical to the original PARameter file but containing the phrase "COVARiance matrix exists" at the end of the file (after the final blank line signifying the end of the previous card set, or immediately after card set 2 if there are no other card sets). This new file, and the now-renamed SAMMY.COV file from the run that created the retroactive parameter covariance file, are used as the input *.par and *.cov file for this run. See test case tr083, step r, for which the PARameter file t083r.par is identical to the original file ../tr082/tr082a.par except for the final line.

Variations on this procedure are possible. Instead of assuming that the *u*- PCM is correct, one could assume that the *p*-PCM is correct. (For a discussion of *u*- vs. *p*-parameters, see the end of

Section IV.C.) Ideally, there should be virtually no differences in results obtained from the two assumptions, since only insignificant changes should occur to the value of the parameters in the retroactive process. In practice there will be small differences. To use the *p*-PCM instead of the *u*-PCM from the *.cov file, include the command

```
P COVARIANCE MATRIX is correct, u is not
```

The user may wish to modify (increase) the uncertainties on some of the parameters. To give explicit values for the uncertainties, while maintaining the correlation matrix currently in the *.cov file, include both of these commands in the INPut file:

```
P COVARIANCE MATRIX is correct, u is not     and
MODIFY P COVARIANCE matrix before using
```

In addition, create a file named "uncer.new" (which must be stored in the same subdirectory in which you will be making the SAMMY runs). This file contains, in free format, the values you want for the uncertainties for all of the varied parameters (*p*-parameters), in the numerical order as indicated in the LPT file. An uncertainty equal to zero in the uncer.new file indicates that SAMMY should use the uncertainty from the *.cov file.

It is possible to use the MODIFY P COVARIANCE option with U COVARIANCE MATRIX rather than P COVARIANCE MATRIX. In this case, the *u*-PCM is taken from the *.cov file and transformation is made to give the associated *p*-PCM; this matrix is then modified using the uncertainties from the uncer.new file. The reverse transformation then gives the *u*-PCM to be used in the SAMMY calculations.

For additional details on modifying the SAMMY-produced PCMs, see Section IV.E.6.

IV.E.3. Least Squares and Other Extensions of SAMMY's Methodology

The least-squares method can be considered as a special case of Bayes' equations, in which the initial parameter covariance matrix (PCM) M is diagonal and infinite (so that the inverse M^{-1} is zero). Nonetheless, in practice it is not easy to reach that limit when creating input for SAMMY. The usual technique is to provide a very large prior uncertainty for each parameter, large enough to be "effectively infinite." Using this technique, however, can lead to numerical problems. In particular, large prior uncertainties on resonance energies will often permit two resonances to interchange positions – an untenable feature.

To circumvent this difficulty and to facilitate comparisons with other codes that do assume a diagonal and infinite prior PCM, several options have been added to SAMMY. The relevant test case is tr163; the procedure is outlined below.

Step a. For each of the data sets, generate Y_i and W_i as described in the previous section. The command line

```
GENERATE Y AND W MATrices      or     YW
```

must be in the input file for each run.

Step b. Fit the data sets using the M+W scheme, including the following commands in the INPut file:

```
USE LEAST SQUARES TO give pcm for initial parameters
REMEMBER ORIGINAL PArameter values
READ Y AND W MATRICEs        or      WY
```

The first of these directs SAMMY to assume that the inverse of the prior covariance matrix is zero; this command is optional (though required if one wishes to do least squares). The second command causes a file REMORI.PAR to be created; this file contains values for $P^{(0)}$ and M^{-1}, as needed in the iterative form of Bayes' equations for M+W [Eq. (IV A3.3)]. The third command is always needed when invoking the M+W method in the resolved resonance region.

If values of starting parameters are not extremely close to the "true" results, there may be divergence problems. In that case, it may also be necessary to include the command

```
TAKE BABY STEPS WITH least squares method
```

in the INPut file. This command will cause the change in the parameter increment $(P' - P)$ to be 1/10 the calculated value of $M'Y$ [see Eq. (IV A3.1) or Eq. (IV B3.1)], and will often alleviate the divergence problems.

Step c. For each data set, generate a new Y_i and W_i using the parameter values determined in step b. Include these command lines

```
GENERATE Y AND W MATrices   or     YW
USE REMEMBERED ORIGInal parameter values
```

The second of these lines does not tell SAMMY to calculate theoretical cross sections at the original parameter values but rather to use $P^{(0)}$, as specified in the REMORI.PAR file, for generating Y via the iterative form of Bayes' equations [Eq. (IV A3.3)]. That file (with that name) must be available in the subdirectory in which these runs are made.

Step d. Fit the data sets using the M+W scheme, with the commands

```
USE REMEMBERED ORIGInal parameter values
READ Y AND W MATRICEs    or       WY
```

The "use remembered . . ." command will cause SAMMY to use the $P^{(0)}$ and M^{-1} from REMORI.PAR when solving for updated parameter values and covariance matrix, as in Eq. (IV A3.3). Again, it may be necessary to include the "take baby steps . . ." command.

Step e. Repeat steps c and d, as many times as desired, or until convergence (i.e., until there are no more changes in the χ^2 values for any of the data sets).

Test case tr163 has been set up to repeat steps c and d twice more (steps e and f, h and i). In addition, two command files (test163_many and test163hi) allow the user to rerun steps h and i 20 more times, each time overwriting the previous results (to avoid keeping so many intermediate files) while keeping track of the changes in the χ^2 values.

These options were implemented by the author to facilitate intercomparisons among three R-matrix codes (SAMMY, EDA [GH75], and RAC [CZ95]), as part of an IAEA Cooperative Research Project on Light-Element Standards [AC05, INDC02, INDC03, INDC04,VP04].

IV.E.4. Covariances for Calculated Cross Sections

Let T_i represent the theoretical cross section (or transmission), at energy point E_i, as calculated from the "final" set of resonance parameters and parameter covariance matrix. The covariance matrix element connecting theory point T_i with point T_j is found from

$$\sum_{k,n} \frac{\partial T_i}{\partial u_k} M_{kn} \frac{\partial T_j}{\partial u_n} \quad , \qquad \text{(IV E4.1)}$$

where M_{kn} is the covariance matrix element connecting parameter u_k with parameter u_n . The theoretical uncertainty on theory T_i is the square root of the diagonal element; that is,

$$\Delta T_i = \sqrt{\Delta^2 T_i} = \sqrt{\sum_{k,n} \frac{\partial T_i}{\partial u_k} M_{kn} \frac{\partial T_i}{\partial u_n}} \quad . \qquad \text{(IV E4.2)}$$

When the phrase

```
INCLUDE THEORETICAL uncertainties in plot file
```

is given in the command section of the INPut file, values of ΔT_i will be reported in the plot file. See Section VII.C for specific details about where to find which uncertainties.

To create an ASCII listing of cross section (or transmission), uncertainty, and correlation matrix, include the phrase

```
CROSS SECTION COVARIance matrix is wanted
```

in the command section of the INPut file. The desired listing will be given in the SAMMY.LPT file. This is a no-Bayes run (i.e., no fitting can be accomplished in the same SAMMY run).

Using this command will also give the cross-section covariance matrix formatted into a "publishable" file named SAMCOV.PUB. This file is formatted with values separated by tabs so that it can be easily ported to a spreadsheet or other program, for example, to be plotted in three dimensions. This SAMCOV.PUB file contains the following information:

Row 1: three tabs, followed by the T_i separated by tabs
Row 2: three tabs, followed by the ΔT_i separated by tabs
Row 3: three tabs, followed by the E_i separated by tabs
Row 4: T_1, ΔT_1, E_1, followed by the first row of the covariance matrix separated by tabs
Row 5: T_2, ΔT_2, E_2, followed by the second row of the covariance matrix separated by tabs
. . .
Row N+3: T_N, ΔT_N, E_N, followed by the Nth row of the covariance matrix separated by tabs

In this format, it is easily possible to manipulate the results in a spreadsheet program. For example, the correlation matrix is found by dividing the covariance matrix element by the uncertainty in the same column in Row 2 and by the uncertainty in the same row in Column 2. See test case tr010, run e, for an example of this. (Caution: The user should exercise caution in porting this file to a spreadsheet, as the number of data points can easily become too large to fit into a normal spreadsheet.)

IV.E.5. Calculating Average Values and Uncertainties for Resonance Widths

In the SAMMY.LPT file (discussed in Section VII.A), the average value and uncertainty are reported for the various channel widths for every spin group. These averages are generated from the *p*-parameter covariance matrix by invoking Bayes' equations over a different set of variables from those used in earlier sections of this manual.

To calculate an average over a set of correlated parameters, we recognize that "average" can be interpreted as "most likely value for a group of numbers." Bayes' equations therefore are applicable, where the theoretical model is a simple function equal to the average whose value is needed. Explicitly, we can rewrite Bayes' equations [see, for example, Eq. (IV A 1.1)] into the form

$$A' = K' G^t \, M^{-1} \Gamma \qquad \text{(IV E5.1)}$$

and

$$K' = \left(G^t \, M^{-1} G \right)^{-1} \quad . \qquad \text{(IV E5.2)}$$

Here A' represents the needed average (for example, for the neutron widths for spin group number 3), and Γ represents the individual values (for each of those widths). The prior value for the average is set to zero. K' is the needed variance for the average, and the prior variance is set to infinity. M represents that portion of the parameter covariance matrix which corresponds to this set of widths. Finally, G is the partial derivative of the function to be fitted with respect to the average A, so that G is 1 for parameters in the set of interest and 0 for all other parameters. With these definitions, Eq. (IV E5.2) reduces to

$$K' = \left[\sum_{i\,j} \left(M^{-1} \right)_{i\,j} \right]^{-1} \quad , \qquad \text{(IV E5.3)}$$

in which the summation includes all parameters within the set to be averaged. The average value from Eq. (IV E5.1) then becomes

$$A' = K' \sum_{i\,j} \left(M^{-1} \right)_{i\,j} \Gamma_j \quad , \qquad \text{(IV E5.4)}$$

again summing over only the relevant parameters.

In the SAMMY.LPT file, two different average values and uncertainties are reported for each channel width for each spin group:

> The first is labeled "Expected Value" in the LPT file and includes all varied widths in the summations in Eqs. (IV E5.3) and (IV E5.4).
>
> The second is labeled "EV changed parameters" and attempts to include only those widths whose values have been affected (changed) by the data analysis. However, the criterion used to determine which parameters are to be included is rather naive: the uncertainty on the individual widths must be less than 9% of the value of the parameter.

In either case, if there are no parameters fitting the requirements, the printed average and uncertainty are zero.

IV.E.6. Modifying the Parameter Uncertainties

While the posterior (output) parameter covariance matrix (PCM) generated by SAMMY in principle includes all possible sources of uncertainty, in practice there are sources of uncertainty that have been omitted from every analysis.

One source is the uncertainty in the theory itself. For example, there is currently no procedure for including the uncertainty associated with an incorrect spin assignment, with the approximation of an infinite number of outlier resonances with a few large ones, or with the crudeness of the approximation used in calculation of the double-plus portion of the multiple-scattering correction. In addition, scattering theory itself is based on several assumptions which have an unquantified uncertainty associated with them, for example, the pretence that all reactions proceed via a compound nucleus.

Another source of uncertainty is the implementation of the theory. For example, any numerical integration scheme used for Doppler or resolution broadening cannot give a completely accurate result. As is well known, there is always one more bug in any large computer code, and this, too, contributes uncertainty.

Inclusion of these, and many other neglected sources of uncertainty, could have the effect of increasing the SAMMY-reported covariance values.

There is also the perception by many nuclear data experts that resonance-parameter uncertainties are too small, in that they lead to exceedingly small uncertainties on reconstructed cross sections.

In response to analysts' requests for automated methods to increase the uncertainties on the resonance parameters, a variety of options have been created. With the exception of Option #2 below, these will be used with runs that perform post-processing operations (e.g., calculate multigroup averages as described in Section V.C, or create ENDF File 32 descriptions of the PCM as discussed in Section IX). All of these methods assume that uncertainties are to be modified but the correlation coefficients will remain the same.

<u>Option #1</u>. A simple INPut file command will cause every uncertainty for every resonance parameter to be multiplied by the same value, that is, every element of the PCM to be multiplied by the square of that value. This command is

```
INITIAL UNCERTAINTY multiplier = value
```

The equal sign must be present, and "value" is replaced by a positive real number. At the beginning of this SAMMY run, each element of the PCM obtained from the input COVariance file is multiplied by the square of the value. See test case tr019, run d.

Option #2. A related command is

```
FINAL UNCERTAINTY MUltiplier = value
```

Here it is the output PCM that is modified; see test case tr019, run e, for an example of the use of this command. Use of this option is not recommended because it requires the analyst to decide before viewing the PCM that the PCM must be changed. Option #1 can be used to produce the same result without permanently changing the SAMMY.COV file (produced directly from the data analysis process) via multiplication by a preconceived value.

Option #3. To multiply the PCM by a value which varies with energy, and may also be spin group dependent, use the command

```
E-DEPENDENT INITIAL uncertainty multiplier    or
E-DEPENDENT UNCERTAInty multiplier.
```

(The hyphen is optional here.) A separate EDU (energy-dependent uncertainty) file is needed with this command; the EDU file contains the following information:

1. Alphanumeric title
2. Second title line, or blank
3. Spin group = 1 [only the equal sign and the number are absolutely necessary]
4. Energy, value of multiplier in 2F10.1 format (i.e., one value in the first ten columns and the second in the next ten columns)
5. Repeat line 4 as many times as needed
6. End with a blank line
7. Repeat lines 3 through 6 as many times as needed

Energies (line 4) must be in order of increasing energy. For resonances in the specified spin group, SAMMY will linearly interpolate to give the value of the multiplier at the resonance energy. If the resonance energy is outside the specified energies (below the first or above the last), the multiplier is assumed to be unity. Likewise, if a spin group is omitted from this listing, the multiplier will be unity for all resonances in that group. Note that the same multiplier is used for all parameters (energy and widths) for a particular resonance.

The name of the EDU file is given after the name of the COVariance file in the input stream. Note that this option works only if you are using a pre-existing COVariance file, not if starting from scratch. Examples are given in test case tr019, runs f and g.

Option #4. To modify the uncertainty on each parameter separately and independently from the modification of the uncertainties on other parameters (while maintaining the original correlation coefficients), insert the commands

```
P COVARIANCE MATRIX is correct, u is not
MODIFY P COVARIANCE matrix before using
```

into the INPut file. Create a file containing the new values for the uncertainties, in the same order in which they appear in the LPT file, in free format. For those parameters for which you

do not wish to change the uncertainty, it is not necessary to copy the value of the uncertainty into this file; instead, the value in this file can be set to zero. The name of this file is given to SAMMY directly following the name of the COVariance file. For examples, see test case tr149, runs l, m, o, and p.

Option #5. The RSAP program [RS03] contains options to read the SAMMY-produced SAMMY.PUB file (see Section VII.F) and create plots showing the effects of modifying the parameter values within the bounds of the uncertainties on the parameters. The uncertainties can be scaled, in which case RSAP produces a new file rsap.PUB in the same format as SAMMY.PUT, containing, however, the scaled uncertainties.

To report the scaled uncertainties back to SAMMY for additional computations, an auxiliary code PUB2COV was written by D. Wiarda. (This code will be made available as part of the RADCOP program under development by R. O. Sayer. [RS06a]) Input to the PUB2COV code consists of the original SAMMY PARameter and COVariance files, the original PUB file, and the modified PUB file. Output is a hybrid SAMMY COVariance file containing the original parameter values, the modified *p*-PCM and the original *u*-PCM. (The modified *p*-PCM has the new uncertainties but the original correlation coefficients.)

To use the hybrid SAMMY COVariance file in a new SAMMY run (e.g., to generate ENDF Files 2 and 32), include the command

```
P COVARIANCE MATRIX is correct, u is not
```

in the INPut file.

V. POST-PROCESSORS AND OTHER MISCELLANEOUS TOPICS

In addition to fitting energy- and angle-differential data in the resolved (and unresolved) resonance region, SAMMY has capabilities for other tasks such as reproducing cross sections directly from resonance parameters, calculating average cross sections, or creating portions of ENDF files. Some of these features are described in this section. For a discussion of SAMMY's interactions with ENDF files, see Section IX.

Methods for reconstructing point-wise cross sections without having to specify an energy grid are given in Section V.A.

Section V.B includes a discussion SAMMY's calculation of certain integral quantities. The code can also fit to these quantities where data or standard values are available.

Section V.C describes how SAMMY may be used to average cross sections (both theoretical and experimental) over particular energy range. The corresponding covariance matrix is also generated.

SAMMY's calculation of Maxwellian averages of capture cross sections (sometimes called "stellar averages") is discussed in Section V.D.

Section V.E describes various "pseudo cross sections" (simple functional forms) that can be generated by SAMMY, for use primarily in debugging Doppler or resolution functions.

Section V.F describes a method for generating the summed strength function for resonance parameters in a particular spin group.

V.A. RECONSTRUCTING POINT-WISE CROSS SECTIONS

SAMMY'S main purpose is to analyze neutron-induced cross section data by fitting to R-matrix parameters; in that mode, the user provides an energy grid (the experimental grid) from which an auxiliary grid can be constructed as discussed in Sections III.A.1 and III.A.2. To calculate a cross section directly from the resonance parameters without any pre-defined energy grid, one would use a nuclear data processor code such as AMPX [MD02], NJOY [RM82], or PREPRO [DC04]; these codes were designed to create energy grids that would describe the unbroadened cross sections with sufficient accuracy for essentially any purpose.

Occasionally, however, it is desirable to have SAMMY generate point-wise cross sections without a pre-existing energy grid. SAMMY has two methods of accomplishing this, as described below. The user should be aware that the energy grids generated in SAMMY will provide a means of viewing the cross sections but are not intended to be highly accurate representations of all the structure in the cross sections.

The first method, borrowed almost directly from the processing code NJOY [RM82], uses a convergence algorithm to choose an energy grid sufficiently dense to properly define total, elastic, and capture cross sections, as well as fission if needed. The output ODF (plot) file SAMMY.ODF contains energies in Section 1, total cross section in Section 2, elastic cross section in Section 3, capture cross section in Section 4, and fission cross section in Sections 5 if needed; Section 6 holds the absorption cross section (sum of capture plus fission cross sections). These cross sections are unbroadened (zero temperature). To invoke this option, include the phrase

```
RECONSTRUCT CROSS SEctions from resonance parameters
```

in card set 3 of the INPut file (see Section VI.A of this report). SAMMY will ask for the data file name, as always, but a dummy name may be given since that information is never used.

Caveat: The method described above makes use of the Reich-Moore approximation to R-Matrix theory. Thus it cannot be used with MLBW or SLBW resonance parameters.

The second option for generating point-wise cross sections without specifying an energy grid *a priori* makes use of SAMMY's ability to choose an auxiliary grid that properly defines the unbroadened cross section (see Section III.A). The user must provide some kind of a "data file," but it need not necessarily be appropriate for the nuclide(s) being considered; it is used only as a starting point for the auxiliary grid. SAMMY first sets up a grid of NEPNTS from EMIN to EMAX; NEPNTS is specified on card set 2 of the INPut file (see Table VI A.1). This grid is evenly spaced in velocity space (i.e., in the square root of energy). SAMMY then chooses additional points for the auxiliary grid as though broadening were to occur.

To invoke this option include the phrases

```
ARTIFICIAL ENERGY GRid is needed
```

and

```
PUT UNBROADENED CROSs sections into plot file
```

in the INPut file. An output plot file SAMMY.UNB contains energies in section 1 and cross section in section 2. (Note that the name of this file is no longer SAMXAC.ODF, to avoid confusion about

which file is produced when.) A second file, SAMMY.DAT, contains the same information in SAMMY's TWENTY data format.

Unlike the RECONSTRUCT method of generating an energy grid, this method evaluates only the one type of cross section specified in the INPut file. Also unlike the first method, any of the several R-matrix approximations may be used, as specified in the INPut file.

Examples of reconstructing point-wise cross sections using both of these methods can be found in several test cases. See, specifically, tr037 for "pure" reconstruction, and tr042 and tr049 for reconstruction followed by computation of stellar (Maxwellian) averages (see Section V.D).

V.B. INTEGRAL QUANTITIES

Although SAMMY was designed for calculating and fitting "differential" quantities such as cross section as a function of energy, nevertheless it often is useful to have the code calculate integral quantities for comparison with integral data. These integral quantities can also be included in the fitting procedure, if desired.* Details of the methods used to calculate these quantities are given in [NL97]. Additional features have been added to the code after publication of that report in order to facilitate direct comparisons between calculations made by SAMMY and those made by NJOY [RM82]; see items 9 and 10 below.

A single SAMMY run is used to calculate a variety of integral quantities. The first four quantities listed below are calculated for x = capture, fission, and absorption (as appropriate for the nuclide under consideration); the others are calculated only for fissile nuclides.

It should be noted that this option works only with the Reich-Moore formalism, not with either of the Breit-Wigner formalisms nor with SAMMY's original implementation of the Reich-Moore formalism. Also, the cross section for the unresolved resonance region is not included here.

1. Thermal cross section,

$$\sigma_{0x} = \sigma_x\left(E_0\right) \quad \text{for } E_0 = 0.0253 \text{ eV} \quad . \tag{V B.1}$$

2. Maxwellian average at thermal energy. This quantity is defined with somewhat different normalization from that used in Section V.D, that is, as

$$\bar{\sigma}_x = \int_{E_1}^{E_2} \sigma_x\left(E\right)\frac{E}{E_0}e^{-E/E_0}dE \Bigg/ \int_{E_1}^{E_2} \frac{E}{E_0}e^{-E/E_0}dE \quad , \tag{V B.2}$$

where $E_1 = 10^{-5}$ eV and $E_2 = 3$ eV.

3. Westcott's g-factor,

$$g_x = \frac{2}{\sqrt{\pi}}\frac{\bar{\sigma}_x}{\sigma_{0x}} \quad . \tag{V B.3}$$

---

* Integral quantities may be calculated and fitted only for the resolved resonance region. In the future, this capability will be made available for the unresolved resonance region as well.

4. Resonance integral,

$$I_x = \int_{E_3}^{E_4} \sigma_x(E) \frac{dE}{E} + X_{4x} \quad , \tag{V B.4}$$

in which E_3 = 0.5 eV, and E_4 and X_{4x} are specified by the user.

5. Average integral,

$$\hat{\sigma}_x = \int_{E_5}^{E_6} \sigma_x(E)\, dE \Big/ (E_6 - E_5) \quad . \tag{V B.5}$$

6. Watt spectrum average,

$$\bar{\sigma}_{Wf} = \int_{E_1}^{E_7} \sigma_f(E) \Phi(E)\, dE \Big/ \int_{E_1}^{E_7} \Phi(E)\, dE \quad , \tag{V B.6}$$

in which the upper limit E_7 = 20 MeV. The Watt fission spectrum, $\Phi(E)$, is given by the function

$$\Phi(E) = e^{-E/a} \sinh\left(\sqrt{bE}\right) = e^{-E/a}\left(e^{\sqrt{bE}} - e^{-\sqrt{bE}}\right)/2 \quad . \tag{V B.7}$$

Here *a* and *b* are constants to be supplied by the user. For ^{235}U, values of *a* and *b* are 0.988 MeV and 2.249 MeV^{-1}, respectively.

An alternative formulation to Eq. (V B.7) for the flux is discussed in Section V.B.1.

7. K1,

$$K1 = \nu\, \sigma_{0f}\, g_f - \sigma_{0a}\, g_a = \left(\nu\sigma_f - \sigma_a\right) \frac{2}{\sqrt{\pi}} \quad , \tag{V B.8}$$

where ν, the total number of neutrons per fission, is a constant whose value is provided by the user.

8. Alpha, or α,

$$\alpha = I_c / I_f \quad . \tag{V B.9}$$

9. Thermal alpha integral (NJOY's α) [RM98],

$$\alpha_{NJOY} = \int_{E_1}^{E_2} \frac{\sigma_c(E)}{\sigma_f(E)} \frac{E}{E_0} e^{-E/E_0} dE \Bigg/ \int_{E_1}^{E_2} \frac{E}{E_0} e^{-E/E_0} dE \quad . \qquad \text{(V B.10)}$$

10. Thermal eta integral (NJOY's η) [RM98],

$$\eta_{NJOY} = \int_{E_1}^{E_2} \frac{\nu\sigma_f(E)}{\sigma_a(E)} \frac{E}{E_0} e^{-E/E_0} dE \Bigg/ \int_{E_1}^{E_2} \frac{E}{E_0} e^{-E/E_0} dE \quad . \qquad \text{(V B.11)}$$

Input to SAMMY for fitting integral quantities is essentially the same as input for fitting differential quantities, with a few minor changes and one additional file. Please see Section VI.D for details. Test cases tr069, tr077, and tr082 have examples of fitting to integral quantities.

V.B.1. User-Supplied Flux for Watt Spectrum Average

For the Watt spectrum average of Eq. (V B.6) with user-supplied flux, it is necessary to evaluate integrals of the form

$$\int_{\alpha}^{\beta} \sigma(E)\,\varphi(E)\,dE \quad , \tag{V B1.1}$$

in which $\sigma(E)$ is given by one of two types of interpolation (defined below), and $\varphi(E)$ is a linear interpolation between energy points provided by the user. That is, the flux has the form

$$\varphi(E) = d + cE \quad , \tag{V B1.2}$$

and the constants d and c are found by setting the flux equal to the given values at two neighboring points. Specifically, if the set of points $\{E_j^{\varphi}, \varphi_j\}$ are given, then for $E_j^{\varphi} \le E \le E_{j+1}^{\varphi}$, these values are found from

$$\varphi_j = d + cE_j^{\varphi} \quad \text{and} \quad \varphi_{j+1} = d + cE_{j+1}^{\varphi} \quad , \tag{V B1.3}$$

which gives

$$c = \frac{\varphi_{j+1} - \varphi_j}{E_{j+1}^{\varphi} - E_j^{\varphi}} \tag{V B1.4}$$

and

$$d = \frac{E_{j+1}^{\varphi}\varphi_j - E_j^{\varphi}\varphi_{j+1}}{E_{j+1}^{\varphi} - E_j^{\varphi}} \quad . \tag{V B1.5}$$

At sufficiently low energies, far below the lowest resonance, the cross section is generally assumed to be $1/V$, where "velocity" V is the square root of the energy E. In this case, we may approximate the cross section between grid points E_k and E_{k+1} by

$$\sigma(E) = \frac{a}{V} + b \quad , \tag{V B1.6}$$

where a and b are given by

$$a = \frac{V_k V_{k+1}}{V_{k+1} - V_k}\left(\sigma_k - \sigma_{k+1}\right) \tag{V B1.7}$$

and

$$b = \frac{V_{k+1}\sigma_{k+1} - V_k \sigma_k}{V_{k+1} - V_k} \quad , \tag{V B1.8}$$

in which we have set

$$\sigma_k = \sigma(E_k) \quad , \quad \sigma_{k+1} = \sigma(E_{k+1}) \quad , \quad V_k = \sqrt{E_k} \quad , \quad \text{and} \quad V_{k+1} = \sqrt{E_{k+1}} \quad . \tag{V B1.9}$$

Inserting Eqs. (V B1.6) and (V B1.2) into the expression (V B1.1) gives

$$\begin{aligned}
\int_{\alpha}^{\beta} \sigma(E)\,\varphi(E)\,dE &= \int_{\alpha}^{\beta} \left\{\frac{a}{V}+b\right\}\left\{d+cE\right\}\,dE = \int_{\sqrt{\alpha}}^{\sqrt{\beta}} \left\{\frac{a}{V}+b\right\}\left\{d+cV^2\right\}\,2VdV \\
&= 2\int_{\sqrt{\alpha}}^{\sqrt{\beta}} \left\{a+bV\right\}\left\{d+cV^2\right\}\,dV \\
&= 2\int_{\sqrt{\alpha}}^{\sqrt{\beta}} \left\{d\left(a+bV\right)+c\left(aV^2+bV^3\right)\right\}\,dV \qquad \text{(V B1.10)} \\
&= 2\left[d\left(aV+\tfrac{1}{2}bV^2\right)+c\left(\tfrac{1}{3}aV^3+\tfrac{1}{4}bV^4\right)\right]_{\sqrt{\alpha}}^{\sqrt{\beta}} \\
&= d\left[2a\left(\sqrt{\beta}-\sqrt{\alpha}\right)+b\left(\beta-\alpha\right)\right]+c\left[\tfrac{2}{3}a\left(\beta^{3/2}-\alpha^{3/2}\right)+\tfrac{1}{2}b\left(\beta^2-\alpha^2\right)\right] \quad .
\end{aligned}$$

Replacing *a* and *b* with their values from Eqs. (V B1.7) and (V B1.8) gives

$$\begin{aligned}
&\int_{\alpha}^{\beta} \sigma(E)\,\varphi(E)\,dE = \\
&\quad d\left[2\frac{V_K\,V_{k+1}}{V_k-V_k}\left(\sigma_k-\sigma_{k+1}\right)\left(\sqrt{\beta}-\sqrt{\alpha}\right)+\frac{V_{k+1}\,\sigma_{k+1}-V_k\sigma_k}{V_{k+1}-V_k}\left(\beta-\alpha\right)\right] \qquad \text{(V B1.11)} \\
&\quad +c\left[\frac{2}{3}\frac{V_k\,V_{k+1}}{V_{k+1}-V_k}\left(\sigma_k-\sigma_{k+1}\right)\left(\beta^{3/2}-\alpha^{3/2}\right)+\frac{1}{2}\frac{V_{k+1}\,\sigma_{k+1}-V_k\sigma_k}{V_{k+1}-V_k}\left(\beta^2-\alpha^2\right)\right] \quad ,
\end{aligned}$$

which can be rearranged in terms of coefficients of σ_k as

$$\begin{aligned}
&\int_{\alpha}^{\beta} \sigma(E)\,\varphi(E)\,dE = \\
&\quad \left[d\left\{2V_{k+1}\left(\sqrt{\beta}-\sqrt{\alpha}\right)-\left(\beta-\alpha\right)\right\}+c\left\{\tfrac{2}{3}V_{k+1}\left(\beta^{3/2}-\alpha^{3/2}\right)-\tfrac{1}{2}\left(\beta^2-\alpha^2\right)\right\}\right] \\
&\qquad\qquad \times\frac{\sigma_k\,V_k}{V_{k+1}-V_k} \qquad \text{(V B1.12)} \\
&\quad +\left[d\left\{-2V_k\left(\sqrt{\beta}-\sqrt{\alpha}\right)+\left(\beta-\alpha\right)\right\}+c\left\{-\tfrac{2}{3}V_k\left(\beta^{3/2}-\alpha^{3/2}\right)+\tfrac{1}{2}\left(\beta^2-\alpha^2\right)\right\}\right] \\
&\qquad\qquad \times\frac{\sigma_{k+1}\,V_{k+1}}{V_{k+1}-V_k} \quad .
\end{aligned}$$

This is the form used in SAMMY to evaluate the integral, with the limit α given by either $\alpha = E_k$ = point on energy grid for the cross section or $\alpha = E_j^{\varphi}$ = grid point for the flux generation. Similarly β is either $\beta = E_{k+1}$ or $\beta = E_{j+1}^{\varphi}$.

At higher energies, the cross section is no longer 1/*V*. In this case, the cross section between grid points is assumed to be of the form

$$\sigma(E) = a + bE \quad , \tag{V B1.13}$$

where *a* and *b* are given by

$$a = \frac{E_{k+1}\,\sigma_k - E_k\,\sigma_{k+1}}{E_{k+1} - E_k} \tag{V B1.14}$$

and

$$b = \frac{\left(\sigma_{k+1} - \sigma_k\right)}{E_{k+1} - E_k} \quad . \tag{V B1.15}$$

Substituting Eqs. (V B1.13) and (V B1.2) into the expression for the integral in Eq. (V B1.1) gives

$$\begin{aligned}
\int_\alpha^\beta \sigma(E)\,\varphi(E)\,dE &= \int_\alpha^\beta \{a + bE\}\,\{d + cE\}\,dE \\
&= \int_\alpha^\beta \left\{ad + acE + bdE + bcE^2\right\}\,dE \\
&= \left[adE + \tfrac{1}{2}(ac + bd)E^2 + \tfrac{1}{3}bcE^3\right]_\alpha^\beta \\
&= ad(\beta - \alpha) + \tfrac{1}{2}(ac + bd)\left(\beta^2 - \alpha^2\right) + \tfrac{1}{3}bc\left(\beta^3 - \alpha^3\right) \quad .
\end{aligned} \tag{V B1.16}$$

Inserting the expressions for *a* and *b* from Eqs. (V B1.14) and (V B1.15) gives

$$\begin{aligned}
&\int_\alpha^\beta \sigma(E)\,\varphi(E)\,dE = \\
&\quad \frac{E_{k+1}\,\sigma_k - E_k\sigma_{k+1}}{E_{k+1} - E_k}\left[d(\beta - \alpha) + \tfrac{1}{2}c\left(\beta^2 - \alpha^2\right)\right] \\
&\quad + \frac{\left(\sigma_{k+1} - \sigma_k\right)}{E_{k+1} - E_k}\left[\tfrac{1}{2}d\left(\beta^2 - \alpha^2\right) + \tfrac{1}{3}c\left(\beta^3 - \alpha^3\right)\right] \quad .
\end{aligned} \tag{V B1.17}$$

Reorganizing gives coefficients of σ_k:

$$\int_{\alpha}^{\beta} \sigma(E)\,\varphi(E)\,dE =$$

$$\left\{d\left[E_{k+1}(\beta-\alpha)-\tfrac{1}{2}\left(\beta^2-\alpha^2\right)\right]+c\left[\tfrac{1}{2}E_{k+1}\left(\beta^2-\alpha^2\right)-\tfrac{1}{3}\left(\beta^3-\alpha^3\right)\right]\right\} \times \frac{\sigma_k}{E_{k+1}-E_k} \qquad \text{(V B1.18)}$$

$$-\left\{d\left[E_k(\beta-\alpha)-\tfrac{1}{2}\left(\beta^2-\alpha^2\right)\right]+c\left[\tfrac{1}{2}E_k\left(\beta^2-\alpha^2\right)-\tfrac{1}{3}\left(\beta^3-\alpha^3\right)\right]\right\} \times \frac{\sigma_{k+1}}{E_{k+1}-E_k} \quad .$$

V. C. AVERAGING THE CROSS SECTIONS

Once the SAMMY analysis is completed, the analyst may wish to average the theoretical curves produced by SAMMY over an energy range (or ranges) in order to more directly compare results with those from other experiments or analyses. Alternatively, the analyst may wish to produce multi-group cross sections plus covariance matrix for use in further calculations.

Three options are available in SAMMY for averaging the cross section:

The original option uses an energy or time average and treats the quantity to be averaged as a histogram. Hence it is useful for averaging experimental data that have been binned into channels but is not so useful for accurate averaging of theoretical cross sections. See Section V.C.1 for details on this option.

The second option uses the Bondarenko [IB64] narrow-resonance scheme for weighting the cross section. Sophisticated integration techniques are used to accurately and rapidly calculate the averages. See Section V.C.2 for details.

The third is an unweighted energy average similar to the first option but uses the same techniques to evaluate the integrals as are used in the Bondarenko option; see Section V.C.3.

In all cases, uncertainties are propagated through the entire procedure. Uncertainties and correlation matrix are printed for the multi-group cross sections.

V.C.1. Energy- or Time-Weighted Averages for Experimental Data

SAMMY's energy-averaged or time-averaged cross section is an average over a specific energy range or time-of-flight range, with no additional weighting. The implementation of this option assumes that the unaveraged cross section has already been "binned," as would occur during the data-collection process. Hence, this option cannot be used for accurate calculation of averaged theoretical cross sections.

The energy-averaged cross section is of the form

$$\bar{\sigma} = \frac{1}{N} \int_{Emin}^{Emax} \sigma\left(E'\right) dE' \quad , \tag{V C1.1}$$

with the normalization N given by

$$N = \int_{Emin}^{Emax} dE' \; = \; Emax - Emin \quad . \tag{V C1.2}$$

Similarly, the time-averaged cross section has the form

$$\bar{\sigma} = \frac{1}{N} \int_{tmin}^{tmax} \sigma\left(E\left(t'\right)\right) dt' \quad , \tag{V C1.3}$$

with the normalization N given by

$$N = \int_{tmin}^{tmax} dt' \; = \; tmax - tmin \quad . \tag{V C1.4}$$

In practice the integrals in Eqs. (V C1.1) through (V C1.4) are replaced by sums over discrete intervals of the form

$$\bar{\sigma} = \frac{1}{N} \sum_{Imin}^{Imax} \sigma_i \, \Delta_i \quad ; \tag{V C1.5}$$

N is given by the same formula with the σ_i term omitted inside the summation.

For energy averaging, the Δ_i are given by

$$\Delta_i = \frac{1}{2}\left[E_{i+1} - E_{i-1}\right] \quad ; \tag{V C1.6}$$

this is equivalent to assuming that the channel endpoints are exactly halfway between the energies specified as channel energy.

For time-average cross sections, the Δ_i are given by the difference between the time at the end of a channel and the time at the beginning. This assumes that the specified experimental energies are stated at the center of the channel, that is, that the time associated with channel *i* is

$$t_i = \sqrt{\frac{m}{2}\frac{L^2}{E_i}} \qquad \text{(V C1.7)}$$

and Δ_i is given by

$$\Delta_i = \frac{1}{2}\left[t_{i+1} - t_{i-1}\right] \quad . \qquad \text{(V C1.8)}$$

In both cases described above, corrections are made to ensure that the range included in the summation does not extend beyond the minimum and maximum energies, which are not likely to be channel boundaries. Note that neither of these approximations is exactly correct when compared to the experimental situation, since the endpoints of the time-of-flight channels are estimated based on center-time information. A more correct procedure would be to use the exact information from the experimental time-of-flight channels; unfortunately such information is not available to the analysis.

To determine the uncertainties associated with $\bar{\sigma}$, we consider a small increment in $\bar{\sigma}$, which can be written as

$$\delta\bar{\sigma} = \frac{1}{N}\sum_j \sum_i \frac{\partial \sigma_i}{\partial u_j}\Delta_i\, \delta u_j \quad , \qquad \text{(V C1.9)}$$

where u_j are the *u*-parameters (see Section IV.C). Squaring this quantity and taking expectation values give the variance on $\bar{\sigma}$ as

$$Var\left(\bar{\sigma}\right) = \left\langle \left(\delta\bar{\sigma}\right)^2 \right\rangle = \frac{1}{N}\sum_i \sum_{i'} \sum_j \sum_{j'} \frac{\partial \sigma_i}{\partial u_j}\frac{\partial \sigma_{i'}}{\partial u_{j'}}\Delta_i\, \Delta_{i'} \left\langle \delta u_j\, \delta u_{j'} \right\rangle \quad . \qquad \text{(V C1.10)}$$

Note that the quantity $\left\langle \delta u_j\, \delta u_{j'} \right\rangle$ is just the parameter covariance matrix $M_{jj'}$, which is known from the earlier analysis. The partial derivatives in Eq. (V C1.10) are readily evaluated within SAMMY, and the Δ_i are known. Thus, the uncertainty on the average cross section $\bar{\sigma}$ may be found directly from this equation.

The input needed to use this option is described in Section VI.F.1. Examples are given in test cases tr014 and tr075.

V.C.2. Bondarenko-Weighted Averages

The general definition of the flux-weighted multigroup cross section is

$$\bar{\sigma}_{x,i} = \int_{E_i^t}^{E_{i+1}^g} \sigma_x(E)\Phi(E)\,dE \Bigg/ \int_{E_i^t}^{E_{i+1}^g} \Phi(E)\,dE \quad , \qquad \text{(V C2.1)}$$

in which subscript x indicates the particular type of cross section (e.g. capture, fission, total). (Superscript g on the energy limits is used to distinguish these energies from the energies E_i of the experimental grid.) The flux $\Phi(E)$ is the energy-dependent neutron flux. Since this flux is not known, the Bondarenko narrow-resonance scheme [IB64] is often used. This scheme is defined as

$$\bar{\sigma}_{x,i} = \int_{E_i^g}^{E_{i+1}^g} \frac{\sigma_x(E)C(E)}{\sigma_{tot}(E)+\sigma_0}\,dE \Bigg/ \int_{E_i^g}^{E_{i+1}^g} \frac{C(E)}{\sigma_{tot}(E)+\sigma_0}\,dE \quad , \qquad \text{(V C2.2)}$$

in which σ_{tot} is the total cross section, σ_0 is an energy-independent constant, and $C(E)$ is a smooth function of energy. Currently in SAMMY, $C(E)$ may be expressed as a piece-wise linear function of energy; see Section VI.F.1 for input options.

(The limit in which C is constant and σ_0 is effectively infinite, while it has little practical application, may be useful for comparison purpose. This limit may be written as

$$\bar{\sigma}_{x,i} = \int_{E_i^g}^{E_{i+1}^g} \sigma_x(E)\,dE \Bigg/ \int_{E_i^g}^{E_{i+1}^g} dE \quad ; \qquad \text{(V C2.3)}$$

this is the form discussed in Section V.C.3 as the "unweighted energy average" option. While a large value of σ_0 and constant C can be used with the Bondarenko option to calculate this quantity, that method is highly inefficient. Instead, it is recommended that the option described in Section V.C.3 be used.)

Evaluation of the integrals in Eq. (V C2.2) is performed in similar manner to that described in Section III.A for numerical integration of the Doppler and resolution-broadening functions. However, unlike the integrations needed for those operations, here the integrand does not approach zero at the end points. The integration scheme is therefore modified at the end points to use the exact limit.

In addition to the calculating the multigroup cross sections, it is also necessary to generate the associated covariance matrix. This is accomplished by first taking small increments

$$\delta\bar{\sigma}_{x,i} = \sum_k \frac{\partial\bar{\sigma}_{x,i}}{\partial u_k}\,\delta u_k \quad , \qquad \text{(V C2.4)}$$

where u represents the resonance parameters. The covariance matrix is then found by taking expectation values

$$C_{xx'ij} = \left\langle \delta\,\bar{\sigma}_{x,i}\ \delta\,\bar{\sigma}_{x',j} \right\rangle = \sum_{k,k'} \frac{\partial \bar{\sigma}_{x,i}}{\partial u_k} \left\langle \delta u_k\ \delta u_{k'} \right\rangle \frac{\partial \bar{\sigma}_{x',j}}{\partial u_{k'}}$$
$$= \sum_{k,k'} \frac{\partial \bar{\sigma}_{x,i}}{\partial u_k} M_{kk'} \frac{\partial \bar{\sigma}_{x',j}}{\partial u_{k'}} \quad , \qquad \text{(V C2.5)}$$

in which

$$M_{kk'} = \left\langle \delta u_k\ \delta u_{k'} \right\rangle \qquad \text{(V C2.6)}$$

is the (known) covariance matrix for the resonance parameters.

Derivatives of the multigroup cross sections with respect to the resonance parameters are found using the chain rule, in the usual fashion.

Input needed to generate Bondarenko-weighted averages (multigroup cross sections) and the associated covariance matrix using SAMMY is described in Section VI.F.1 of this document. Examples are given in test cases tr083 and tr085; included in these examples are validity tests where the Bondarenko scheme of Eq. (V C2.2) is used to mimic the energy-average scheme of Section V.C.1 and the unweighted average of Section V.C.3.

V.C.3. Unweighted Energy Average

The unweighted energy average is defined as

$$\bar{\sigma}_{x,i} = \int_{E_i^g}^{E_{i+1}^g} \sigma_x\left(E\right) dE \Bigg/ \int_{E_i^g}^{E_{i+1}^g} dE \quad . \qquad \text{(V C3.1)}$$

This form is mathematically equivalent to the limit of Eq. (V C2.2) in which C is constant and σ_0 is effectively infinite. However, it would be highly inefficient to use Eq. (V C2.1) to calculate Eq. (V C3.1), because in the Bondarenko method, (a) the total cross section (as well as the cross section of interest) must be computed and (b) not only the numerator but also the denominator requires numerical integration. Hence, the unweighted energy average is calculated via a separate implementation in SAMMY.

The multigroup covariance matrix is calculated in the same fashion as described in Section V.C.2 for the Bondarenko averaging scheme.

Input details are presented in Section VI.F.1. For examples, see test cases tr071, tr085, and tr146.

V.D. STELLAR-AVERAGED CAPTURE CROSS SECTIONS

Stellar-averaged capture cross sections∗ may be generated for nuclear astrophysics applications. These are similar to the Maxwellian average used in reactor applications (see Section V.B on Integral Quantities) but defined in a somewhat different fashion. They are obtained from the stellar reaction rate formula [KW84],

$$\left\langle \sigma(E)\sqrt{E} \right\rangle_{kT} = \int_0^\infty \sigma_{capture}(E)\sqrt{E}\, W(E,kT)\, dE \quad , \qquad \text{(V D.1)}$$

where *W(E,kT)* is the Maxwellian weighting factor

$$W(E,kT) = \frac{2\sqrt{E}\, e^{-E/kT}}{\sqrt{\pi}\,(kT)^2} \quad , \qquad \text{(V D.2)}$$

and the capture cross section $\sigma_{capture}$ is generated from the resolved resonance parameters. The integration is performed numerically in SAMMY, using techniques similar to those described in Section III.A for the broadening integrals.

Energies in the above equations are center of mass. The cross sections generated from resonance parameters are, however, expressed in terms of laboratory energy. The conversion from center of mass to laboratory is

$$E = \frac{M}{m+M} E_{lab} \quad , \qquad \text{(V D.3)}$$

where m is the mass of the incident neutron and M is the mass of the target nucleus. The integration variable is changed from E to E_{lab} before the integral is evaluated.

The numerical integration technique is used to evaluate Eq. (V D.1) instead of the analytical approximation which may be more familiar to nuclear astrophysicists, because the assumptions underlying the analytical approximation are not always valid (see below). SAMMY does, however, calculate and print the approximate value in addition to the numerical result and provides a comparison between the two. (In addition to printing these in the LPT file output, SAMMY also generates an output file SAM16.DAT which contains only the table of stellar averages.)

The assumptions under which the analytical approximation is derived are the following: (1) The function $e^{-E/kT}$ is constant across the width of a resonance. (2) The neutron width $\Gamma_{n\lambda}$ is constant across the width of a resonance. (3) The multilevel Breit-Wigner approximation provides an adequate description for the cross section. (4) The lower-energy limit may be extended from 0 to negative infinity. Under these assumptions, the Maxwellian average has the approximate value

∗ Only the resolved resonance parameters, not the unresolved, are used in the calculation of Eq. (V D.1). However, point-wise cross sections from ENDF File 3 may be added, as described at the end of this section.

$$\left\langle \sigma(E)\sqrt{E} \right\rangle \cong \frac{\pi^{3/2}}{m}\left(\frac{1}{kT}\right)^2 \sum_{\lambda} e^{-\frac{M}{m+M}\frac{E_\lambda}{kT}} \frac{2g_\lambda \Gamma_{\lambda n}\Gamma_{\lambda\gamma}}{\Gamma_\lambda} + \sqrt{\frac{E_{thermal}}{kT}}\sigma_{capture}\left(E_{thermal}\right) \quad , \tag{V D.4}$$

where the summation includes only those resonances that have positive energies, and the "thermal" energy is somewhat arbitrarily taken to be the lowest energy for which the differential cross sections are calculated. [This is sufficient, since results are the same so long as the energy is low enough that the energy-dependence is $1/V$ (i.e., $1/\sqrt{E}$).]

To generate Maxwellian averages [both the numerically integrated values of Eq. (V D.1) and the analytic approximation values of Eq. (V D.4)], include a line in the INPut file specifying one of the following two statements; note that these are treated identically within SAMMY:

```
MAXWELLIAN AVERAGED capture cross sections are wanted
STELLAR AVERAGED CAPture cross sections are wanted
```

It is also necessary to provide an additional input file, the MXW file, containing values for the temperatures at which the calculation is to be performed. See Section VI.F.4, for details.

There are several options in SAMMY for specifying the energy grid on which the numerical integration of Eq. (V D.1) will take place. Because the precision with which the results are calculated may depend upon the method chosen, the user is encouraged to try different options to ensure that the desired accuracy is achieved. The first option is to use an experimental (i.e., user-provided) grid. A better alternative is to begin with the experimental grid, but the user should also specify

```
BROADENING IS WANTED
```

and give values for at least one broadening parameter. (This might be considered the "default," since this is what would apply if stellar averages were requested but no other thought was given to the specifics.) If the Doppler temperature is specified, it is used only to calculate an energy grid; the cross sections in the Maxwellian average are of course evaluated at zero temperature.

The purpose of specifying that broadening is wanted is to force SAMMY to choose a sufficiently dense auxiliary grid (see Section III.A) to properly describe the structure in the cross section, and thus to ensure accurate integration. Additionally the user may wish to request extra points added between experimental points (see variable NXTRA in card set 2 of the INPut file, Table VI A.1).

Two other options permit SAMMY to choose the energy grid automatically. The first uses the (NJOY) reconstruct option via the command

```
RECONSTRUCT CROSS SEction from resonance parameters
```

(This command can be used only with the Reich-Moore approximation.) The other option (which can be used also with Breit-Wigner) begins with a uniformly spaced grid, then adds points as needed to describe the structure. This option is invoked with the command

```
ARTIFICIAL ENERGY GRid is needed
```

The number of energy points in the initial (uniformly spaced) grid is given by variable NEPNTS on card set 2 in the INPut file (Table VI A.1).

In all cases, the user specifies EMIN and EMAX as limits for the differential data. Within those energy limits, SAMMY will generate the capture cross section on the chosen energy grid and use those data points for the numerical integration process. External to those limits (i.e., below EMIN and above EMAX), SAMMY will extrapolate in an appropriate fashion in order to reach the integration limits (0 to infinity). SAMMY will issue warnings if the limits seem too confining (i.e., if the integrand does not approach zero at high energy).

Estimates of the covariance matrix for the stellar-averaged capture cross section may be found by using default specifications for solving Bayes' equations (i.e., by <u>not</u> specifying

```
DO NOT SOLVE BAYES EQUATIONS
```

in the INPut file) and assigning uncertainties (and possibly correlations) to the flagged parameters. Those uncertainties will then be propagated through the averaging process, and the covariance matrix for the stellar-averaged capture cross section will be generated. <u>Caveat</u>: Only those uncertainties included, either implicitly or explicitly, on the flagged parameters will contribute to the uncertainties on the averages. This may result in an underestimation of the uncertainties on the averages, since not all resonance parameter uncertainties can be included.

Often it is important to include values for the capture cross section at higher energies than those described by the resolved resonance parameters (i.e., in the unresolved resonance region). Currently the only way to accomplish this within SAMMY is to present this data as an ENDF file and include the phrase

```
ADD CROSS SECTIONS From endf/b file 3
```

in the INPut file. SAMMY will ask for the name of this file immediately following the name of the MXW file. For the numerical integration results, the File-3 values are added directly to the resonance cross section before integration; in this case, the differential data are still extrapolated to zero, but the extrapolation beyond EMAX is based on the File-3 values. For the analytic approximation, the File-3 cross sections are integrated (numerically) separately and the results reported both separately and summed with the approximation results.

Test case tr051 contains examples of the various options described above.

V.E. PSEUDO CROSS SECTIONS FOR TESTING

It is possible to generate a fictitious theoretical "cross section" that exhibits constant, linear, delta-function, or $1/V$ (inverse velocity) behavior. These pseudo cross sections are useful for testing the effect of resolution functions or Doppler broadening.

To invoke these functions, in the INPut file, in the location where you would normally provide the data type ("transmission", "capture", "differential elastic", etc.), give one of the following phrases:

```
CONSTANT
LINEAR
QUADRATIC
DIRAC
1/V
```

SAMMY will then calculate, instead of the Reich-Moore cross section, the following:

- a constant cross section [everywhere equal to 1]
- a linear-in-energy cross section [=1 at Emin, 2 at Emax, but see below]
- a quadratic-in-energy cross section [=1 at Emin, 2 at Emid=(Emin+Emax)/2, 1 at Emax]
- an approximation to the Dirac delta function [= 0 everywhere except 1 at Emid]
- a $1/V$ cross section [where $V = \sqrt{E}$ with E = Energy]

In the output plot file (SAMMY.ODF or SAMMY.PLT , as described in Section VII.C of this document), the pseudo cross section is stored in section 2 (which would normally contain the experimental data). Section 4 contains the "corrected" cross sections that have been Doppler or resolution broadened, normalized, or otherwise corrected as specified in the user's INPut and PARameter file.

Along with these pseudo cross sections, it is often useful to have SAMMY choose an energy grid according to certain well-defined specifications (such as uniform in energy or uniform in flight time). To invoke these options, include one of the following lines in the alphanumeric command section of the INPut file:

```
UNIFORM ENERGY GRID
UNIFORM VELOCITY GRId
UNIFORM TIME GRID
```

In the first case, the code will provide an "experimental" energy grid that is equally spaced in energy E. The default number of points in this grid is 1001, though you may overwrite this number by specifying NEPNTS in Columns 41 to 45 of line 2 of the INPut file.

For the uniform velocity grid, SAMMY uses 1001 points equally spaced in $V = \sqrt{E}$; for the uniform time grid there will be 1001 points equally spaced in $T = 1/\sqrt{E}$ (which is proportional to time of flight *t*). Again, NEPNTS can be specified if you wish a different number of points.

(Note that, for the SAMMY run, you must include a name for a data file, but the file does not need to exist; it will be ignored.)

When using a fictitious cross section with a uniform grid (in energy, velocity, or time), SAMMY assumes that you want the LINEAR or QUADRATIC or whatever cross section to be LINEAR or QUADRATIC , etc., in the variable in which the grid is given. That is, if you specify for a example a "UNIFORM TIME GRID" and ask for QUADRATIC cross section, it will be quadratic in the time variable (in $T = 1/V = 1/\sqrt{E}$).

See test case tr115 for examples of these features.

[CAVEAT: While using the DIRAC delta function option with only resolution broadening, the calculated curve in section 4 of the SAMMY.ODF or SAMMY.PLT file will closely resemble the resolution function. The user should, however, be aware that it is NOT the resolution function. If the resolution function has discontinuities (as, for example, a square function in time whose width changes abruptly at a certain energy between Emin and Emax), those discontinuities will manifest themselves as odd shapes in the calculated curve.]

V.F. SUMMED STRENGTH FUNCTION

The summed strength function, as defined by Mughabghab [SM06] for incident neutrons and converted to SAMMY notation, is

$$
\begin{aligned}
S\left(\Lambda\right) &= \frac{g_c}{\left(2l+1\right)\Delta E_\Lambda} \sum_{\lambda=1}^{\Lambda} \sqrt{\frac{1}{E_\lambda}} \frac{\rho}{P_l\left(\rho\right)} \Gamma_{\lambda n} \\
&= \frac{2g_c}{\left(2l+1\right)\Delta E_\Lambda} \sum_{\lambda=1}^{\Lambda} \frac{\rho}{\sqrt{E_\lambda}} \gamma_{\lambda n}^2 \quad .
\end{aligned}
\tag{V F.1}
$$

Only the first elastic (neutron) channel $c = n$ is considered here. The summation is over all resonances of the one or two particular spin groups (where Λ is the total number of such resonances) in an energy interval ΔE_Λ. The convention for ΔE_Λ, taken from [HD02], is that ΔE is the energy difference between the first and last resonances, plus one average spacing between resonances, that is,

$$
\Delta E_\Lambda = \left(E_\Lambda - E_1\right) + \frac{1}{\Lambda - 1}\left(E_\Lambda - E_1\right) = \frac{\Lambda}{\Lambda - 1}\left(E_\Lambda - E_1\right) \quad . \tag{V F.2}
$$

To calculate $S\left(1\right)$ through $S\left(N\right)$, for resonances within a specified energy range in one or two spin groups (for which the first elastic channels must have the same value of *l*), include the following command in card set 3 of the INPut file:

```
SUMMED STRENGTH FUNCtion is wanted
```

In the interactive input, immediately following the name of the PARameter file, give the name of the COVariance file. On the next line, give two spin group numbers (the second of which can be zero if only one is required) and the energy range (minimum and maximum energies) for which you want the summed strength function to be calculated, in free format. Subsequent lines may contain the same information for other combinations of spin groups and energy ranges, if desired. See test case tr019, run h, for examples.

[There are two differences here from the usual SAMMY input: (1) No DATa file is needed, and no dummy name should be supplied. (2) This option works ONLY when a previous SAMMY run has generated a SAMMY.COV file.]

For each input line, SAMMY will calculate $S\left(\Lambda\right)$ for Λ=1 to N, where N is the total number of resonances in the energy interval specified. SAMMY will also calculate the uncertainties for each $S\left(\Lambda\right)$, and the covariance matrix for the set of $S\left(\Lambda\right)$. See test case tr019, run h.

VI. INPUT TO SAMMY

Input to SAMMY consists of three or more files, which may be user generated or (sometimes) produced by earlier SAMMY runs. These files are summarized in Table VI.1 and described in detail in the sections listed in the table. Test case numbers (see Section XII.B) are given for those files that are infrequently used.

Table VI.1. SAMMY input files

Description	Contents	Section(s) / table(s) containing details	Test case using this file
Interactive input	Interactive input to SAMMY (file names, energy ranges)	Section VI.E	
INPut file	Details about the interaction being studied, including SAMMY control information	Section VI.A Tables VI A.1 and VI A.2	
PARameter file	Initial values for resonance and other parameters, flags defining which are to be varied, uncertainty information	Section VI.B Table VI B.2	
DATa file	Experimental data, including energy, cross section (or transmission, for example), and uncertainty	Section VI.C.1 Table VI C1.1	
COVariance file	Covariance matrix for the parameters as output by an earlier SAMMY run	Section VII.B	
DCV (Data CoVariance)	Covariance information for the data	Section VI.C.2	tr007, tr118
IDC (Implicit Data Covariance) for normalization and backgrounds only	Information on data-reduction parameters to be used to generate implicit data covariance matrix	Section VI.C.3.c	tr070
IDC (User supplied)	Information on data-reduction parameters to be used to generate implicit data covariance matrix	Section VI.C.3.b	tr118 tr140 (*.dcv)
NTG file	Integral data file	Section VI.D	tr069, tr077

Table VI.1 (continued)

Description	Contents	Section(s) / table(s) containing details	Test case using this file
AVG file or BON file	Information needed by SAMMY in order to produce energy-averaged or Bondarenko-averaged cross sections	Section VI.F.1	tr014, tr083, tr084, tr085
NDF file	Information needed by SAMMY in order to generate an output file in ENDF-6 File 2 format	Section VI.F.2	tr023
ENDF resonance parameter file	File 2 from ENDF, to be used instead of the usual SAMMY PARameter file (and for part of the SAMMY INPut file)	Section VI.F.3	tr049, tr050, tr086, tr091, tr102, tr129
ENDF File 3	Smooth cross sections to be added to the cross section calculated from resonance parameters, for use in calculating the stellar (Maxwellian) averages	Section V.D	tr051
MXW file	Temperatures at which the stellar (Maxwellian) averages are to be evaluated	Sections V.D and VI.F.4	tr042, tr049, tr051
SSM file	Edge-effects corrections to single-scattering correction for capture cross sections (file is generated by a previous SAMMY run)	Section III.D	tr039 and many others
URR PAR file	Input information for unresolved resonance region	Section VIII	tr073, tr088
YWY file	W and Y matrices from a single data set, when analyzing several data sets simultaneously, e.g., for creating a retroactive parameter covariance matrix (files are generated by previous SAMMY runs)	Sections IV.E.1 and IV.E.2	tr082, tr089, tr131, tr149

VI.A. THE INPut FILE

SAMMY's INPut file contains essentially three types of information. The first is a set of command statements that define the particular case to be run; these are discussed in detail in Section VI.A.1. The second type consists of spin group and channel definitions, and the third is miscellaneous other information. Table VI A.1 gives details about the second and third types.

Information in the INPut file is categorized into "card sets." One or more lines of input are included in each card set. The categories are described here, and details are given in Table VI A.1.

Card set 1 of the table contains a title, which is reproduced in the output LPT file (see Section VII.A) but is otherwise unused.

Card set 2 contains miscellaneous information, including the mass of the sample, the energy range, and a flag to indicate how many iterations of Bayes' equations are to be run. Some of the information given here may also be input elsewhere, in which case, values given here are ignored.

Card set 3 contains the command statements; see Section VI.A.1 for details.

Card set 4 contains particle-pair definitions, an alternative method of providing information (masses, spins and parities, charges, threshold values) for the two particles in the channel, in key-word format. This is the preferred format.

Card set 4a contains the same information as in card set 4, but in fixed format.

Card set 4.5 exists only if the command "`PLOT RESOLUTION FUNCtion`" is given in card set 3.

Card sets 5 and 6 describe the original input for the Doppler- and resolution-broadening functions (see Sections III B.1 and III C.1). (See also card set P4.)

Card set 7 gives the matching radius for the R-matrix formalism, sample thickness, and various other parameters. Values for many of these parameters may, however, be superseded by values specified in the PARameter file (Section VI.B) or elsewhere in the INPut file (card set P4).

Card set 8 specifies the type of data to be analyzed (e.g., capture cross section, transmission). When the data are angular distributions, angles are also specified here.

Card set 9 was originally used to specify the spin and parity of the nucleus in the sample. For Version M6 and subsequent versions, this card is no longer required and should be removed from INPut files. Currently, this card set will be ignored if it exists in the INPut file; however, future versions of SAMMY may *require* that this line be removed.

Card set 10 had previously been used to describe the quantum numbers for the various spin groups. For Version M6 and subsequent versions, the original format is deemed to be obsolete and is no longer supported. Users should convert their INPut files to use either the "NEW SPIN GROUP FORMAT" (previously called "Alternative to card set 10" and now denoted "card set 10.1" in Table VIA.1) or the new "card set 10.2," which makes use of the particle-pair definitions given in card set 4 or 4a. In either case, SAMMY provides assistance in converting the INPut files; users can simply begin a SAMMY run using the obsolete INPut file and follow the instructions on the screen.

Card set 11 is needed only when analyzing capture cross sections using self-shielding and multiple-scattering corrections. Dimensions of the sample, plus interpolation and integration parameters, are specified in this card set.

Finally, many of the parameter types that are normally given in the PARameter file (see Table VI B.2) may now be given in the INPut file instead. This is convenient, for example, when an evaluation involves data from many different experiments, so that the same resonance parameters but different measurement-specific parameters are needed for each data set. Caution: Parameters that are specified in the INPut file cannot be varied; any flags equal to 1 will be ignored here. The parameters can, however, be PUP'd (see Section IV.D.2 for a discussion of the Propagated Uncertainty Parameter option). Flags equal to 3 will be understood in both the INPut and the PARameter files. Note that each of these card sets can occur in at most one of the two files; SAMMY will abort with an error message if the same card set is found in both files.

Table VI A.1. Format of the INPut File

Comment 1: Numbers in the first column (labeled "C:L") represent the card set number (before the colon) and the line number within that card set (after the colon).

Comment 2: Numbers in the second column (labeled "P,T") indicate position number (columns) within the line. Letters indicate format type: integer format ("I", which implies a number without a decimal point and requires that the number be in the right-most columns), real format ("F", which requires a number with a decimal point), or alphanumeric ("A", which can be numbers or letters or symbols).

C:L	P,T	Variable name	Meaning (units)	Notes
1:1	1-80, A	TITLE		
2:1	1-10, A	ELMNT	Sample element's name	
	11-20, F	AW	Atomic weight (amu)	
	21-30, F	EMIN	Minimum energy for this data set (eV)	These values for EMIN and EMAX will be ignored if values are given in the interactive input (see Section VI.E)
	31-40, F	EMAX	Maximum energy (eV)	
	41-45, I	NEPNTS	1. Number of points to be used in generating artificial energy grid (default = 10001) 2. Maximum number of points to be analyzed at one time (default = 500). Use of this option is discouraged.	1. See Section V.A for a discussion of the artificial energy grid. 2. NEPNTS is the number of data points to be included in each region when "DIVIDE DATA INTO REGions" is specified in card set 3.
	46-50, I	ITMAX	Number of iterations (default = 2)	Use a negative number for values > 9; see Section IV.A.3 for details.
	51-52, I	ICORR	Correlations smaller than this value (divided by 100) are not to be printed. $0 \le \text{ICORR} \le 100$ Default = 50	ICORR is ignored unless the phrase "DO NOT PRINT SMALL Correlation coefficients" occurs in card set 3. ICORR relates only to what is printed in SAMMY.LPT, not to what is used in calculations.

Table VI A.1 (continued)

C:L	P,T	Variable name	Meaning (units)	Notes
2:1, cont.	53-55, I	NXTRA	Number of extra points to be added between each pair of data points for auxiliary energy grid $0 \leq \text{NXTRA} \leq 999$ Default = 0	The minimum number of points in the auxiliary grid is (NXTRA+1) × NDAT, where NDAT is the number of points in the data grid.
	56-57, I	IPTDOP	Number of points to be added to auxiliary energy grid across small resonances	See Section III.A.2. Default = 9; range is $1 \leq \text{IPTDOP} \leq 21$
	59-60, I	IPTWID	Determines the number of points to be added to auxiliary grid in tails of small resonances	Default = 5
	61-70, I	IXXCHN	1. Number of energy channels in ODF-type data file to be ignored 2. When MATNUM (below) is not zero, then IXXCHN = ZA for use in an output ENDF file	1. When reading experimental data from an ODF file (as discussed in Section VI.C.1), usually the first data point is in channel 1. To start at a later channel, set IXXCHN equal to the number of channels to be skipped. 2. This option is almost never used. See Section IX for more appropriate input for creating ENDF files.
	71-72, I	NDIGIT	Number of digits for compact format for covariance matrix	See Section VII.E for details. Value: 1 to 6 Default = 2

Table VI A.1 (continued)

C:L	P,T	Variable name	Meaning (units)	Notes
2:1, cont.	73-74, I	IDROPP	The input resonance-parameter covariance matrix will be modified before being used in the fitting procedure. Correlations smaller than this % will be set to zero.	Value: 1 to 99; default = 2 This variable is ignored unless the phrase "`DROP SMALL VALUES OF covariance matrix`" occurs in the command section of the INPut file (card set 3).
	75-80, I	MATNUM	ENDF Material Number	This value is almost never used. See Section IX for more appropriate input for creating ENDF files.
3:?	1-20, A	WHAT	Alphanumeric information concerning program options.	See Table VI A1.2 for a listing of valid commands.
3:Last		(blank)		

Table VI A.1 (continued)

C:L	Notes
4:?	This card set is present only when the phrase "`KEY WORD PARTICLE PAir definitions are given`" occurs in card set 3 above. The same information is given here as in card set 4a, but here the format is not in columns. Instead, SAMMY's key-word format is used: The key word is printed, followed by an equal sign, followed by the value of the parameter. Spaces before or after the equal sign are optional. For each key word, characters given in CAPs are required, and those in lowercase are optional. Either caps or lowercase may be used in the INPut file. The information for a particle pair begins with the NAme key word and terminates either with another NAme key word (for another particle pair) or with a blank line. As many parameters as desired may be on a line (separated by either commas or blanks); spacing on the line is arbitrary. For each particle pair, any number of lines can be used. Valid key words are as follows. Values that are zero need not be explicitly specified.

Key word	Notes
Name	Equal sign must be followed by a unique eight-character name for this particle pair
"`Particle A`" or "`PA`"	An arbitrary eight-character name for this particle. SAMMY recognizes a few special types, for which it will automatically set the mass, charge, spin, and parity. These values do not need to be given in the INPut file; values that are given in the INPut file override the default values for these particles. The recognized particle types are listed below. Characters in caps (and the digit "3") are required; alternatively, use the first character followed immediately by a space. "`NEUtron`" or "`N `" ➔ neutron "`PROtron`" or "`P `" ➔ protron "DEUteron" or "`D `" ➔ deuteron "`ALPha`" or "`A `" ➔ alpha particle "`HE3`" or "`H `" ➔ helium 3 "`TRIton`" or "`T `" ➔ triton When this particle pair occurs in an incident channel, particle A is assumed to be the incident particle rather than the target particle.

Table VI A.1 (continued)

C:L	Notes	
4:?, cont.	"Particle B" or "PB"	When this particle pair occurs in an incident channel, particle B is the target particle.
	"Mass A" or "MA"	Mass of particle A, in amu
	"Mass B" or "MB"	Mass of particle B, in amu
	"Charge A" or "ZA"	Charge of particle A
	"Charge B" or "ZB"	Charge of particle B
	"Spin A" or "SA"	Spin of particle A; if non-zero, may include sign for parity
	"Spin B" or "SB"	Spin of particle B; if non-zero, may include sign for parity
	"PARIty A"	Parity of particle A; needed only if the spin of particle A is zero and the parity is negative
	"PARIty B"	Parity of particle B; needed only if the spin of particle B is zero and the parity is negative
	"PEnetrability"	"Yes" or "No" or "1" or "0"
	"Shift"	"Yes" or "No" or "1" or "0"
	"Q-value" or "THreshold"	Note: If the Q-value is given, it is implicitly assumed to be in the center-of-mass system. If, instead, the excitation energy (threshold energy) is given, it is assumed to be in the laboratory unless overridden with one of the commands "CM NON COULOMB EXCITation" or "CM COULOMB EXCITATIOn".
	"EFfective radius" or "RE"	Channel radii may be given here if they are appropriate for all channels in which this particle pair appears. However, if channel radii are given in card set 7 or 7a of the parameter file, the values given here are ignored.
	"TRue radius" or "RT"	
4:Last	(end this card set with one blank line)	

Table VI A.1 (continued)

C:L	P,T	Variable name	Meaning (units)	Notes
4a:1	1- 8, A	NAMPP	Alphanumeric name for this particle pair	This card set is present only when the command "`PARTICLE-PAIR DEFINitions are given`" occurs in card set 3 above.
	9-10, A	Aa	Type of particle for first particle in pair (incident particle, if appropriate)	For special particle types, charge, mass, spin, and parity do not need to be given in the INPut file. These types include " n", " p", "de", "he", "h3", "tr", and "al".
	11-12, A	Ab	Type of particle for second particle in pair	ditto
	13-15, I	Za	Charge number for first particle	(not needed if one of the special particle types is used, or if the other particle is a neutron, or if this is a fission pair)
	16-18, I	Zb	Charge number for second particle	
	19, I	Lpent	1 to calculate penetrabilities 0 if penetrability = 1	(required)
	20, I	Ishift	1 to calculate shift 0 if S - B = 0.0	(required)
	21-25, F	Sa	Spin and parity for P1	(not needed if one of the special particle types is used, or if this is a fission pair)
	26-30, F	Sb	Spin and parity for P2	
	31-40, F	Ma	Mass of Particle 1 (amu)	
	41-50, F	Mb	Mass of Particle 2 (amu)	
	51-60, F	Ex	Excitation energy (eV) (Zero for ground state)	Asssumed to be defined in the laboratory system. Override with card-set 3 commands "`CM NON COULOMB EXCITation`" or "`CM COULOMB EXCITATIOn`".
	61-70, F	Re	Effective radius for channels of this particle pair (fermi)	These are the "default" values, but they may be overwritten for some channels.
	71-80, F	Rt	True radius for for channels of this particle pair (fermi)	
4a: 2,3,etc. Repeat previous line once for each set of particle pairs				
4a: Last (end this card set with a blank line)				

Table VI A.1 (continued)

C:L	P,T	Variable name	Meaning (units)	Notes
4.5:1	1-10, F 11-20, F … 71-80, F	ERESOL	Energies at which to plot the resolution function	This card set is present only if "`PLOT RESOLUTION FUNC`tion" is specified in card set 3. See Section X.L for details.

Table VI A.1 (continued)

C:L	P,T	Variable name	Meaning (units)	Notes
5:1	1-10, F	TEMP	Effective temperature of the sample (K); zero for no Doppler broadening. This value may be overwritten in PARameter card set 4 (see Table VI B.2).	This card set is omitted when "`BROADENING IS NOT WA`nted" is specified in card set 3. (SAMMY will abort if this rule not followed.)
	11-20, F	DIST	Flight-path length (m)	
	21-30, F	DELTAL	That portion of the Gaussian resolution width attributed to the flight-path length (m).	Value may be overwritten in PARameter card set 4 (see Table VI B.2).
	31-40, F	DELTAE	E-folding width of exponential resolution function (μs); (0 for pure Gaussian resolution function). This value may be overwritten in PARameter card set 4 (see Table VI B.2).	See Section III.C.1.b. If the line "`EXPONENTIAL FOLDING` width is energy-dependent" is specified in card set 3 of the INPut file, then see Eq. (III C1 b.6) for details of the energy dependence.
	41-50, F	DELTAG	The absolute value of DELTAG is the FWHM (μs) of a Gaussian resolution function representing the burst width. (DELTAG = 0 for a purely exponential resolution function.)	See Section III.C.1.a, Eqs. (III C1 a.13) and (III C1 a.15). If DELTAG is negative, channel widths are given in card set 6.
	51-60, F	DELTTT	Approximate step size for the Effective Temperature for the Leal-Hwang method of Doppler broadening (K). Value > 0; default = 5.0	See Section III.B.2. If DELTTT < 0.0, an error message will be printed and the code will cease operation.
	61-70, F	ELOWBR	The energy below which no broadening is wanted, for high-energy Gaussian approximation to Doppler broadening (eV)	Default = 0.0
	71-80, F	DDDEEE	Range for straight-line energy average resolution function (eV)	See Section III.C.4.

Table VI A.1 (continued)

C:L	P,T	Variable name	Meaning (units)	Notes
6:1	1-10, F	DELTAB	Minimum channel width for interval from EMIN to EMAX (μs)	This card set is included only if DELTAG< 0 in card set 5.
	11-15, I	NCF	Number of crunch boundaries (energy intervals)	
6:2	1-10, F 11-20, F etc.	(BCF(I), CF(I), I=1,NCF)	BCF(I) = maximum energy for this crunch factor (read in order of increasing energy) (eV) CF(I) = crunch factors (integer units of DELTAB)	The value of Δt_c to be used in the energy range BCF(I-1) < E < BCF(I) is CF(I)×DELTAB. See Eq. (IIIC1a.7) and the following.
7:1	1-10, F	CRFN	Channel radius (fermi) If CRFN is input as zero, its value is computed as 1.45×(1.008665 +AW)1/3.	Value may be overwritten in card set 4 or 7 of the PARameter file (see Table VI B.2).
	11-20, F	THICK	Sample thickness (atoms/barn).	Needed only for TRANSmission or for TOTAL cross section or for multiple-scattering corrections.
	21-30, F	DCOVA	Constant term in data covariance (default = 0.0)	Data covariance matrix has additional term of the form (DCOVA + Ei × DCOVB) × (DCOVA+ EJ×DCOVB). Usually these terms will be set to zero.
	31-40, F	DCOVB	Linear term (default = 0.0)	
	41-50, F	VMIN	Minimum absolute uncertainty (standard deviation) on experimental data Often set to zero	If an experimental uncertainty in the DATa file is smaller than VMIN, SAMMY will increase the value to VMIN.

Table VI A.1 (continued)

C:L	P,T	Variable name	Meaning (units)	Notes
8:1	1-80, A	CROSS	Type of data, which must begin in first column on the line. Only those characters in CAPITAL letters are required.	
			TRANSmission	Use of transmission data rather than total cross section data is recommended; see Section XI.A for details.
			TOTAL cross section	
			ELASTic or SCATTering	
			DIFFErential elastic	Elastic angular distribution
			DIFFErentiAL REaction	Reaction angular distribution
			REACTion , or INELAstic scattering, or FISSion	These three data types produce the same computation, unless further information is given. For details regarding the use of individual REACTion types, see Section II.B.1.c. See also card set 10.1:2 and 10.2:2, parameter IFEXCL.
			FINAL state pairs = PAIRS in final state =	Using one of these two options is the preferred means of indicating the reaction data type. The equal sign must be followed by the names (from card set 4 or 4a) of the particle pairs to be included in the final state.
			CAPTUre	
			SELF-indication	Section III.E.6
			ABSORption	$\sigma_{absorption} = \sigma_{fission} + \sigma_{capture}$
			ETA (“ETA” followed by 2 spaces)	Defined as $\eta = \sigma_{fission} \big/ \left(\sigma_{fission} + \sigma_{capture}\right)$
			INTEGral	Section V.B
			COMBInation	This option is no longer available.
			CONSTant LINEAr QUADRatic DIRAC delta function 1/V	See Section V.E for details on these pseudo cross section types.

Table VI A.1 (continued)

C:L	P,T	Variable name	Meaning (units)	Notes
8:2	1- 5, I	NANGLE	Number of angles	This line and those following are present only for data types "DIFFErential elastic cross sections" or "DIFFErentiAL REaction." See Section II.B.1.b for details.
	11-20, F	ANGLE(1)	First angle, in laboratory; between 0 and 180 degrees	
	21-30, F	ANGLE(2)	Second angle (degrees)	
	...			
	71-80, F	ANGLE(7)	Seventh angle	
8:3 etc.	1-10, F 11-20, F etc.	ANGLE(8) ANGLE(9) etc.	Other angles, for a total of NANGLE	These lines are absent if NANGLE < 8.
8:4	11-20, F	DANGLE(1)	Angular spread of detector at ANGLE(1) (degrees)	
	...	DANGLE(7)	Spread at ANGLE(7)	
8:6 etc.	1-10, F 11-20, F etc.	DANGLE(8) DANGLE(9) etc.	Spread at other angles, for a total of NANGLE	These lines are absent if NANGLE < 8.
9	This card set, which originally contained the spin of the target nuclide, is no longer needed and should be removed from INPut files. The spin of the target nuclide is now given either in card set 10.1 or in card set 4 or 4a. Currently, SAMMY will ignore this card if it is present. However, that capability will not necessarily be maintained in future releases of the code.			
10	The original card set 10 is obsolete and must be replaced by either card set 10.1 or card set 10.2. To convert your old INPut files, begin a SAMMY run using that file; SAMMY will generate a file INPUT.NEW containing card set 10.1. <u>Caution</u>: Information in INPUT.NEW may not be entirely correct, as information in the obsolete format can be misinterpreted. It is the user's responsibility to ensure that the conversion is correct.			

Table VI A.1 (continued)

C:L	P,T	Variable name	Meaning (units)	Notes
10.1:1	It is no longer necessary to have "USE NEW SPIN GROUP Format" in card set 3 in order to use this alternative; card set 10.1 is now the default. The *recommended* version, however, is card set 10.2 in conjunction with card set 4.			
	1-3, I	JJ	Spin group number: 1,2,3, ...	
	5, A	EXCL	Flag to exclude this spin group from calculation of cross section	blank = include "X" = exclude
	6-10, I	NENT(JJ)	Number of entrance channels (must be > 0)	NENT + NEXT is the total number of particle channels for this spin group.
	11-15, I	NEXT(JJ)	Number of exit channels, excluding those that are also entrance channels (can be zero)	
	16-20, F	SPINJ(JJ)	Integer or half-integer spin for resonances in group JJ	Positive for even parity and negative for odd
	21-30, F	ABNDNC (JJ)	Isotopic abundance for this spin group	These values may be over-written in the PARameter file, card set 10
	31-35, F	SPINI	Ground-state spin for the nuclide (i.e., for the target particle)	Integer or half-integer; positive for even parity and negative for odd
10.1:2	4-5, I	N	Channel number	One line is needed for each channel.
	6-8, I	KZ1(N,JJ)	Charge number Z1 for the first particle in this channel	(blank if only neutron channels are present)
	10, I	LPENT (N,JJ)	Is SAMMY to calculate the penetrability for channel N, spin group JJ?	1 if calculate penetrability 0 if penetrability is not to be calculated (i.e., if P = 1)
	11-13, I	KZ2(N,JJ)	Charge number Z2 for the second particle in this channel	(blank if only neutron channels are present)
	15, I	ISHIFT (N,JJ)	1 if calculate shift; 0 if assume S - B = 0	

Table VI A.1 (continued)

C:L	P,T	Variable name	Meaning (units)	Notes
10.1: 2 cont.	18, I	IFEXCL (N,JJ)	1 if exclude this channel from final-state calculation for reaction cross section; 0 if include	This flag defines the particular reaction to be calculated. (See card set 8 above.)
	19-20, I	LSPIN (N,JJ)	Orbital angular momentum for channel	Non-negative integer
	21-30, F	CHSPIN (N,JJ)	Channel spin (integer or half-integer, sign implies parity)	Channel spin is the vector sum of the spins of the two particles in the channel.
	31-40, F	ENBND (N,JJ)	Boundary condition (eV) Used only if ISHIFT = 1 Default: ENBND = - l, where l is orbital angular momentum	If ENBND > 0, then $B = S_l(\rho)$, where $\rho = ka$ and $\hbar k$ is the center-of-mass momentum for energy ENBND (See Section III.A.1). If ENBND < 0, then B = ENBND.
	41-50, F	ECHAN (N,JJ)	Excitation energy of residual nucleus in an inelastic channel (eV)	Assumed to be defined in the laboratory system. Override with card-set-3 commands "CM NON COULOMB EXCITation" or "CM COULOMB EXCITATIOn"
	51-55, F	RDEFF (N,JJ)	Effective radius (fermi) (Value may be overwritten in the PARameter file.)	As defined by ENDF; used in calculating phase shift only. This value is used only in the absence of card set 7 (and 7a) of the PARameter file.
	56-60, F	RDTRU (N,JJ)	True radius (fermi) (Value may be overwritten in the PARameter file.)	As defined by ENDF; used in calculating penetrabilities and phase shifts. This value is used only in the absence of card set 7 (and 7a) of the PAR file.

Table VI A.1 (continued)

C:L	P,T	Variable name	Meaning (units)	Notes
10.1: 2 cont.	61-70, F	EMM1 (N,JJ)	Mass of first particle in this channel (that is, of the target nuclide, in the case of an incident channel) (amu)	If zero, SAMMY uses AW from card set 2.
	71-80, F	EMM2 (N,JJ)	Mass of second particle in the channel (that is, of the neutron or other incident particle, for entrance channels) (amu)	If given as zero, SAMMY uses the atomic weight of the neutron.
10.1: 3,4,etc.	Repeat Line 2 for a total of (NENT + NEXT) lines			
10.1: 5,6,etc.	Repeat Lines 1, 2, 3, 4, etc., once for each spin group			
10.1: Last	(blank)			

Table VI A.1 (continued)

C:L	P,T	Variable name	Meaning (units)	Notes
10.2:1	Use this option for defining the spin groups only when one of the phrases `"KEY-WORD PARTICLE-PAir definitions are given"` or `"PARTICLE-PAIR DEFINItions are given"` occurs in card set 3, and when card set 4 or 4a is present.			
	1-3, I	JJ	Spin group number (consecutive, beginning with 1)	
	5, A	EXCL(JJ)	Flag to exclude this spin group from calculation	blank = include "X" = exclude
	8-10, I	NENT(JJ)	Number of entrance channels (must be > 0)	NENT + NEXT is the total number of particle channels for this spin group.
	13-15, I	NEXT(JJ)	Number of exit channels, excluding those which are also entrance channels (can be zero)	
	16-20, F	SPINJ(JJ)	Integer or half-integer spin for resonances in group J	Positive for even parity and negative for odd
	21-30, F	ABNDNC (JJ)	Isotopic abundance for this spin group	(May be overwritten in PARameter file)
10.2:2	3-5, I	N	Channel number	
	6-7	(blank)		
	8-15, A	PPTYPE	Name of particle pair	Must be identical to one of the particle-pair names given in card set 4 or 4a
	18, I or A	IFEXCL (N,JJ)	1 if exclude this channel from final-state calculation for reaction cross section; 0 or blank if include. X (or x) to exclude this channel from inclusion anywhere in the calculation.	This flag defines the particular reaction to be calculated. (See card set 8 above.) This option ("X") should be used only for purposes of testing your input; it should not be used for regular production runs. See test case tr152 for examples using this feature.
	19-20, I	LSPIN (N,JJ)	Orbital angular momentum for channel	Non-negative integer

Table VI A.1 (continued)

C:L	P,T	Variable name	Meaning (units)	Notes
10.2: 2 cont.	21-30, F	CHSPIN (N,JJ)	Channel spin (integer or half-integer, sign implies parity)	Channel spin is the vector sum of the spins of the two particles in the channel.
	31-40, F	ENBND (N,JJ)	Boundary condition (eV) Used only if ISHIFT = 1 or SHift = Yes. Default: ENBND = - LSPIN	If ENBND > 0, then $B = S_l(\rho)$, where $\rho = ka$ and $\hbar k$ is the center-of-mass momentum for energy ENBND (Section II). If ENBND < 0, then B = ENBND.
	41-50, F	RDEFF (N,JJ)	Effective radius (fermi)	Needed here only if different from the value of the effective radius given in the particle-pair definitions. Is ignored if Radius parameters are given in the PARameter file.
	51-60, F	RDTRU (N,JJ)	True radius (fermi)	Needed here only if different from the value of the true radius given in the particle-pair definitions. Is ignored if Radius parameters are given in the PARameter file.
10.2: 3,4,etc.	Repeat Line 2 for a total of (NENT + NEXT) lines			
10.2: 5,6,etc.	Repeat Lines 1,2,3,4,etc, once for each spin group			
10.2: Last	(blank)			

Table VI A.1 (continued)

C:L	P,T	Variable name	Meaning (units)	Notes
11: 1	This card set is present only if self-shielding and multiple-scattering corrections are mentioned in card set 3. See Section III.D.			
	1-10, F	THSAMP	Sample thickness (cm) This may be calculated as the thickness in atoms/barn, multiplied by the atomic mass in amu, multiplied by the inverse of Avagadro's number (i.e., by 1.66053886 in the appropriate units), divided by the density for the material in g/cm^3. See, for example, the web site http://www.chemicool.com/ for values for density.	
	11-20, F	XSAMP	Sample height (cm) or sample radius (cm)	
	21-30, F	YSAMP		Currently unused
	31-40, F	XBEAM	Beam height (cm) or beam radius (cm), or zero if beam is larger than sample	If XSAMP is given as zero here but XBEAM is positive, the code will set XSAMP = XBEAM, and vice versa.
	41-50, F	YBEAM		Currently unused
	51-55, I	NTHETA	Number of points for parts of theta integration	Default = 33
	56-60, I	NGAUSZ	Number of points for pieces of z integration	4, 8, or 16 Default = 16
	61-65, I	NGAUS	Number of points for pieces of integration over cross section of beam	4, 8, or 16 Default = 16
	66-70, I	MTHETA	Number of points for the remainder of theta integration	Default = 16
	71-75, I	NXTPT	Number of points for integration and/or interpolation over σ; see Eq. (III D.8) and following	Default = 16
	76-80, I	MXTPT	Number of points for integration over σ'; see Eq. (III D.8) *ff*	Default = 64

Table VI A.1 (continued)

Card set	Meaning (units)	Notes

The remaining card sets in the INPut file are exact duplicates of corresponding card sets in the PARameter file. Any given card set can be in at most one location (i.e., it may be either in the INPut file, in the PARameter file, or in neither, but not in both).

A flag to vary a parameter (flag = 1) is ignored when the card set is in the INPut file. A flag equal to 3 will, however, cause the parameter to be PUP'd (see Section IV.D.2 for a discussion of propagated uncertainty parameters).

If no multiple-scattering size parameters (card set 11) are given in the INPut file, two blank lines must precede the beginning of these card sets.

The ordering of these card sets does not matter; however, they must follow everything else in the INPut file.

P4	BROADening parameters	
P6	NORMAlization and background	Section III.E.3.a
P8	DATA reduction parameters	See Section III.E.3.b
P9	ORRES (Oak Ridge Resolution Function)	Section III.C.2
P10	ISOTOpic or NUCLIde abundances	
P11	MISCEllaneous parameters	
P12	PARAMagnetic cross section parameters	Section III.E.4
P13	BACKGround functions	Section III.E.3.a
P14	RPI R (RPI Resolution Function), or GEEL , or GELINa, or NTOF	Section III.C.3
P14a	RPI T or RPI C (note the blank space after "RPI" in both cases) GEEL DEFAULts, or GELINa DEFAULts, or NTOF DEFAULts	RPI Resolution Function with either the relevant default values Section III.C.3
P15	DETECtor efficiencies.	Section III.E.5
P16	USER- (USER-Defined Resolution Function)	Section III.C.5

VI.A.1. Alphanumeric Commands

SAMMY relies on the use of alphanumeric commands to govern the operations it will perform. These commands, which are in English, are located in card set 3 of the INPut file. Commands are divided into 23 different categories, which are summarized in Table VI A1.1.

Valid commands are listed by category in Table VI A1.2; some commands may be listed in more than one category. A second listing, with the commands in alphabetical order, is given in Table VI A1.3.

Any of the valid statements listed in Tables VI A1.2 and VI A1.3 may be included in card set 3 of the INPut file, in any order. Usually only the first 20 characters of the statement are required; occasionally other information must be given either in specific columns or following an equal sign, as indicated in the "notes" column of the table. Characters shown in lowercase letters are optional in the INPut file but are included here for clarity.

In Table VI A1.2, mutually exclusive options are grouped together, and groups are divided by a solid line. Options within a group are divided by dashed lines.

In the event that contradictory statements are included in an INPut file, the last to appear is the instruction that SAMMY will honor. Default instructions (denoted by "D" in the appropriate column) need not be included explicitly. Options that are described "for debug purposes" (denoted "B" in Table VI A1.3) should generally be avoided because these cause considerable output to be generated, especially when many data points are included. Improper commands (misspellings, etc.) will be noted as such both in the LPT file and on screen, but will otherwise be ignored.

The first 20 characters of a command are shown in the table in uppercase; nevertheless, they may be included as either uppercase or lowercase in the INPut file. Cases may be intermixed within a command (early releases of the code required consistent case within a command).

A command may be "commented out" by insertion of a pound sign (#) in the first column; in that case, SAMMY will simply ignore the command. Hyphens within a command can be replaced by a blank, except when preceded or followed by a number; similarly, a blank between two letters may be replaced by hyphen.

An entire row (20 characters) of hyphens indicates that the next rows are to be treated as comments; a second row of twenty hyphens is needed to end this comment section.

Numbers in the final column of Table VI A1.2 relate to the position of the command in the common block, as stored in program file blk/BGZYX. Generally, the SAMMY user can ignore this column.

Table VI A1.1. Categories for alphanumeric commands

Category	Description of commands in this category	Abbreviation used for this category in Table VI A1.3
General	Is this run to use resolved or unresolved resonance formulae; how to insert comments among the commands	General
R-matrix approximation	Define which approximation to the R-matrix is to be used for this calculation	RM
Parameters – input control for quantum numbers, etc.	Define which type of input is to be used for spin group information and other parameters	Param
Parameters – input control for prior covariance matrix	Define the prior parameter covariance matrix	PCM in
Parameters – output control for parameter covariance matrix	Define the method of output for the parameter covariance matrix	PCM out
Experimental data – input control	Define the format for the experimental data	Data
Experimental data – input control for covariance matrix	Define the format for input of data covariance matrix	DCM
Experimental data – angular distribution	Define frames of references and other details for angle-differential calculations	Angle
Broadening options	Is broadening wanted	Broad
Broadening – Doppler	Define which version of Doppler broadening is to be used	Doppler
Broadening – resolution	Provide some of the details about the resolution broadening function (most information is given along with parameter values rather than here)	Resol
Multiple-scattering corrections	Define how the multiple-scattering corrections are to proceed	MSC
Bayes' solution	Define details of the fitting procedure	Bayes

Table VI A1.1 (continued)

Category	Description of commands in this category	Abbreviation used for this category in Table VI A1.3
Options for printing into SAMMY.LPT	Define what information will be printed in output file SAMMY.LPT	LPT
ENDF as input	Provide details about the ENDF files to be used as input to SAMMY	ENDF in
ENDF output	Provide details about the particular ENDF output that is to be generated	ENDF out
Plot file control	Define units for energy in the plot file; ask for specialized plot-file output	Plot
Averages, etc.	Define which post-processing procedure is to be used	Average
Constants	Define which set of values are to be used for the physical constants	Constant
Cross section calculation details	Give miscellaneous details about the cross section calculation	CS calc
No pre-defined energy grid	Provide instructions concerning the method to be used in generating an energy grid on which the cross section is to be calculated	Grid
Special options	Miscellaneous options that do not fit other categories	Special
URR controls	Give details regarding calculations in the unresolved resonance region	URR

Table VI A1.2. Alphanumeric statements acceptable for use in the INPut file, card set 3.
See text for a description of the columns

Category	D	Statements	Notes	#
General	D	(none needed)	Resolved resonance region (RRR) R-matrix calculation Unless otherwise specified, all alphanumeric commands refer to RRR.	
		`UNRESOLVED RESONANCE region`, or `FRITZ FROEHNERS FITAcs`, or `FITACS`	Use the SAMMY version of Fritz Froehner's code FITACS for analysis of the unresolved resonance region (URR). See Section VIII.	2 3 4
		----------	Two lines of hyphens may be used to separate commands from comments.	5
		#	Alternatively, begin each comment line with a pound sign (#).	

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
R-matrix approx-imation	D	`REICH-MOORE FORMALISm is wanted`, or `MORE ACCURATE REICH-moore`, or `XCT`	See Section II. Note that "more accurate" refers to the computational method, not to the formalism.	171 172 173
		`ORIGINAL REICH-MOORE formalism`, or `CRO`	See Section II. This method of calculating the RM formalism is sometimes inaccurate, particularly at low energies for capture. Probably this option will be eliminated in later releases of the code.	174 175
		`MULTILEVEL BREIT-WIGner is wanted`, or `MLBW FORMALISM IS WAnted`, or `MLBW`	See Section II.B.3. Note that SAMMY's MLBW treatment is identical to that specified in ENDF-102; that is, only elastic cross sections are MLBW, while fission and capture are calculated via SLBW equations.	176 177 178
		`SINGLE LEVEL BREIT-Wigner is wanted`, or `SLBW FORMALISM IS WAnted`, or `SLBW`	See Section II.B.3.	179 180 181
		(No command)	When "type of cross section" (see card set 8 of Table VI A.1) is "1/v", "constant", "linear", "quadratic", or "Dirac delta function", then that designated type is calculated; this overrides any command given in the alphanumeric listing for Reich-Moore, etc. This option is used for debug only; see Section V.E for more details.	

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Parameters – input control for quantum numbers, etc.	D	`USE NEW SPIN GROUP Format`	See card set 10.1 in Table VI A.1. Although this is the default format for input of quantum-number information, it is not the preferred method because the input is awkward for many situations (e.g., charged-particle channels). The preferred method is to use KEY-WORD PARTICLE-PAir defintions (see below) in conjunction with card set 10.2 of the INPut file.	51
		`USE OBSOLETE SPIN GRoup format`	This option is no longer available for running SAMMY. When an INPut file contains this command, SAMMY will create a file called INPUT.NEW, and then cease excution. This file contains a zeroth-order guess at appropriate spin-group definitions in the "new" format. See card set 10 of the Table VI A.1 for more information.	52 53
		`PARTICLE PAIR DEFINItions are used`	See card set 4a in Table VI A.1.	54 55
		`KEY-WORD PARTICLE-PAir definitions are given`	See card set 4 in Table VI A.1. This is the preferred method of input for spin-group information.	56
		`QUANTUM NUMBERS ARE in parameter file`	Key-word particle-pair definitions and spin-group definitions can now be given in the PARameter file rather than in the INPut file. See Table VI B.3 for details.	57
		`PUT QUANTUM NUMBERS into parameter file`	The initial spin-group definitions for this run will be converted into key-word particle-pair format and written to a PARameter file SAMQUA.PAR (which contains the initial values for resonance and other parameters).	58

Table VI A1.2 (continued)

Category	D	Statements	Notes	#

Parameters – input control for quantum numbers, etc. (cont.)		`SPIN OF INCIDENT PARticle is +`
		or
		`SPIN OF INCIDENT PARticle is -`
			If using the "new spin group format," and the incident particle is not a neutron, the spin and parity of the incident particle must be specified here. The sign (indicating parity) must appear in column 30, and the integer or half-integer value of the spin (written as a decimal) must appear in the next columns.
			
			<u>Eample:</u>
			SPIN OF INCIDENT PARTICLE IS -1.5
				59

		`USE I4 FORMAT TO REAd spin group number`	The default PARameter file format does not permit specifying more than 50 spin groups. If more than 50 are needed, include this command and use four columns rather than two for each spin group number in the PAR file.	60
		`INPUT IS ENDF/B FILE 2`	Resonance parameters and spin-group quantum number information is taken from an ENDF/B file; see Section VI.F.3.	61
		`USE ENERGY RANGE FROm endf/b file 2`	If this command is not included, SAMMY will use the energy range from INPut file or from interactive input instead of using the range specified in the ENDF file. If the PARameter file is not an ENDF file, this command is ignored.	62
		`FLAG ALL RESONANCE Parameters`	Use this command if all resonance parameters are to be varied (equivalent to setting the "flags" to "1" in the PARameter file).	63

Table VI A1.2 (continued)

Category	D	Statements	Notes	#

Parameters – input control for prior covariance matrix		`IGNORE INPUT BINARY covariance file,`
		or
		`IGNORE`
			Your PARameter file specifies that the parameter covariance matrix is kept in a separate file. For this particular run, however, you wish to pretend that there were no previous runs generating such a file; instead you wish to use the large (ideally infinite) uncertainties that indicate no prior knowledge of parameter values. The name of the COVariance file should not be included in the input stream when this command is used.	65
				66

		`ENERGY UNCERTAINTIES are at end of line in par file`	See Table VI B.2, card set 1, columns 68–80, second alternative.	64

		`RETROACTIVE OLD PARAmeter file new covariance,`
		or
		`RETROACTIVE,`
		or
		`U COVARIANCE MATRIX is correct, p is not`
			An approximate parameter covariance matrix has been created retroactively (see Section IV.E.2 for details). For this run, the original PARameter file is to be used with the new COVariance file. The *u*-parameter covariance matrix is assumed to be correct in this file.	71
				72
				73

		`P COVARIANCE MATRIX is correct, u is not`	The *p*-parameter covariance matrix is assumed to be correct in the initial (retroactive) covariance file. See Section IV.E.2.	74
		`MODIFY P COVARIANCE matrix before using`	The correlation matrix in the covariance file is correct, but the uncertainties will be modified. See Section IV.E.2 for details.	75
		`INITIAL DIAGONAL U Covariance`	The initial *u*-parameter covariance matrix is assumed to be diagonal; the *p*-parameter covariance matrix is not. Details are in Section IV.E.6.	76
		`INITIAL DIAGONAL P Covariance`	The initial *p*-parameter covariance matrix is assumed to be diagonal; the *u*-parameter covariance matrix is not. See Section IV.E.6.	77

Table VI A1.2 (continued)

Category	D	Statements	Notes	#

Parameters – input control for prior covariance matrix (continued)		`PERMIT NON POSITIVE definite parameter covariance matrices,`
		or
		`PERMIT ZERO UNCERTAInties on parameters`
			This option should be used only for purposes like calculating multigroup cross sections and covariances, not for fitting data.	78
				
				79

		`READ COMPACT COVARIAnces for parameter priors,`
		or
		`READ COMPACT CORRELAtions for parameter priors,`
		or
		`COMPACT CORRELATIONS are to be read and used,`
		or
		`COMPACT COVARIANCES are to be read and used`
			See Section VII.E.	87
				
				88
				
				83
				
				84

		`PARAMETER COVARIANCE matrix is in endf format,`
		or
		`ENDF COVARIANCE MATRix is to be read and Used`
			See Section VI.F.3.	89
				
				90

		`USE LEAST SQUARES TO define prior parameter covariance matrix`	This command overrides any other information about the prior parameter covariance matrix. See Section IV.E.3 for details regarding use of the infinite-prior-uncertainty option that distinguishes least squares from Bayes' equations.	36

Table VI A1.2 (continued)

Category	D	Statements	Notes	#

Parameters – output control for parameter covariance matrix		`WRITE CORRELATIONS Into compact format,`
		or
		`WRITE COVARIANCES INto compact format,`
		or
		`PUT CORRELATIONS INTo compact format,`
		or
		`PUT COVARIANCES INTO compact format`
			Create an output file SAMMY.CCV which contains an abbreviated (compact) version of the initial parameter correlation matrix. See Section VII.E for details.	85
				86
				81
				82

		`PUT COVARIANCE MATRIx into endf file 32`	See Section VI.F.2 for details.	296

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Experimental data – input control	D	`DATA ARE IN ORIGINAL multi-style format`	Three points per line, relative uncertainties, in 3(2F15.5,F7.3) format. See Section VI.C.1.	11

		`DATA FORMAT IS ONE Point per line,`
		or
		`USE CSISRS FORMAT FOr data,`
		or
		`CSISRS`
			The ASCII data file contains one point per line, in (3G11.8) format, with uncertainties being absolute rather than relative.	12
				13
				14

		`USE TWENTY SIGNIFICAnt digits,`
		or
		`TWENTY`
			The ASCII data file contains one point per line in (3F20.10) format. Uncertainties are absolute.	15
				16

		`DATA ARE IN STANDARD odf format`	The DATa file includes information about the data-reduction parameters and is the "standard" ODF file with energy in section 1, data in section 2, absolute uncertainty in section 3, and partial derivatives with respect to data-reduction parameters in section 4 and following. See Section III.E.3.b of this manual for details.	17
		`DATA ARE IN ODF FILE`	The DATa file is in ORELA Data Format. Section 1 contains energies, 2 the data, and 3 the (absolute) uncertainties. See Section VI.C.1 of this report for details, and test case tr005 for examples.	18

		`DATA ARE ENDF/B FILE,`
		or
		`USE ENDF/B ENERGIES and data, with MAT=9999`
			The DATa file is an ENDF file containing File 3, that is, containing point-wise cross sections of the same type as specified in the INPut file. Following this command, anywhere after column 20 on the same line, write "MAT=" and then give the ENDF MAT number.	19
				20

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Experimental data – input control (cont.)		`DIFFERENTIAL DATA Are in ascii file`	See Section VI.C.1 for details; note that the default for angle-differential data is ODF file.	22
	D	`DO NOT DIVIDE DATA Into regions`	Include entire energy range in a single SAMMY run.	23
		`DIVIDE DATA INTO REGions with a fixed number of data points per region`	SAMMY will automatically choose energy regions of NEPNTS data points each, for sequential analysis. (See card set 2, Table VI A.1 for input for NEPNTS.) Warning: SAMMY merely counts; it does not consider carefully whether a dividing point is located in a region where the theoretical values (σ or *T*) are nonlinear with respect to the parameters. Dividing in such a location (at or near a resonance) will invalidate the linearity assumption used in deriving Bayes' equation, and thus lead to spurious results. Users are urged to use this option only on the "zeroth pass," as an aid in deciding where to divide the data, and not for final runs. With high-capacity computer systems available today, this option is seldom needed.	24

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Experimental data – input control for covariance matrix		`IMPLICIT DATA COVARIance is wanted,` or `IDC`	See Section VI.C.3.c.	31 32
		`USER SUPPLIED IMPLICit data covariance matrix,` or `USER IDC`	See Section VI.C.3.b.	33 34
		`PUP COVARIANCE IS IN an ascii file`	The covariance matrix for all or some of the Propagated Uncertainty Parameters (PUPs) is in an ASCII file. See Sections IV.D.2 and VI.C.3.a for details.	35
		`CREATE PUP FILE FROM varied parameters used in this run`	Use this run, in which only parameters to be PUP'd in later runs are varied, to generate a file containing the PUP covariance matrix for future runs. See Sections IV.D.2 and VI.C.3.a for additional information.	21
		`ADD CONSTANT TERM TO data covariance` or `ADD CONSTANT TO DATA covariance matrix`	These three statements refer to the option of adding a constant to the data covariance matrix, both on- and off-diagonal, over the energy region in which the effect of the non-*s*-wave resonance is felt. The magnitude of this constant is specified in columns 68–80 in the PARameter file, for each resonance. For the third option, the default value of this constant is set at 1.0E−6 for every non-*s*-wave resonance.	39 40
	D	`DO NOT ADD CONSTANT term to data covariance`		41
		`USE DEFAULT FOR CONStant term to add to data covariance`		42

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Experimental data – input control for covariance matrix (cont.)		`USE TEN PERCENT DATA uncertainty,` or `ADD TEN PERCENT DATA uncertainty`	The "experimental uncertainty" is assumed by SAMMY to be 10% of the "measured value". This option should not be used for analyses of real data.	43 44
	D	`DATA COVARIANCE IS Diagonal`	The *explicit* data covariance matrix is diagonal. Nevertheless, the *actual* data covariance matrix may include *implicit* contributions, either from propagated uncertainty parameters (see Section IV.D.2 or VI.C.3.a) or from a user-supplied implicit data covariance matrix (see Section VI.C.3.b).	45
		`DATA HAS OFF-DIAGONAl contribution to covariance matrix of the form` $(a+bE_i)\ (a+bE_j)$	*a* and *b* are specified as DCOVA and DCOVB in the INP file, card set 7 in Table VI A.1.	46
		`DATA COVARIANCE FILE is named YYYYYY.YYY`	Substitute your own file name for YYYYYY.YYY in columns 31–40. See Table VI C2.1 for the format for this file. Note that only ten characters are allowed for this file name.	47

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Experimental data – angular distribution	D	`USE LABORATORY CROSS sections`	For angle-differential elastic or reaction data; see Section II.B.1.b.	281
		`USE CENTER-OF-MASS Cross sections`		282
		`DIFFERENTIAL DATA ARe in ascii file`	See Section VI.C.1 for details; note that the default for input of angle-differential data is ODF file.	22
		`PREPARE LEGENDRE COEfficients in endf format`	Generate the file SAMMY.N04, which contains the ENDF File-4 Legendre coefficients for elastic angular distributions.	283
		`OMIT FINITE SIZE CORrections`		284
		`INCIDENT NEUTRON ATTenuation is included`	See Section III.E.7.	285
		`APPROXIMATE SCATTEREd neutron attenuation is wanted,` or `SCATTERED NEUTRON ATtenuation is included`	See Section III.E.7.	286 287
		`ANGLE-AVERAGE FOR DIfferential cross section`	See Section III.E.7.	288

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Broadening options	D	`BROADENING IS WANTED`	Some form of broadening is to be used; see Sections III.B and III.C.	201
		`BROADENING IS NOT WAnted`	If you do not wish to have SAMMY Doppler or resolution broaden the theoretical values, be sure to remove card sets 5 and 6 (see Table VI A.1) from the INP file, as well as include this line.	202

Table VI A1.2 (continued)

Category	D	Statements	Notes	#

Broadening – Doppler	D	`USE FREE GAS MODEL Of doppler broadening,`
		or
		`FGM`
			The free-gas model of Doppler broadening, as described in Section III.B.1, is to be used.	211
				212

		`USE LEAL-HWANG DOPPLer broadening`	The Doppler-broadening method of Leal and Hwang, as described in Section III.B.2, is to be used.	213 214

		`HIGH ENERGY GAUSSIAN approximation for Doppler broadening,`
		or
		`USE MULTI-STYLE DOPPler broadening,`
		or
		`HEGA`
			High-energy Gaussian approximation to the free-gas model is to be used for Doppler broadening, as described in Section III.B.3.	215
				216
				217
				218

		`USE CRYSTAL LATTICE model of doppler broadening,`
		or
		`CLM`
			Use the crystal lattice (DOPUSH) model of Doppler broadening, as described in Section III.B.4.	219
				220

		`NO LOW-ENERGY BROADEning is to be used`	Theoretical values are not to be broadened below the energy value ELOWBR given in card set 5 of Table VI A.1 (the INPut file). This option works only with the high-energy Gaussian approximation for Doppler broadening.	221

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Broadening – resolution		`TWO RESOLUTION FUNCTions together`	It is possible to use more than one type of resolution function in the same run. See Section III.C.	231
		`USE TRUE TOTAL CROSS section for resolution broadening`	Usually total cross sections will be converted to transmissions after Doppler broadening, before resolution broadening. This command forces the use of the total cross section rather than the transmission for resolution broadening and is useful in comparing the true total cross section with the effective total cross section. See Section III.E.1 for details, and test case tr081 for an example.	232
		`EXPONENTIAL FOLDING width is energy-dependent`	See Section III.C.1.b, Eq. (III C1 b.6).	233
	D	`SHIFT ENERGY FOR EXPonential tail on resolution broadening`	See Section III.C.1.c; the energy shift ΔE_s is chosen to give a maximum of the integrand at the resonance energy.	234
		`DO NOT SHIFT ENERGY for exponential tail on resolution broadening`	See Section III.C.1.c; the energy shift ΔE_s is assumed zero here.	235
		`PLOT RESOLUTION FUNCtion`	See Section X.L. This command is used to make plots of the original (Gaussian and/or exponential) resolution function.	236
		`RPI DEBUG`	Used to obtain extra printouts when debugging the RPI resolution function.	239
		`CENTER THE CONSTANT energy resolution function`	See Section III.C.4.	240

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Broadening – resolution (cont.)		(No command)	When using the RPI/GELINA/ nTOF resolution function, the user must specify whether or not the centroid of the resolution function is to be shifted.	

		`SHIFT RPI RESOLUTION function to center,`
		or
		`SHIFT GEEL RESOLUTIOn function to center,`
		or
		`SHIFT GELINA RESOLUTion`
		or
		`SHIFT NTOF RESOLUTIOn`
			The RPI/GELINA/nTOF resolution function will be centered so as not to shift the peak energies of resonances. See Section III.C.3.	237
				241
				243
				245

		`DO NOT SHIFT RPI RESolution function to center,`
		or
		`DO NOT SHIFT GEEL REsolution function to center,`
		or
		`DO NOT SHIFT GELINA resolution function to center,`
		or
		`DO NOT SHIFT NTOF REsolution function to center`
			The RPI/GELINA/nTOF resolution function is to be used exactly as input with no centering.	238
				242
				244
				246

Table VI A1.2 (continued)

Category	D	Statements	Notes	#

Multiple-scattering corrections	D	`DO NOT INCLUDE SELF-shielding or multiple-scattering corrections,`
		or
		`NO SELF-SHIELDING ANd multiple-scattering corrections`
			Calculate the cross section but do not include any self-shielding or multiple-scattering corrections.	251
				252

		`USE SELF SHIELDING Only, no scattering,` or `SELF SHIELD,`
		or
		`INCLUDE ONLY SELF SHielding and not Multiple scattering`
			Only self-shielding is to be included; no single- or double-scattering (see Section III.D).	253
				254
				255

		`USE SINGLE SCATTERINg plus self shielding,`
		or
		`SINGLE`
			Include self-shielding plus single-scattering corrections.	256
				257

		`INCLUDE DOUBLE SCATTering corrections,`
		or
		`USE MULTIPLE SCATTERing plus single scattering,`
		or
		`DOUBLE,`
		or
		`MULTIPLE`
			Include self-shielding, single-scattering, and double-scattering corrections (see Section III.D).	258
				259
				261
				260

		`INFINITE SLAB,`
		or
		`NO FINITE-SIZE CORREctions to single scattering`
			Single-scattering correction does not include edge effects.	263
				262

	D	`FINITE SLAB,`
		or
		`FINITE SIZE CORRECTIons to single scattering`
			Edge effects corrections are included for single scattering.	265
				264

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Multiple-scattering corrections (cont.)	D	`MAKE NEW FILE WITH Edge effects`	See Section III.D. This statement is ignored if "INFINITE SLAB" is specified. Be sure to rename and save the SAMMY.SSM file if you wish to reuse it.	266
		`FILE WITH EDGE EFFECts already exists`	Use this option to conserve run time. Include the name of this file (which was generated by a previous SAMMY run) after the name of your DATa file.	267
		`MAKE PLOT FILE OF MUltiple scattering pieces`	Store Y_0, Y_1, and Y_2 in file SAM53.DAT, to be read by program SAMCPR.	268 269

		`NORMALIZE AS CROSS Section rather than yield,`
		or
		`CROSS SECTION`
			See Section III.D.
			
			Note than normalization *must* be specified explicitly. SAMMY will abort if the INPut file does not specify which normalization is to be used.
				270
				
				271

		`NORMALIZE AS YIELD Rather than cross section,`
		or
		`YIELD`
				272
				
				273

		`NORMALIZE AS (1-E)SIgma`		274
		`PRINT MULTIPLE SCATTering corrections`	Create a table of E, Y_0, Y_1, Y_2, and Y (energy plus components of the corrected yield) in file SAM012.DAT.	275

		`PREPARE INPUT FOR MOnte carlo simulation,`
		or
		`MONTE CARLO`
			This is the initial SAMMY run to generate cross sections for use in Monte Carlo simulation of multiple-scattering effects.	276
				277

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Bayes' solution	D	SOLVE BAYES EQUATIONs	Update the parameter values and covariances via Bayes' equations, for those parameters that are flagged in the PARameter file.	151
		DO NOT SOLVE BAYES Equations	Parameter values are not updated but remain fixed. Theoretical values of transmission or cross section are evaluated for each energy region specified, using these fixed parameter values.	152
	D	LET SAMMY CHOOSE WHIch inversion scheme to use		153
		USE (N+V) INVERSION scheme, or NPV	Original method; Section IV.B.1.	154 155
		USE (I+Q) INVERSION scheme, or IPQ	See Section IV.B.2.	156 157
		USE (M+W) INVERSION scheme, or MPW	See Section IV.B.3.	158 159
		USE LEAST SQUARES TO define prior parameter covariance matrix	This command overrides any other information about the prior parameter covariance matrix. See Section IV.E.3.	36
		TAKE BABY STEPS WITH least-squares method	See Section IV.E.3.	49
		REMEMBER ORIGINAL PArameter values	See Section IV.E.3.	37
		USE REMEMBERED ORIGInal parameter values	See Section IV.E.3.	38

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Options for printing into SAMMY.LPT	D	`DO NOT PRINT ANY INPut parameters`		91 92
		`PRINT ALL INPUT PARAmeters`	All resonances parameters are printed in SAMMY.LPT.	93
		`PRINT VARIED INPUT Parameters`	Resonances for which no parameters are flagged will not be printed. Use this option for direct comparison with output parameters, which are always printed in this mode.	94
	D	`DO NOT PRINT INPUT Data`	"Input data" refers to experimental values of the measured cross section (or transmission, etc.), as read from the DATa file (see Section VI.C). "Theoretical values" refers to the calculated cross sections (as broadened and otherwise corrected). Often these are available in the plot file (see Table VII C.1), so they need not be printed in the LPT file.	95
		`PRINT INPUT DATA`, or `PRINT EXPERIMENTAL Values`		96 97
	D	`DO NOT PRINT THEORETical values`		98
		`PRINT THEORETICAL VAlues`, or `PRINT THEORETICAL CRoss sections`		99 100
	D	`DO NOT PRINT PARTIAL derivatives`		101
		`PRINT PARTIAL DERIVAtives`	Use this option only for debug purposes.	102
		`SUPPRESS INTERMEDIATe printout`	Updated parameter values and covariance matrix elements are printed only upon completion of entire run.	103
		`DO NOT SUPPRESS INTErmediate printout`	Updated parameter values and covariance matrix elements are printed after completion of each energy region.	104
	D	`DO NOT SUPPRESS ANY intermediate printout`	Updated parameter values are printed after each iteration of Bayes' equations (i.e., typically twice for each energy region). Updated covariance matrix elements are evaluated and printed only upon completion of an energy region.	105

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Options for printing into SAMMY.LPT (cont.)	D	`DO NOT USE SHORT FORmat for output`		106
		`USE SHORT FORMAT FOR output`	Resonance parameters are printed in the LPT file (Section VII.A), in F12.4 format rather than E format. Although this may produce more legible output, fewer significant digits may be printed.	107
	D	`DO NOT PRINT REDUCED widths`		108
		`PRINT REDUCED WIDTHS`	Reduced width amplitudes will be printed in the LPT file (Section VII.A), along with the square root of the resonance energies. That is, what are printed are the "*u*-parameters" as described in Section IV.C.	109
		`DO NOT PRINT SMALL Correlation coefficients`	Any line of the correlation matrix whose off-diagonal elements are small will not be printed. "Small" is defined as less than ICORR/100 in absolute value, where ICORR is given in card set 2 of Table VI A.1.	110
	D	`DO NOT PRINT DEBUG Info`		112
		`PRINT DEBUG INFORMATion,` or `DEBUG`	Use for debug purposes only on short runs.	113 114
		`PRINT CAPTURE AREA In lpt file`	The capture area, defined as $A = g\Gamma_n\Gamma_\gamma / \Gamma$, is printed in the SAMMY.LPT file.	115
		`CHI SQUARED IS NOT Wanted,` *or* `DO NOT PRINT LS CHI squared`	See Section IV.A.2 for definitions of both χ^2_{LS} and χ^2_B. Independent of which commands are given, both χ^2 values are printed whenever they can be calculated without excess effort.	116 117
	D	`CHI SQUARED IS WANTEd,` or `PRINT LS CHI SQUARED`		118 119
	D	`PRINT BAYES CHI SQUAred`		121
		`DO NOT PRINT BAYES Chi squared`		120

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Options for printing into SAMMY. LPT (cont.)	D	`DO NOT PRINT WEIGHTEd Residuals,`	See Section IV.A.2 for definitions of weighted residuals.	122
		or `DO NOT PRINT LS WEIGhted residuals`		123
		`PRINT WEIGHTED RESIDuals,`		124
		or `PRINT LS WEIGHTED REsiduals`		125
		`PRINT BAYES WEIGHTED residuals`		126
	D	`DO NOT PRINT BAYES Weighted residuals`		127
	D	`DO NOT PRINT PHASE Shifts`		130
		`PRINT PHASE SHIFTS For input parameters`	Hard-sphere phase shifts are defined in Section II.A.	131

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
ENDF as input		`INPUT IS ENDF/B FILE 2`	Resonance parameter values and spin-group quantum number information are taken from an ENDF/B file; see Section VI.F.3.	61
		`USE ENERGY RANGE FROm endf/b file 2`	If this command is not included, SAMMY will use the energy range from INPut file or from interactive input instead of using the range specified in the ENDF file. If the PARameter file is not an ENDF file, this command is ignored.	62

		`PARAMETER COVARIANCE matrix is in endf format,`
		or
		`ENDF COVARIANCE MATRix is to be read and used`
			See Section VI.F.3.	89
				
				90

		`DATA ARE ENDF/B FILE,`
		or
		`USE ENDF/B ENERGIES and data, with MAT=9999`
			The DATa file is an ENDF file containing File 3, that is, containing point-wise cross sections of the same type as specified in the INPut file. Following this command, anywhere after column 20 on the same line write "MAT=" and then give the ENDF MAT number.	19
				20

		`PRESERVE GAMMA_N NOT g_gamma_n from endf`	Some older ENDF files used AJ = I (the spin of the target nuclide) rather than AJ = I + ½ or I - ½ when the spin J was not well determined. In such a case SAMMY, by default, assumes the ENDF value for the neutron width is really $g\Gamma_n$. Include this command if you wish to assume that the ENDF value is Γ_n.	301

Table VI A1.2 (continued)

Category	D	Statements	Notes	#

ENDF output		`ENDF/B-VI FILE 2 IS wanted`
		or
		`ENDF`
			Resonance parameters are to be provided in the format required for ENDF/B-VI File 2. See Section VI.F.2 for details for the resolved resonance region, and VIII.C for the unresolved.	291
				292

		`NDF FILE IS IN KEY-Word Format`	The "NDF file" contains extra input required for generating ENDF File 2 output; see Section VI.F.2. This file can be in fixed format (default) or key word based if this command is present.	293

		`GENERATE FILE 3 POINt-wise cross section,`
		or
		`FILE 3`
			For either RRR or URR. See Section IX for details.	294
				295

		`PUT COVARIANCE MATRIx into endf file 32`	Parameter covariance matrix is to be printed into File 32 format. See Section IX for details.	296

		`FILE 33 LB=1 COVARIAnce is wanted,`
		or
		`FILE 33`
			Write group average cross sections into file SAMMY.CRS (which is ENDF-like) and the associated covariance matrix into SAMMY.N33 (which resembles ENDF File 33). See Section IX for details.	297
				298

		`PREPARE LEGENDRE COEfficients in endf format`	Generate the file SAMMY.N04 which contains the ENDF File-4 Legendre coefficients for elastic angular distributions. See Section IX.	283
		`AUTOMATIC NDF FILE Creation`	When input resonance parameters are from an ENDF file, SAMMY will automatically create the *.ndf file needed for creating an output ENDF File 32; see Section IX.	299
		`INCLUDE MIN & MAX ENergies in endf file`	For URR only. See Section VIII.	379

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Plot file control	D	`DO NOT GENERATE PLOT file automatically`		349 350
		`GENERATE PLOT FILE Automatically`, or `GENERATE ODF FILE AUtomatically`	See Table VII C.1 for a description of the plot file.	352 351

		`EV = UNITS ON ENERGY in plot file,`
		or
		`EV`
			Units for energies in the plot file should be eV. (This is the default only if Emax < 1 keV.)
			[NOTE: Angular distribution plot files always use eV.]
				356
				357

		`KEV = UNITS ON ENERGy in plot file,`
		or
		`KEV`
			Units for energies in the plot file should be keV. (This is the default if Emax > 1 keV.)
			[NOTE: Angular distribution plot files always use eV.]
				358
				359

		`MEV = UNITS ON ENERGy in plot file,`
		or
		`MEV`
			Units for energies in the plot file should be MeV.
			[NOTE: Angular distribution plot files always use eV.]
				360
				361

		`ODF FILE IS WANTED-- XXXXXX.XXX,ZEROth order calculation`
		
		`ODF FILE IS WANTED-- XXXXXX.XXX,FINAl calculation`
			Most SAMMY users will not need these commands, because they are ignored when GENERATE PLOT FILE Automatically is used.
			
			To use these options, replace XXXXXX.XXX (columns 21–30) with the name of your ODF file. Be sure that file already contains energies and data (sections 1, 2, 3, and possibly 6 and 7; see Table VII C.1).
			
			Note that file names are arbitrary, extensions are optional, but the name must use ten columns. No space is permitted after the comma.
				353
				354

		Eamples
		`ODF FILE IS WANTED--FILE00.ODF,ZEROth order calculation`
		`ODF FILE IS WANTED--FILE01.ODF,FINAl calculation`		

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Plot file control (cont.)	D	`DO NOT INCLUDE THEORetical uncertainties in plot file`	Uncertainties ΔT_i on theoretical values T_i are reported in sections 10 and 11 (or 6 & 7) of the plot file. See Section IV.E.4 for a detailed description and derivation of these uncertainties.	362
		`INCLUDE THEORETICAL uncertainties in plot file`		363

		`PLOT UNBROADENED CROss sections,`
		or
		`PUT UNBROADENED CROSs sections into plot file`
			Generate file SAMMY.UNB which contains the auxiliary energy grid in Section 1 and the unbroadened theoretical values in Sections 2 etc. SAMMY also generates an ASCII file SAMUNB.DAT with the same information in CSISRS format.	364
				365

		`PLOT RESOLUTION FUNCtion`	See Section X.L to make plots of the original resolution function.	236

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Averages, etc.	D	`(none needed )`	Do not average over energy ranges.	

		`AVERAGE OVER ENERGY Ranges`
		or
		`AVERAGE OVER ENERGIEs`
			Produce energy-averaged experimental data and theoretical values, using output parameters from an earlier SAMMY analysis. See Section V.C.1 for details.	311
				
				312

			CAUTION: The integration scheme used here is histogram based, suitable for averaging experimental data but not suitable for averaging theoretical cross sections. Use "`ENERGY AVERAGE USING constant flux`" option instead.	

		`GROUP AVERAGE OVER Energy ranges,`
		or
		`GROUP`
		or
		`BONDARENKO AVERAGE Over energy ranges`
			Produce Bondarenko averages, using output parameters from an earlier SAMMY analysis. See Section V.C.2 for details.	313
				
				314
				
				315

		`ENERGY AVERAGE USING constant flux,`
		or
		`UNWEIGHTED ENERGY AVerage`
			This is the appropriate scheme to use when averaging theoretical cross sections with constant flux; see Section V.C.3.	325

		`MAXWELLIAN-AVERAGED capture cross sections are wanted,`
		or
		`STELLAR-AVERAGED CAPture cross sections are wanted,`
		or
		`MXW`
			Generate stellar averaged capture cross section; see Section V.D.	316
				
				317
				
				318

		`CALCULATE MAXWELLIAN averages after reconstructing cross sections`	This option provides stellar averaged capture cross sections (Section V.D) using reconstructed energy grid (Section V.A, NJOY method).	319

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Averages, etc. (cont.)		`MAKE NO CORRECTIONS to theoretical values`	Do not perform Doppler or resolution-broadening corrections, nor include normalizations or backgrounds, before averaging.	321
		`ADD CROSS SECTIONS From endf/b file 3`	For use in generating Maxwellian averages; see Table VI F4.1.	320
		`PRINT AVERAGED SENSItivities for endf variables`	For comparison with other codes calculating multigroup cross sections and covariances.	324

Table VI A1.2 (continued)

Category	D	Statements	Notes	#

Constants	D	`USE ENDF VALUES FOR constants,`
		or
		`USE 1999 ENDF-102 Constant values`
			SAMMY is now using those values for the physical constants that have been "blessed" by ENDF.
			See Section IX.A for details.
				141
				142

		`USE 1995 ENDF-102 COnstant values,`
		or
		`USE OLDER VALUES OF constants`
				144
				143

		`USE SAMMY-K1 DEFAULTs for constants`	This will give the values that the command "USE PRECISE VALUES Of constants" used to give with version K1 of SAMMY. This option should be used for comparison purposes only and not for new analyses.	145

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Cross section calculation details		`USE POLAR COORDINATEs for fission widths`	When there are two channels for fission, the pair may be treated as a vector, in which case the two independent variables are the magnitude of the vector and the polar angle, rather than the two widths. Compare, for example, with the Vogt formalism [EV58].	191
		`NUMERICAL DERIVATIVEs for resonance parameters`	Debug command, to be used only for testing that analytic derivatives are correct.	193
	D	`DO NOT USE S-WAVE CUtoff`	See Section II.D.1.b for a description of these options.	194
		`USE S-WAVE CUTOFF`		195
		`USE NO CUTOFF FOR DErivatives or cross sections`		186
		`USE ALTERNATIVE COULomb functions`	Use the more-accurate (but also more time-consuming) version of the Coulomb penetrabilities and shift factors. See Section II.C.4 for details.	196
		`ADD DIRECT CAPTURE Component to cross section`	See Section II.B.4 for details.	197
	D	`LAB NON COULOMB EXCItation energies`	The excitation energy (for channels for which there is no Coulomb interaction) is defined in the laboratory rather than the center-of-mass system. See parameter ECHAN in card set 10.1 or 10.2 of the INPut file, Table VIA.1.	67
		`CM NON COULOMB EXCITation energies`	The non-Coulomb excitation energy is given in the cm system rather than the laboratory system.	68
	D	`LAB COULOMB EXCITATIon energies`	For Coulomb channels, the excitation energy ECHAN (card set 4 or 4a or 10.1 of the INPut file) is in the laboratory system.	69
		`CM COULOMB EXCITATIOn energies`	For Coulomb channels, the excitation energy is in the center-of-mass system.	70

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
No pre-defined energy grid		`RECONSTRUCT CROSS SEction from resonance parameters`	SAMMY will automatically choose an appropriate grid and evaluate total, elastic, capture, and fission cross sections on that grid, using NJOY method. See Section V.A.	306
		`ARTIFICIAL ENERGY Grid is needed`	SAMMY will automatically choose an appropriate grid and evaluate, using SAMMY method. See Section V.A.	307

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Special options		`RELEVANT PARAMETERS are chosen via uncertainty ratio`	Solve Bayes' equations one time. Then, based on the ratio of *u*-parameter uncertainties, choose which of the R-matrix parameters are relevant. Create file SAMMY.REL, which contains the original parameter values with only the relevant parameters flagged to be varied. See test case tr166 for examples.	327
		`CROSS SECTION COVARIance matrix is wanted`	Calculate the covariance matrix for the theoretical cross sections.	328
		`INITIAL UNCERTAINTY multiplier =`	All prior parameter uncertainties (square roots of diagonal elements of parameter covariance matrix) are to be multiplied by the specified number. See Section IV.E.6 for further discussion, and test case tr019 for examples.	329
		`FINAL UNCERTAINTY MUltiplier =`	All output parameter uncertainties (square roots of diagonal elements of parameter covariance matrix) are to be multiplied by the specified number. See Section IV.E.6 for further discussion, and test case tr019 for examples.	330

		`E-DEPENDENT INITIAL Uncertainty multiplier,`
		or
		`E-DEPENDENT UNCERTAInty multiplier`
			All prior parameter uncertainties are to be multiplied by an energy- and spin-group-dependent multiplier. Details are give in Section IV.E.6, and test case tr019 contains examples.	6
				7

		`SUMMED STRENGTH FUNCtion is wanted`	Evaluate and print the summed strength function and corresponding covariance matrix. See Section V.F for details.	331

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Special options (cont.)		`GENERATE PARTIAL DERivatives only`	SAMMY will assume all resonance parameters, and only resonance parameters, are to be varied; that Bayes' equations are not to be solved; and that the partial derivatives of the theoretical values with respect to those parameters are to be written into file SAMMY.PDS .	332
		`GENERATE SPIN GROUP cross sections`	Generate the ODF (Plot) file containing the energy (from auxiliary grid) in section 1, the unbroadened cross section in section 2, the spin-group-1 contribution to the unbroadened cross section in section 3, spin-group-2 contribution in section 4, etc.	333
		`REFORMULATE DATA FOR implicit data covariances`	See Sections IV.D.3 and VI.C.3.	334
		`COMPARE EXPERIMENT To theory`	See Section X.E; results are reported in binary file SAM53.DAT.	335

		`GENERATE Y AND W MATrices,`
		or
		`YW`
			See Section IV for a description of the M+W form of Bayes' Equations. See test case tr089 for examples of the use of this option.	336
				337

		`READ Y AND W MATRICEs,`
		or
		`WY`
				338
				339

		`STOP abc` *n* (Note that there are two spaces before "*n*" in this command; *n* is replaced with an integer value.)	Cease execution prior to the *n*th occurrence of segment abc. Used only for debug (Section XI.B) and for preparation for Monte Carlo calculations (Section X.M).	340
		`WRITE CALCULATED CROss sections into ascii file`	Write energies and theoretical values into ascii file SAMTHE.DAT in 2F20.10 format.	341

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
Special options (cont.)		`PRINT MULTIPLE SCATTering corrections`	Create a table of E, Y_0, Y_1, Y_2, and Y (energy plus components of the corrected yield) in file SAM012.DAT.	275
		`UNIFORM ENERGY GRID`	Instead of using the energies from the experimental data set to define the energy grid, SAMMY will create a grid of 1001 points uniformly space in energy. This is for testing purposes only, so this grid must be used only for "no Bayes" runs. See Section V.E for details.	342
		`UNIFORM VELOCITY GRId`	SAMMY will create a grid of 1001 points uniformly spaced in velocity (square root of energy). To be used for testing purposes only. See Section V.E.	343
		`UNIFORM TIME GRID`	SAMMY will create a grid of 1001 points uniformly spaced in time (1 over the square root of energy). To be used for testing purposes only. See Section V.E for details.	344

		`CREATE PUBLISHABLE List of parameters,`
		or
		`PUBLISH`
			The file SAMMY.PUB will be created, which contains resonance parameters and uncertainties in columns, with each value separated by tabs. This file can be ported to spreadsheet programs to be formatted for publication purposes. See Section VII.F for details.	345
				346

		`DO NOT TEST FOR EIGEnvalues`	Do not test whether the parameter covariance matrix is positive-definite (i.e., whether all eigenvalues are greater than zero).	347

Table VI A1.2 (continued)

Category	D	Statements	Notes	#
URR controls		`EXPERIMENTAL DATA ARe in separate files`	See Section VIII.B for details of input to unresolved resonance region (URR) calculations.	371
		`NO ANNOTATED PARAMETer file for urr input`	Input for URR is essentially the original format as in the FITACS code; see Table VIII.B.1.	372

	D	`ANNOTATED PARAMETER file for urr,`
		or
		`ANNOTATED`
			Input for URR is "annotated file", which contains key words and phrases to make the input more human-legible. See Section VIII.B and Table VIII.B.2 for details.	373
				374

	D	`OUTPUT IN ANNOTATED parameter file for urr`	Output parameter file is annotated. (This is always true; SAMMY now contains no option for writing non-annotated output, although that can still be used as input).	375

		`ENDF/B-VI FILE 2 IS wanted,`
		or
		`ENDF`
			Resonance parameters are to be written into the format required for ENDF/B-VI File 2. See Section VI.F.2 for details.	291
				292

	D	`USE ALL EXPERIMENTAL data points,`
		or
		`DO NOT USE ENERGY LImits as given in the input file`
			All data points appearing in the initial URR PARameter file (see Section VIII.B) are to be fitted during the analysis. Energy limits given in the INPut file will be ignored.	376
				377

		`USE ENERGY LIMITS AS Given in the input file`	The energy range specified in card set 2 of the INPut file will be used to define which data points are to be included in the analysis.	378
		`INCLUDE MIN & MAX ENergies in endf file`	When creating ENDF File 2 for LRU = 2, include Emin and Emax from the SAMMY run as part of the energy list. Examples are in test cases tr127, tr128, tr133, and tr134.	379

Table VI A1.2 (continued)

Category	D	Statements	Notes	#

URR controls (cont.)		`CALCULATE WIDTH FLUCtuation factors more accurately,`
		or
		`CALCULATE DRESNER INtegrals more accurately`
			Use 1001 grid points rather than the default 101 points for calculating the Dresner integrals. See tr073 for examples.	380
				370

		`MOLDAUER PRESCRIPTIOn is to be used,`
		or
		`MOLDAUER`
			Moldauer's "effective degree of freedom" is to be used, to compensate for strong overlap of resonances. See page 352 of FF00.	322
				323

Table VI A1.3. Alphabetic list of acceptable commands for card set 3

Abbreviations in the "Category" column are defined in Table VI A1.1 and refer to the location in Table VI A1.2 in which a description of this command can be found. "P" in the column labeled "Parameter" indicates that additional values are required on this line. "D" in the column labeled "Default" indicates that this is a default command and so may be safely omitted. "B" in the "deBug" column indicates that this command should be only for debugging and not for production runs. "A" in "Archaic" column indicates a command that will likely soon be eliminated.

Command statement	Category	Parameter	Default	deBug	Archaic
ADD CONSTANT TERM TO data covariance	DCM				
ADD CROSS SECTIONS From endf/b file 3	Average				
ADD DIRECT CAPTURE Component…	CS calc				
ADD TEN PERCENT DATA uncertainty	DCM				
ANGLE-AVERAGE FOR DIfferential cross section	Angle				
ANNOTATED	URR		D		
ANNOTATED PARAMETER file for urr	URR		D		
APPROXIMATE SCATTEREd neutron attenuation…	Angle				
ARTIFICIAL ENERGY GRid is needed	Grid				
AUTOMATIC NDF FILE Creation	ENDF out				
AVERAGE OVER ENERGY ranges	Average				
BONDARENKO AVERAGE Over energy ranges	Average				
BROADENING IS NOT WAnted	Broad				
BROADENING IS WANTED	Broad		D		
CALCULATE DRESNER INtegrals more accurately	URR				
CALCULATE MAXWELLIAN averages after reconst…	Average				
CALCULATE WIDTH FLUCtuation factors more…	URR				
CENTER THE CONSTANT energy resolution function	Resol				
CHI SQUARED IS NOT Wanted	LPT				
CHI SQUARED IS WANTEd	LPT		D		
CLM	Doppler				
CM COULOMB EXCITATIOn energies	CS calc				
CM NON COULOMB EXCITation energies	CS calc				
COMPACT CORRELATIONS are to be read and used	PCM in				
COMPACT COVARIANCES are to be read and used	PCM in				

Table VI A1.3 (continued)

Command statement	Category	Parameter	Default	deBug	Archaic
COMPARE EXPERIMENT To theory	Special				
CREATE PUBLISHABLE List of parameters	Special				
CREATE PUP FILE FROM varied parameters used…	DCM				
CRO	RM				A
CROSS SECTION	MSC				
CROSS SECTION COVARIance matrix is wanted	Special				
CSISRS	Data				
DATA ARE ENDF/B FILE	Data				
DATA ARE IN ODF FILE	Data				
DATA ARE IN ORIGINAL multi-style format	Data		D		
DATA ARE IN STANDARD odf format	Data				
DATA COVARIANCE FILE is named YYYYYY.YYY	DCM	P			
DATA COVARIANCE IS Diagonal	DCM		D		
DATA FORMAT IS ONE Point per line	Data				
DATA HAS OFF-DIAGONAl contribution to cov...	DCM				
DEBUG	LPT			B	
DIFFERENTIAL DATA ARE In ascii file	Data				
DIFFERENTIAL DATA ARe in ascii file	Angle				
DIVIDE DATA INTO REGions with a fixed number…	Data				
DO NOT ADD CONSTANT term to data covariance	DCM		D		
DO NOT ALLOW VALUES for data-related param…	Special				
DO NOT DIVIDE DATA Into regions	Data		D		
DO NOT GENERATE PLOT file automatically	Plot		D		
DO NOT INCLUDE SELF-shielding or multiple-scat…	MSC		D		
DO NOT INCLUDE THEORetical uncertainties in…	Plot				
DO NOT PRINT ANY INPut parameters	LPT		D		
DO NOT PRINT BAYES Chi squared	LPT				
DO NOT PRINT BAYES Weighted residuals	LPT		D		
DO NOT PRINT DEBUG Info	LPT		D		
DO NOT PRINT INPUT Data	LPT				
DO NOT PRINT LS CHI squared	LPT				

Table VI A1.3 (continued)

Command statement	Category	Parameter	Default	deBug	Archaic
DO NOT PRINT LS WEIGhted residuals	LPT		D		
DO NOT PRINT PARTIAL derivatives	LPT		D		
DO NOT PRINT PHASE Shifts	LPT		D		
DO NOT PRINT REDUCED widths	LPT		D		
DO NOT PRINT SMALL Correlation coefficients	LPT		D		
DO NOT PRINT THEORETical values	LPT				
DO NOT PRINT WEIGHTEd residuals	LPT		D		
DO NOT SHIFT ENERGY for exponential tail…	Resol				
DO NOT SHIFT GEEL REsolution function…	Resol				
DO NOT SHIFT GELINA resolution function…	Resol				
DO NOT SHIFT NTOF REsolution function…	Resol				
DO NOT SHIFT RPI RESolution function…	Resol				
DO NOT SOLVE BAYES Equations	Bayes				
DO NOT SUPPRESS ANY intermediate printout	LPT		D		
DO NOT SUPPRESS INTErmediate printout	LPT				
DO NOT TEST FOR EIGEnvalues	Special				
DO NOT USE ENERGY LImits as given in the…	URR				
DO NOT USE SHORT FORmat for output	LPT		D		
DO NOT USE S-WAVE CUtoff	CS calc		D		
DOUBLE	MSC				
E-DEPENDENT INITIAL uncertainty multiplier	Special				
E-DEPENDENT UNCERTAInty multiplier	Special				
ENDF	ENDF out				
ENDF	URR				
ENDF COVARIANCE MATRix is to be read and used	PCM in				
ENDF/B-VI FILE 2 IS wanted	ENDF out				
ENDF/B-VI FILE 2 IS wanted	URR				
ENERGY AVERAGE USING constant flux	Average				
ENERGY UNCERTAINTIES are at end of line…	PCM in				
EV	Plot				
EV = UNITS ON ENERGY in plot file	Plot				

Table VI A1.3 (continued)

Command statement	Category	Parameter	Default	deBug	Archaic
EXPERIMENTAL DATA ARe in separate files	URR				
EXPONENTIAL FOLDING width is energy-dependent	Resol				
FGM	Doppler		D		
FILE 3	ENDF out				
FILE 33	ENDF out				
FILE 33 LB=1 COVARIAnce is wanted	ENDF out				
FILE WITH EDGE EFFECts already exists	MSC				
FINAL UNCERTAINTY MUltiplier =	Special	P			
FINITE SIZE CORRECTIons to single scattering	MSC		D		
FINITE SLAB	MSC		D		
FITACS	General				
FLAG ALL RESONANCE Parameters	Param				
FRITZ FROEHNERS FITAcs	General				
GENERATE FILE 3 POINt-wise cross section	ENDF out				
GENERATE ODF FILE AUtomatically	Plot				
GENERATE PARTIAL DERivatives only	Special				
GENERATE PLOT FILE Automatically; or	Plot				
GENERATE SPIN GROUP cross sections	Special				
GENERATE Y AND W MATrices	Special				
GROUP AVERAGE OVER Energy ranges	Average				
HEGA	Doppler				
HIGH ENERGY GAUSSIAN approximation for Doppler…	Doppler				
IDC	DCM				
IGNORE	PCM in				
IGNORE INPUT BINARY covariance file	PCM in				
IMPLICIT DATA COVARIance is wanted	DCM				
INCIDENT NEUTRON ATTenuation is included	Angle				
INCLUDE DOUBLE SCATTering corrections	MSC				
INCLUDE MIN & MAX ENergies in endf file	ENDF out				
INCLUDE MIN & MAX ENergies in endf file	URR				
INCLUDE ONLY SELF SHielding and not multiple…	MSC				

Table VI A1.3 (continued)

Command statement	Category	Parameter	Default	deBug	Archaic
INCLUDE THEORETICAL uncertainties in plot file	Plot				
INFINITE SLAB	MSC				
INITIAL DIAGONAL P Covariance	PCM in				
INITIAL DIAGONAL U Covariance	PCM in				
INITIAL UNCERTAINTY multiplier =	Special	P			
INPUT IS ENDF/B FILE 2	Param				
INPUT IS ENDF/B FILE 2	ENDF in				
IPQ	Bayes				
KEV	Plot				
KEV = UNITS ON ENERGy in plot file	Plot				
KEY-WORD PARTICLE-PAir definitions are given	Param				
LAB COULOMB EXCITATIon energies	CS calc		D		
LAB NON COULOMB EXCItation energies	CS calc		D		
LET SAMMY CHOOSE WHIch inversion scheme…	Bayes		D		
MAKE NEW FILE WITH Edge effects	MSC		D		
MAKE NO CORRECTIONS to theoretical values	Average				
MAKE PLOT FILE OF MUltiple scattering pieces	MSC				
MAXWELLIAN AVERAGED capture cross sections…	Average				
MEV	Plot				
MEV = UNITS ON ENERGy in plot file	Plot				
MLBW	RM				
MLBW FORMALISM IS WAnted	RM				
MODIFY P COVARIANCE matrix before using	PCM in				
MOLDAUER	URR				
MOLDAUER PRESCRIPTIOn is to be used	URR				
MONTE CARLO	MSC				
MORE ACCURATE REICH-moore	RM				
MPW	Bayes				
MULTILEVEL BREIT-WIGner is wanted	RM				
MULTIPLE	MSC				
MXW	Average				

Table VI A1.3 (continued)

Command statement	Category	Parameter	Default	deBug	Archaic
NDF FILE IS IN KEY-Word Format	ENDF out				
NO ANNOTATED PARAMETer file for urr input	URR				
NO FINITE-SIZE CORREctions to single scattering	MSC				
NO LOW-ENERGY BROADEning is to be used	Doppler				
NO SELF-SHIELDING ANd multiple-scattering…	MSC		D		
NORMALIZE AS (1-E)SIgma	MSC				
NORMALIZE AS CROSS Section rather than yield	MSC				
NORMALIZE AS YIELD Rather than cross section	MSC				
NPV	Bayes				
NUMERICAL DERIVATIVEs for resonance parameters	CS calc			B	
ODF FILE IS WANTED-- XXXXXX.XXX, FINAl guess	Plot	P			
ODF FILE IS WANTED-- XXXXXX.XXX, ZEROth order…	Plot	P			
OMIT FINITE SIZE CORrections	Angle				
ORIGINAL REICH-MOORE formalism	RM				A
OUTPUT IN ANNOTATED parameter file for urr	URR		D		
P COVARIANCE MATRIX is correct, U is not	PCM in				
PARAMETER COVARIANCE matrix is in endf format	PCM in				
PARTICLE PAIR DEFINItions are given	Param				
PERFORM SUMMARY ANALysis	Special				
PERMIT NON POSITIVE definite parameter cov…	PCM in				
PERMIT ZERO UNCERTAInties on parameters	PCM in				
PLOT RESOLUTION FUNCtion	Resol				
PLOT RESOLUTION FUNCtion	Plot				
PLOT UNBROADENED CROss sections	Plot				
PREPARE INPUT FOR MOnte carlo simulation	MSC				
PREPARE LEGENDRE COEfficients in endf format	Angle				
PREPARE LEGENDRE COEfficients in endf format	ENDF out				
PRESERVE GAMMA_N NOT g_gamma_n from endf	ENDF in				
PRINT ALL INPUT PARAmeters	LPT				
PRINT AVERAGED SENSItivities for endf variables	Average				
PRINT BAYES CHI SQUAred	LPT		D		

Table VI A1.3 (continued)

Command statement	Category	Parameter	Default	deBug	Archaic
PRINT BAYES WEIGHTED residuals	LPT				
PRINT CAPTURE AREA In lpt file	LPT				
PRINT DEBUG INFORMATion	LPT			B	
PRINT EXPERIMENTAL Values	LPT				
PRINT INPUT DATA	LPT				
PRINT LS CHI SQUARED	LPT		D		
PRINT LS WEIGHTED REsiduals	LPT				
PRINT MULTIPLE SCATTering corrections	MSC				
PRINT MULTIPLE SCATTering corrections	Special				
PRINT PARTIAL DERIVAtives	LPT			B	
PRINT PHASE SHIFTS For input parameters	LPT				
PRINT REDUCED WIDTHS	LPT				
PRINT THEORETICAL CRoss sections	LPT				
PRINT THEORETICAL VAlues	LPT				
PRINT VARIED INPUT Parameters	LPT				
PRINT WEIGHTED RESIDuals	LPT				
PUBLISH	Special				
PUP COVARIANCE IS IN an ascii file	DCM				
PUT CORRELATIONS INTo compact format	PCM out				
PUT COVARIANCES INTO compact format	PCM out				
PUT COVARIANCE MATRIx into endf file 32	PCM out				
PUT COVARIANCE MATRIx into endf file 32	ENDF out				
PUT QUANTUM NUMBERS into parameter file	Param				
PUT UNBROADENED CROSs sections into plot file	Plot				
QUANTUM NUMBERS ARE in parameter file	Param				
READ COMPACT CORRELAtions for parameter priors	PCM in				
READ COMPACT COVARIAnces for parameter priors	PCM in				
READ Y AND W MATRICEs	Special				
RECONSTRUCT CROSS SEction from resonance…	Grid				
REFORMULATE DATA FOR implicit data covariances	Special				
REICH-MOORE FORMALISm is wanted	RM		D		

Table VI A1.3 (continued)

Command statement	Category	Parameter	Default	deBug	Archaic
RELEVANT PARAMETERS are chosen via uncert…	Special				
REMEMBER ORIGINAL PArameter values	Bayes				
RETROACTIVE	PCM in				
RETROACTIVE OLD PARAmeter file new cov…	PCM in				
RPI DEBUG	Resol			B	
SCATTERED NEUTRON ATtenuation is included	Angle				
SELF SHIELD	MSC				
SHIFT ENERGY FOR EXPonential tail on resolution…	Resol		D		
SHIFT GEEL RESOLUTIOn function to center	Resol				
SHIFT GELINA RESOLUTion	Resol				
SHIFT NTOF RESOLUTIOn	Resol				
SHIFT RPI RESOLUTION function to center	Resol				
SINGLE	MSC				
SINGLE LEVEL BREIT-Wigner is wanted	RM				
SLBW	RM				
SLBW FORMALISM IS WAnted	RM				
SOLVE BAYES EQUATIONs	Bayes		D		
SPIN OF INCIDENT PARTICLE IS -	Param	P			
SPIN OF INCIDENT PARTICLE IS +	Param	P			
STELLAR AVERAGED CAPture cross sections…	Average				
STOP abc n	Special			B	
SUMMED STRENGTH FUNCtion is wanted	Special				
SUPPRESS INTERMEDIATe printout	LPT				
TAKE BABY STEPS WITH least squares method	Bayes				
TWENTY	Data				
TWO RESOLUTION FUNCTions together	Resol				
U COVARIANCE MATRIX is correct, P is not	PCM in				
UNIFORM ENERGY GRID	Special				
UNIFORM TIME GRID	Special				
UNIFORM VELOCITY GRId	Special				
UNRESOLVED RESONANCE region	General				

Table VI A1.3 (continued)

Command statement	Category	Parameter	Default	deBug	Archaic
UNWEIGHTED ENERGY AVerage	Average				
USE (I+Q) INVERSION scheme	Bayes				
USE (M+W) INVERSION scheme	Bayes				
USE (N+V) INVERSION scheme	Bayes				
USE 1995 ENDF-102 COnstant values	Constant				
USE 1999 ENDF-102 COnstant values	Constant				
USE ALL EXPERIMENTAL data points	URR		D		
USE ALTERNATIVE COULomb functions	CS calc				
USE ALTERNATIVE COULomb functions	CS calc				
USE CENTER-OF-MASS Cross sections	Angle		D		
USE CRYSTAL LATTICE model of doppler broadening	Doppler				
USE CSISRS FORMAT For data	Data				
USE DEFAULT FOR CONStant term to add to…	DCM				
USE ENDF VALUES FOR constants	Constant		D		
USE ENDF/B ENERGIES and data, with MAT=9999	Data	P			
USE ENERGY LIMITS AS given in the input file	URR				
USE ENERGY RANGE FROm endf/b file 2	Param				
USE ENERGY RANGE FROm endf/b file 2	ENDF in				
USE FREE GAS MODEL Of doppler broadening	Doppler		D		
USE I4 FORMAT TO REAd spin group number	Param				
USE LABORATORY CROSS sections	Angle				
USE LEAL-HWANG DOPPLer broadening	Doppler				
USE LEAST SQUARES TO define prior par cov…	Bayes				
USE LEAST SQUARES TO define prior par… cov…	PCM in				
USE MULTIPLE SCATTERing plus single scattering	MSC				
USE MULTI-STYLE DOPPler broadening	Doppler				
USE NEW SPIN GROUP Format	Param		D		
USE NO CUTOFF FOR DErivatives or cross sections	CS calc				
USE OBSOLETE SPIN GRoup format	Param				A
USE OLDER VALUES OF constants	Constant				
USE POLAR COORDINATEs for fission widths	CS calc				

Table VI A1.3 (continued)

Command statement	Category	Parameter	Default	deBug	Archaic
USE REMEMBERED ORIGInal parameter values	Bayes				
USE SAMMY-K1 DEFAULTs for constants	Constant				
USE SELF SHIELDING Only, no scattering	MSC				
USE SHORT FORMAT FOR output	LPT				
USE SINGLE SCATTERINg plus self shielding	MSC				
USE S-WAVE CUTOFF	CS calc				
USE TEN PERCENT DATA uncertainty	DCM				
USE TRUE TOTAL CROSS section for resolution…	Resol				
USE TWENTY SIGNIFICAnt digits	Data				
USER IDC	DCM				
USER SUPPLIED IMPLICit data covariance matrix	DCM				
WRITE CALCULATED CROss sections into ascii file	Special				
WRITE CORRELATIONS Into compact format	PCM out				
WRITE COVARIANCES INto compact format	PCM out				
WY	Special				
XCT	RM				
YIELD	MSC				
YW	Special				

VI.B. THE PARameter FILE

The PARameter file contains initial values for all those parameters that are to be varied, as well as others that may be held fixed or treated as propagated-uncertainty parameters (see Section IV.D.2 for details concerning PUPs). In addition, this file may contain *a priori* uncertainties or covariances for the varied parameters.

Various types of data can be included in the PARameter file. These are organized into "card sets," with each card set consisting of one or more lines of information. Most card sets begin with a header line and end with a blank line. The header lines are listed in Table VI B.1, along with key words for some of the card sets. Details about each card set are given in Table VI B.2 and summarized here.

Card set 1 contains resonance parameters, ending in a blank line. Card set 2 contains a single number, called FUDGE, which is the "fudge factor" by which a parameter is multiplied to give the initial uncertainty for that parameter, unless that uncertainty is specified elsewhere.

Only card set 1 is required to be in the file. If any of card sets 3 through "Last" are present, then card set 2 must also be present.

Card set 3 gives values for parameters of the external R-function (see Section II.B.1.d). Two alternate formats are available for this.

Card set 4 gives values for some broadening (and other) parameters.

Card set 5 gives values of "unused" parameters, that is, of those data-reduction parameters that are not directly affected by the data set to be analyzed but that are coupled via the covariance matrix to other parameters that *are* directly affected. An example of such a parameter would be the thickness of a thin sample, for which the data have already been analyzed via SAMMY, while the current data set is from a measurement with a thick sample. The auxiliary code SAMAMR must be used between the two SAMMY runs to ensure that the correct thickness is used with the appropriate data set (see Section X.C).

Card set 6 gives values for normalization and background parameters, as described in Eqs. (III E3a.1) and (III E3 a.2) of Section III.E.3.a

Card set 7 contains values for the two channel radii (as used for potential scattering and for penetrability and shift factor). Key-word format for the channel radii is described in card set 7a. See item 3 in Section III.E.2 for discussion of effective vs. true radius.

Card set 8 gives names and values for data reduction parameters, as described in Section III.E.3.b.

Card set 9 gives values of parameters for the Oak Ridge resolution function (ORR) parameters, as described in Section III.C.2.

Card set 10 contains isotopic mass and abundance values, as described in Section III.E.2.

Card set 11 contains values for miscellaneous parameters, described in various locations throughout this manual.

Card set 12 provides parameter values for paramagnetic cross sections; see Section III.E.4.

Card set 13 contains values for parameters of the background functions described in Section III.E.3.a.

Card set 14 gives parameters of the RPI resolution function, Section III.C.3.

Card set 15 provides values for *l*- and isotope-dependent detector efficiencies, Section III.E.5.

Card set 16 gives input for the numerical user-defined resolution function. This is described in more detail in Section III.C.5.

The last card set defines the prior covariance matrix for the parameters. Three alternative methods are given: Card set *Last A* assumes a covariance matrix has been prepared by a previous SAMMY run; the presence of this card set eliminates the possibility of any others being used. Card sets *Last B* ("explicit uncertainties") and *Last C* ("relative uncertainties") may be interchanged at will, as long as each occurs at most once in any given PARameter file. A fourth alternative is available for resonance energies only (see card set 1, columns 68-80, option 3). A fifth is to omit this card set entirely, in which case, default uncertainties are used for every parameter.

Note that each card set in the PAR file (except for card sets 1 and 2) begins with an alphanumeric description of what follows. Note also that each card set (except card set 2) terminates with a blank card. A blank line at the very end of the file may be omitted, but all others must be present.

<u>Quantum numbers included in PARameter file</u>

Beginning with Release M6 of the SAMMY code, it is possible to include all information relevant to the R-matrix within the PARameter file rather than have partial information (spin group definitions) in the INPut file. Details are given in Table VI B.3.

Table VI B.1. Header lines for card sets in the PARameter file

Card set	Alphanumeric header line	Notes
1		Resonance parameters. No header line; card set ends in a blank line.
2		Fudge factor for default uncertainties; no header line, no blank line.
3	`EXTERnal R-function parameters follow`	Only one of card sets 3 and 3a is permitted.
3a	`R-EXTernal parameters follow`	
4	`BROADening parameters may be varied`	
5	`UNUSEd but correlated variables`	Card set is created by SAMAMR run.
6	`NORMAlization and background`	
7	`RADIUs parameters follow` (two versions: usual for fewer than 99 channels and spin groups, alternative version for greater than 99 channels or spin groups.	Card set 7a is the preferred method.

7a	`RADII are in KEY-WORD format`
	or
	`CHANNel radius parameters follow`
	
	<u>Valid key words for channel radius</u>:
	`RADIus` or `RADIi`
	`EFfective radius`
	`TRue radius`
	<u>Valid key words for uncertainty</u>:
	`RElative`
	`ABsolute` or `UNcertainty`
	<u>Valid key words for particle-pair names</u>:
	`PARTicle-pair` or `PP`
	<u>Valid key words for orbital angular momentum:</u>
	`L` or `ORbital angular momentum`
	with `ODd`, `EVen`, or `ALl` after equal sign
	<u>Valid key word for flags</u>:
	`FLags` with `Yes`, `1`, `No`, `0`, `2`, or `-1`
	<u>Valid key word for spin groups</u>:
	`GRoup` followed by a group number or `All`
	`CHannels =`, followed by channel numbers	

8	`DATA reduction parameters are next`	Seldom used

Table VI B.1 (continued)

Card set	Alphanumeric header line	Notes
9	ORRES Valid subheadings for first five columns of subsequent lines: BURST WATER or TANTA (not both) LITHI or NE110 (not both) CHANN	
10	ISOTOpic abundances and masses, or NUCLIde abundances and masses	
11	MISCEllaneous parameters follow Valid subheadings for first five columns of subsequent lines: DELTA ETA FINIT GAMMA TZERO SIABN SELFI EFFIC DELTE DRCAP	
12	PARAMagnetic cross section parameters follow	In first five columns of next line, use one of "TM ", "ER ", "HO "
13	BACKGround functions Valid subheadings for first five columns of subsequent lines: CONST EXPON POWER EXPLN T-PNT E-PNT TFILE EFILE	
14	RPI Resolution function, or GEEL resolution function, or GELINa resolution, or NTOF resolution function Valid subheadings for first five columns of subsequent lines: BURST TAU LAMBD A1 EXPON A3 A5 XXPON BINS CHANN	
14a	RPI Transmission resolution function, or RPI Capture resolution function, or GEEL DEFAUlts, or GELINa DEFAUlts, or NTOF DEFAUlts Valid subheadings for first five columns of subsequent lines: BURST BINS CHANN	
15	DETECtor efficiencies	

Table VI B.1 (continued)

Card set	Alphanumeric header line	Notes

16	`USER-Defined resolution function`
	Valid subheadings for first five columns of subsequent lines:
	`BURST  CHANN  FILE=`	

Last	`COVARiance matrix is in binary form in another file`	
Last B	`EXPLIcit uncertainties and correlations follow`	
Last C	`RELATive uncertainties follow`	

Last D	`PRIOR uncertainties follow in key-word format`
	See Table VI B.2 for details.
	Valid key words are:
	`RELAtive, ABSOlute,` or `UNCErtainty`
	`EMIN` or `EMAX`
	`GRoup` with number or `All`
	`Channel` with number or `All`
	`Energy` or `Gamma`
	`PP` or `PARTicle pair`
	`L` or `Orbital angular momentum`	

Table VI B.2. Format of the PARameter file

Comment 1: The two numbers in the first column (labeled "C:L") represent the card set number (before the colon) and the line number within that card set (after the colon).

Comment 2: Numbers in the second column (labeled "P, T") indicate position number within the line. Letters indicate format type: integer format ("I", which implies a number without a decimal point and requires that the number be in the right-most columns), real format ("F", which requires a number with a decimal point), or alphanumeric ("A", which can be numbers or letters or symbols).

C:L	P, T	Variable Name	Meaning (units)	Notes
1:1	1-11, F	E_λ	Resonance energy E_λ (eV)	
	12-22, F	$\Gamma\gamma$	Capture width (milli-eV)	
	23-33, F	Γ_{c1}	Particle width for channel 1 (milli-eV)	If any particle width Γ is negative, SAMMY uses $\lvert\Gamma\rvert$ for the width and set the associated amplitude γ to be negative. That is, SAMMY uses $\gamma = -\alpha\sqrt{\lvert\Gamma\rvert}$, where α is the appropriate factor (see Section II.A.1).
	34-44, F	Γ_{c2}	Particle width for channel 2 (milli-eV)	
	45-55, F	Γ_{c3}	Particle width for channel 3 (milli-eV)	
	56-57, I	IS_E	Vary E_λ?	0 = no, 1 = yes, 3 = PUP (See Section IV for meanings of "vary" and "PUP".)
	58-59, I	IS_γ	Vary $\Gamma\gamma$?	0 = no, 1 = yes, 3 = PUP
	60-61, I	IS_{c1}	Vary Γ_{c1}?	0 = no, 1 = yes, 3 = PUP
	62-63, I	IS_{c2}	Vary Γ_{c2}?	0 = no, 1 = yes, 3 = PUP
	64-65, I	IS_{c3}	Vary Γ_{c3}?	0 = no, 1 = yes, 3 = PUP
	66-67, I	IGROUP	Quantum numbers for this resonance are those of group number IGROUP (card set 10.1 or 10.2 in Table VIA.1)	If IGROUP is negative or greater than 50, this resonance will be omitted from the calculation.
			(To use more than 50 spin groups, include the phrase "`USE I4 FORMAT TO REAd spin group number`" in the INPut file card set 3. Then use Columns 66-68 for IGROUP, and columns 70-82 for X. The maximum number of spin groups is then 500; values greater than 500 indicate omitted resonances.)	

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
1:1 cont.	68-80, F	X	For many cases, this variable is not used (columns may be left blank). However, there are three possible uses for this variable: (1) If X < 0, then values of Γ for other particle channels are included on the following line. (2) If X is positive and the statement "`ENERGY UNCERTAINTIES are at end of line`" is included in card set 3 of the INPut file (see Table VI A1.2), then X is the prior absolute uncertainty on E_λ (eV). (3) If X is positive, and the expression "`ADD CONSTANT TERM TO data covariance`" is included in the INPut file (see Table VI A1.2), then a constant on-and-off diagonal contribution to the data covariance matrix (DCM) is to be used under this resonance. In this case X should be $\leq (\Delta d)^2$, where Δd is the absolute uncertainty on data near this resonance. NOTE: This option is seldom used.	
1:2	1-11, F	Γ_{c4}	Particle width for channel 4 (milli-eV)	This line is present only if X < 0 on the preceding line
	12-22, F	Γ_{c5}	Width for ch 5 (milli-eV)	
	23-33, F	Γ_{c6}	Width for ch 6 (milli-eV)	
	34-44, F	Γ_{c7}	Width for ch 7 (milli-eV)	
	45-55, F	Γ_{c8}	Width for ch 8 (milli-eV)	
	56-57, I	IS_{c4}	Vary Γ_{c4}?	0 = no, 1 = yes, 3 = PUP
	58-59, I	IS_{c5}	Vary Γ_{c5}?	0 = no, 1 = yes, 3 = PUP
	60-61, I	IS_{c6}	Vary Γ_{c6}?	0 = no, 1 = yes, 3 = PUP
	62-63, I	IS_{c7}	Vary Γ_{c7}?	0 = no, 1 = yes, 3 = PUP
	64-65, I	IS_{c8}	Vary Γ_{c8}?	0 = no, 1 = yes, 3 = PUP
	66-67, I	IGROUP	must be same as previous line	
	68-80, F	X	As above, negative to indicate continuation line. Positive for uncertainty on resonance energy, or for off-diagonal DCM.	
1:3,4, etc	Repeat line 2 as needed, until all non-zero channel widths have been defined.			
1:5 etc,	Repeat lines 1 – 4 as many times as needed, until all resonances are specified.			
1:Last	End with a blank line.			

Table VI B.2 (continued)

C:L	P,T	Variable Name	Meaning (units)	Notes
2:1	1-11, F	Fudge	Fudge = initial relative uncertainty for varied parameters whose initial uncertainty is not specified elsewhere. Default = 0.1	One exception: The value of FUDGE will not affect the resonance energy E_λ. The default initial uncertainty for E_λ is set at ½ times the sum of all widths (including Doppler and resolution widths).
3:1	1-80, A	WHAT	"`EXTERnal R-function parameters follow`"	Alphanumeric indicator of what comes next; only the first five characters are read.
3:2	1-3, I	IGROUP	Spin group number	
	4-5, I	ICHN	Channel number	If zero, SAMMY assumes 1.
	6-16, F	E_α^{down}	Logarithmic singularity below energy range (eV)	Parameters of the logarithmic parameterization of the external R-matrix for quantum numbers α (i.e., for IGROUP and ICHN), of the form given in Eq. (II B1 d.1).
	17-27, F	E_α^{up}	Logarithmic singularity above energy range (eV)	
	28-38, F	$R_{con,\,\alpha}$	Constant term	
	39-49, F	$R_{lin,\,\alpha}$	Linear Term	
	50-60, F	s_α	Coefficient of logarithmic term (must be non-negative)	
	62, I	ISE_α^{down}	Vary E_α^{down} ?	0 = no, 1 = yes, 3 = PUP
	64, I	ISE_α^{up}	Vary E_α^{up} ?	0 = no, 1 = yes, 3 = PUP
	66, I	$ISR_{con,\,\alpha}$	Vary $R_{con,\,\alpha}$?	0 = no, 1 = yes, 3 = PUP
	68, I	$ISR_{lin,\,\alpha}$	Vary $R_{lin,\,\alpha}$?	0 = no, 1 = yes, 3 = PUP
	70, I	ISs_α	Vary s_α ?	0 = no, 1 = yes, 3 = PUP
3:3 etc.	Repeat line 2 as many times as desired. Include only those spin groups and channels for which you wish to parameterize the external R-matrix in this manner.			
3:Last	(blank)			

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
3a:1	1-80, A	WHAT	"`R-EXTernal parameters follow`". This card set 3a is an alternative, not a supplement, to card set 3. It is not permitted to use both.	
3a:2	1-2, I	IGROUP	Spin group number	
	3, I	ICHN	Channel number	If zero, SAMMY assumes 1.
	4, I	ISE_{α}^{down}	Vary E_{α}^{down} ?	0 = no, 1 = yes, 3 = PUP
	5, I	ISE_{α}^{up}	Vary E_{α}^{up} ?	0 = no, 1 = yes, 3 = PUP
	6, I	$ISR_{con,\alpha}$	Vary $R_{con,\alpha}$?	0 = no, 1 = yes, 3 = PUP
	7, I	$ISR_{lin,\alpha}$	Vary $R_{lin,\alpha}$?	0 = no, 1 = yes, 3 = PUP
	8, I	$ISs_{con,\alpha}$	Vary $s_{con,\alpha}$?	0 = no, 1 = yes, 3 = PUP
	9, I	$ISs_{lin,\alpha}$	Vary $s_{lin,\alpha}$?	0 = no, 1 = yes, 3 = PUP
	10, I	$ISR_{q,\alpha}$	Vary $R_{q,\alpha}$?	0 = no, 1 = yes, 3 = PUP
	11-20, F	E_{α}^{down}	Logarithmic singularity below energy range (eV)	Parameters of the logarithmic parameterization of the external R-matrix for quantum numbers α (i.e., for IGROUP and ICHN), of the form given in Eq. (IIB1d.1).
	21-30, F	E_{α}^{up}	Logarithmic singularity above energy range (eV)	
	31-40, F	$R_{con,\alpha}$	Constant term	
	41-50, F	$R_{lin,\alpha}$	Linear Term (eV^{-1})	
	51-60, F	$s_{con,\alpha}$	Constant coefficient of logarithmic term (must be non-negative)	
	61-70, F	$s_{lin,\alpha}$	Linear coefficient of logarithmic term	
	71-80, F	$R_{q,\alpha}$	Quadratic term	
3a:3 etc.	Repeat line 2 as many times as desired. Include only those spin groups and channels for which you wish to parameterize the external R-matrix in this manner.			
3a: Last (blank)				

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
4:1	1-80, A	WHAT	"`BROADening parameters may be varied`"	Values for parameters in this card set may be specified in the INPut file if they are not to be varied (card sets 5 and 7 of Table VIA.1). Alternatively, this entire card set may be inserted at the end of the INPut file when parameters are treated as PUPs.
4:2	1-10, F	CRFN	Matching readius (F)	In many cases this value is overruled (e.g., card set 7 or 7a).
	11-20, F	TEMP	Effective temperature of the sample (K)	
	21-30, F	THICK	Sample thickness (atoms/barn)	
	31-40, F	DELTAL	Spread in flight-path length (m)	
	41-50, F	DELTAG	The absolute value of DELTAG is the full width at half max of a Gaussian resolution function whose variance is equivalent to that of the square pulse (μs). See Section III.C.1.a for details.	In card set 5 of the INPut file, a negative value of DELTAG is used as a marker to indicate that channel widths and crunch boundaries are included in card set 6. Here in card set 4 of the PAR file, DELTAG can be either negative or positive, but only |DELTAG| has any meaning. It is acceptable to have a negative value of DELTAG in the INPut file, so that crunch boundaries and channel widths will be read, and then have a completely different value of DELTAG in the PARameter file. SAMMY computations will make use of (1) the crunch boundaries and channel widths from the INPut file and (2) the absolute value of DELTAG from the PARameter file. See test case tr048 for examples.

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
4:2 cont.	51-60, F	DELTAE	e-folding width of exponential resolution function (μs)	
	61-62, I	Icrfn	Flag to vary this parameter; values -2, 0, and 1 may be used, but -1 and 3 may not (see below for meanings of these values).	
	63-64, I	Itemp	Flags to vary these parameter. Meanings are as follows:	
	65-66, I	Ithick	-2 → do not vary this parameter. Use the value given in card sets 5, 6, or 7 of the INPut file rather than the value given here.	
	67-68, I	Ideltal		
	69-70, I	Ideltag		
	71-72, I	Ideltae	-1 → do not vary this parameter. Use the value given here in the PARameter file rather than the value given in the COVariance file (if it exists). (Note that only those parameters that were not varied in earlier runs can be changed in this manner.) 0 → do not vary this parameter. Use the value given in the COVariance file if it exists; otherwise, use this value. 1 → do vary this parameter. For the starting value, use the value given in the COVariance file if it exists. 3 → PUP this parameter. Use the value given here. (See Section IV.D.2 for a description of propagated uncertainty parameters.)	
4:3	1-10 11-20 … 51-60	dCRFN dTEMP … dDE	Uncertainty on CRFN Uncertainty on TEMP … Uncertainty on DELTAE	This line is optional. If absent, prior uncertainties are set to FUDGE × value of parameter.
4:4	(blank)			

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
5:1	1-80, A	WHAT	"`UNUSEd but correlated variables come next`"	Parameter files using this card set are never generated directly by a SAMMY user; rather, they result from using the code SAMAMR (see Section X.C).
5:2	1-5, A	NUSED_1	Name of first unused variable	
	11-15, A	NUSED_2	Name of 2nd unused variable	
	. . .			
	71-75, A	NUSED_8	Name of 8th unused variable	
5:3	1-10, F	UNUSED_1	Value of first unused variable	
	11-20, F	UNUSED_2	Value of 2nd unused variable	
	. . .			
	71-80, F	UNUSED_8	Value of 8th unused variable	
5:4, 5, etc.	Repeat lines 2 and 3 as many times as needed			
5:Last	(blank)			

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
6:1	1-80, A	WHAT	"`NORMAlization and background are next`"	See Section III.E.3.a. This card set could be put into the INPut file rather than PARameter file if no values are to be varied.
6:2	1-10, F	ANORM	a = normalization (dimensionless)	Value ~ 1
	11-20, F	BACKA	B_a = constant background (dimensionless if data are transmission, barns if c.s.)	
	21-30, F	BACKB	B_b = background proportional to $1/\sqrt{E}$ or linear in time ($\sqrt{\text{eV}}$ or $\text{barns}\times\sqrt{\text{eV}}$)	
	31-40, F	BACKC	B_c = background proportional to $\sqrt{E}$ or linear in inverse time ($1/\sqrt{\text{eV}}$ or $\text{barns}/\sqrt{\text{eV}}$)	
	41-50, F	BACKD	B_d = coefficient for exponential background (dimensionless or barns)	
	51-60, F	BACKF	B_f = exponential decay constant ($\sqrt{\text{eV}}$)	
	61-62, I	Ianorm	Flag for these parameters: -1, 0, 1, or 3	
	63-64, I	Ibacka	-1 → do not vary or PUP this parameter. Use the value given here in the PAR file rather than the value given in the COVariance file if it exists. (Note that only those parameters that were not varied in earlier runs can be changed in this manner).	
	65-66, I	Ibackb		
	67-68, I	Ibackc		
	69-70, I	Ibackd		
	71-72, I	Ibackf	0 → do not vary or PUP this parameter. Use the value given in the COVariance file if it exists; otherwise, use the value given here. 1 → do vary this parameter. For the starting value, use the value given in the COVariance file if it exists. 3 → PUP this parameter, using this value.	

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
6:3	1-10, F	Danorm	uncertainty on ANORM	This line is optional for angle-integrated data but not for angular distributions. When the line is omitted, the uncertainty is assumed to be FUDGE × value of parameter.
	11-20, F	Dbacka	uncertainty on BACKA	
	21-30, F	Dbackb	uncertainty on BACKB	
	31-40, F	Dbackc	uncertainty on BACKC	
	41-50, F	Dbackd	uncertainty on BACKD	
	51-60, F	Dbackf	uncertainty on BACKF	
6:4, 6:5, etc.	When the data are angular distributions, line 2 contains normalization and backgrounds for the first angle and line 3 the corresponding uncertainties. Line 4 contains values for the second angle, etc.			
6:Last	(blank)			

Table VI B.2 (continued)

C: L	P, T	Variable Name	Meaning (units)	Notes
7:1	1-80, A	WHAT	"`RADIUs parameters follow`" For more than 99 spin groups, see card set "7 alternate." For a more flexible, key-word-based format, see card set 7a.	
7:2	1-10, F	PAREFF	Radius (Fermi) to be used for potential scattering	
	11-20, F	PARTRU	Radius (Fermi) to be used for penetrabilities and shifts (1) If > 0, use this value. (2) If = 0 and IFLTRU is not negative, SAMMY uses the value of CRFN from the INPut file or from card set 4 of the PARameter file for PARTRU. (3) If < 0, the absolute value of the number given is the ratio of the mass of the sample nucleus to that of a neutron. SAMMY then calculates PARTRU as 1.23 $(AWRI)^{1/3}$ + 0.8, which is the ENDF formula, converted to units of Fermi.	
	21, I	ICHAN	Channel indicator	0 → applies to all channels 1 → applies only to specified channels
	22, I	IFLEFF	Flag to indicate how PAREFF is to be treated	= 0 → not varied = 1 → varied = 3 → treated as PUP (Section IV.D.2)
	23-24, I	IFLTRU	Flag to indicate how PARTRU is to be treated	= −1 → treated as identical to PAREFF = 0 → not varied = 1 → varied independently of PAREFF = 3 → treated as PUP (Section IV.D.2)
	25-26, I	IG1	The number of a spin group using these radii	As many spin groups as needed are given in columns 25-80, 2 columns per group.
	27-28, I	IG2	Second spin group for these radii	
	. . .			
	?, I	IG_Last	Final spin group for these radii	
	?, I	IX	Zero, denoting end of spin group list	When ICHAN=1, specify channel numbers by inserting a zero (IX = 0) after the string of spin group numbers, and follow with the string of channel numbers.
	?, I	IC1	First channel number	
	?, I	IC2	Second channel number	
	. . .			
	?, I	IC_Last	Last channel number	
7:Last		(blank)		

Table VI B.2 (continued)

C: L	P, T	Variable Name	Meaning (units)	Notes
7:1 alternative	1-80, A	WHAT	"`RADIUs parameters follow`" For fewer than 99 spin groups, see card set 7 on previous page. For a more flexible, key-word-based format, see card set 7a.	
7:2	1-10, F	PAREFF	Radius (Fermi) to be used for potential scattering	
	11-20, F	PARTRU	Radius (Fermi) to be used for penetrabilities and shifts (1) If > 0, use this value. (2) If = 0 and IFLTRU is not negative, SAMMY uses the value of CRFN from the INPut file or from card set 4 of the PARameter file for PARTRU. (3) If < 0, the absolute value of the number given is the ratio of the mass of the sample nucleus to that of a neutron. SAMMY then calculates PARTRU as 1.23 $(AWRI)^{1/3}$ + 0.8, which is the ENDF formula, converted to units of Fermi.	
	21-25, I	ICHAN	Channel indicator	0 → applies to all channels 1 → applies only to specified channels
	26-30, I	IFLEFF	Flag to indicate how PAREFF is to be treated	= 0 → not varied = 1 → varied = 3 → treated as PUP (Section IV.D.2)
	31-35, I	IFLTRU	Flag to indicate how PARTRU is to be treated	= −1 → treated as identical to PAREFF = 0 → not varied = 1 → varied independently of PAREFF = 3 → treated as PUP (Section IV.D.2)
	36-40, I	IG1	The number of a spin group using these radii	As many spin groups as needed are given in columns 36-80, 5 columns per group.
	41-45, I	IG2	Next spin group for these radii	
	. . .			
	?, I	IG_Last	Final spin group for these radii	
	?, I	IX	Zero, denoting end of spin group list	When ICHAN=1, specify channel numbers by inserting a zero (IX = 0) after the string of IG's, and follow with the string of channel numbers.
	?, I	IC1	First channel number	
	?, I	IC2	Second channel number	
	. . .			
	?, I	IC_Last	Last channel number	
7: Last		(blank)		

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
7a:1	1-80, A	WHAT	"`RADII are in KEY-WORD format`", or "`CHANNel radius parameters follow`"	If using the first option, the phrase "key-word" must occur somewhere on the line.

See Table VI B.1 for an itemized list of the valid key words used in this card set.

Many test cases contain examples of this card set: tr041,tr043,tr119, tr151. Below is one example from test case tr059, file t059cz.par :

```
Channel RADIUS PARAMETERS FOLLOW
 Radius=   3.200   3.200  Flags=1  3
   PP=n+16O     L=all
 Radius=   3.200   3.200  Flags=3 -1
   PP=alf+13C   L=all
 Radius=   3.200   3.200  Flags=3  1
   PP=n+16O  1  L=all
 Radius=   3.200   3.200  Flags=3  3
   PP=n+16O  2  L=all
```

7a:2 Channel radii parameters are given in key word format, with the key word followed by an equal sign followed by the value. Radii values must be specified first, prior to the information regarding which channels are associated with these radii.

Valid key words for radii: `RADIus`, `RADIi`, `EFfective radius`, `TRue radius`. Only those letters in caps must be included; they may be either caps or lowercase in the file. If key word `RADIus` is used, it can be followed by one or two values (separated by space or comma); the first is the effective radius, and the second is the true radius. In any case, if only one radius value is specified, the other is assumed to be equal to that same value.

No other key words may be included on this line.

7a:3 Uncertainties may be given for the radii. Use the key word `RElative` to specify relative uncertainties, and `ABsolute` or `UNcertainty` to provide absolute uncertainties. Give two values after the equal sign, the first for the effective radius and the second for the true radius. It is permitted to give only one value, in which case that value is used for both radii. However, if only one value is given, it must be the last item on this line.

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
7a:4, 7a:5, etc.	Valid key words for particle-pair names: `PARTicle-pair`, `PP`. Particle-pair names must be specified before the orbital angular momenta values, and must be *exactly* as in the INPut file, card set 4 or 4a. Valid key words for orbital angular momentum: `L`, `ORbital angular momentum`. After the equal sign, values may be given as `ODd`, `EVen`, or `ALl`. In addition (or instead), specific values of *l* can be specified (separated by commas or blank spaces). The orbital angular momentum specification can be on the same line or a following line after the particle-pair specification. In principle more than one particle pair can be specified for a given pair of channel radii. In practice this is not recommended, since different particle pairs correspond to different physical situations, and hence the radii are intrinsically different (though the *value* may be the same).			
7a:6	Valid key word for flags: FLags. One or two values are given, separated by blanks or commas. If only one flag is given, it applies to the effective radius; the true radius is assumed to be held fixed. If two flags are given, the first applies to the effective radius and the second to the true radius. Values may be "`Y`" or "1" (indicating that the radius is to be varied) or "`N`" or "0" (indicating that the value for the radius is fixed), or 3 (indicating that the radius is to be treated as a PUP). For the effective radius, a value "−1" indicates that the two radii are to be treated as identical. If both radii are listed explicitly, the key word `FLags` may be given on the same line with the radii.			
7a:7 etc.	Valid key word for spin groups: `GRoup`. Following the equal sign, a single group number is given, or "`All`" may be specified. After the group number, give the key word `CHannels`. Following the equal sign, appropriate channel numbers are listed, separated by commas and/or blanks. NOTE: Channels *must* be specified on the same line as groups. More than one group can be assigned to the same radii values; each group must be given on a separate line.			
7a: last	(blank)			

Table VI B.2 (continued)

C:L	P,T	Variable Name	Meaning (units)	Notes
8:1	1-80, A	WHAT	"`DATA reduction parameters are next`"	See Section III.E.3.b for a discussion of data-reduction parameters. This card set could be put into the INPut file rather than PARameter file if no values are to be varied.
8:2	1-5, A	NAMDTP	Alphanumeric name for the first data-reduction parameter	
	7, I	Iff	Flag to indicate how this parameter is to be treated	1 if varied 3 if PUP (see Section IV.D.2) 0 otherwise
	11-20, F	PARDTP	Current value of parameter	
	21-30, F	UNCDTP	Absolute uncertainty for this parameter	
	31-40, F	PTILDE	Value of parameter used to generate partial derivatives	If zero, SAMMY assumes PTILDE = PARDTP
8:5,6 etc.	Repeat lines 2,3,4... as required			
8:Last	(blank)			

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
9:1	1-80, A	WHAT	"ORRES"	Oak Ridge Resolution function (Section III.C.2). Card set may be in INPut file instead of here.
9:2	1-5, A	WHAT	"BURST"	Burst width is on this line.
	7, I	Iff	Flag to indicate how burst width is to be treated	1 if varied, 3 if PUP, 0 otherwise
	11-20, F	BURST	Value of square burst width (ns)	
	21-30, F	DBURST	Uncertainty on BURST (ns)	
9.3	1-5, A	WHAT	"WATER"	Information about water moderator is on this line and the next line.
	7, I	IF0	Flag to indicate treatment for WATR0	1 if varied, 3 if PUP, 0 otherwise
	8, I	IF1	Flag for WATR1	1 if varied, 3 if PUP, 0 otherwise
	9, I	IF2	Flag for WATR2	1 if varied, 3 if PUP, 0 otherwise
	10, I	m	Degrees of freedom for chi-squared distribution	Integer, > 0 (default = 4)
	11-20, F	WATR0	Constant term Λ_0 in expression for the mean free path Λ for the water moderator (mm)	Default = 3.614
	21-30, F	WATR1	Coefficient of linear term Λ_1 in expression for Λ (mm)	Default = -0.089
	31-40, F	WATR2	Coefficient of quadratic term Λ_2 in expression for Λ (mm)	Default = 0.037
9:4	11-20, F	DW0	Uncertainty on WATR0	Use this line only if previous line specified "WATER".
	21-30, F	DW1	Uncertainty on WATR1	
	31-40, F	DW2	Uncertainty on WATR2	
9:3a	1-5, A	WHAT	"TANTA"	Tantalum target is used instead of water moderator; see Section III.C.2 for precise meaning of variables. Note that you cannot have both WATER and TANTA.
	7, I	IFTANT	Flag to indicate whether TANTA is to be varied	
	11-20, F	TANTA	ε` (mm^{-1})	
	21-30, F	Dtanta	Uncertainty on TANTA	

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
9:4a	7, I	IFX1	Flag for X1	Include this line only for tantalum target. Flags are 1 if varied, 3 if PUP, 0 otherwise. See Section IV.D.2 for information about PUPs.
	8, I	IFX2	Flag for X2	
	9, I	IFX3	Flag for X3	
	10, I	IFX0	Flag for X0	
	11-20, F	X1	x'_1 (mm)	
	21-30, F	X2	x'_2 (mm)	
	31-40, F	X3	x'_3 (mm)	
	41-50, F	X0	x'_0 (mm)	
9:5	11-20, F	DX1	Uncertainty on x'_1 (mm)	Include this line only for tantalum target.
	21-30, F	DX2	Uncertainty on x'_2 (mm)	
	31-40, F	DX3	Uncertainty on x'_3 (mm)	
	41-50, F	DX0	Uncertainty on x'_0 (mm)	
9:6	7, I	Ifwww	Flag for β'	Use this line only for tantalum target. Flags are 1 if varied, 3 if PUP, 0 otherwise.
	8, I	Ifalpha	Flag for α'	
	11-20, F	WWW	β' (mm^{-1})	
	21-30, F	ALPHA	α' (dimensionless)	
9:7	11-20, F	Dwww	Uncertainty on β' (mm^{-1})	Use this line only for tantalum target.
	21-30, F	Dalpha	Uncertainty on α' (dimensionless)	
9:8	1-5, A	WHAT	"`LITHI`"	Lithium-glass detector is used.
	7, I	IFD	Flag for *d*	Flags are 1 if varied, 3 if PUP, 0 otherwise.
	8, I	IFF	Flag for *f*	
	9, I	IFG	Flag for *g*	
	11-20, F	D	*d* (nsec)	
	21-30, F	F	*f* ($nsec^{-1}$)	
	31-40, F	G	*g* (dimensionless)	
9:9	11-20, F	DD	Uncertainty on *d* (nsec)	Include this line only for lithium-glass detector.
	21-30, F	DF	Uncertainty on *f* ($nsec^{-1}$)	
	31-40, F	DG	Uncertainty on *g*	

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
9:8a	1-5, A	WHAT	"`NE110`"	NE110 detector is used.
	7, I	IFDEL	Flag for δ	(Note that you cannot use both LITHI and NE110).
	8-10, I	NMDETS	Number of cross-section values and energies to be included (i.e., number of line # 9's to be read)	If zero, default values are used; default material is $CH_{1.104}$.
	11-20, F	DELTA	δ (mm)	
	21-30, F	dDELTA	Uncertainty on δ (mm)	
	31-40, F	DENSTY	λ (number of molecules per mm.b of detector)	Default is 0.0047
9:9a	11-20, F	ENDETS(i)	Maximum energy for this value of SIGDTS (eV)	These lines occur only with the NE110 detector, and only when NMDETS > 0. Repeat this line a total of NMDETS times.
	21-30, F	SIGDTS(i)	Total cross section for detector material (barns)	
9.10	1-5, A	WHAT	"`CHANN`"	Channel widths and crunch boundaries are given here.
	7, I	Ifchnn	Flag if CHANN is varied	0 if fixed, 1 if vary, 2 if PUP
	11-20, F	ECRNCH(i)	Maximum energy for this channel width (eV)	
	21-30, F	CHANN(i)	Channel width *c* (nsec)	
	31-40, F	DCHANN(i)	Uncertainty on channel width *c* (nsec)	
9:11	Repeat this line as many times as needed			
9:12	(blank)			

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
10:1	1-80, A	WHAT	"`ISOTOpic abundances and masses`", or "`NUCLIde abundances and masses`"	Each nuclide in the sample should have an entry here.
10:2	1-10, F	AMUISO (1)	Atomic mass (amu)	
	11-20, F	PARISO (1)	Fractional abundance for this nuclide (dimensionless)	
	21-30, F	DELISO (1)	Uncertainty on abundance (dimensionless)	
	31-32, I (or 31-35, I if > 99 groups)	IFLISO (1)	Flag whether treatment for the abundance	−2 → use value of isotopic abundance given in INPut file 1 → vary 0 → do not vary 3 → treat as PUP (Section IV.D.2)
	33-34, I or 36-40, I	IGRISO (1,1)	Number of the first spin group belonging to this nuclide	If more than 24 spin groups are needed, insert "-1" in Columns 79-80, and continue on the next line.
	35-36, I or 41-50, I	IGRISO (2,1)	Number of second spin group	When there are more than 99 spin groups altogether, each integer entry on this line requires five columns.
	etc.			
10:3	1-5, I	IGRISO (24,1) or (9,1)	Number of the next spin group belonging to this nuclide	This line is needed only if the final entry on the previous line was −1.
	6-10, I	etc.		As many as needed
10:4	Repeat previous line as many times as needed.			
10:5 etc. Repeat Lines 2 – 4 as many times as needed.				
10:6	(blank)			

Table VI B.2 (continued)

C:L	P,T	Variable Name	Meaning (units)	Notes
11:1	1-80, A	WHAT	"`MISCEllaneous parameters follow`"	Any line in this card set may be omitted when not needed. This card set may be in INPut file.
11:2	1-5, A	WHAT	"`DELTA`"	$\Delta L = E\,\Delta L_1 + \Delta L_0$ is used instead of DELTAL from card set 4 of this file, or instead of DELTAL from card set 5 of the INPut file.
	7, I	IFLAG1	Flag to indicate treatment for parameter ΔL_1	Flags = 1 to vary, 3 to PUP, and 0 to hold fixed.
	9, I	IFLAG0	Flag to indicate treatment for parameter ΔL_0	
	11-20, F	DELL11	ΔL_1 = Coeff. of E (m/eV)	
	21-30, F	D1	Uncertainty on ΔL_1 (m/eV)	
	31-40, F	DELL00	ΔL_0 = Constant term (m)	
	41-50, F	D0	Uncertainty on ΔL_0 (m)	
11:3	1-5, A	WHAT	"`ETA  `" ("eta" plus two blank spaces)	Use if type of data (see card set 8 of INput file) is ETA.
	7, I	IFLAGN	Flag to indicate treatment for parameter ν	
	11-20, F	NU	Normalization coefficient	NU = ν (dimensionless) as in ETA = NU $\times$ (fission /absorption)
	21-30, F	DNU	Uncertainty on NU	
11:4	1-5, A	WHAT	"`FINIT`"	Finite-size corrections for angular distributions; See Section III.E.7.
	7, I	IFLAGI	Flag to indicate treatment for parameter ATTNI	Repeat this line once for each angle. If the line occurs only once, the same attenuations are used for each angle.
	9, I	IFLAGO	Flag to indicate treatment for parameter ATTNO	
	11:20, F	ATTNI	Incident-particle attenuation (atoms/barn)	Flags = 1 to vary, 3 to PUP, 0 to hold fixed.
	21:30, F	DTTNI	Uncertainty on ATTNI	
	31:40, F	ATTNO	Exit-particle attenuation (atom/b)	
	41:50, F	DTTNO	Uncertainty on ATTNO	

Table VI B.2 (continued)

C:L	P,T	Variable Name	Meaning (units)	Notes
11:5	1-5, A	WHAT	"GAMMA"	Use the same Γ_γ for all resonances in this spin group; assumed to be varied.
	6-7, I	IG	Spin group number	
	11-20, F	GAMGAM	Radiation width Γ_γ for all resonances in spin group IG	
	21-30, F	DGAM	Uncertainty on GAMGAM	
11:6	1-5, A	WHAT	"TZERO"	See Section III.E.8.
	7, I	IFTZER	Flag for t_0	
	9, I	IFLZER	Flag for L_0	
	11-20, F	TZERO	t_0 (μs)	
	21-30, F	DTZERO	Uncertainty on t_0 (μs)	
	31-40, F	LZERO	L_0 (dimensionless)	
	41-50, F	DLZERO	Uncertainty on L_0 (dimensionless)	
	51-60, F	FPL	Flight-path length (m)	This value for the flight-path length is used only if DIST is zero (INPut File, card set 5).
11:7	1-5, A	WHAT	"SIABN"	Abundances for self-indication transmission sample. See Section III.E.6.
	7, I	IF1	Flag for SIABN(1)	
	9, I	IF2	Flag for SIABN(2)	
	10, I	IF3	Flag for SIABN(3)	
	11-20, F	SIABN(1)	Abundance for nuclide # 1	Note that nuclides are defined in card set 10, which <u>must</u> occur before card set 11 in the PARameter file.
	21-30, F	DS(1)	Uncertainty on SIABN(1)	
	31-40, F	SIABN(2)	Abundance for nuclide # 2	
	41-50, F	DS(2)	Uncertainty on SIABN(2)	
	51-60, F	SIABN(3)	Abundance for nuclide # 3	Repeat this line until all nuclides have been included.
	61-70, F	DS(3)	Uncertainty on SIABN(3)	

Table VI B.2 (continued)

C:L	P,T	Variable Name	Meaning (units)	Notes
11:8	1-5, A	WHAT	"SELFI"	Temperature and thickness for transmission sample for self-indication experiment. See Section III.E.6.
	7, I	IFTEMP	Flag for temperature	
	9, I	IFTHCK	Flag for thickness	
	11-20, F	SITEM	Effective temperature (K) for self-indication transmission sample	
	21-30, F	dSITEM	Uncertainty on SITEM	
	31-40, F	SITHC	Thickness (atoms/barn)	
	41-50, F	dSITHC	Uncertainty on SITHC	
11:9	1-5, A	WHAT	"EFFIC"	Efficiencies for capture and for fission for eta calculation.
	7, I	IFCAPE	Flag for capture efficiency	
	9, I	IFFISE	Flag for fission efficiency	
	11-20, F	EFCAP	Efficiency for detecting capture events	
	21-30, F	EFFIS	Efficiency for detecting fission events	
	31-40, F	dEFCAP	Uncertainty on EFCAP	
	41-50, F	dEFFIS	Uncertainty on EFFIS	
11:10	1-5, A	WHAT	"DELTE"	Delta-E is energy dependent, as described in Section III.C.1.b, Eq. (III C1 b.7).
	7, I	IFLAG1	Flag for DELE1	
	9, I	IFLAG0	Flag for DELE0	
	10, I	IFLAGL	Flag for DELEL	
	11-20, F	DELE1	Coefficient of *E* in Eq. (III A2b.7) (m / eV)	
	21-30, F	DD1	Uncertainty on DELE1	
	31-40, F	DELE0	Constant term in Eq. (III A 2b.7) (m)	
	41-50, F	DD0	Uncertainty on DELE0	
	51-60, F	DELEL	Coefficient of log term in Eq. (III A 2b.7) (m / ln(eV))	
	61-70, F	DDL	Uncertainty on DELEL	

Table VI B.2 (continued)

C:L	P,T	Variable Name	Meaning (units)	Notes
11:11	1-5, A	WHAT	"DRCAP"	Numerical direct capture component for nuclide number NUC is read from DRC file; COEF (NUC) multiplies that value. Note that this line may be included as many times as needed, to a maximum of once per nuclide. See Section II.B.4 for details.
	7, I	IFLAG1	Flag to vary COEF(Nuc)	
	9, I	NUC	Nuclide Number	
	11-20, F	COEF	Coefficient of the value given in the DRC file	
	21-30, F	dCOEF	Uncertainty on COEF	
11:12	1-5, A	WHAT	"NSENS"	This line must be present when neutron sensitivity calculations are to be included with self-shielding and multiple-scattering corrections. See Section III.D, Eq. (III D.17), for details.
	7, I	IFNEUT	Flag for neutron sensitivity	
	11-20, F	SENSIN	*A* = multiplier for neutron-sensitivity calculation; value is equal to the binding energy of the target nucleus. (SAMMY will automatically set this to a positive value, even if a negative value is given.)	
	21-30, F	DSENSN	Uncertainty on *A*	
11:Last	(blank)			

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
12:1	1-80, A	WHAT	"`PARAMagnetic cross section parameters follow`"	See Section III.E.4. This card set could be put into the INPut file rather than PARameter file if no values are to be varied.
12:2	1-5, A	WHAT	"`TM  `", "`ER  `", "`HO  `" (2 letters plus 3 blanks)	Which particular nuclide is to be used
	7, I	IFA	Flag to vary A	1 to vary, 3 to PUP, 0 otherwise
	9, I	IFB	Flag to vary B	1 to vary, 3 to PUP, 0 otherwise
	10, I	IFP	Flag to vary P	1 to vary, 3 to PUP, 0 otherwise
	11-20, F	A	*A* of Eq. (VH.1)	See Section III.E.4 for default values.
	21-30, F	dA	Uncertainty on *A*	
	31-40, F	B	*B* of Eq. (VH.1)	
	41-50, F	dB	Uncertainty on *B*	
	51-60, F	P	*P* of Eq. (VH.1)	
	61-70, F	dP	Uncertainty on *P*	
12:3	7, I	ISO	Isoptope (nuclide) number for this paramagnetic cross section	
	9, I	IFC	Flag to vary *C*	1 to vary, 3 to PUP, 0 otherwise
	11-20, F	C	*C* of Eq. (VH.1)	
	21-30, F	dC	Uncertainty on *C*	
12:4	(blank)			

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
13:1	1-80, A	WHAT	"`BACKGround functions`"	See Section III.E.3.a. This card set could be put into the INPut file rather than PARameter file if no values are to be varied.
13:2	1-5, A	WHAT	"`CONST`"	Line is present only if needed and may be repeated as needed.
	7, I	IFA	Flag to vary or PUP A	1 to vary, 3 to PUP, 0 otherwise
	11-20, F	A	Constant background (same units as data)	
	21-30, F	dA	Uncertainty on background	
	31-40, F	Emin	Minimum energy for which this background applies (eV)	Default energies are entire range of analysis.
	41-50, F	Emax	Maximum energy (eV)	
	51-60, F	FPL	Flight-path length (m)	This value of the flight-path length is used only if DIST was not given in card set 5 of INPut file or elsewhere.
13:3	1-5, A	WHAT	"`EXPON`"	This line is present only if needed, and may be repeated as needed.
	7, I	IFA	Flag to vary or PUP A	
	9, I	IFB	Flag to vary or PUP B	
	11-20, F	A	Coefficient of exponential (units same as data)	See Section III.E.3.a for an explanation of this background function.
	21-30, F	dA	A priori uncertainty on A	
	31-40, F	B	Coefficient of time in exp (ns)	
	41-50, F	dB	A priori uncertainty on B	
	51-60, F	Emin	Minimum energy for which this background applies (eV)	Default energies are entire range of analysis.
	61-70, F	Emax	Maximum energy (eV)	
	71-80, F	FPL	Flight-path length (m)	This value of the flight-path length is used only if DIST was not given in card set 5 of the INPut file (or elsewhere).

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
13:4	1-5, A	WHAT	"POWER"	This line is present only if needed and may be repeated as needed.
	7, I	IFA	Flag to vary or PUP A	
	9, I	IFB	Flag to vary or PUP B	
	11-20, F	A	Coeff. of power of time (units are [data]×[ns^{-B}])	See Section III.E.3.a for an explanation of this background function.
	21-30, F	dA	A priori uncertainty on A	
	31-40, F	B	Power (dimensionless)	
	41-50, F	dB	A priori uncertainty on B	
	51-60, F	Emin	Minimum energy for which this background applies (eV)	Default energies are entire range of analysis.
	61-70, F	Emax	Maximum energy (eV)	
	71-80, F	FPL	Flight-path length (m)	This value of *L* is used only if flight-path length was not given earlier.
13:5	1-5, A	WHAT	"EXPLN"	This line is present only if needed and is always followed by line # 6. The pair of lines may be repeated as needed.
	7, I	IFA	Flag to vary or PUP A	
	9, I	IFB	Flag to vary or PUP B	
	10, I	IFC	Flag to vary or PUP C	
	11-20, F	A	Constant term in exponential (dimensionless)	See Section III.E.3.a for an explanation of this background function.
	21-30, F	dA	A priori uncertainty on A	
	31-40, F	B	Coef. of *t* in exponential (ns^{-1})	
	41-50, F	dB	A priori uncertainty on B	
	51-60, F	C	Coefficient of $[\ln(t)]^{-1}$ in exponential (ln(nsec))	
	61-70, F	dC	A priori uncertainty on C	
13:6	11-20, F	Emin	Minimum energy for which this background applies (eV)	Line 6 must follow each and every occurrence of line 5.
	21-30, F	Emax	Maximum energy (eV)	
	31-40, F	FPL	Flight-path length (m)	This value of *L* is used only if flight-path length was not given earlier.

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
13:7	1-5, A	WHAT	"T-PNT"	Point-wise linear function of time. If this line is present, it must occur at least twice. All occurrences must be contiguous in the file, and the times "T" must be increasing monotonically.
	7, I	IFA	Flag to vary or PUP A	1 to vary, 3 to PUP, 0 otherwise
	11-20, F	A	Value of this background at time T (same units as data)	Section III.E.3.a provides an explanation of this background function.
	21-30, F	dA	Uncertainty on A	
	31-40, F	T	Flight time for which this value of A applies (ns)	
	41-50, F	FPL	Flight-path length (m)	This value of the flight-path length is used only if DIST was not given in card set 5 of INPut file or elsewhere.
13:8	1-5, A, F	WHAT	"E-PNT"	Point-wise linear function of energy. If this line is present, it must occur at least twice. All occurrences must be contiguous in the file, and the energies "E" must be increasing monotonically.
	7, I	IFA	Flag to vary or PUP A	1 to vary, 3 to PUP, 0 otherwise
	11-20, F	A	Value of this background at energy E (same units as data)	Section III.E.3.a provides an explanation of this background function.
	21-30, F	dA	Uncertainty on A	
	31-40, F	E	Energy for which this value of A applies (eV)	

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
13:9	1-5, A	WHAT	"`TFILE`"	Point-wise linear function of time t_i, with times and values A_i to be stored in a separate file. Line 10 must follow this line; the two lines may be repeated as needed.
	7, I	IFB	Flag to vary or PUP B	1 to vary, 3 to PUP, 0 otherwise
	11-20, F	B	Multiplier for this background	Section III.E.3.a provides an explanation of this background function.
	21-30, F	dB	Uncertainty on B	
	31-40, F	FPL	Flight-path length (m)	This value of the flight-path length is used only if DIST was not given in card set 5 of INPut file or elsewhere.
13: 10	1-70, A	FILE	Name of file containing the point-wise background. The first line in this file is a title, the other lines each contain values for two parameters (t_i and A_i), in free format.	A file name on line 10 must follow every occurrence of line 9.
13: 11	1-5, A	WHAT	"`EFILE`"	Point-wise linear function of energy E_i, with times and values A_i to be stored in a separate file. Line 12 must follow this line; the two lines may be repeated as needed.
	7, I	IFB	Flag to vary or PUP B	1 to vary, 3 to PUP, 0 otherwise
	11-20, F	B	Multiplier for this background	See Section III.E.3.a for details.
	21-30, F	dB	Uncertainty on B	
13: 12	1-70, A	FILE	Name of file containing the point-wise background. The first line in this file is a title; the other lines each contain values for two parameters (E_i and A_i), in free format.	A file name on line 12 must follow every occurrence of line 11.
13:Last (blank)				

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
14:1	1-80, A	WHAT	"RPI Resolution" "GEEL resolution" "GELINa resolution" "NTOF resolution"	See Section III.C.3. This card set could be put into the INPut file rather than PARameter file if no values are to be varied.
14:2	1-5, A	WHAT	"BURST"	This line may be omitted.
	7, I	IP	Flag to vary P	0, 1, or 3 to keep, vary, or PUP.
	11-20, F	P	Full width at half max of burst (ns)	
	21-30, F	dP	Uncertainty on P	
14:3	1-5, A	WHAT	"TAU " (two spaces needed)	This line may be omitted, in which case line 4 is also omitted.
	6, I to 10, I	Iτ1 to Iτ5	Flags to vary τ_1 to τ_5 one flag per column	0, 1, or 3 to keep, vary, or PUP.
	11-20, F to 71-80, F	TAU1 to TAU7	τ_1 through τ_7 10 spaces for each value	These lines give parameters for τ from Eq. (III C3 a.4).
14:4	6, I	Iτ6	Flag to vary τ_6	This line is present if and only if line 3 is also present.
	7, I	Iτ7	Flag to vary τ_7	0, 1, or 3 to keep, vary, or PUP.
	11-20, F to 71-80, F	dTAU1 to dTAU7	Uncertainty on τ_1 through τ_7 10 spaces for each value	
14:5	1-5, A	WHAT	"LAMBD"	This line may be omitted, in which case line 6 is also omitted.
	6, I to 10, I	IΛ0	Flag to vary Λ_0, Λ_1, Λ_2, Λ_3, Λ_4 One space per flag	0, 1, or 3 to keep, vary, or PUP.
	11-20, F to 51-60, F	LAM0 to LAM4	Λ_0, Λ_1, Λ_2, Λ_3, Λ_4 10 spaces for each value	See Eq. (III C3 a.3) and Tables III C3 b.1 and 2 for details.
14:6	11-20, F to 51-60, F	dLAM0 to dLAM4	Uncertainties on Λ_0, Λ_1, Λ_2, Λ_3, Λ_4	This line is present if and only if line 5 is also present.

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
14:7	1-5, A	WHAT	"A1 " (That's "A One, blank blank blank")	This line may be omitted, in which case line 8 is also omitted.
	6, I to 10, I	IAA1 to IAA5	Flag to vary a_1, a_2, a_3, a_4, a_5 (one space per flag)	0, 1, or 3 to keep, vary, or PUP.
	11-20, F to 71-80, F	AA1 to AA7	Values for a_1, a_2, a_3, a_4, a_5, a_6, a_7 from Eq. (III C3 a.5) 10 spaces for each value	See Eq. (III C3 a.5) and Tables III C3 b.1 and 2 for details.
14:8	6, I	IAA6	Flag to vary a_6	This line is present if and only if line 7 is also present.
	7, I	IAA7	Flag to vary a_7	
	11-20, F to 71-80, F	dAA1 to dAA7	Uncertainties on a_1, a_2, a_3, a_4, a_5, a_6, a_7	
14:9	1-5, A	WHAT	"EXPON"	This line may be omitted (in which case line 10 is also omitted).
	6, I to 10, I	IT0, IA1 to IA5	Flag to vary t_0, A_2, A_3, A_4, A_5 One space per flag	
	11-20, F to 51-60, F	T0, A2 to A5	Values for t_0, A_2, A_3, A_4, A_5 from Eq. (III C3 a.2) 10 spaces for each value	See Eq. (III C3 a.2) and Tables III C3 b.1 and 2 for details. If lines 11 and 12 are present, the value for A_3 given here will be ignored. Likewise, when lines 13 and 14 are present, the value for A_5 given here will be ignored.
14: 10	11-20, F to 51-60, F	dT0, dA2 to dA5	Uncertainties on t_0, A_2, A_3, A_4, A_5 10 spaces for each value	This line is present if and only if line 9 is also present.
14: 11	1-5, A	WHAT	"A3SQE" or "A3 " ("A 3 blank blank blank")	This line may be omitted, in which case line 12 is also omitted and A_3 is equal to the value given in line 9.
	6, I to 10, I	IAA31 to IAA35	Flag to vary a_{31}, a_{32}, a_{33}, a_{34}, a_{35}. One space per flag	With WHAT="A3SQE", the value of α_3 is sqrt(E).
	11-20, F to 71-80, F	AA31 to AA37	Values for a_{31}, a_{32}, a_{33}, a_{34}, a_{35}, a_{36}, and a_{37} from Eq. (III C3 a.5), 10 spaces for each.	With WHAT="A3 ", $\alpha_3 = 1$. See Eq. (III C3 a.5) for details.

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
14: 12	6, I	IAA36	Flag to vary a_{36}	This line is present if and only if line 11 is also present.
	7, I	IAA37	Flag to vary a_{37}	0, 1, or 3 to keep, vary, or PUP.
	8, I	indicator	2 ➔ multiply A3 by sqrt(E) 0 ➔ do not	
	11-20, F to 71-80, F	dAA31 to dAA37	Uncertainties on a_{31}, a_{32}, a_{33}, a_{34}, a_{35}, a_{36}, and a_{37}	
14: 13	1-5, A	WHAT	"A5SQE" or "A5 " ("A 5 blank blank blank") See notes in next column.	This line may be omitted, in which case line 14 is also omitted and A_5 is assumed to be energy independent.
	6, I to 10, I	IAA31 to IAA35	Flag to vary a_{51}, a_{52}, a_{53}, a_{54}, a_{55}. One space per flag	With WHAT="A5SQE", the value of α_5 is sqrt(E). With WHAT="A5 ", $\alpha_5 = 1$. See Eq. (III C3 a.5) for details.
	11-20, F to 71-80, F	AA51 to AA57	Values for a_{51}, a_{52}, a_{53}, a_{54}, a_{55}, a_{56}, and a_{57} from Eq. (III C3 a.5), 10 spaces each	
14: 14	6, I	IAA56	Flag to vary a_{56}	This line is present if and only if line 13 is also present.
	7, I	IAA57	Flag to vary a_{57}	
	8, I	indicator	2 ➔ multiply A5 by sqrt(E) 0 ➔ do not	
	11-20, F to 71-80, F	dAA51 to dAA57	Uncertainties on a_{51}, a_{52}, a_{53}, a_{54}, a_{55}, a_{56}, and a_{57}	
14: 15	1-5, A	WHAT	"XXPON"	This line may be omitted. Line gives values for extra exponential terms Eq. (III C3 a.2).
	6, I	IB1	Flag to vary B_1	
	7, I	IB2	Flag to vary B_2	0, 1, or 3 to keep, vary, or PUP.
	11-20	B1	Value for B_1	See Section III.C.3.a.
	21-30	B2	Value for B_2	If zero, lines 16 and 17 must be given. If not zero, this is the value for B_2.
	31-40	dB1	Uncertainty for B_1	
	41-50	dB2	Uncertainty for B_2	

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
14: 16	1-5, A	WHAT	"XXPON"	This line and the next are present only if B_2 is zero in line 15.
	6, I to 10, I	IBI1 to IBI5	Flag to vary b_{i1}, b_{i2}, b_{i3}, b_{i4}, b_{i5}. One space per flag	0, 1, or 3 to keep, vary, or PUP.
	11-20, F to 71-80, F	BI1 to BI7	Values for b_{i1}, b_{i2}, b_{i3}, b_{i4}, b_{i5}. b_{i6}, and b_{i7}, 10 spaces for each.	See Eq. (III C3 a.2) for details.
14: 17	6, I	IBI6	Flag to vary b_{i6}	This line is present if and only if line 16 is also present.
	7, I	IBI7	Flag to vary b_{i7}	
	11-20, F to 71-80, F	dBI1 to dBI7	Uncertainties on b_{i1}, b_{i2}, b_{i3}, b_{i4}, b_{i5}. b_{i6}, and b_{i7}	
14: 18 etc.	Repeat Lines 15-17 for a total of 5 times at most.			
14: 19	1-5,A	WHAT	"BINS "	Continuously varying channel width (bins per decade of energy). (Line may be omitted; line must be omitted if line 20 is included.) See Section III.C.3.a.
	6-10, I	Nbinpd	1 < Nbinpd < 99999	
14: 20	1-5, A	WHAT	"CHANN"	Channel crunch boundaries. (Line may be omitted. Line cannot be present if line 19 is present.)
	7, I	ICH	Flag to vary c	0, 1, or 3 to keep, vary, or PUP.
	11-20	ECRNCH	Highest energy for this channel width c (eV)	See Section III.C.3.a.
	21-30	CH	Values for c (ns)	
	31-40	dCH	Uncertainty for c (ns)	
14:21... Repeat line 20 as many times as needed. Lines 19 and 20 cannot be used together.				
14:Last (blank)				

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
14a:1	1-80, A	WHAT	"`RPI Transmission resolution function`", or "`RPI Capture resolution function`", or "`GEEL DEFAUlts`", or "`GELINa DEFAUlts`", or "`NTOF DEFAUlts`"	See Section III.C.3. This card set could be put into the INPut file rather than PARameter file if no values are to be varied
14a:2	1-5, A	WHAT	"`BURST`"	This line may be omitted.
	7, I	IP	Flag to vary P	0, 1, or 3 to keep, vary, or PUP.
	11-20, F	P	Full width at half max of burst (ns)	
	21-30, F	dP	Uncertainty on P	
14a:3 to 14a:18		Default values for RPI transmission or capture (as defined in Table III C3 b.1), or for Geel or nTOF (as defined in Table III C3 b.2), will be used. No input is needed here.		
14a: 19	1-5,A	WHAT	"`BINS` "	Continuously varying channel width (bins per decade of energy). (Line may be omitted; line must be omitted if line 20 is included.) See Section III.C.3.a.
	6-10, I	Nbinpd	1 < Nbinpd < 99999	
14a: 20	1-5, A	WHAT	"`CHANN`"	Channel crunch boundaries. (Line may be omitted; line cannot be used if line 19 is used.)
	7, I	ICH	Flag to vary *c*	0, 1, or 3 to keep, vary, or PUP.
	11-20	ECRNCH	Highest energy for this channel width *c* (eV)	See Section III.C.3.a.
	21-30	CH	Values for *c* (ns)	
	31-40	dCH	Uncertainty for *c* (ns)	
14a:21...Repeat Line 20 as many times as needed. Lines 19 and 20 cannot both be included.				
14a:Last (blank)				

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
15:1	1-80, A	WHAT	"`DETECtor efficiencies`"	See Section III.E.5. This card set could be put into the INPut file rather than PARameter file if no values are to be varied.
15:2	1-10, F	PARDET (1)	Detector efficiency appropriate for these spin groups	If more than 29 spin groups are needed, insert "−1" in Columns 79-80 and continue on the next line with five columns for each entry. When there are more than 99 spin groups altogether, use 5 columns for each integer entry in this line .
	11-20, F	DELDET (1)	Uncertainty on this detector efficiency	
	21-22, I or 21-25, I	IFLDET (1)	Flag whether to vary this detector efficiency	
	23-24, I or 26-30, I	IGRDET (1,1)	Number of the first spin group belonging to this isotope	
	25-26, I or 31-35, I	IGRDET (2,1)	Number of second spin group belonging to this isotope	
	etc.			
15:3	1-5, I	IGRDET (29,1)	Number of next spin group belonging to this isotope	This line is present only if the final entry on line 3 is "−1"
	2-10, I	IGRDET (30,1)		
	Etc.			
15:4	Repeat line 2 (and 3 if needed) for second (third, etc.) detector efficiency. Any spin groups which are not included in this listing will be assigned the final efficiency given in the list.			
15:Last	(blank)			

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
16:1	1-80, A	WHAT	"`USER-Defined resolution function`"	See Section III.C.5. This card set could be put into the INPut file rather than PARameter file if no values are to be varied.
16:2	1-5, A	WHAT	"`BURST`"	Line is optional.
	7, I	IFBRST	Flag to indicate whether burst width is to be varied	0, 1, or 3 to keep, vary, or PUP.
	11-20, F	BURST	Value of square burst width (ns)	
	21-30, F	dBURST	Uncertainty on burst (ns)	
16:3	1-5, A	WHAT	"`CHANN`"	Channel crunch boundaries. (Line is optional.)
	7, I	ICH	Flag to vary *c*	0, 1, or 3 to keep, vary, or PUP.
	11-20	ECRNCH	Highest energy for this channel width *c* (eV)	See Section III.C.5.
	21-30	CH	Values for *c* (ns)	
	31-40	dCH	Uncertainty for *c* (ns)	
16:4,5...	Repeat Line 3 as many times as needed			
16:6	1-5, A	WHAT	"`FILE=`"	
	6-75, A	NAME	Name of file containing user-defined resolution function	
16:7,8...	Repeat Line 6 as many times as needed			
16:Last	(blank)			

Table VI B.2 (continued)

C:L	P, T	Variable Name	Meaning (units)	Notes
Last A :1	1-80, A	WHAT	"`COVARiance matrix is in binary form in another file`" (See Table VIIB.1)	The *output* parameter file makes use of this alternative. An *input* parameter file using this alternative must be accompanied by an input covariance file, either generated by an earlier SAMMY run or read from an ENDF File 32. NOTE: If card set "Last A" is used, it is the only version of card set "Last" that is permitted.
Last B :1	1-80, A	WHAT	"`EXPLIcit uncertainties and correlations follow`"	NOTE: It is permissible to use card sets "Last B", "Last C", and "Last D" together in the same SAMMY PARameter file. If card set "Last B" is used, values specified here will override any uncertainty values given anywhere else. It is recommended that this card set *not* be used for PUPped parameters, because information given here will be lost once Bayes' equations are solved and a SAMMY.COV file has been made. In particular, a misleading value will be generated for the final chi-squared value after fitting a data set. Use this card set only for varied parameters, not for PUPs.
Last B:2	1-5, I	NN		See notes at the end of this section for detailed meaning of these parameters.
	6-10, I	MM		
	11-15, I	KK		
	16-20, I	LL		
	21-30, I	VV		
Last B:3 etc		Repeat line 2 as many times as needed		
Last B:Last		(blank)		

Table VI B.2 (continued)

C:L	P,S	Variable Name	Meaning (units)	Notes
Last C:1	1-80, A	WHAT	"`RELATive uncertainties follow`"	Give uncertainties for some resonance parameters. If card set "Last C" is used, values specified here will override uncertainty values given anywhere else except those in "Last B".
Last C:2	1-11, F	E_λ (1)	Resonance energy, *exactly* as it appears in card set 1 above	
	12-22, F	RU(1,1)	Relative uncertainty on resonance energy	
	23-33, F	RU(2,1)	Relative uncertainty on Γ_γ	
	34-44, F	RU(3,1)	Relative uncertainty on Γ_{c1}	
	45-55, F	RU(4,1)	Relative uncertainty on Γ_{c2}	
	56-66, F	RU(5,1)	Relative uncertainty on Γ_{c3}	
	68, I	JU(1,1)	Flag specifying whether to use this uncertainty for E_λ	= 1 [use relative uncertainty given by RU(i,1)]. = 0 [use either the uncertainty given elsewhere, or use the default value].
	70, I	JU(2,1)	Flag to use this unc. for Γ_γ	
	72, I to 76, I	JU(3,1) to (5,1)	Flag to use this unc. for Γ_{cx}	
	77-86	x	If negative, there is a continuation line for more channels	
Last C:3	12-22, F	RU(6,1)	Relative uncertainty on Γ_{c4}	Include as many as of the channels as needed here; there is no need to include trailing lines which contain only zeros.
	23-33, F	RU(7,1)	Relative uncertainty on Γ_{c5}	
	34-44, F	RU(8,1)	Relative uncertainty on Γ_{c6}	
	45-55, F	RU(9,1)	Relative uncertainty on Γ_{c7}	
	56-66, F	RU(10,1)	Relative uncertainty on Γ_{c8}	
	68, I to 76, I	JU(7,1) to (10,1)	Flag to use this unc. for Γ_{cx}	Repeat this line as needed.
Last C:4 etc		Repeat Lines 2,3 as many times as needed		
Last C:Last		(blank)		

Table VI B.2 (continued)

C:L	P,S	Variable Name	Meaning (units)	Notes
Last D:1	1-80, A	WHAT	"`PRIOR uncertainties follow in key word format`"	Give uncertainties for some resonance parameters, in key word format. Examples are given in test case tr151. In all cases below, an equal sign must appear between the key word and the value of the parameter.
Last D:2	Valid key word for uncertainty: `RELAtive uncertainty`. The absolute uncertainty will be the product of this value times the absolute value of the parameter. Other valid key words for uncertainty: `ABSOlute uncertainty` or `UNCErtainty`. These are both treated as absolute uncertainties. To give an energy range, use key words `EMIN` or `EMAX` followed by equal sign and value. This uncertainty will be applied only to parameters for resonances within this energy range. (Warning: a zero-value will be interpreted as undefined. To give values of `EMIN` or `EMAX` as zero, use instead a small but non-zero value.) To specify which parameters will have this uncertainty, two options are available; one or more of these can be used with each value of uncertainty. (1) Use key word `GRoup` followed (after equal sign) by a single group number, or by the word "All" (which indicates that this uncertainty applies to resonances in all spin groups). On the same line, use key word `CHannel` followed (after equal sign) by one or more channel numbers, and/or by the key word `Energy` or `Gamma` (indicating, respectively, the resonance energy and the capture width). <u>Caution</u>: SAMMY will not read beyond column 80 on a line. If there are too many channels to fit everything on the same line, it is possible to simply repeat the `GRoup` information with the remainder of the `CHannel` numbers on an additional line. Another option is to put all of the `GRoup` and `CHannel` information on a line separate from the other key word information.				

Table VI B.2 (continued)

C:L	P,S	Variable Name	Meaning (units)	Notes
Last D:2 cont.	(2) If quantum numbers were defined using the particle-pair option, then it is possible to use the key word `PP` or `PARTicle pair` followed (after equal sign) by the name of the particle pair exactly as given in the INPut (or PARameter) file. Use key word "`L`" or "`Orbital angular momentum`" followed by an equal sign and one or more integer values (separated by commas or spaces), to specify the spin groups and channels (those with this particle pair and these values of angular momentum) for which this uncertainty should apply. It is possible (though not necessarily practical!) to use `PP=Energy` or `PP=gamma` to give the uncertainty on resonance energies or capture widths. In this case, values of *l* need not be given, and the uncertainty is assumed to apply to all spin groups. Conflicting input is permitted here. In the case of conflicts, SAMMY will assume that the **first** uncertainty to be specified is the one to be used. See Table VI B.1 for a simple itemization of valid key words.			
Last D:3 etc	Repeat Line 2 as many times as needed.			
Last D:Last	(blank)			

Table VI B.2 (continued)

NOTES for card set "Last B", `Explicit covariance` information.

For `EXPLIcit` input of parameter uncertainties, values for variables NN, MM, KK, LL, and VV are described here. Explicit uncertainties need not be given for every parameter, but only for those for which the default value appears inadequate. Also note that uncertainties associated with parameters of most card sets may be provided along with values for those parameters. When that option is available, it is the preferred method of input.

(a) To explicitly input the initial (prior) uncertainty on resonance parameters, find the number of the resonance (i.e., count lines in card set 1 in this file). That number is "NN" and goes in columns 1-5, right-adjusted. The value of MM for columns 6-10 is 1 if the parameter of interest is E_λ, 2 if $\Gamma\gamma$, 3 if Γ_{c1}, 4 if Γ_{c2}, , and so on. KK and LL are zero. VV then represents the *absolute* value of the uncertainty for this parameter, in the same units as the parameter itself.

(b) To explicitly input the prior uncertainty on R-external parameters, set NN = (100 plus IGROUP), where IGROUP is the group number. Let MM = 1 for E_α^{down} , 2 for E_α^{up}, 3 for $R_{con,\alpha}$, 4 for $R_{lin,\alpha}$, 5 for $c_{con,\alpha}$, 6 for $c_{lin,\alpha}$, and 7 for $R_{q,\alpha}$, all for channel 1. If using "card set 3" to input R-external for channel 2, use MM = 6, 7, 8, 9, 10, and for channel 3, use MM = 11, 12, 13, 14, 15. If using "card set 3a," use MM = 8, 9, 10, 11, 12, 13, 14; for channel 3, use 15 through 21. The absolute value of the uncertainty on that parameter is then given by VV.

(c) To explicitly input the prior uncertainty on broadening parameters, the preferred method is to specify uncertainties along with values in card set 4. To use the EXPLIcit option, set NN = 2000 + n, where n = 1 for radius, 2 for effective temperature, 3 for sample thickness, and so on. (MM is irrelevant here.) The absolute uncertainty on that parameter is VV.

(d) To explicitly input the prior uncertainty on normalization or background parameters , the preferred method is to use card set 6. To use the EXPLIcit option, set NN = 3000 + n, where n = 1 for ANORM, n = 2 for BACKA, and so on. VV is the absolute uncertainty on that parameter.

(e) To explicitly input the prior uncertainty on the radii, the preferred method is to use card set 7a. To use the EXPLIcit option with card set 7, set NN = 4000 + n, where n is the radius pair number (i.e., the "line number," minus one, in card set 7). Also set MM = 1 for potential scattering radius, MM = 2 for the channel radius, or MM = 1 if the two radii are treated as identical. VV is the absolute uncertainty on the radius. (No uncertainty is permitted on the mass AWRI.)

(f) To explicitly input correlations between the uncertainties on two parameters, let NN and MM indicate the first parameter, as in (a) through (e) above. The second parameter is indicated by KK and LL (analogous to NN and MM, respectively). The correlation coefficient is then given by VV. Note that VV is in the range from −1 to +1.

Table VI B.3. Format of the PARameter file when spin group information is included here

Comment 1: Except for header lines, all information in this file can be found either in the table describing the INPut file or in the table describing the original PARameter file.

Comment 2: When this option is used, the command "`QUANTUM NUMBERS ARE in parameter file`" must be present in card set 3 of the INPut file.

Header Line?	Contents of line
yes	`PARTIcle pair definitions` (first five characters required)
	Card set 4 from the INPut file (Table VI.A.1), ending with a blank line.
yes	`SPIN GROUPs` (first ten characters required)
	Card set 10.2 from INPut file, ending with a blank line
yes	`RESONances are listed next` (first five characters required)
Remainder of the file is identical to original PARameter file (starting with card set 1)	

VI.C. THE DATa and Data CoVariance FILES

Several possible formats are offered for inputting experimental data into the current version of SAMMY; these are described in Subsection VI.C.1. ASCII versions include the original (MULTI-style) data file with three data points per line, a format consistent with CSISRS data, and a 20-significant-digit format to meet the need for high precision.

Several different options are provided for input of the data covariance matrix (DCM). One commonly used method is to assume that the DCM contains only diagonal components, in which case the uncertainty (square root of the diagonal covariance matrix element) provided in the DATa file is used. As discussed in Section IV, this is not the optimal treatment of data uncertainties, as it is not the correct treatment for the important systematic experimental uncertainties. Instead, the user is encouraged to use one or another of several forms for including off-diagonal data covariance information.

The DCM may be calculated external to SAMMY and provided explicitly in ASCII format, as described in Section VI.C.2. When using this "explicit DCM" option, the user must take great care to ensure that as many significant digits as possible are printed in the file in order to avoid numerical difficulties in the calculations.

A better option is for the user to provide the components of the DCM, as discussed in Section VI.C.3. This is preferable to the explicit DCM, for two reasons: (1) The input is both shorter and simpler for the user to generate. (2) Internal to SAMMY, matrix manipulation can be accomplished via the efficient "implicit data covariance" treatment as described in Section IV.

Finally, components of the off-diagonal DCM often are derived from uncertainties on parameters that are directly involved in the SAMMY analysis (e.g., the normalization or the resolution-function parameters might be viewed as contributing to the DCM). In these cases, there is now an option in SAMMY to simply flag these parameters with the number "3" to indicated that these are PUPs (Propagated Uncertainty Parameters). SAMMY will then make use of the uncertainties on the PUP'd parameters in deriving the implicit data covariance matrix. Details are discussed in Section IV.D.2.

VI.C.1. Experimental Data

The original format for the DATa file is shown in Table VI C1.1; this version is borrowed directly from MULTI [GA74]. Three data points, including energy, experimental value for cross section (or transmission, eta, etc.), and relative uncertainty appear on each line. Energies may be ordered from high to low or low to high, but the ordering must be monotonic. The data file may contain points that are not within the range [EMIN,EMAX] specified for this run; such points will be ignored (or, possibly, used for determining the auxiliary grid. See Section III.A).

A second ASCII format permits one data point per line, in (3F11) or (3E11) format, with uncertainties being absolute (rather than relative as in the "original" format). To use this option, the phrase "`USE CSISRS FORMAT FOr data`" or an equivalent must appear in card set 3 of the INPut file (See Table VI A1.2).

A third ASCII format is useful when many significant digits are needed (e.g., when comparing cross sections calculated by SAMMY with those calculated by other codes). This format has one data point per line, in (3F20) or (3E20) format, and uncertainties are absolute. The phrase "`USE TWENTY SIGNIFICAnt digits for experimental data`" (or simply "`TWENTY`") must appear in card set 3 of the INPut file (Table VI A1.2).

The energies and cross sections from an ENDF/B File 3 listing may be used for the "experimental data" in a SAMMY run. The command for this option is "`USE ENDF/B ENERGIES and cross sections MAT=`abcd", in which "abcd" is replaced by the ENDF MAT (material) number. See test case tr086 for examples.

For ORNL-ORELA staff and others who use the plotting package FORODF [JC78] with their version of SAMMY, there are several possible methods of supplying data in ORELA Data Format (ODF): For the first, you must specify "`DATA ARE IN ODF FILE`" in card set 3 of the INPut file (see Tables VI A.1 and VI A1.2). In this ODF data file, section 1 contains the energy (which can be either high-to-low or low-to-high), section 2 contains the data, and 3 contains the absolute uncertainty. Use of this alternative is discouraged, because SAMMY handles it awkwardly, copying to a temporary file in the usual DATa file format of Table VI C1.1. See test case tr005 for an example using this option.

The second ODF format is the "standard ODF format," for which you must specify "`DATA ARE IN STANDARD odf format`" in your input file. In this ODF file, unlike the version in the previous paragraph, the energies must be ordered high to low. Again energies are stored in section 1, data in section 2, and absolute uncertainties in section 3. The standard ODF file contains additional sections not in the other version: sections 4, 5, and so forth are used to store the partial derivatives of the data with respect to the data-reduction parameters. (See Section III.E.3 of this report for a discussion of data-reduction parameters.) Note that section 4 of the ODF file must correspond to data-reduction parameter number 1, section 5 to parameter number 2, etc. As with all varied parameters, initial values are given in the PARameter file (card set 8 of Table VI B.2). This method has not been used very much and will likely be dropped in future releases.

Two options are available for specifying differential elastic scattering data. The first is via an ODF file. Section 1 of this file contains the energy; section 2, the measured cross sections for the first angle; section 3, the absolute uncertainties on the cross sections in section 2; sections 4 and 5, the cross sections and uncertainties for the second angle; and so forth. In general, section $2n$ contains data for the nth angle; and section $2n+1$ contains the uncertainties. Angles are specified in the INPut file, card set 8 (see Table VI A.1). (This option has seen little use and will likely be dropped in future revisions.)

The second option for differential elastic data is via an ASCII file, all in (8F10.1) format, with at least two lines per energy. The first line contains the energy in the first ten columns, cross section at first angle in columns 11-20, cross section at second angle in columns 21-30, etc.; if there are more than seven angles, the eighth appears in columns 1-10 of the next line. The second line (or set of lines) is blank in columns 1-10, contains the (absolute) uncertainty in the cross section at the first angle in columns 11-20, uncertainty for the second angle in columns 11-20, etc.; again, if there are more than seven angles, then values for the 8th and subsequent angles are on additional lines, beginning in column 1. These two (sets of) lines are repeated once for each energy. To use this option, it is necessary to include the phrase "`DIFFERENTIAL DATA ARE IN ascii file`" in the INPut file. See test cases tr033, tr043, tr109, and others for examples.

Table VI C 1.1. MULTI-Style Format for the DATa file

Line	Column	Variable	Format	Meaning (units)
1,2,etc.	1-15	$ENERGY_1$	F15	Energy (eV)
	16-30	$DATA_1$	F15	Experimental cross section (barns), transmission, yield, or other type of data
	31-37	$FRACT_1$	F7	Fractional uncertainty in $DATA_1$
	38-52	$ENERGY_2$	F15	
	53-67	$DATA_2$	F15	
	68-74	$FRACT_2$	F7	
	75-89	$ENERGY_3$	F15	
	90-104	$DATA_3$	F15	
	105-111	$FRACT_3$	F7	

Note that although F formats are specified above, input can be in either E or F format. Numbers must, however, be within the columns specified, and a decimal point is required. If using E format, the exponent is in the right-most columns.

VI.C.2. Explicit Data Covariance Matrices

Two types of options for off-diagonal data covariance matrices (DCM) are available within SAMMY. The first, which is labeled "explicit," is treated as a regular off-diagonal covariance matrix; see the description of Bayes' equations, Section IV. Use of the explicit data covariance matrix thus requires inversion of an $N \times N$ array, where N is the number of data points.

The second, "implicit" data covariance matrix (described in Section IV.A.1.a), makes use of the specific mathematical form for the covariance matrix,

$$V = v + g\, m\, g^t \quad , \qquad \text{(VI C2.1)}$$

where v is the diagonal statistical portion, m is the covariance matrix for the data-reduction parameters, and g represents the partial derivatives of the theoretical values with respect to the data-reduction parameters. (See Section IV.D for more details.) With the implicit DCM, the components (v, g, and m) are provided to the code; V itself is not needed. The implicit DCM is treated by a more sophisticated mathematical process that does not require inversion of such a large matrix. See Section VI.C.3 for input details for the implicit DCM.

When either formulation could be used, the implicit is recommended because the implementation is far more efficient and often more accurate.

Table VI C2.1 shows the format for a Data CoVariance (DCV) file, to be included when each covariance matrix element is given explicitly. The name of this file must be specified in card set 3 of the INPut file (Tables VI A.1 and VI A1.2) in columns 31-40 of the line reading "`DATA COVARIANCE FILE is named ...`" Because the matrix is symmetric, only the lower triangular half of this matrix is given in the file; matrix elements are read across the columns, as illustrated here.

V11				
V21 ➔	V22			
V31 ➔	V32 ➔	V33		
V41 ➔	V42 ➔	V43 ➔	V44	
V51 ➔	V52 ➔	V53 ➔	V54 ➔	V55

When creating an explicit DCV file, it is important to provide as many significant digits as possible for each matrix element, in order to ensure reasonably accurate results and avoid numerical problems associated with singular matrices.

Occasionally it may be convenient to introduce a constant on- and off-diagonal data covariance in the neighborhood of a non-*s*-wave resonance, permitting effective decoupling of any underlying l = 0 state from the non-*s* waves. This is effective because an additive constant covariance is mathematically equivalent to a constant, coherent correction term for either the data or the theory. (Algebraic details are presented in Appendix A of the original SAMMY report [NL80].) This type of off-diagonal data covariance matrix can be generated automatically by SAMMY; details for input are given in Table VI A1.2 under the category "Experimental data – input control for covariance matrix" and in card set 1, columns 68 to 80, of Table VI B.2.

Another type of explicit off-diagonal data covariance matrix that can be automatically generated by SAMMY is of the form

$$V_{ij} = \bar{V}_{ij} + \left(a + bE_i\right)\left(a + bE_j\right) \quad , \qquad \text{(VI C2.2)}$$

where $\bar{V}_{ij}$ is provided by the user, E_i is the energy for data point i, and a and b are constants chosen by the user. This type of covariance is useful if there are energy-dependent coherent uncertainties in the data, for example, if a subtracted background is imperfectly known. Input for this option is given in card set 7 of Table VI A.2, and the "Input Control" statement "`DATA HAS OFF-DIAGONAL contribution ...`" of Table VI A1.2.

Table VI C2.1. Format of the data covariance file

This file contains the lower triangular half of the matrix, reading across the columns

Line	Column	Variable	Format	Meaning
1	1-10	VARDAT(1,1)	F10.1	Variance for data point 1
2	1-10	VARDAT(2,1)	F10.1	Covariance between data points 1 and 2
	11-20	VARDAT(2,2)	F10.1	Variance for data point 2
3	1-10	VARDAT(3,1)	F10.1	Covariance between data points 1 and 3
	11-20	VARDAT(3,2)	F10.1	Covariance between data points 2 and 3
	21-30	VARDAT(3,3)	F10.1	Variance for data point 3
4	1-10 ...	VARDAT(4,1)	F10.1	
		etc.		
…				
Last	1-10 ...	VARDAT(Last,1)	F10.1	
		etc.		

Note that the ordering of data points is **low** to **high** (independent of the ordering in the DATa file), and <u>only</u> those data points actually used in the calculation can be referenced in the DCV file. A maximum of eight matrix elements are to be included on one line; thus, "line number 11," for example, will actually be two lines, with eight numbers on the first and three on the second.

VI.C.3. Implicit Data Covariance (IDC) Matrices

The data-reduction process, which is generally performed by the experimentalist who measured the data, includes background subtraction and normalization, as well as other corrections (for deadtime, self-shielding, etc.). This process introduces systematic errors, which lead to an off-diagonal data covariance matrix (DCM). This off-diagonal portion of the DCM should be included along with the diagonal portion (statistical errors) in the analysis process.

As described in Section IV (*The Fitting Procedure*) and, in particular, Section IV.D.3 (*Implicit Data Covariance Matrix*), it is possible for SAMMY to treat data covariances without actually ever generating, storing, or inverting the complete off-diagonal DCM. There are several possibilities for inputting the necessary information into SAMMY.

The Propagated Uncertainty Parameter (PUP) option is described in detail in Sections IV.D.1 and IV.D.2. Input for PUPs is discussed in Section VI.C.3.a.

A second option for input of data covariance information is for the user to externally generate the pieces *g* (derivatives with respect to data-reduction parameters) and *m* (covariance matrix for the data-reduction parameters) of the DCM. See Section VI.C.3.b for details.

Finally, in Section VI.C.3.c, SAMMY's original version of IDC methodology is discussed. Though this option is still available, in practice it provides the exact same results as the PUP method and is somewhat more awkward to use.

VI.C.3.a. Input for propagated uncertainty parameters

The Propagated Uncertainty Parameter (PUP) option is described in detail in Sections IV.D.1 and IV.D.2. Essentially, the PUP method takes any of the SAMMY parameters (either R-matrix parameters or parameters from the experiment-related corrections to the cross sections) and incorporates the uncertainty on that parameter into the data covariance matrix (DCM). The value of the parameter is held fixed.

As indicated in Table VI B.2, SAMMY input parameters generally have both a flag and an uncertainty associated with them. If that flag is zero, the parameter is treated as a constant and the uncertainty is ignored. When the flag is 1, the value of that parameter is refined ("fitted" or "searched on") during the analysis process; the uncertainty is taken as the "prior" uncertainty on that parameter (unless, of course, a prior COVariance file is used). If the flag is 3, the parameter value remains fixed, but the uncertainty becomes a component of the DCM.

Nearly all the data-related card sets of the PARameter file (Table VI B.2) can now be inserted into the INPut file (see the end of Table VI A.1). When the card set is in the INPut file, flags = 1 will be ignored but flags = 3 will be honored.

Sometimes it is desirable to provide an off-diagonal covariance matrix for the PUP'd parameters. For example, the set of resolution-function parameters may be determined altogether, by fitting a functional form to measured data; those parameters are then correlated. To input such information to SAMMY, create an ASCII file containing the following information:

1. A title on the first line.
2. A line containing "Number of parameters = #", where # is replaced by the integer number of PUP parameters for which covariances will be provided. [In fact, only the equal sign and the number are absolutely necessary on this line.]
3. One or more lines containing the exact values of the PUPs, in free-format. These values must be within 0.1 % of the actual value of the parameters as given in the PARameter or INPut file. (Caution: if there are two PUPs whose values are nearly identical, and it is the second one that you are intending to use here, SAMMY might misinterpret the information. To avoid this problem, include the first PUP, and all in between, in the PUP covariance matrix.)
4. One or more lines containing the lower triangular covariance matrix elements for those parameters (reading across the matrix from the left-hand side to the diagonal in the usual SAMMY fashion), in free format.

It is NOT necessary to include every PUP in this file, but those that are included must be consecutively located in the SAMMY.LPT listing; that is, the PUP numbers inside the pointed brackets must be consecutive, as in <6> and <7>. For example, one might have a covariance matrix for the resolution-function parameters but wish to PUP the Doppler width plus the normalization and background parameters as well. See test case tr168 for examples.

To use the PUP covariance file in a SAMMY run, include the phrase "PUP COVARIANCE IS IN an ascii file" in the command section of the INPut file.

It is possible to use SAMMY to generate PUP covariance information and write it into a file to be used as input for subsequent runs. For example, to predetermine resolution-function parameters, a SAMMY run (or series of runs) might be made on "clean" data with well-defined resonance parameters. Only the resolution parameters would be flagged. The command "CREATE PUP FILE FROM varied parameters used in this run" would be included in the INPut file for this run (or for the final run of the series). The output file SAMPUP.COV is in the appropriate format for use as the input PUP covariance file for future runs. Again, see test case tr168 for an example of this.

Caveat: The implementation of the PUP covariance input option is new and has not been extensively tested. Because there are so many possibilities for parameters to be PUP'd, it has not been possible for the author to test each and every potential combination. The user is therefore strongly advised to carefully examine the SAMMY.LPT output file to be sure that the PUP covariance matrix information has been properly interpreted by the code. In particular, look at the array printed following the phrase "Correlation matrix for PUPped parameters" and check that the uncertainties and correlations correspond to the appropriate PUPs.

For sequential runs in which the varied-parameter COVariance file from one run is used as input to the next run, values and uncertainties for varied parameters cannot be modified. (The exception is via the use of program SAMAMR; see Section X.C.) However, values and uncertainties for PUPs can be modified, since they are associated with the data set rather than with the parameters whose values are being determined. (The exception is that the treatment of R-matrix parameters may not be changed during a sequence of runs.) If the user wishes to be certain that values for PUPs do not change, s/he can insert the command "DO NOT ALLOW VALUES for data-related parameters to change" into the INPut file.

R-matrix parameters should <u>not</u> be PUP'd during sequential runs: One of the assumptions underlying the use of sequential analysis is that the data sets being analyzed are completely independent of each other, that is, they are not united via a common DCM. Therefore, if a parameter (e.g., a channel radius) is PUP'd for two data sets, the associated components of the DCM uniting the two data sets will be ignored. This would violate the assumption of independent data sets. The same is also true for simultaneous runs of two or more data sets, as described in Section IV.E.1, because the scheme described there also assumes that the data sets are independent.

It is expected that future development work will provide a means of properly including the effect of a PUP'd variable that connects two otherwise-independent data sets.

VI.C.3.b. User-supplied implicit data covariance matrix

After reducing experimental data from raw counts to a form resembling a cross section, the experimentalist has available all information needed to produce the covariance matrix for the reduced data. This covariance matrix would have the form given in Eq. (IVD.1):

$$V_{ij} = v_i \, \delta_{ij} + \sum_{kk'} g_{ik} \, m_{kk'} \, g_{jk'} \qquad \text{(VI C3 b.1)}$$

where g_{ik} is the partial derivative of the expression for data point *i* (in terms of the measured quantity and the data-reduction parameters) with respect to data-reduction parameter *k*. The covariance matrix for the data-reduction parameters is *m*. (For a concrete example of this, see the paper by Gunsing [FG98] detailing the derivation of the covariance matrix for data measured at the GELINA facility.)

Rather than generating the entire covariance matrix *V*, the SAMMY user can prepare a file containing the partial derivatives that SAMMY will then use for the Implicit Data Covariance Matrix. The SAMMY INPut file should contain the command "USER-SUPPLIED IMPLICIt data covariance matrix", and the name of the file must be given directly after the name of the data file.

The format for the user-supplied implicit data covariance file is as shown in Table VI C3 b.1.

Examples

For examples on the use of IDC, see test cases tr070, tr118, and tr140. Case tr118 contains equivalent examples of normalization and background included in the fitting (case a), implicit covariance matrix (cases c and i), user-supplied implicit data covariance matrix (cases g and h), and explicit data covariance matrix (case j).

Table VI C3 b.1. Format for user-supplied IDC file

Card set: Line	Variable	Meaning
1:1	Alpha	At least the first two characters (and the equal sign) of the phrase "`NUmber of data-reduction parameters =`", followed by an integer number *K* which indicates how many partial derivatives are to be read. Example: NU=7
1:2	(blank)	
2:1	Alpha	At least the first ten characters of the phrase "`PARTIAL DErivatives`" or "`FREE-FORMAt partial derivatives`"
2:2	X(i,1)	If "`PARTIAL DErivatives`", then the *K* partial derivatives for the first data point, eight values per line, continuing on the next lines if needed, in 8F10 format, or If "`FREE-FORMAt partial derivatives`", then this line contains the energy, the statistical uncertainty on the first data point, and the *K* partial derivatives for the first data point, in free format
2:3	X(i,2)	The *K* partial derivatives for the second data point in 8F10 format, or Energy, statistical uncertainty, and partial derivatives in free format
etc.		
2: *N* + 1	X(i,*N*)	The *K* partial derivatives for the *N*th data point (where *N* is the total number of data points in the SAMMY run), in 8F10 format. Energy, statistical uncertainty, and *K* partial derivatives, in free format.
2: *N* + 2	(blank)	
3:1	Alpha	At least the first ten characters of the phrase "`UNCERTAINTies on data-reduction parameters`". NOTE: This card set is optional and may be omitted if the uncertainties are multiplied into X, that is, if X(i,k) from card set 2 contains X_k^i times the square root of w_k rather than just X_k^i itself.
3:2	X(i,1)	Uncertainties for the *K* data-reduction parameters, continuing on the next lines if needed. Format is 8F10 or free-format as specified in card set 2, line 1.
3: 3	(blank)	
4:1	Alpha	At least the first ten characters of the phrase "`CORRELATIOns for data-reduction parameters`". This card set is optional and may be omitted if values for the data-reduction parameters were independently determined (i.e., if parameters are uncorrelated).
4:2	C(1,2)	Correlation between parameter number 1 and parameter number 2. Format is F10 or free format, as specified in card set 2 line 1.
4:3	C(1,3), C(2,3)	Correlation between parameters 1 and 3, and between 2 and 3; format is 2F10 or free format.
etc.		
4: *K* + 1	C(*i*,*K*)	Correlation between parameters *i* (for *i* = 1 to *K*−1) and *K*, in 8F10 format or free format, continuing on additional lines if needed.
4: *K* + 2	(blank)	

VI.C.3.c. Implicit data covariance for normalization and background

To determine the covariance matrix due to the background and normalization corrections, SAMMY assumes that the "corrected" data *D* and the "original" data *R* are related via

$$D(E) = \frac{R(E) - b(E)}{a} \quad , \qquad \text{(VI C3 c.1)}$$

in which *a* and *b* are defined as in Section III.E.3.a (*Explicit Normalization and/or Background Functions*). Note that for the IDC, corrections are applied to the experimental data and therefore are opposite to those applied to the theory as in Section III.E.3.a.

Values and uncertainties (as well as possible correlations) for the normalization and background parameters should be determined by the experimentalist. However, the analyst may find it necessary to apply further corrections to the data. In this case, the analyst can run SAMMY, including normalization and/or background functions in the parameter file with the parameters flagged (varied) in order to determine the correct values for the parameters. The next step would be to produce a modified data file; this step can be accomplished with SAMMY by including a command line "`REFORMULATE DATA FOR implicit data covariance`" in the INPut file. SAMMY will then produce a file SAMMY.DA2 in the same format as the analyst's DATa file, with the data values corrected according to Eq. (VI C3 c.1). Note that uncertainties in this data file will not be changed (except to divide by the normalization *a*, if the uncertainties in the file are absolute rather than relative): This file, like the original, contains only statistical, but not systematic, errors. SAMMY will also produce a file SAMMY.IDC that contains the normalization and broadening information, and a new parameter file SAMMY.PA2 identical to the analyst's PAR file except for the absence of the normalization and broadening information. The uncertainties in SAMMY.IDC can then be modified (or added) to be the proper experimental uncertainties on the normalization and broadening parameters, to be used in further SAMMY runs.

In subsequent SAMMY runs for that data set, the INPut file contains the command line "`IMPLICIT DATA COVARIance matrix is to be used`." SAMMY then looks for the IDC file, which uses the same formats as portions of the PARameter file. In particular, card set 6 (`NORMAlization and background`) and card set 13 (`BACKGround functions`) can be included in this file; see Section III.E.3.a for a description of these functions. Any correlations between values should also be given here, using again the formats of the PARameter file for `EXPLIcit uncertainties` (card set Last, alternative B).

NOTE: This use of the implicit data covariance (IDC) with normalization and background parameters was the earliest implementation of the more general IDC construction, as outlined in Section IV.D.3. The PUP concept (Section IV.D.2) is applicable to more parameter types, and is easier for the analyst to use but (when used with the same parameters) gives identical results to the original normalization-and-background IDC described in this section. It is likely, therefore, that this original version will eventually be phased out. Analysts are encouraged to use the PUP option instead.

VI.D. INTEGRAL DATA FILE

When the data type is specified as "INTEGral quantities" (see card set 8 of the INPut file), two kinds of data files are needed. The first is an experimental *differential* data file, which is used only to generate the energy grid on which the integrals are to be calculated; the type of data and values of the cross sections in this file are ignored. The second kind of data file contains the experimental integral data and is designated as the "NTG" file.

In the NTG file, each type of integral data is specified by a unique five-character name, which is given in Columns 1 to 5 of the appropriate line. Names can be either uppercase or lowercase, and the ordering is arbitrary. Only those data types for which experimental measurements exist need to be specified; others can simply be omitted from this file.

Table VI D.1 shows the various types of integral data available in SAMMY. Note that underscore _ in a name denotes a blank space.

When the INPut and PARameter files specify more than one nuclide (isotope), SAMMY will calculate the integral quantities for each nuclide separately, ignoring the abundances specified in INPut and/or PARameter files. Integral data are assumed to be for a specific nuclide; *it is important to note that the ordering of the nuclides must be the same in the NTG file as in the PAR file.*

Correlations between experimental data are also given in the NTG file.

Table VI D.1. Types of integral data

Name as used in NTG file	Description
THABS, THFIS, THCAP	Absorption, fission, or capture cross section, respectively, at thermal energy (E = 0.0253 eV)
MXABS, MXFIS, MXCAP	Maxwellian average absorption, fission, or capture cross section
WGABS, WGFIS, WGCAP	Westcott's *g* factor for absorption, fission, or capture cross section
RIABS, RIFIS, RICAP	Resonance integral for absorption, fission, or capture cross section
AVABS, AVFIS, AVCAP	Average integral for absorption, fission, or capture cross section
WATTS	Watt spectrum average
K1_ _ _	[v (MXFIS) - (MXABS)] 2 / $\sqrt{\pi}$
ALPHA	α = (RICAP) / (RIFIS)
NJALF	NJOY's α
NJETA	NJOY's η

The name of the integral data file is given directly after the name of the differential data file, in the "interactive input to SAMMY." Details for the format of the NTG file are given in Table VI D.2.

Table VI D.2. Format of the NTG file

Line No.	Column	Variable Name	Meaning
1	1-70	TITLE	Title for the file; is printed in LPT file but never used
2	1-5	NUCLID	Nuclide number (default = 1); nuclides must be in the same order as in PAR file
3, 4, etc.	1- 5	WHAT	Type of integral data, from list in Table VI D.1
	11-20	DATA	Experimental value for this data type
	21-30	UNC	Experimental uncertainty for this data type
	31-40	CONST	For resonance integral data, CONST is the maximum energy for integrand, and CONST2 is the remainder to be added to the integrated value For average integral data, CONST is the lower limit on the integral and CONST2 the upper For K1, CONST is the value of v For Watt spectrum average, CONST = *a* and CONST2 = *b*
	41-50	CONST2	
5		(blank)	
6, etc.			Repeat lines 2 through 5 as many times as needed
7		(blank)	
8	1-5	WHAT	CORRElations follow
9	1-5	WHAT1	Type of integral data
	6-10	NUC1	Nuclide number
	11-15	WHAT2	Type of integral data
	16-20	NUC2	Nuclide number
	21-30	CORR	Correlation between data of type WHAT1 for nuclide number NUC1, and WHAT2 for Nuc2
10, 11, etc.			Repeat line 9 as many times as needed
12		(blank)	

VI.E. INTERACTIVE INPUT TO SAMMY

SAMMY was designed to run interactively, with the user supplying appropriate responses to questions asked by the code. A command file may be prepared, containing the interactive input.

Table VI E.1 lists the questions asked by SAMMY for a simple run and describes appropriate responses. For detailed examples of more complicated runs, see the SAMMY test cases as discussed in Section XII.B. For each test case, the command file for Unix or Linux runs is "testxyz" (where "xyz" is the 3-digit test case number). Equivalent command files for Windows runs are called "test.bat".

The maximum length for a file name to be used as input to SAMMY is 70 characters.

Table VI E.1. Input for a typical SAMMY run starting with a new parameter file

SAMMY Prompt	User Response
1. What is the name of the input file?	INPut file name plus extension, for example, AAAAAA.INP*. Maximum number of characters is 70.
2. What is the name of the parameter file?	PARameter file name, for example, AAAAAA.PAR*. Maximum number of characters is 70.
3. What is the first data file name? EMIN? EMAX?	DATa file name, for example AAAAAA.DAT*, followed by the minimum and maximum energies (in EV) for this step in F format, separated by commas or spaces. The decimal point must be included, or the program may misinterpret your input. EMIN and EMAX need not be repeated here if they are given in the INPut file, card set 2, Table VI A.1. If they are in both places, values given here are used.
4. What is new EMIN? EMAX? Data file name?	Energy range (in eV) for the next step, in F format, separated by commas or spaces. If EMIN = 0.0 and EMAX = 0.0 (i.e., if you simply hit "return" or include a blank line in the command file), then the program will terminate. If the data file name is blank, the previous DATa file is assumed.
5. Repeat Step 4 as needed, ending with a blank line.	

* File names are chosen for convenience, with extensions INP, PAR, and DAT used to indicate the type of file. SAMMY users may make different choices for extensions, or use none at all.

VI.F. OTHER INPUT FILES FOR SAMMY

In addition to the INPut, PARameter, and DATa files, several special-purpose input files exist for various options available in SAMMY. These are discussed in the following sections:

1. The AVG file, described in Section VI.F.1, contains the energy ranges for calculation of multigroup cross sections.

2. In order for SAMMY to generate output in appropriate formats for the Evaluated Nuclear Data Files (ENDF), ENDF-specific information is required. This is provided in the NDF file, described in Section VI.F.2.

3. ENDF Files 2 and/or 32 are sometimes used as input to SAMMY. See Section VI.F.3 for details.

4. The calculation of Maxwellian or stellar-averaged capture cross sections requires information about which temperatures are to be used for the calculation. Section VI.F.4 provides information about this input file.

5. The Crystal Lattice Model of Doppler broadening requires additional input, as shown in Section VI.F.5.

VI.F.1. The AVeraGe File

In Section V.C, descriptions are given of the way SAMMY can be used to produce energy-averaged, time-averaged, Bondarenko-averaged, or unweighted energy-averaged cross sections and the associated covariance matrix. To invoke these options, alphanumeric command lines must be included in the INPut file. For energy- or time-averaging (Section V.C.1), the command is

```
AVERAGE OVER ENERGY ranges.
```

For Bondarenko averaging, the command is

```
GROUP AVERAGE OVER Energy ranges, or
BONDARENKO AVERAGE Over energy ranges.
```

For unweighted energy-averaging, the command is

```
UNWEIGHTED ENERGY Average, or
ENERGY-AVERAGE USINg constant flux
```

One or more additional files are required, which are denoted the AVG (AVeraGe) files or BON (BONdarenko) files; their names are given to SAMMY as interactive input (see Table VI E .1), directly following the name of the first data file, or, if a COVariance file is used, directly after the name of the COVariance file . Formats for AVG files are given in Table VI F1.1, and for the BON files in Table VI F1.2. The two types of files follow very much the same format, except the BON files require additional input parameter values. For unweighted energy-averaging, either file may be used (the "TYPE" line is ignored).

For all types of multigroup averaging, it is possible to print the partial derivatives (sensitivities) of the multigroup cross sections with respect to the resonance parameters and to print the associated multigroup covariance matrix. The command

```
PRINT AVERAGED SENSItivities for endf parameters
```

will cause the creation of several files, all in ASCII format:

SAMAVG.COV contains the multigroup covariance matrix.

SAMSEN.DAT contains partial derivatives of all multigroup cross sections with respect to resonance parameters of the five lowest-lying resonances. These derivatives are with respect to the *p*-parameters (see Section IV.C) rather than *u*-parameters, that is, with respect to the "endf parameters" as suggested in the command line.

SAMMY.LLL contains the same information as the multigroup-average portion of the SAMMY.LPT file, but in reverse energy order to facilitate comparison with results from some processor codes.

SAMMY.MGS contains the multigroup cross section (and nothing else), again in reverse energy order, to facilitate porting to spreadsheets for comparisons with output from other codes.

Table VI F1.1. Format of the AVG file

Line Number	Col-umn	Variable Name	Format	Meaning (units)	Possible Values	Notes
1	1-80	TITLE	A80			
2	1-10	TYPE	A10	Type of averaging to be used	"`ENERGY-AVErage`" or "`TIME-AVERAge`"	energy- or time- average
3	1-10	EMIN	F10	Minimum energy for this range (eV)		
	11-20	EMAX	F10	Maximum energy for this range (eV)		If EMAX = 0, use EMAX equal to the value given for EMIN on the next line
4, 5, ...	(repeat line 3 as many times as needed)					
last	(blank)					

Table VI F1.2. Format of the BONdarenko file

Line Number	Col-umn	Variable Name	For-mat	Meaning (units)	Possible Values	Notes
1	1-80	TITLE	A80			
2	1-10	TYPE	A10	Type of averaging to be used	"BONDA RENKO"	Currently this is the only option; others may be added later
3	1-10	EMIN	F10	Minimum energy for this range (eV)		
	11-20	EMAX	F10	Maximum energy for this range (eV)		If EMAX = 0, use EMAX equal to the value given for EMIN on the next line
4,5,...	(repeat Line 3 as many times as needed)					
6	(blank)					
7	1-10	TYPE	A10	Type of parameters to be used	"BONDA RENKO"	Again this is the only option; others may be added later
8	1-10	EBONDA(1)	F10	Energy (eV)		
	11-20	BONDAR(1)	F10	Value of $C(E)$ at E = EBONDA(1)		Eq. (VC2.2)
	21-30	SIG000	F10	σ_0		Eq. (VC2.2)
9	1-10	EBONDA(2)	F10	Energy (eV)		
	11-20	BONDAR(2)	F10	Value of $C(E)$ at E = EBONDA(2)		
10, 11,...	(Repeat line 9 as many times as needed. Value of $C(E)$ is interpolated linearly between the points specified.)					
last	(blank)					

VI.F.2. Input to Produce Files in ENDF File 2 or File 32 Format

SAMMY is capable of converting information obtained from the usual SAMMY INPut and PARameter files (plus a modest amount of additional input) into ENDF File 2 format, in several of the many versions of that format. To invoke this option, the following line must be included in the INPut file:

```
ENDF/B-VI FILE 2 IS wanted
```

(This may be shortened to "ENDF" if desired.)

One additional file is required, denoted the "ndf" file, whose name is supplied to SAMMY in the site in which SAMMY would normally expect the DATa file name (see Section VI.E). Contents of this file are shown in Table VI F2.1.

There is a more convenient version of the ndf file, which is used when the INPut file contains the command line

```
NDF FILE IS IN KEY-Word format
```

This is the preferred version for the ndf file. Formats for the file are key word based; see Table VI F2.2 for details. Below are two examples of key word files:

^{235}U	^{23}Na
Z=92 A=235 Isotope # 1 Spi=7.5 L=0,Group=1,2	Z=11 A=23 Mat=1125 Isotope=1 Spin=1.5 L=0,GROUP=1,2 L=1,GROUP=3,4,5,6,7,8 L=2,GROUP=9,10,11,12,13,14,15,16

In either case, SAMMY will produce a file called SAMMY.NDF, which contains the appropriate lines for ENDF/B File 2. See test cases tr023, tr086, tr126, tr137, tr154 for examples.

In SAMMY.NDF, resonance energies are given in F format, to as many significant digits as possible within the limitation of eleven columns. Widths are given in E format, with, however, the "E" suppressed and the exponent given as one digit if possible.

To produce ENDF File 32 (covariance matrix for resonance parameters), include the command

```
PUT COVARIANCE MATRIx into endf file 32
```

Only the key word version of the ndf file is acceptable for this option. Parameters such as "`LCOmp`", "`DIAgonal`" and "`DEfault uncertainty`" are relevant here; see Table VI F2.2. The output file, to be used as ENDF File 32, is called SAMMY.N32.

When the command DEBUG is given in the INPut file, then additional "annotated" files will be produced by SAMMY, to aid the reader in understanding what is where in the ENDF file. The file SAMMY.NDX is identical to file SAMMY.NDF, except that it also contains annotations (lines beginning with #) describing the information in the file. Similarly, the file SAMMY.N3X is identical to the first portion of SAMMY.N32 except for the annotations.

NOTE: The ENDF File 2 LRF=3 convention for the angular momentum parameter AJ is as follows: AJ is defined as $\pm J$, where the sign denotes the channel spin s; AJ = $-J$ denotes $s = I - i$, with $i = 1/2$ for neutron; AJ = $+J$ denotes $s = I + i$. This is in compliance with the format change approved by the Cross Section Evaluation Working Group at the 1999 meeting [ENDF 99].

CAUTION: SAMMY's original implementation of the LRF=7 format was not entirely correct for 0^- nuclides; the negative parity was not specified properly. To the best of the author's knowledge, no official ENDF files were created with this version of SAMMY. Nevertheless, anyone using very early examples of LRF=7 ENDF files for 0^- nuclides should check to be certain that the file behaves as expected.

Table VI F2.1. File needed for generating ENDF File 2 output

Card Set	Line number	Variable	Format	Notes
1	1	ZA AWR	F F	These are ENDF variables, and thus follow the ENDF-6 rules for determining their values. Often, but not always, ZA has the value (1000 * Z + A). AWR is the ratio of the mass of the sample to the neutron mass; the default value is AW/*aneutron*, where AW is the mass as given in the SAMMY INPut file and *aneutron* is the mass of the neutron. In general, it is recommended that the default value be used for AWR.
		LRF	I	LRF specifies which ENDF format and which R-matrix approximation are to be used; LRF = 3 (Reich-Moore) is default. Caution: The ENDF LRF=3 format permits only a limited subset of the Reich-Moore capability as implemented in SAMMY.
		MAT	I	ENDF MAT number (default = 9999).
2	1	SPI(1) ZAI(1) ABN(1) AWRI(1)	F	These are also ENDF-6 variables and are defined, respectively, as the ground-state spin, the (Z,A) value, the abundance, and the ratio of the isotopic mass to that of a neutron. Use of the default for AWRI(i) is again recommended: AW/*aneutron*, where AW is the value given in the SAMMY files and *aneutron* is the mass of a neutron.
	2	LENDFG(1,1)	I	Angular momentum for the first ENDF spin group
		KENDFG(1,1,1) KENDFG(2,1,1) . . .	I I	SAMMY spin groups belonging to this ENDF spin group. There may be more than one SAMMY group per ENDF group, since ENDF LRF = 3 groups consist of energy-ordered sets of all resonances with the same *l*, while SAMMY groups are defined by both J and *l*. SAMMY will check that the specified groups have the correct *l*, and print an error message if they do not.
	3	LENDFG(i,1)	I	Angular momentum *l* for ith group (2nd, 3rd, etc.)
		KENDFG(1,i,1) KENDFG(2,i,1) . . .	I I	SAMMY groups belonging to this ENDF group
	4	Repeat Line 3 as many times as necessary		
	Last	(blank)		
3	Repeat card set 2 as many times as necessary, once for each nuclide/isotope			

Table VI F2.2. Key-word-based file needed for generating ENDF File 2 output

For each key word used, only those few characters written as capitals in the table are required; those in lowercase are optional. Key words may be given as capitals or in lower-case or in mixed case

Card set	Key word variable	Notes
1	`Z`	Z for target nucleus
	`A`	Atomic mass number
	`ZA`	If different from (1000 * Z + A), then this value must be inserted directly
	`AWr`	Ratio of the mass of the sample nucleus to the neutron mass. AWR is the ratio of the mass of the sample to the neutron mass; the default value is AW/*aneutron*, where AW is the mass as given in the SAMMY INPut file and *aneutron* is the mass of the neutron. In general, it is recommended that the default value be used for AWR.
	`Mat`	ENDF MAT number (default = 9999)
	`MT`	ENDF reaction number, for file 3 output
	`LRF`	Which ENDF file 2 format and which R-matrix approximation are to be used (1=SLBW, 2=MLBW, 3=RM, 7=RML). If LRF is not specified, SAMMY will choose the appropriate value.
	`LCOmp`	Which ENDF file 32 format is to be used: LCOMP = 0 can be used only for LRF = 1 or 2; results are not guaranteed to be correct. Use of this format is discouraged. LCOMP = 1 can be used for LRF = 1, 2, 3, or 7, or for URR. LCOMP = 2 (“compact”) can be used for LRF = 1, 2, 3, or 7, or for URR. However, this format should be used with extreme caution as it is a relatively crude approximation. Caution: The format for LCOMP = 1, LRF = 7, is not yet an official ENDF format.
	`NDigit`	Number of digits to be used for LCOMP = 2. Only NDigit = 2 is an approved ENDF format.
	`DIAgonal`	If LCOmp = 1 and DIAgonal = `Yes`, then only the diagonal pieces of the covariance matrix will be specified in File 32.
	`NUmber`	Number of energies to be included (for URR only)
	`E`	Energy (for URR)

Table VIF.2 (continued)

Card set	Key word variable	Notes
1 cont.	`DEfault uncertainty` *`or`* `DU`	Relative uncertainty for unflagged parameters. The value of the uncertainty to be printed in File 32 is this value times the value of the parameter.
	`FLagged`	Only resonances with flagged parameters (flag = 1) will be included in file 32. (No value needs to be given here.)
	`ALl`	All resonances are to be included in file 32. (No value needs to be given here.)
	`(blank)`	Terminate this card set with a blank line.
2	`ISOtope or NUClide`	(No value needs to be given here.)
3	`Z`	Z for target nucleus (this isotope)
	`A`	Atomic mass number (this isotope)
	`ZA`	If different from (1000 * Z + A), then this value must be inserted directly.
	`AWr`	Ratio of the mass of the sample nucleus (this isotope) to the neutron mass. Again, it is recommended that the default value be used rather than giving the value here explicitly.
	`ABn`	Abundance for this isotope
	`SPin`	Ground state spin for this isotope
	(blank)	Terminate this card set with a blank line.
4	`L`	Orbital angular momentum for this ENDF spin group. On the same line, give key word "`GROUP`" and specify the SAMMY group numbers that contribute to this *l* for this isotope. Example: `L=0, Group=1,2,3`
5	Repeat card set 4 as many times as needed, ending with a blank line.	
6	Repeat from card set 2 through 5, as many times as needed. (CAUTION: The author does not guarantee that the program will work properly for more than one isotope.)	
7	`SHort`	For LCOMP = 1, LRF = 3, the "short-range section information" follows this line; see the ENDF-102 description of File 32 input for details. Be sure that at least two blank lines precede this line.

Table VIF.2 (continued)

Card set	Key word variable	Notes
8	`N`	Ordinal number for this short-range section. (This number is for your use only, so the value need not be correct.) On the same line, give key word "`Spin group`" and specify the ordinal numbers for the spin groups to be included in this section. Example: `N=1  S=1,3,4`
9	energy range	On the line immediately following card set 8, give the energy range (minimum to maximum) for resonances to be included in the short-range section. No key word is required, but an equal sign must be present. Example: `Energy range = -10.  20.`
10	Repeat card sets 8-9 as many times as needed. End with a blank line.	

VI.F.3. Using ENDF File 2 as input to SAMMY

Instead of manually creating a SAMMY-type PARameter file and an entire SAMMY-type INPut file, a user may retrieve resonance parameters (File 2) from the Evaluated Nuclear Data Files (ENDF) Library at the National Nuclear Data Center [NNDC] and use that file directly as input to SAMMY. The first portion of a SAMMY-type INPut file is still required; this file contains card sets 1–8 but no others (see Table VI A.1). Included in card set 3 of the INPut file must be the line

```
INPUT IS ENDF/B FILE  MAT=abcd  ,
```

in which "`abcd`" is to be replaced by the ENDF MAT (material) number. The name of the ENDF/B file is included in the input stream where the name of the PARameter file is called for.

Prior to Release M6 of the SAMMY code, it was necessary for the user to edit the ENDF file and extract File 2 for the material of interest. This is no longer needed; SAMMY will now search through a long ENDF file and use the relevant portion. However, if the command line reads only

```
INPUT IS ENDF/B FILE
```

without the MAT number, then SAMMY will assume (as in the past) that the ENDF file contains only File 2 for the material of interest.

With either of the commands given above, only resonance parameters and spin-group quantum numbers are retrieved from the ENDF File 2. If the energy range from the ENDF file is to be used for the SAMMY run, then the command

```
USE ENERGY RANGE FROm endf/b file 2
```

is given in the INPut file.

(Note that additional commands may be required for the experimental data and associated energy grid. In general, the user must provide a separate file for the experimental data in the customary fashion as described in Section VI C.1.)

Output from a run using an ENDF file for input includes several additional files not usually found in SAMMY output. The first is SAMNDF.INP which is a SAMMY-type INPut file containing the spin group information in card set 10.1 format. The second, SAMNDF.PAR, is a SAMMY-type PARameter file containing the resonance parameter information from the ENDF file, translated into SAMMY formats. These two files can then be modified as needed and used for subsequent SAMMY runs.

A third member of this list of additional output files is SAMQUA.PAR, a PARameter file that contains quantum number information as well as resonance parameters. See Table VI B.2 for a detailed explanation of this file.

Caveat # 1: Only isotopic ENDF files can be used as input for SAMMY runs. For example, one could use the file for ^{28}Si but not the file for natural silicon.

Caveat # 2: The file SAMNDF.INP contains a command (card set 3) specifying which type of R-matrix approximation was used for the ENDF file. For example, if the ENDF File 2 indicates LRF=1, then the resonance parameters were determined by a procedure that used the single-level Breit-Wigner approximation; SAMNDF.INP therefore will contain the command line "`SLBW FORMALISM IS WANTED`". Similarly LRF = 2 indicates multilevel Breit Wigner, and LRF = 3 indicates the ENDF Reich-Moore approximation.

If the intent of the user is simply to use SAMMY to create a plot of the evaluated cross sections, then the SAMMY runs should indeed use the same approximation as was used to define the ENDF file.

However, if the intent is to use the ENDF File 2 parameters as starting values for analysis of new data, or for a new evaluation, then the user is encouraged to modify (or remove) the command in the INPut file for subsequent runs. New analyses should use the Reich-Moore approximation, which is the default option for SAMMY.

VI.F.4. Format of the MXW File

In order to generate stellar (Maxwellian) averages of capture cross sections (see Section V.D), two pieces of input are needed. In the alphanumeric portion (card set 3) of the INPut file, the line

```
MAXWELLIAN AVERAGED capture cross sections are wanted
```

or

```
STELLAR AVERAGED CAPture cross sections are wanted
```

must be included (the two phrases are treated identically within the code). It is also necessary to specify the temperatures at which the stellar averages are to be calculated; these are given in a "MXW" file whose name is specified immediately following the name of the DATa file in the input stream. The format of the MXW file is one temperature per line, in F10.1 format, in units of eV.

When calculating stellar averages, it is often desirable to include cross sections at energies above the resolved resonance region. In SAMMY, this may be done by providing the "smooth cross section" in the ENDF File 3 format. Users must also include the following line

```
ADD CROSS SECTIONS From endf/b file 3
```

in the alphanumeric portion of the INPut file.

For users unfamiliar with ENDF formats, a description of the relevant portions of File 3 is presented in Table VI F4.1. Note that the parameter INT specifies an interpolation scheme for NBT energy points. For INT = 1, the cross section from E_i to E_{i+1} is constant and equal to C_i. For INT = 2, the cross section for $E_i < E < E_{i+1}$ is linearly interpolated between the two values. (Note that other options are available in ENDF but only these two have been implemented in SAMMY.)

Examples for stellar averaging are given in test cases tr042, tr049, and tr051.

Table VI F4.1. Format for File 3 cross sections to be added for stellar averages
A decimal point must occur somewhere with an F format

Line Number	Variable	Col-umns	Format	Notes
1	(Nothing on this line is important to SAMMY runs)			
2	NR	45-55	I11	Number of energy regions
	NP	56-66	I11	Total number of energy points to be specified
3	NBT(1)	1-11	I11	Number of energy points in region 1
	INT(1)	12-22	I11	Interpolation type for region 1 (INT=1 implies constant, INT=2 implies linear; contact the SAMMY author if other options are needed.)
	NBT(2)	23-33	I11	Number of energy points in region 2
	INT(2)	34-44	I11	Interpolation type for region 2
	NBT(3)	45-55	I11	Number of energy points in region 3
	INT(3)	56-66	I11	Interpolation type for region 3
4,5, ...	Repeat Line 3 until all NR regions have been specified. Note that the sum of the NBT values must equal NP.			
6	E(1)	1-11	F11	First energy value
	C(1)	12-22	F11	Value of cross section at energy E(1)
	E(2)	23-33	F11	Next energy value
	C(2)	23-44	F11	Value of cross section at energy E(2)
	E(3)	45-55	F11	Next energy value
	C(4)	56-66	F11	Value of cross section at energy E(3)
7,8,...	Repeat Line 6 until all NP energy points have been specified			

VI.F.5. Crystal-Lattice Model File

The crystal-lattice model of Doppler broadening, discussed in Section III.B.4, requires additional input beyond that needed by other Doppler models:

(1) In the INPut file, include one of these alphanumeric commands:
`USE CRYSTAL LATTICE model of doppler broadening` or `CLM`

(2) Provide the location/name of the CLM file in the input stream, directly after the name of the DATa file.

The format for the CLM file is given in Table VI F5.1, where we have again used the convention that "C:L" implies "card set number: line number" and the notation "f-f " refers to "free format."

Table VI F5.1. Format of the SAMMY CLM file (crystal-lattice model)
Note: "f-f" indicates "free-format"

C:L	Variable Name	Format	Possible Values	Default Value	Meaning
1:1	Title	A80			Alphanumeric title
2:1	Mode_ S_Norm	f-f integer	0 or 1	0	Mode of normalization 0 ➔ do not correct the S function 1 ➔ correct the S function
	Nphon	f-f integer	> 0		Phonon-expansion order
	Sub	f-f real	> 0.0	1.0	Number of subdivisions between the spectrum points for beta mesh
	Xdop	f-f real	> 0.0	1.0	Initial Doppler cut of beta mesh
	Eps	f-f real	> 0.0, small	0.08	Precision over normalization and sum rule check of scattering law
	Epsc	f-f real	> 0.0, small	0.001	Precision of convolution integral calculation
2:2	(blank)				
3:1	What	A5	CONTI		Continuous distribution parameters follow
3:2	Del_Phonon	f-f real	> 0.0		Interval (in eV) between points of the phonon distribution

Table VI F5.1 (continued)

C:L	Variable Name	Format	Possible Values	Default Value	Meaning
3:2, cont.	N_Cont	f-f integer	0 or > 0		If greater than zero, line 3 in card set 3 is in free-form real; N_Cont is the number of points to be read. If equal to zero, line 3 is in fixed format (8F10.1); SAMMY will count the number of points.
3:3	Phonon(i)	f-f real, or 8F10.1			Phonon distribution, uniformly spaced in energy
3:4	(blank)				
4:1	What	A5	`DISCR`		Discrete mode parameters follow. (This card set may be omitted.)
4:2	N_Osc	f-f integer	0 or > 0		If > 0, lines 3 and 4 are free-form real and there are N_Osc values to be read. If = 0, or if this card is absent, Lines 3 and 4 are fixed format (8F10.1) and SAMMY will count how many values there are.
4:3	Osc_Eng(i)	f-f real or 8F10.1			Energies (eV) for discrete mode oscillators
4:4	Osc_Wts(i)	f-f real or 8F10.1			Weights for discrete mode oscillators
4:5	(blank)				
5:1	What	A5	`TRANS`		Translational parameters follow (This card set may be omitted.)
5:2	Twt	f-f real			Translational weight
	C_Trans	f-f real			Diffusion constant
	Tbeta	f-f real		1.0	Normalization for continuous part

VII. OUTPUT FROM SAMMY

The output from SAMMY is presented in two or more files, depending on the control parameters set in the INPut file (card set 3 of Table VI A.1). Table VII.1 summarizes those output files; no guarantees are made that the list is complete. The ordering in the table is somewhat arbitrary, beginning with the most commonly used files.

In the table, unit numbers correspond to those used within the FORTRAN of SAMMY. Most SAMMY users will have no need for this information, which is included for completeness' sake. The final column of the table tells which sections and/or tables contain details about the file listed in the first column.

Table VII.1. SAMMY output files

File name and unit number	Contents	Location of details
(log file) 6	What appears on the screen in the interactive mode; system information	
SAMMY.LPT 21	Descriptive output, to be carefully examined by the analyst. ("LPT" stands for "line printer", a concept which clearly dates the origin of this code!)	Section VII.A
SAMMY.IO 70	Initial and final values of varied parameters	
SAMMY.PAR 32	PARameter output file, in same format as the initial PARameter file, in which values have been updated for the varied parameters	Table VI B.2 Section VI.B
SAMMY.COV 64	Updated COVariance matrix for the updated parameters, in binary form. Updated parameter values and other information are also included here.	Table VII B.1 Section VII.B
SAMMY.ODF 72	This is the plot file in ORELA Data Format (ODF), from which plots can be produced using utility program FORODF	Section VII.C
SAMMY.PLT 61	A "generic" binary file containing the same information as in SAMMY.ODF	Section VII.C
SAMMY.DAT 72	ODF file containing experimental data and uncertainties for angular distribution data	Section X.A

Table VII.1 (continued)

File name and unit number	Contents	Location of details
SAMMY.NDF 75	ASCII file containing resonance parameters in the format required for File 2 of the Evaluated Nuclear Data Files (ENDF/B-6)	Section VI.F.2
SAMMY.NDX 56	ASCII file identical to SAMMY.NDF, with additional descriptive information	Section VI.F.2
SAMMY.N32 55	ASCII file containing the resonance parameters in the format required for File 32 of the Evaluated Nuclear Data Files (ENDF/B-6)	Section VI.F.2
SAMMY.N3X 56	ASCII file identical to SAMMY.N32, with additional descriptive information	Section VI.F.2
SAMMY.FL3 55	ENDF File 3 (point-wise cross sections)	Section VIII.B
SAMMY.FLX 56	ENDF File 3 with additional descriptive information	Section VIII.B
SAMNDF.INP 13	SAMMY-type INPut file produced when an ENDF/B File 2 is used for resonance parameter input	Section VI.F.3
SAMNDF.PAR 12	SAMMY-type PARameter file produced when an ENDF/B File 2 is used for resonance parameter input	Section VI.F.3
SAMQUA. PAR 12	PARameter file containing spin group information, created when "PUT QUANTUM NUMBERS into parameter file" command is used. The spin group information here is in key-word particle-pair format.	
SAMMY.CCV 77	Compact parameter CoVariance matrix (uncertainties, plus correlation matrix in integer format)	Section VII.E
SAMMY.SSM 25	A binary file containing edge-effects corrections (the function Q) to single-scattering correction for capture cross sections	Section III.D
SAM012.DAT 60	Table with energy, self-shielded cross section, single-scattering correction, double-plus correction, and full multiple-scattering-corrected cross section (sum of the other three); generated via the command "`PRINT MULTIPLE SCATTering corrections`"	

Table VII.1 (continued)

File name and unit number	Contents	Location of details
SAMMY.MCR 12	Input information for Monte Carlo simulation of multiple-scattering corrections	Section X.M
SAMXAC.ODF	No longer available (replaced with SAMMY.UNB, to eliminate redundancy in the code)	
SAMMY.UNB 9	Binary file in ODF format, containing energy in Section 1 and unbroadened cross sections in other sections, created when command "`PUT UNBROADENED CROSs sections into plot file`" is invoked	
SAMUNB.DAT 9	ASCII file containing auxiliary energy grid and unbroadened cross sections in `TWENTY` format, created when command "`PUT UNBROADENED CROSs sections into plot file`" is invoked	
SAMUNX.DAT 9	ASCII file containing auxiliary energy grid and unbroadened cross sections in CSISRS format, for those cases where more than one type of cross section is available (e.g., when multiple-scattering corrections are needed)	
SAMMY.LEG 99	ASCII file containing energy and Legendre coefficients for all possible *L* for each energy in the auxiliary grid. In older versions, this file was called "legendre.dat"	
SAMMY.N04 97	Legendre coefficients in format for ENDF File 4. In older versions, this file was called "endf_legendre.dat"	Section IX
SAMJNK.DAT 96	The same information as SAMMY.LEG or SAMMY.N04, in expanded format	Section IX
SAMMY.LLL 69	Average cross sections and uncertainties	Section VI.F.1
SAMAVG.COV 29	ASCII file containing covariance matrix for multigroup average cross sections	Section VI.F.1
SAMSEN.DAT 29	Partial derivatives of averaged cross section with respect to some of the R-matrix parameters	Section VI.F.1
SAMMY.CRS 55	Multigroup average cross sections, in ENDF-like file	Section IX
SAMMY.N33 55	Covariance matrix for multigroup average cross sections, in ENDF File 33 format	Section IX

Table VII.1 (continued)

File name and unit number	Contents	Location of details
SAMMY.PUB 37	Tabulated file containing all resonance parameters and uncertainties, in a form suitable for porting to spreadsheets for formatting for publication	Section VII.F
SAMCOV.PUB 37	Tabulated file containing the calculated cross sections and the associated covariance matrix. The cross sections are "point-wise" (i.e., given at specific energies).	Section IV.E.4
SAMMY.PA2 33	Modified PARameter file when "`REFORMULATE DATA FOR implicit data covariance`"	Section VI.C.3.c
SAMMY.IDC 34	File containing normalization and background information when "`REFORMULATE DATA FOR implicit data covariance`"	Section VI.C.3.c
SAMMY.DA2 15	Modified DATa file in which normalization and background corrections have been made, when "`REFORMULATE DATA FOR implicit data covariance`"	Section VI.C.3.c
SAMCOV.PUP 40	File containing values and covariances for varied *u*-parameters (to be used as PUPs in later runs), created when the command "`CREATE PUP FILE FROM varied parameters used in this run`" is given in the INPut file	Section VI.C.3.a
SAMMY.REL 12	PARameter file in which only the "relevant" parameters have been flagged	Table VI A1.2
INPUT.NEW 22	Spin group information in the format of card set 10.1, provided as a possible alternative to the obsolete format used in the INPut file	
REMORI.PAR 25	Binary file containing original parameter file and inverse of original parameter covariance matrix, when needed for iterations with M+W method of solution of Bayes' equations	Section IV.E.3
SAMMY.YWY 32	Binary file containing contribution of one data set to the *Y* and *W* matrices needed in M+W method of solution of Bayes' equations	Section IV.E.1
SAMMY.PDS 71	Partial derivatives of the theoretical values with respect to every resonance parameter	Section VII.D

VII.A. LINE-PRINTER OUTPUT

The first two output files (the “LPT” and the “IO” files) are intended for visual inspection. The LPT file contains full output, detailed to the extent specified by the user in the INPut file (see Tables VI A.1 and VI A1.2).

The IO file merely lists initial and final parameter values.

The LPT file contains a wealth of information with which users should become familiar. Here you find, among other things,

- Input file names;
- Title for the run (taken from your INPut file);
- Values for varied and fixed parameters;
- Verbatim alphanumeric commands (with notification if the command is not recognized);
- Chronological listing of the SAMMY segments used in the run;
- Updated parameter values, uncertainties, and correlation values;
- Chi-squared values;
- Error messages, if applicable.

Sample LPT files may be found among the output for the test cases or tutorial exercises; see Section XII.

It is strongly recommended that novice SAMMY users examine the LPT file for each run, to be sure SAMMY is interpreting input as the user intended. Even experienced SAMMY users should regularly look at the LPT file, especially when output parameter values or chi-squared values are puzzling or when the run ends abnormally. Such problems are often the result of user input errors, which can frequently be discovered by comparing intended input values with the values as listed in the LPT file. In addition, the LPT file often provides error messages to guide the user into fixing an input error. Error messages are also provided for abnormal aborts for common input errors. (Please notify the author if you have suggestions for a more informative error message for your favorite mistake.)

VII.B. OUTPUT TO BE USED AS INPUT

Two output files (the "PAR" and the "COV" files) are intended to be used as input to another SAMMY run. The PAR file is as described in Section VI.B, with the "Last A" alternative chosen for the "last" card set of Table VI B.2.

In very early versions of SAMMY, the output "binary COVariance file" contained only the new (updated) covariance matrix for physical parameters (i.e., **not** for the *u*-parameters; see Section IV.C). Output parameter values were stored in the output PARameter file. When these two files were used as input to another run, the covariance matrix for the *u*-parameters was generated from Eq. (IV C.1).

Two drawbacks to this scheme led to expansion of the COV file. First, unnecessary computer time was spent in making the conversion back to *u*-parameters. Second, and more important, was the loss of precision between runs. In converting from *u*-parameters to physical parameters, storing these in ASCII format, reading them back in for the next run, and converting back to *u*-parameters, often the last several significant digits were lost. One would expect that analysis of two energy regions, first in two separate executions of SAMMY, then in one execution but still analyzing the two regions sequentially, should give identical results. With the early storage scheme, small differences occurred; with the current scheme, no discrepancies are found.

SAMMY users should keep in mind the following:

If a COVariance file is specified, SAMMY will use parameter values given in the (binary) COVariance file rather than those given in the PARameter file.

That is, all parameter values are taken from the values stored in the binary COVariance file; these values are more precise than those in the PARameter file. (See, however, the end of this section for exceptions to this rule.)

Table VII B.1 shows which variables are written in what order in the COVariance file. Dotted lines separate values kept in separate records.

Occasionally a user may wish to modify the contents of the COVariance file (and associated PARameter file), in order to de-activate a measurement-related parameter (e.g., sample thickness or Doppler temperature) and activate the comparable parameter for the measurement to be analyzed next. This may be accomplished using the program SAMAMR; see Section X.C for details.

Table VII B.1. Binary COVariance file

Variable names (with dimension in parenthesis)	Meaning
TITLE	test which version of the SAMMY code wrote this COV file
JJJJJJ(300)	array dimensions, etc.
ALLVR(NVPALL)	covariance matrix for physical parameters (*p*-parameters), stored in NVPALL separate records
VRPR(NVPALL)	covariance matrix for *u*-parameters, stored in NVPALL separate records
U(NVPALL)	values of *u*-parameters
PKEN(NRES)	resonance energies
GGA(NRES)	gamma widths
GSI(NTOTC,NRES)	particle widths
IFLRES(NTOTC2,NRES)	flags for resonance parameters. Flags are 0 if fixed, 1 ≤ flag ≤ NVPALL if parameter is varied, and NVPALL < flag ≤ NFPALL if PUP'd
IGROUP(NRES)	number of the spin group to which the resonance belongs
BETAPR(NTOTC,NRES)	(related to particle widths)
GBETPR(3,NRES)	(related to gamma widths)
BETA(NTRIAG,NRES)	(related to particle widths)
POLAR(2,NRES)	optional; fission width in polar coordinate system
IFLPOL(2,NRES)	optional; flags for polar fission widths
IFLEXT(NREXT,NTOTC,NGROUP)	flags for R-external parameters
PAREXT(NREXT,NTOTC,NGROUP)	R-external parameters
IGRRAD(NTOTC,NGROUP), PAREFF(NUMRAD), IFLEFF(NUMRAD), PARTRU(NUMRAD), IFLTRU(NUMRAD)	values of the several radii, spin groups to which they apply, and flags for radii

Table VII B.1 (continued)

Variable names (with dimension in parenthesis)	Meaning
AMUISO(NUMISO), PARISO(NUMISO), IFLISO(NUMISO), IGRISO(NGROUP)	atomic weight, fractional abundance, flags for abundances, spin groups which correspond to this isotope
PARDET(NUMDET), IFLDET(NUMDET), IGRDET(NGROUP)	detector efficiency parameters for eta measurements, flags for detector efficiencies, which detector efficiency applies to this spin group
PARBRD(NUMBRD)	"broadening" parameters
IFLBRD(NUMBRD)	flags for broadening parameters
DUM(19)	related to broadening parameters
PARMSC(NUMMSC)	values of miscellaneous parameters
NAMMSC(NUMMSC)	names of miscellaneous parameters
IFLMSC(NUMMSC)	flags for miscellaneous parameters
IRADMS(NGROUP)	radiation width number for this spin group
IJKMSC(NUMMSC-KDRCAP+1)	index for direct capture component
PARPMC(NUMPMC), IFLPMC(NUMPMC), ISOPMC(NUMPMC)	paramagnetic parameters, flags for paramagnetic parameters, which isotopes these apply to
PARORR(NUMORR)	parameters related to the Oak Ridge resolution function option
IFLORR(NUMORR)	
ECRNCH(NUMORR-11)	
ENDETS(NMDETS)	
SESESE(NMDETS)	
ESESES(NMDETS)	
SIGDTS(NMDETS)	
PARRPI(NUMRPI), IFLRPI(NUMRPI), ECRNCH(NUMRPI-NNNRPI)	parameters related to the RPI resolution function option

Table VII B.1 (continued)

Variable names (with dimension in parenthesis)	Meaning
PARUDR(NUMUDR), IFLUDR(NUMUDR), ECRNCH(NUMUDR-NNNUDR)	parameters related to the user-defined numerical resolution function option
PARBGF(NUMBGF), IFLBGF(NUMBGF), KNDBGF(NUMBGF), BGFMIN(NUMBGF), BGFMAX(NUMBGF), DIST	parameters related to the background function option
PARDTP(NUMDTP)	values of data reduction parameters
NAMDTP(NUMDTP)	names of data reduction parameters
IFLDTP(NUMDTP)	ordinal numbers for varied data reduction parameters
PARUSD(NUMUSD)	values of "unused" parameters
NAMUSD(NUMUSD)	names of unused parameters
IFLUSD(NUMUSD)	ordinal numbers for unused parameters
PARBAG(NUMBAG)	values of "baggage" parameters
NAMBAG(NUMBAG)	names of baggage parameters
IFLBAG(NUMBAG)	ordinal numbers for baggage parameters

Exceptions:

The rule that parameter values are taken from the COVariance file (if it exists) rather than from the PARameter file is violated under certain conditions:

- Certain unvaried parameters can be flagged to use values from the PAR file; see Table VI B.2 for specifics.
- Exceptions can also occur for most of the PUP'd parameters, as discussed in Section IV.D.2.
- The user may overwrite the rule, as discussed in Sections IV.E.2 and IV.E.6. The rule is often, but not always, violated when modifications are to be made to the parameter covariance matrix. To ascertain exactly which parameter values have been used, look through the LPT file for the phrase "`SAMMY-NEW`". If this phrase occurs, then the PARameter file values were used. If this phrase does not occur, then the COVariance file parameter values were used.

VII.C. PLOT OUTPUT

The output file SAMMY.ODF is in the ORELA DATA FORMAT [JC78] and is intended for use with the plotting program FORODF to produce plots of the results of SAMMY calculations. Table VII C.1 shows what is stored in each section of the SAMMY.ODF file, for the case when the experimental data are either total cross section or transmission. Table VII C.2 describes the ODF file for other types of energy-differential data, and Table VII C.3 shows the SAMMY.ODF file for angular-distribution (angle- and energy-differential) data. In the case of angular-distribution data, when the input data are provided in an ASCII file, SAMMY will produce a second output ODF file (SAMMY.DAT) that contains the experimental values; if the input data are given in an ODF file, the SAMMY.DAT file is not generated. A description of the SAMMY.DAT file is shown in Table VII C.4.

For computer systems using other plotting routines, SAMMY also provides a "generic" binary file containing the same information as that in the ODF file. See Section X.I for details on the use of this SAMMY.PLT file.

Table VII C.1. Sections of the ODF file generated by SAMMY, for transmission or total cross-section data

Sect. No.	Contents and units
1	Energy (Units are as specified by input command. If not specified, then units are eV if appropriate, otherwise keV)
2	Experimental cross section (barns)
3	Absolute uncertainty in experimental cross section (barns)
4	Zeroth-order theoretical cross section as evaluated by SAMMY (barns)
5	Final theoretical cross section as evaluated by SAMMY (barns)
6	Experimental transmission (dimensionless)
7	Absolute uncertainty in experimental transmission
8	Zeroth-order theoretical transmission as evaluated by SAMMY
9	Final theoretical transmission as evaluated by SAMMY
10 [a]	Theoretical uncertainty on section 4 if data were total cross section, or on section 8 if data were transmission
11 [a]	Theoretical uncertainty on section 5 or section 9
12 [b]	Adjusted energy initially, when t_0 and L_0 are to be varied
13 [b]	Adjusted energy finally, when t_0 and L_0 are to be varied

[a] These sections are filled only if the phrase "`INCLUDE THEORETICAL errors`" occurs in the INPut file (Table VI A1.2).
[b] These sections are filled only if t_0 and L_0 are to be varied.

Table VII C.2. Sections of the ODF file generated by SAMMY, for energy-differential data that are neither transmission nor total cross section

Sect. No.	Contents and units
1	Energy (Units are as specified by input command. If not specified, then units are eV if appropriate, otherwise keV)
2	Experimental cross section (barns)
3	Absolute uncertainty in experimental cross section (barns)
4	Zeroth-order theoretical cross section as evaluated by SAMMY (barns)
5	Final theoretical cross section as evaluated by SAMMY (barns)
6 [a]	Theoretical uncertainty on section 4 (barns)
7 [a]	Theoretical uncertainty on section 5 (barns)
8 [b]	Adjusted energy initially, when t_0 and L_0 are to be varied. See Section III.E.8 of this report
9 [b]	Adjusted energy finally, when t_0 and L_0 are to be varied. See Section III.E.8 of this report

[a] These sections are filled only if the phrase "`INCLUDE THEORETICAL errors`" occurs in the INPut file (Table VI A1.2).
[b] These sections are filled only if t_0 and L_0 are to be varied.

Table VIIC.3. Sections of SAMMY.ODF when data are angular distributions (energy- and angle-differential elastic scattering or reaction data)

Sect. No.	Contents and units
1	Energy (eV)
2	Zeroth-order theoretical cross section for the first angle (barns)
3	Final theoretical cross section for the first angle (barns)
4	Zeroth-order theoretical cross section for the second angle (barns)
5	Final theoretical cross section for the second angle (barns)
...	
$2n$	Zeroth-order theoretical cross section for the nth angle (barns)
$2n + 1$	Final theoretical cross section for the nth angle (barns)

Table VIIC.4. Sections of the ODF file SAMMY.DAT generated by SAMMY when data are angular distributions

Sect. No.	Contents and units
1	Energy (eV)
2	Experimental cross section for the first angle (barns)
3	Uncertainty on experimental cross section for the first angle (barns)
4	Experimental cross section for the second angle (barns)
5	Uncertainty on experimental cross section for the second angle (barns)
...	
$2n$	Experimental cross section for the nth angle (barns)
$2n + 1$	Uncertainty on experimental cross section for the nth angle (barns)

VII.D. COMPLETE SET OF PARTIAL DERIVATIVES FOR RESONANCE PARAMETERS

It is possible for SAMMY to generate an ASCII file containing partial derivatives of the cross sections with respect to all resonance parameters. This option was added to SAMMY for one specialized application, when the results of a SAMMY analysis were to be used as the starting point for a study of integral quantities; it is not expected to be a generally useful option for other applications.

To invoke this SAMMY option, include the statement

```
GENERATE PARTIAL DERIVATIVES ONLY
```

in the INPut file. The output file SAMMY.PDS will then be produced; contents of this file are shown in Table VII D.1.

For this file, resonance parameters are numbered as follows: First, resonances are ordered according to spin groups. Next, resonances are energy ordered within spin groups. Finally, for each resonance, the *u*-parameters associated with the energy, the reduced-gamma-width amplitude, the reduced-neutron-width amplitude, and other reduced width amplitudes (if they exist), are, respectively, the first, second, third, and possibly fourth and fifth parameters. (See Section II.D.1.e for a description of *u*-parameters for the Reich-Moore approximation.)

Table VII D.1. Contents of output file SAMMY.PDS

Line Number	Variable	Columns	Format	Meaning
1	NPAR	1-10	I10	total number of resonance parameters
2, etc.	U(1) to U(NPAR)		6G13.6	value of the parameters
3	DATA(1)	1-13	F	first experimental data value
	DELD(1)	14-26	F	uncertainty on data
	THEORY(1)	27-39	F	theoretical value for first data point
	G(1,1)	40-52	F	partial derivative of THEORY with respect to parameter number 1
	G(1,2)	53-65	F	partial derivative of THEORY with respect to parameter number 2
	G(1,3)	66-79	F	partial derivative of THEORY with respect to parameter number 3
4 etc.	G(1,4) to G(1,NPAR)		6G13.6	partial derivative of THEORY with respect to parameter number 4
5	DATA(i)	1-13	F	*i*th experimental data value
	DELD(i)	14-26	F	uncertainty on data
	THEORY(i)	27-39	F	theoretical value for *i*th data point
	G(i,1)	40-52	F	partial derivative of THEORY with respect to parameter number 1
	G(i,2)	53-65	F	partial derivative of THEORY with respect to parameter number 2
	G(i,3)	66-79	F	partial derivative of THEORY with respect to parameter number 3
6 etc	G(i,4) to G(i,NPAR)		6G13.6	partial derivative of THEORY with respect to parameter number 4
Repeat lines 5 and 6 for each data point.				

VII.E. COMPACT FORMAT FOR PARAMETER COVARIANCE INFORMATION

Existing formats for communication of covariance information are often inadequate. The sheer quantity of numbers in a typical covariance matrix prohibits storage of this information in ASCII format, and binary files are generally not transportable from one computer to another. This issue is discussed at greater length elsewhere [HD97]. SAMMY has an option for abbreviated formats for parameter covariance matrices, designated the "compact" format. This option is also available for use in the transmission of covariance information from one code to another via ENDF files; see Section IX for details.

When a binary covariance file from an earlier SAMMY run is specified as input for another run, then the inclusion of an appropriate command line will cause the creation of an output file SAMMY.CCV. (The characters CCV suggest Compact CoVariance.)

Important: It is the initial (prior) parameter covariance matrix that is written into this file. The final (posterior) parameter covariance matrix, if created by this run, is written in the usual binary format into file SAMMY.COV.

To create SAMMY.CCV in compact format, include any one of the following equivalent alphanumeric commands:

```
PUT COVARIANCES INTO compact format
PUT CORRELATIONS INTo compact format
WRITE CORRELATIONS Into compact format
WRITE COVARIANCES INto compact format
```

Within the CCV file, the covariance matrix is expressed as uncertainties plus correlation matrix. At the beginning of the CCV file, absolute uncertainties are listed for each varied parameter, in (6(1PG11.5)) format. The rest of the file specifies the non-negligible correlation matrix elements, converted to integer format.

The SAMMY compact format is directly analogous to the ENDF Compact Format (file 32, LRU=0, LCOMP=2; see Section IX). In this format, off-diagonal correlation coefficients C are mapped to integers M (which range from -99 to + 99) as follows: Define *small* as IDROPP/100, where IDROPP is an input parameter (card set 2 of the INPut file, Table VI A.1) with default value 2. Correlation coefficients in the range $-small < C < small$ are mapped to zero. Positive correlation coefficients in the range $M / 100 < C \leq (M + 1) / 100$ are mapped to M. Negative coefficients in the range $(M + 1) / 100 \leq C < M / 100$ are mapped to $-M$. Diagonal correlation coefficients always have the value +1, so they are not explicitly written in the file.

To reconstruct the (approximate) covariance matrix from the mapped values, all coefficients C mapped to positive integer M are assigned the value $c = (M + 1/2)/100$. All coefficients C mapped to negative integer $-M$ are assigned the value $c = -(M + 1/2)/100$. If $M = 0$, $c = 0$. A partial listing of values for this description is given in Table VII E.1.

Table VII E.1. Map from true correlation coefficient *C* to integer *M* and back to approximate coefficient *c* for compact format

C	M	c	C	M	c
$-1.00 \le C < -0.99$	-99	-0.995	$0.99 < C \le 1.00$	99	0.995
$-0.99 \le C < -0.98$	-98	-0.985	$0.98 < C \le 0.99$	98	0.985
$-0.98 \le C < -0.97$	-97	-0.975	$0.97 < C \le 0.98$	97	0.975
$-0.97 \le C < -0.96$	-96	-0.965	$0.96 < C \le 0.97$	96	0.965
…	…	…	…	…	…
$-0.04 \le C < -0.03$	-3	-0.035	$0.03 < C \le 0.04$	3	0.035
$-0.03 \le C < -0.02$	-2	-0.025	$0.02 < C \le 0.03$	2	0.025
$-0.02 \le C < -0.01$	-1	-0.015	$0.01 < C \le 0.02$	1	0.015
$-0.01 \le C \le 0.01$	0	0.000			

For example, a correlation coefficient whose exact value is $C = 0.7382$ is mapped to $M = 73$ and reconstructed as $c = 0.735$. The value $C = -0.2901$ is mapped to $M = -29$ and reconstructed as $c = -0.295$; if $C = -0.3000$, again $M = -29$ and $c = -0.295$.

Only the lower triangular half of the $n \times n$ correlation matrix C_{ij} is written into the SAMMY.CCV file. The first entry of a row is the row number *i*; the second, the initial column number *j*; and the following entries are the (*M*-style) correlation of parameter *i* with parameters *j* through *k* (where *k* is the lesser of $i - 1$ and $j + m - 1$, and *m* is the maximum number of such correlations that can fit on the line). If all entries on a line are zero, the line is omitted.

Several test cases contain SAMMY runs to produce the output SAMMY.CCV file and/or others that read and use the CCV file to re-generate the covariance matrix. Among them are test cases tr071, tr082, tr083, tr084, tr089, tr131, tr146, and tr149.

Use one of the following equivalent commands to read a compact format and reconstruct the parameter covariance matrix:

```
READ COMPACT COVARIAnces for prior parameters
READ COMPACT CORRELAtions for prior parameters
COMPACT COVARIANCES are to be read and used
COMPACT CORRELATIONS are to be read and used
```

SAMMY has the ability to use other than two digits (1, 2, 3, 4, 5, or 6 digits) for writing and reading the compact format (though this is not an approved ENDF format). To write SAMMY.CCV with a different number of digits, set NDIGIT in column 72 of card set 2 of the INPut file.

VII.F. PUBLICATION AIDS

While the SAMMY.LPT and the SAMMY.PAR output files both contain values for the resonance parameters, neither is presented in a manner that is suitable for publication purposes. To obtain complete resonance-parameter output that can be easily formatted for publication, include the command

`PUBLISH`, *or*

`CREATE PUBLISHABLE List of parameters`

in the INPut file. Use of these commands will cause creation of a file named SAMMY.PUB, which contains resonance parameter values and uncertainties, plus quantum number information, in columns separated by tabs. This file can easily be ported to a spreadsheet program for formatting as required.

The columns headings for the SAMMY.PUB file are shown in Table VII F.1. Within the table, resonances are ordered according to energy, from low to high.

The outline in Table VII F.2 describes (in excruciating detail) one possible method of converting SAMMY.PUB into an Excel spreadsheet formatted in a manner that might be suitable for publication in a technical manual.

Table VII F.1. Columns of SAMMY.PUB file

Column Heading	Meaning
J	πJ = parity and spin of the spin group to which this resonance belongs
L	l = Orbital angular momentum of the first channel in this spin group
Energy	Resonance energy E_λ
Unc_E	Uncertainty on the resonance energy E_λ
W_Capture	$\overline{\Gamma}_{\lambda\gamma}$ = capture width
Unc_Cap	Uncertainty on the capture width
Width_1	$\Gamma_{\lambda 1}$ = width for the incident channel
Uncer_1	Uncertainty on $\Gamma_{\lambda 1}$
Width_2	$\Gamma_{\lambda 2}$ = width for the second channel
Uncer_2	Uncertainty on $\Gamma_{\lambda 2}$
Etc.	Repeat for other widths

Table VII F.2. Converting SAMMY.PUB into a spreadsheet

1. copy SAMMY.PUB onto a Windows directory
2. bring up Excel, perhaps via
    a. Start
        i. Programs
            1. Excel
3. data (one of the menus across top of page)
    a. import external data
        i. import data
            1. all files (box at bottom)
            2. highlight the SAMMY.PUB file
            3. Open
                a. Next
                b. Next
                c. Finish
                d. OK
4. put the curser in the grey box above “1” and to the right of “A”
5. format (another of menus at top)
    a. cells
        i. number
            1. decimal places (2 or 3 or whatever)
                a. OK
6. put the curser above the “J” column
7. format
    a. cells
        i. number
            1. decimal places = 1
                a. OK
8. put the curser above the “L” column
9. format
    a. cells
        i. number
            1. decimal places = 0
                a. OK
10. put the curser in the grey box above “1” and to the right of “A”
11. format
    a. column
        i. autofit selection
12. other options of interest:
    a. to add or delete a row or column … need icons on tool bar
        i. tools/customize/command/edit/ and /insert/; move icons to tool bar
        ii. once icons are there, put curser in column or row to delete (or after position to add column or row), and click the icon
    b. to move a column
        i. highlight the column (click on letter above column)
        ii. click scissors (cut)
        iii. highlight the (empty) column into which you want to move this one
        iv. hit “enter”

VIII. UNRESOLVED RESONANCE REGION

As a first step towards expansion into the unresolved resonance region, Fritz Fröhner's code FITACS [FF89] has been obtained and inserted into SAMMY. FITACS uses Hauser-Feshbach theory with width fluctuations. The adjustable parameters are neutron strength functions, distant-level parameters, average radiation widths (at $E = 0$), and average fission widths (at $E = 0$). The energy dependence of the radiation widths is specified via the giant dipole model, of the fission widths via Hill-Wheeler fission barrier transmission coefficients, and of the mean level spacing for *s*-waves via the Gilbert-Cameron composite formula. Mean spacings for $l > 0$ are given via the Bethe formula. Moldauer's prescription is used for partial cross sections. Details of the theory are presented in Section VIII.A.

Initially (for release M2 of the code), FITACS was incorporated into SAMMY (as segments SAMFFF and SAMACS) in a limited fashion only. Internal changes were made, to be consistent with SAMMY notation and to use dynamic dimensioning of arrays. The M + W version of Bayes' method has replaced the fitting procedure used in FITACS. Calculation of penetrabilities was extended to all l values (FITACS had used only s, p, d, and f-waves). The output included files from which plots can be made. Results were reported in SAMMY.PAR in the same format as is used in the input file (as well as in more human-legible fashion in SAMMY.LPT).

Subsequently, additional modifications, improvements, and new features have been made in the SAMMY URR treatment:

- Partial derivatives with respect to varied parameters are calculated exactly rather than approximately.
- A more efficient integration routine has been written for the Dresner integral, Eq. (VIII A.5).
- It is possible to include (and vary, if desired) a normalization for each data set.
- Elastic cross section data may be fitted.
- There is no limit on the number or type of experimental data sets. Data may be kept in separate files rather than appended to the parameter file.
- The output has been modified to conform more closely to SAMMY conventions.
- An "annotated" PARameter file, including key-word-based input, is the default input option, and the only option available for output. (Files in the original format can still be used for input, but options are limited with that format.)
- Different sets of average resonance parameters can be used in different energy ranges.

- Output can be produced in ENDF/B format, for both File 2 (resonance parameters) and File 32 (covariance matrices). ENDF files cannot be used for input, because the ENDF format requires a more limited theoretical description than does FITACS/SAMMY.

- The fitting procedure can be performed sequentially, in similar fashion as in the resolved resonance region. That is, output PARameter and COVariance files from the fit to one data set may be used as input to another run which fits another data set. [Initially, only simultaneous fitting of all data sets was permitted.]

- "No-Bayes" runs can be made: cross sections will be calculated from the resonance parameters, but no fitting will be done.

Additions being considered for future revisions of the code include the following:

- Multiple nuclides in the sample
- An option to calculate multigroup cross sections and covariances
- An option to include integral quantities in the fit
- Extensions to the theory
- Additional ENDF capability (requiring ENDF format changes)
- A link between the resolved resonance parameters and those for the unresolved region, in order to provide more consistent evaluated cross sections
- Methodologies for retroactive generation of covariance matrices, similar to that used in the resolved resonance region

Input for analysis of data in the unresolved resonance region is described in Section VIII.B. Output is described in Section VIII.C. The relationship between ENDF parameters and SAMMY/URR parameters is discussed in Section VIII.D.

For an example of the use of SAMMY/URR, see [HD00] and test cases 73, 88, 127, 133, 134, 142, and 145.

VIII.A. EQUATIONS FOR UNRESOLVED RESONANCE REGION

The formulae for cross sections in the unresolved resonance region, as implemented in SAMMY, are presented in this section. The implementation is a modified form of that provided by Fritz Fröhner in his FITACS code [FF89]. (Please note that any mistakes in these formulae are attributable only to the author of this manual, not to Fröhner. The author is indebted to Herve Derrien for significant contributions both to the development of the code and to the composition of this section of the manual.)

Elastic cross section

The elastic cross section is given as the difference between the total cross section and the sum of all the non-elastic partial cross sections. The total cross section is given by Eqs. (VIII A.1) through (VIII A.4), and the non-elastic partial cross sections by Eqs. (VIII A.5) through (VIII A.20).

Total cross section

The average total cross section, for a given spin and parity and incident channel *c*, may be written in the form

$$\langle \sigma_c \rangle = \frac{2\pi g_c}{k_c^2}\left(1-\mathrm{Re}\langle S_{cc}\rangle\right) \quad , \qquad \text{(VIII A.1)}$$

where, as usual, g_c is the spin factor and k_c is the center-of-mass momentum. The average scattering matrix $\langle S_{cc}\rangle$ is given by

$$\langle S_{cc}\rangle = e^{-2i\varphi_c}\,\frac{1-\langle R_{cc}\rangle L_c^{0*}}{1-\langle R_{cc}\rangle L_c^{0}} \quad , \qquad \text{(VIII A.2)}$$

and the average R-matrix can be written in the form

$$\langle R_{cc}\rangle = R_c^{\infty} + i\pi s_c \quad , \qquad \text{(VIII A.3)}$$

with parameters defined as follows:

R_c^{∞} = distant-level parameter (an input quantity);

φ_c = hard-sphere scattering phase shift, generated using matching radius *a* (an input quantity);

L_c^0 = $(S_c - B_c) + iP_c$ (see Section II.A), with boundary condition B_c chosen such that $S_c - B_c = 0$;

s_c = pole strength.

The pole strength is defined in terms of input quantities $\tilde{S}_c$ (the strength function, for which we have introduced the tilde to avoid confusion with the shift factor used in definition of L_c^0) and a_c (the R-matrix matching radius) as

$$s_c = \tilde{S}_c \sqrt{E} \big/ 2\rho \quad , \qquad \text{(VIII A.4)}$$

where ρ is the center-of-mass momentum k_c multiplied by the channel radius a_c.

Non-elastic partial cross sections

The non-elastic partial cross sections may be written in terms of transmission coefficients T_x as

$$\left\langle \sigma_{ab} \right\rangle = \frac{\pi g_a}{k_a^2} \frac{T_a T_b}{T} \int_0^\infty dt \; e^{-iT_\gamma/T} \prod_{c \notin \gamma} \left(1 + \frac{2}{\nu_c} \frac{T_c}{T} t \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} \quad , \qquad \text{(VIII A.5)}$$

where the quantities to the left of the integral sign are the Hauser-Feshbach expression, and the integrand is the Moldauer prescription [PM80] for the width fluctuation correction factor. (A derivation of this expression, including the assumptions under which it is derived, is provided in Section VIII.A.1.) Here a represents the incident channel and b the exit channel; ν_c and T_c represent the number of degrees of freedom (multiplicity) and transmission coefficient, respectively, for channel c. Subscript γ refers to photon channels. T is defined as the sum over all channels:

$$T = \sum_c T_c \quad . \qquad \text{(VIII A.6)}$$

The transmission coefficient for neutron channels is given by

$$T_c = 1 - \left| \left\langle S_{cc} \right\rangle \right|^2 = \frac{4\pi \; P_c \, s_c}{\left| 1 - \left\langle R_{cc} \right\rangle L_c \right|^2} \quad , \qquad \text{(VIII A.7)}$$

where c is an incident channel, P and L are as defined in Section II.A, and the other quantities are given above. For photon and fission channels, the transmission coefficients for spin J are

$$T_\gamma = 2\pi \left\langle \Gamma_\gamma \right\rangle \big/ D_J \qquad \text{and} \qquad T_f = 2\pi \left\langle \Gamma_f \right\rangle \big/ D_J \quad , \qquad \text{(VIII A.8)}$$

in which D_J is the mean level spacing for levels with this spin.

The J-dependence of the mean level spacing is set in SAMMY/FITACS via the Bethe formula (e.g., [FF83]):

$$\left(D_J\left(E\right)\right)^{-1} = \left(d\left(E\right)\right)^{-1}\left\{\exp\left[\frac{-J^2}{2\left(\sigma\left(E\right)\right)^2}\right] - \exp\left[\frac{-\left(J+1\right)^2}{2\left(\sigma\left(E\right)\right)^2}\right]\right\} \quad , \qquad \text{(VIII A.9)}$$

where d (E) is independent of J, and σ is the spin cutoff parameter. The spin cutoff parameter is related to the level density parameter a and the energy E by the formula

$$\sigma^2 = \left(0.14592\right)\left(A+1\right)^{2/3}\sqrt{a\left(E+BE-PE\right)} \quad , \qquad \text{(VIII A.10)}$$

in which BE represents the neutron binding energy (an input parameter) and PE the pairing energy (also an input parameter). The value for a is determined from the input quantity D, which is the mean level spacing of the l = 0 resonances at E = 0; note that D includes both $J = I - i$ and $J = I + i$, where I is the spin of the target nucleus and i = ½ is the spin of the neutron. An expression for the inverse of D can be found from Eq. (VIII A.9) to be

$$\begin{aligned} D^{-1} &= \sum_J \left(D_J\left(E=0\right)\right)^{-1} \\ &= \left(d\left(0\right)\right)^{-1}\left\{\exp\left[\frac{-\left(I-\frac{1}{2}\right)^2}{2\sigma^2}\right] - \exp\left[\frac{-\left(I+\frac{3}{2}\right)^2}{2\sigma^2}\right]\right\} \quad ; \end{aligned} \qquad \text{(VIII A.11)}$$

this expression is used to determine the value of σ^2 and hence of the level density parameter a.

The energy dependence of the mean level spacing is calculated with the Gilbert-Cameron composite formula [AG65]. Let E_x represent the excitation energy of the compound nucleus; this energy is equal to the sum of the incident neutron kinetic energy E and the neutron binding energy BE (which is an input quantity). That is to say,

$$E_x = E + BE \quad . \qquad \text{(VIII A.12)}$$

The energy dependence for low excitation energies $\left(E_x < E_0\right)$, where E_0 is a matching energy, is given by the constant-temperature formula

$$D^{-1} \sim C_3 \frac{\exp\left[C_2\sqrt{E_0 - PE}\right]}{\left(E_0 - PE\right)^{3/2}} \exp\left[\frac{E_x - E_0}{2}\left(\frac{C_2}{\sqrt{E_0 - PE}} - \frac{3}{E_0 - PE}\right)\right] \quad . \qquad \text{(VIII A.13)}$$

In the code, the matching energy E_0 is set at

$$E_0 = \left[\frac{5}{2} + \frac{150}{(N+Z+1)} \right] \qquad \text{(VIII A.14)}$$

in units of MeV, with $N + Z$ being the mass number for the target nucleus. Values of the constants C_2 and C_3 are given by

$$C_2 = \sqrt{4a} \quad \text{and} \quad C_3 = \frac{1}{12\sqrt{2aq}} \quad , \qquad \text{(VIII A.15)}$$

with q defined as

$$q = 0.14592(N+Z+1)^{2/3} \quad , \qquad \text{(VIII A.16)}$$

where $N + Z$ is again the mass number for the target nucleus and a is the level density parameter.

At higher energies $(E_x > E_0)$, the energy dependence of the mean level spacing is calculated via the Fermi-Gas formula

$$D^{-1} \propto C_3 \frac{\exp\left[C_2\sqrt{E_x - PE}\right]}{(E_x - PE)^{3/2}} \quad . \qquad \text{(VIII A.17)}$$

Note that the two formulae agree at the matching energy (i.e., at $E_x = E_0$).

Radiation widths $\langle \Gamma_\gamma \rangle$ are assumed to depend only on parity π and on E. The energy dependence is calculated with the giant dipole resonance model.

Fission widths $\langle \Gamma_f \rangle$ may vary with spin as well as parity and incident neutron energy E. Energy dependence is calculated with the Hill-Wheeler fission barrier transmission coefficients [DH53]. For a given J^π, the energy dependence of the fission widths is taken to be

$$\langle \Gamma_f(E) \rangle = \langle \Gamma_f(0) \rangle \frac{1+\exp\left[E_{HW}/W_{HW}\right]}{1+\exp\left[-(E-E_{HW})/W_{HW}\right]} \quad , \qquad \text{(VIII A.18)}$$

where the Hill-Wheeler threshold energy E_{HW} and the Hill-Wheeler threshold width W_{HW} are input quantities. This equation may be written in more "standard" notation as

$$\left\langle \Gamma_f(E) \right\rangle = \left\langle \Gamma_f(0) \right\rangle \frac{1+\exp\left(2\pi\left(E_f - BE\right)/\hbar\omega\right)}{1+\exp\left(-2\pi\left(E_x - \left(E_f - BE\right)\right)/\hbar\omega\right)} \quad , \qquad \text{(VIII A.19)}$$

where, as above, E_x is the excitation energy of the neutron and *BE* is the binding energy. Also, E_f is the fission barrier height, and $\hbar\omega$ the width of the fission barrier.

Finally, a few words regarding the derivation of Eq. (VIII A.5) are warranted. That derivation is based on several assumptions:

(1) The Moldauer prescription [PM80] for width fluctuations is used. That is, the width fluctuation correction factor is introduced to compensate for the non-unity of the ratio

$$\left\langle \frac{T_a T_b}{T} \right\rangle \Bigg/ \frac{\langle T \rangle}{\langle T_a \rangle \langle T_b \rangle} \quad . \qquad \text{(VIII A.20)}$$

(2) Partial widths obey a chi-squared distribution with ν_c degrees of freedom (where the value of ν_c depends on the number of channels of this de-excitation); averages are therefore weighted with this distribution. In the Moldauer prescription for width fluctuations, simple channels have $1 < \nu_c < 1.78$; for lumped channels, ν_c is a function of T_c.

(3) Channels with the same transmission coefficients may be combined by introducing multiplicities.

The integral of Eq. (VIII A.5) is described by Fröhner as the "width fluctuation correction or Dresner factor." One (relatively modest) difference between SAMMY and the original FITACS coding is the algorithm for calculating the Dresner integral; in SAMMY, the coding has been refined to increase both speed and accuracy of calculation by using a non-uniform grid designed specifically for this task.

(Note: Prior to release 7 of the code, the Moldauer correction was inadvertently disabled in code. This has now been fixed.)

VIII.A.1. Derivation of Non-Elastic Average Cross Section

Derivations shown in this section are based on (1) notes provided by Fritz Fröhner [FF99] and (2) discussions with Herve Derrien [HD00a]. Any errors in these pages are the responsibility of the SAMMY author alone.

The interpretation of the transmission coefficient T_c in terms of average resonance parameters is straightforward if one assumes that the resonant cross section can be approximated by the single-level Breit Wigner formula, i.e.,

$$\sigma_{ab} = \frac{\pi g_a}{k_a^2} \sum_{\lambda} \frac{\Gamma_{\lambda a}\, \Gamma_{\lambda b}}{\left(E - E_\lambda\right)^2 + \left(\Gamma_\lambda / 2\right)^2} \quad , \qquad \text{(VIII A1.1)}$$

in which total width Γ_λ is the sum of all partial widths. The corresponding average cross section in an energy interval containing a large number of resonances may be written as

$$\left\langle \sigma_{ab} \right\rangle = \frac{\pi g_a}{k_a^2} 2\pi\, \rho_a \left\langle \frac{\Gamma_a \Gamma_b}{\Gamma} \right\rangle \quad , \qquad \text{(VIII A1.2)}$$

where ρ is the level density, and the brackets refer to averages. (Note that the subscript λ has been dropped for simplicity's sake.) The calculation of the average quantity $\left\langle \Gamma_a \Gamma_b / \Gamma \right\rangle$ is not straightforward, since the known parameters are $\left\langle \Gamma_a \right\rangle$ and $\left\langle \Gamma_b \right\rangle$ (from the statistical properties of the resonance parameters). One has to take into account the fluctuations of the partial widths of the resonances from the chi-squared distribution of the parameters.

A method of calculating the average $\left\langle \Gamma_a \Gamma_b / \Gamma \right\rangle$ from the known entities $\left\langle \Gamma_a \right\rangle \left\langle \Gamma_b \right\rangle / \left\langle \Gamma \right\rangle$ was proposed by Dresner [FF99]. He suggested making the substitution

$$\left\langle \frac{\Gamma_a \Gamma_b}{\Gamma} \right\rangle = \left\langle \frac{\Gamma_a \Gamma_b}{\sum_{all\ c} \Gamma_c} \right\rangle = \left\langle \Gamma_a \Gamma_b \int_0^\infty dq \exp\left(-q \sum_c \Gamma_c \right) \right\rangle \quad , \qquad \text{(VIII A1.3)}$$

which follows from the identity

$$\int_0^\infty d\, q\, e^{-qQ} = \frac{1}{Q} \int_0^\infty d\, y\, e^{-y} = \frac{1}{Q} \quad . \qquad \text{(VIII A1.4)}$$

The product of partial widths in Eq. (VIII A1.3) can be rearranged as

$$\left\langle \Gamma_a \Gamma_b \int_0^\infty d\,q \exp\left(-q \sum_c \Gamma_c \right) \right\rangle = \left\langle \int_0^\infty d\,q \;\; \Gamma_a\, e^{-q\Gamma_a} \;\; \Gamma_b\, e^{-q\Gamma_b} \;\; \prod_{c \neq a,b} e^{-q\Gamma_c} \right\rangle \cdot \quad \text{(VIII A1.5)}$$

Because the channels *a*, *b*, and *c* are independent, the average of the product is equal to the product of the averages. Likewise integration over *q* is independent of the averaging process; hence Eq. (VIII A1.3) can be rewritten as

$$\left\langle \frac{\Gamma_a \Gamma_b}{\Gamma} \right\rangle = \int_0^\infty d\,q \;\; \left\langle \Gamma_a\, e^{-q\Gamma_a} \right\rangle \left\langle \Gamma_b\, e^{-q\Gamma_b} \right\rangle \prod_{c \neq a,b} \left\langle e^{-q\Gamma_c} \right\rangle \quad . \qquad \text{(VIII A1.6)}$$

One assumes the partial widths obey a chi-squared distribution with ν degrees of freedom, which has the form

$$\rho(x, \nu)\,dx = \left[\mathbf{\Gamma}\left(\frac{\nu}{2} \right) \right]^{-1} \left(\frac{\nu x}{2} \right)^{\nu/2-1} e^{-\nu x/2} \; \frac{\nu}{2} \; dx \quad , \qquad \text{(VIII A1.7)}$$

where $\mathbf{\Gamma}$ in this expression refers to the gamma function. Note that $\nu = 1$ corresponds to the Porter-Thomas distribution for a single neutron channel; $\nu = 2$ corresponds to two channels. For fission, the value of ν depends on the number of open or partially open fission channels; ν_f is an input parameter in SAMMY (and in FITACS).

Applying this distribution to the average quantity needed in Eq. (VIII A1.6), with $x = \Gamma_c \big/ \langle \Gamma_c \rangle$, gives

$$\begin{aligned} \left\langle e^{-q\Gamma_c} \right\rangle &= \int_0^\infty e^{-q\langle \Gamma_c \rangle x} \; \rho(x, \nu)\; dx \\ &= \frac{1}{\mathbf{\Gamma}(\nu/2)} \left(\frac{\nu}{2} \right)^{\frac{\nu}{2}-1} \int_0^\infty e^{-q\langle \Gamma_c \rangle x} \; x^{\frac{\nu}{2}-1} \; e^{-\nu x/2} \; \frac{\nu}{2} \; dx \quad , \end{aligned} \qquad \text{(VIII A1.8)}$$

which can be rewritten into the form

$$\left\langle e^{-q\Gamma_c}\right\rangle = \frac{1}{\mathbf{\Gamma}(\nu/2)}\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}} \int_0^\infty e^{-\left(q\langle\Gamma_c\rangle+\nu/2\right)x}\; x^{\frac{\nu}{2}-1}\, dx$$

$$= \frac{1}{\mathbf{\Gamma}(\nu/2)}\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}}\left(\frac{\nu}{2}+q\left\langle\Gamma_c\right\rangle\right)^{-\frac{\nu}{2}} \int_0^\infty e^{-w}\; w^{\frac{\nu}{2}-1}\, dw \qquad \text{(VIII A1.9)}$$

$$= \frac{1}{\mathbf{\Gamma}(\nu/2)}\left(1+\frac{2}{\nu}q\left\langle\Gamma_c\right\rangle\right)^{-\frac{\nu}{2}}\Gamma(\nu/2) = \left(1+\frac{2}{\nu}q\left\langle\Gamma_c\right\rangle\right)^{-\frac{\nu}{2}} \quad .$$

Likewise, $\left\langle \Gamma_a\, e^{-q\Gamma_a}\right\rangle$ from Eq. (VIII A1.6) has the form

$$\left\langle \Gamma_a\, e^{-q\Gamma_a}\right\rangle = \int_0^\infty \left\langle\Gamma_a\right\rangle x\, e^{-q\langle\Gamma_a\rangle x}\; \rho(x,\nu)\, dx$$

$$= \frac{\left\langle\Gamma_a\right\rangle}{\mathbf{\Gamma}(\nu/2)}\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}-1} \int_0^\infty e^{-q\langle\Gamma_a\rangle x}\; x^{\frac{\nu}{2}}\; e^{-\nu x/2}\,\frac{\nu}{2}\, dx$$

$$= \frac{\left\langle\Gamma_a\right\rangle}{\mathbf{\Gamma}(\nu/2)}\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}}\left(\frac{\nu}{2}+q\left\langle\Gamma_a\right\rangle\right)^{-\frac{\nu}{2}-1} \int_0^\infty e^{-w}\; w^{\frac{\nu}{2}}\, d\,w$$

$$= \frac{\left\langle\Gamma_a\right\rangle}{\mathbf{\Gamma}(\nu/2)}\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}}\left(\frac{\nu}{2}+q\left\langle\Gamma_a\right\rangle\right)^{-\frac{\nu}{2}-1} \mathbf{\Gamma}\left(\frac{\nu}{2}+1\right)$$

$$= \frac{\left\langle\Gamma_a\right\rangle}{\mathbf{\Gamma}(\nu/2)}\left(\frac{\nu}{2}\right)^{\frac{\nu}{2}}\left(\frac{\nu}{2}+q\left\langle\Gamma_a\right\rangle\right)^{-\frac{\nu}{2}-1} \frac{\nu}{2}\mathbf{\Gamma}\left(\frac{\nu}{2}\right)$$

$$= \left\langle\Gamma_a\right\rangle\left(1+\frac{2}{\nu}q\left\langle\Gamma_a\right\rangle\right)^{-\frac{\nu}{2}-1} \qquad \text{(VIII A1.10)}$$

and similarly for $\left\langle \Gamma_b\, e^{-q\Gamma_b}\right\rangle$. Hence Eq. (VIII A1.6) can be expressed as

$$\left\langle\frac{\Gamma_a\Gamma_b}{\Gamma}\right\rangle = \left\langle\Gamma_a\right\rangle\left\langle\Gamma_b\right\rangle \int_0^\infty dq\; \prod_c\left(1+\frac{2}{\nu_c}q\left\langle\Gamma_c\right\rangle\right)^{-\nu_c/2-\delta_{ac}-\delta_{bc}} \quad , \qquad \text{(VIII A1.11)}$$

in which the correspondence of ν with channel *c* is made explicit by the addition of the subscript.

Making a change of variable from q to $t = \langle \Gamma \rangle q$ gives

$$\left\langle \frac{\Gamma_a \Gamma_b}{\Gamma} \right\rangle = \frac{\langle \Gamma_a \rangle \langle \Gamma_b \rangle}{\langle \Gamma \rangle} \int_0^\infty dt \prod_c \left(1 + \frac{2}{\nu_c} \frac{\langle \Gamma_c \rangle}{\langle \Gamma \rangle} t \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} \quad . \qquad \text{(VIII A1.12)}$$

The "transmission coefficients" are related to the average widths by

$$T_c = 2\pi \, \rho_c \, \langle \Gamma_c \rangle \quad . \qquad \text{(VIII A1.13)}$$

Note the equality of the level densities, $\rho_a = \rho_b = \rho_c = \rho_J$, since all refer to the same spin and parity. Hence Eq. (VIII A1.12) can be rewritten as

$$2\pi \, \rho_a \left\langle \frac{\Gamma_a \Gamma_b}{\Gamma} \right\rangle = \frac{T_a T_b}{T} \int_0^\infty dt \prod_c \left(1 + \frac{2}{\nu_c} \frac{T_c}{T} t \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} \quad , \qquad \text{(VIII A1.14)}$$

so that the cross section can be expressed as

$$\langle \sigma_{ab} \rangle = \frac{\pi g_a}{k_a^2} \frac{T_a T_b}{T} \int_0^\infty dt \prod_c \left(1 + \frac{2}{\nu_c} \frac{T_c}{T} t \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} \quad . \qquad \text{(VIII A1.15)}$$

For photon channels, the limit of non-fluctuating radiation widths, $\nu_{c=\gamma} \to \infty$ gives

$$\lim_{\nu \to \infty} \left(1 + \frac{2}{\nu_c} \frac{T_c}{T} t \right)^{-\nu_c/2} = e^{-t T_\gamma / T} \quad . \qquad \text{(VIII A1.16)}$$

Therefore our expression for the cross section, Eq. (VIII A1.15), takes the form

$$\langle \sigma_{ab} \rangle = \frac{\pi g_a}{k_a^2} \frac{T_a T_b}{T} \int_0^\infty dt \; e^{-i T_\gamma / T} \prod_{c \notin \gamma} \left(1 + \frac{2}{\nu_c} \frac{T_c}{T} t \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} \quad , \qquad \text{(VIII A1.17)}$$

which is equivalent to Eq. (VIII A1.6) combined with Eq. (VIII A1.2). This concludes the derivation of the formula given in Eq. (VIII A.5).

Evaluation of this expression for the average cross section in SAMMY (and in FITACS) assumes further simplification: First, we make the change of variable from t to $q = t\,T_\gamma / T$:

$$\left\langle \sigma_{ab} \right\rangle = \frac{\pi g_a}{k_a^2} \frac{T_a T_b}{T_\gamma} \int_0^\infty dq \;\; e^{-q} \prod_{c \notin \gamma} \left(1 + \frac{2}{\nu_c} \frac{T_c}{T_\gamma} q \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} \quad \text{(VIII A1.18)}$$

Second, we change variable from q to $u = e^{-q}$ to obtain

$$\left\langle \sigma_{ab} \right\rangle = \frac{\pi g_a}{k_a^2} \frac{T_a T_b}{T_\gamma} \int_0^1 du \;\; \prod_{c \notin \gamma} \left(1 - \frac{2}{\nu_c} \frac{T_c}{T_\gamma} \ln u \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} \quad . \quad \text{(VIII A1.19)}$$

Next, define parameters b_c via

$$b_c = \frac{2}{\nu_c} \frac{T_c}{T_\gamma} \quad , \qquad \text{(VIII A1.20)}$$

substitute into Eq. (VIII A1.19), and sum over incident (neutron) channels a and reaction channels b, to give

$$\left\langle \sigma_{nx} \right\rangle = \frac{\pi g}{k^2} T_\gamma \sum_{a \in n} \sum_{b \in x} \frac{\nu_a b_a}{2} \frac{\nu_b b_b}{2} \int_0^1 du \;\; \prod_{c \notin \gamma} \left(1 - b_c \ln u \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} \quad . \quad \text{(VIII A1.21)}$$

This can be written as

$$\left\langle \sigma_{nx} \right\rangle = \frac{\pi g}{k^2} T_\gamma \, Q_{nx} \quad , \qquad \text{(VIII A1.22)}$$

where Q is defined as

$$Q_{nx} = \sum_{a \in n} \sum_{b \in n} \frac{\nu_a b_a}{2} \frac{\nu_b b_b}{2} \, I_{ab} \qquad \text{(VIII A1.23)}$$

with

$$I_{ab} = \int_0^1 du \;\; \prod_{c \notin \gamma} \left(1 - b_c \ln u \right)^{-\nu_c/2 - \delta_{ac} - \delta_{bc}} \quad . \qquad \text{(VIII A1.24)}$$

This expression for I_{ab} is denoted the "Dresner integral." Evaluation of this integral is accomplished in SAMMY by (1) choosing a grid for u in which the spacing between points increases as the integrand flattens and (2) using a quadratic quadrature scheme. This integration scheme was tested with a wide range of plausible values for b's and ν's, comparing results for various values of N (where N is the number of points in the u-grid). Results were good to six digits of accuracy, for all tested values of b's and v's, using as few as 201 points in the grid.

VIII.B. INPUT FOR ANALYSIS OF DATA IN UNRESOLVED RESONANCE REGION

Two or more input files are required for analysis in the unresolved resonance region (URR). The first is comparable to the usual SAMMY INPut file, which may contain as few as three lines: Card set 1 of Table VIA.1 (the title line), card set 2 (nuclide name, atomic weight, and energy range), and (at least) one line for card set 3 (alphanumeric information). Options for alphanumeric commands in the URR are

```
UNRESOLVED RESONANCE region
EXPERIMENTAL DATA ARe in separate files
ANNOTATED PARAMETER file for urr
NO ANNOTATED PARAMETer file for urr input
ENDF/B-VI FILE 2 IS wanted
PUT COVARIANCE MATRIx into endf file 32
COVARIANCE MATRIX FRom old run is used
GENERATE FILE 3 POINt-wise cross sections
DEBUG
DO NOT SOLVE BAYES Equations
USE ENERGY LIMITS AS given in the input file
PRINT PARTIAL DERIVAtives
INCLUDE MIN & MAX ENergies when creating endf file
```

The first of these is required, as the SAMMY default is the resolved resonance region (RRR). The other alphanumeric commands are optional; their effects are described below.

The second file, the URR PARameter file, contains the unresolved resonance parameters. In the URR, there are several differences from the usual SAMMY conventions: To inform the code that a parameter is to be varied, FITACS assumes that, if the uncertainty is given as zero for a given parameter, then that parameter is not varied. (Hence there is no means of providing a default value for uncertainty.) This procedure is in contrast with the usual SAMMY procedure of assigning a value (generally 1) to a flag for each varied parameter; in the future, the formats for input to the FITACS portion of SAMMY will perhaps be modified to conform to SAMMY standards.

SAMMY permits several types of modifications to the original FITACS-style PARameter file: (1) Experimental data may be kept in separate files. (2) Normalizations can be included (and varied) for each data set. (3) ENDF File 2 and File 32 can be produced. (4) ENDF File 3 can be produced. (5) The PARameter file itself may be “annotated” in order to be more legible to humans. (6) Units may be specified for various quantities. (7) Different parameters may be specified in different energy regions. (8) Direct inelastic and/or direct capture components may be added. (9) Sequential analyses may be performed. (10) The analysis may be restricted to an energy range smaller than that for which the data are defined. Options (6) through (9) are available only with the annotated PARameter file.

Each of the 10 options is described separately below; details are given in Tables VIII B.1 and VIII B.2. Table VIII B.3 provides a guide for the various types of energy ranges encountered during a URR analysis.

(1) When the INPut file contains the phrase

```
EXPERIMENTAL DATA ARe in separate files,
```

experimental data are kept in separate file(s) rather than included as a portion of the URR PARameter file. Files names for individual data sets are given on the lines immediately following the INPut and PARameter file names in the interactive input stream. See, for example, test case tr073 run y.

(2) Normalizations can be included and varied (i.e., fitted) for each data set. That is, the theoretical calculation of the cross section is modified by

$$Theory = norm \times \sigma_{calculated} \quad , \qquad \text{(VIII B.1)}$$

where *norm* is given by the formula

$$norm = a + bE^{c} \qquad \text{(VIII B.2)}$$

and *a*, *b*, and *c* are input parameters, specified in the PARameter file. Note that one set of values for *a*, *b*, and *c* is given for each data set. Note also that there is no possibility to specify *b* and *c* unless

```
EXPERIMENTAL DATA ARe in separate files.
```

See tr073 for examples.

(3) When output in ENDF File 2 format is wanted, the phrase

```
ENDF/B-VI FILE 2 IS wanted
```

must be present in the INPut file. Also include the command

```
DEBUG
```

if you wish to create an annotated file SAMMY.NDX. This annotated file contains comments that define which parameters' values are given; except for the annotations, this file is identical to the SAMMY.NDF.

One additional SAMMY input file must be provided; the name for this file is given in the input stream after the name of the PARameter file (or after the COVariance file if it exists) and before the name(s) of any data files. This NDF file provides information regarding the specifics of the ENDF file to be created. The NDF file is in key word format, and contains only the following parameters:

`Z` = charge
`A` = atomic number
`Mat` = ENDF material number
`NUmber` of energy points = number
`Energy` number 1 = value of energy-point

Only the one or two characters in capitals are required; others are optional. The value is given following the equal sign. One or the other of "`NU...=`" and "`E...=`" must be present. (If both are present, "`NU...=`" will be ignored.)

The number of energy points specifies at how many equally spaced points per energy region the parameter values will be printed into the ENDF file. Values may also be printed at Emin and Emax, the limits of the analysis, if the phrase

```
INCLUDE MIN & MAX ENergies in endf file
```

is given in the INPut file. For example, for 3 points per region and 5 regions, a total of $3 \times 5 + 2 = 17$ sets of values would be given in the ENDF file.

If, instead of having a certain number of points for each energy range, specific values of energy are wanted in the ENDF file, then the alternative "`E...=`" should be specified. Subsequent energies are given one per line, with or without the key word "`E...=`" prior to the value. These energy values should be the last entries in this file.

See test cases tr073 and tr127 for examples. Runs a, b, e, and f of tr127 use "`NU...=`" key word, while run g uses the "`E...=`" key word.

To also obtain the associated covariance file (ENDF File 32), include the phrase

```
PUT COVARIANCE MATRix into endf file 32
```

in the INPut file. See test case tr128 runs j and k for examples.

(4) ENDF File 3 output (point-wise cross sections, in file SAMMY.FL3) can be generated when the command

```
GENERATE FILE 3 POINt-wise cross sections
```

is included in the INPut file. The energy grid for this cross section is as defined by the input data sets. If the `DEBUG` command is also used, an annotated ENDF File 3 (SAMMY.FLX) output file is also produced. See test case tr073, runs n through t, for examples.

(5) Two modes, annotated and unannotated, are available for the URR PARameter file:

The unannotated mode is essentially equivalent to Fröhner's original FITACS file (which includes both parameters and data). Formats for this file are described in Table VIII B .1; all numbers, both integer and real, are specified with F10 formats. To use this mode, the INPut file must contain the command

```
NO ANNOTATED PARAMETer file for urr input
```

Test case tr073 has examples of this input mode.

The annotated PARameter file is described in detail in Table VIII B.2; this is the default mode for SAMMY. With this option, some parameters are entered by key word; other parameter lists have headings to define which parameters are in the list. See, for example, test case tr073 run g, or test cases tr128.

(6) Units may be specified for various energy-related quantities by including the phrase "`in eV`", "`in keV`", or "`in MeV`" in the appropriate location in the PARameter file. (Note that, as always with SAMMY input, capitalization is irrelevant.) If units are not specified, defaults are as given in Table VIII B.2 (i.e., MeV for binding energy and pairing energy, eV for all others). The quantities for which units may be specified are as follows:

excitation energies for inelastic states
binding energy
pairing energy
energy maxima for the different ranges (see (7) below)
energies for direct inelastic contribution (see (8) below)

See in particular tr128 run l (letter "l" not number "one") for examples.

(7) Different parameter values may be used in different energy ranges; see Table VIII.B.2, card sets 4-7, for input details. See test case tr128 for examples.

(8) A direct inelastic component may be added to the inelastic and total cross sections, and/or a direct capture component added to the capture and total cross sections. These components are specified numerically on grids chosen by the user; SAMMY interpolates linearly between grid points. See card set 11 of Table VIII B.2 for details. Examples are in tr088 and tr134.

(9) Although many data sets can be analyzed simultaneously in URR, SAMMY also permits sequential runs similar to those used in the RRR. For details, see the description of the SAMMY.COV file in the next section. For examples, see test case tr073 runs a and g.

(10) The default choice for energy range in the URR is to include all energies for which data are available. However, the analysis may be restricted to a smaller energy range by including the command

```
USE ENERGY LIMITS AS given in the input file
```

in the INPut file. See test case tr073 runs j,k,l for examples.

Table VIII B.1. Formats for original PARameter file for treatment of the unresolved resonance region

Card set	Line No.	Description
1	1–4	First four lines are alphanumeric title
2	1	Number of iterations, fitting tolerance (essentially delta chi squared). Note that integers are to be specified as real numbers. All formats are F10.
	2	Mass in amu, radius in Fermi (or use default), neutron binding energy in MeV, pairing energy *PE* in MeV. Again, formats are F10; note that the energy units are MeV, as opposed to the usual SAMMY standard of eV.
3	1,2,...	Center-of-mass excitation energy (in eV), spin, and parity for the *n*th target level (beginning with ground state). Repeat as many times as needed.
	Last	(Blank)
4	1	Strength function S_c, uncertainty, distant-level parameter R_c^{∞}, uncertainty, radiation width $\langle \Gamma_\gamma \rangle$ in eV, uncertainty, mean level spacing D in eV for $l = 0$
	2	Strength function, uncertainty, distant-level parameter, uncertainty, radiation width in eV, uncertainty, for $l = 1$
	3	Strength function, uncertainty, distant-level parameter, uncertainty, radiation width in eV, uncertainty, for $l = 2$
	4,5,...	As above, for higher l values as needed
	Last	(Blank)
5	1	For the lowest J value for $l = 0$, Average fission width $\langle \Gamma_f \rangle$ (eV) Degree of freedom ν_f for fission width distribution Hill-Wheeler threshold energy E_{HW} Hill-Wheeler threshold width W_{HW} Uncertainty on the average fission width
	2,3,…	Repeat line 1 for each possible value of J for $l = 0$.

Table VIII B.1 (continued)

Card set	Line No.	Description
5, cont.	4,5,…	Repeat lines 1-3 for each possible value of J for l = 1, 2, ... For a given spin J and parity (even or odd l), only one set of values is actually used for $\langle \Gamma_f \rangle$ and the other parameters. Nevertheless, all J and l must be included in this list. Only the values associated with the lowest l value will be used for the calculations; the other values will be ignored. For example, the ground state of ^{235}U is $7/2^-$. For $l = 0$, J^π = $3^-, 4^-$. For $l = 1$, J^π = $2^+, 3^+, 4^+, 5^+$. For $l = 2$, J^π = $1^-, 2^-, 3^-, 4^-, 5^-, 6^-$. The 3^- and 4^- values used in the calculations will be those given for $l = 0$. The values given for $J^\pi = 3^-$ and 4^- with $l = 2$ will be ignored.
	Last	(Blank)
6	1	Type of cross-section data (`TOTAl`, `CAPTure`, `FISSion`, or `INELastic`)
	2	Uncertainties are `RELAtive` or `ABSOlute`
	3	Energy, cross section, and uncertainty for first data point. Normalization and uncertainty (a and Δa) for this data set.
	4,...	Energy, cross section, uncertainty. (Note: if `RELAtive` then these need to be specified only for first data point; the others are assumed to be the same.)
	Last	(Blank)
6x	All	Repeat card set 6 as many times as needed, in any order
7	1	The single word "`NORMALIZATION`". (Card set 7 is present only if the command "`EXPERIMENTAL DATA ARe in separate files`" appears in card set 3 of the INPut file.)
	2	Type of cross section, normalization parameters a, Δa, b, Δb, c, Δc, where the normalization for this data set is given by $norm = a + b\ E^c$
	3,etc.	Repeat Line 2 once for each data set. Normalizations must appear in the same order in which the data sets appear. SAMMY will check to be sure the data types are consistent.

Table VIII B.2. Formats for annotated PARameter file for treatment of the unresolved resonance region

Card set	Line No.	Description
1	1,2,...	Alphanumeric title, as many lines as desired. Printed but otherwise ignored.
	Last	----- (First four characters must be hyphens [minus signs]; this ends the title. Other characters on this line are printed but ignored.)
2	1,2,...	Key word = Value. Possible keywords here are Key word — Meaning — Default `ITErations` — number of iterations — 3 `TOLerance` — fitting tolerance — 0.005 `RADius` — radius in F — 1.23 $AW^{1/3}$+0.8 `AW` (atomic weight) — mass in amu — (no default) Only the letters in capitals are required; the values may be in any format.
	Last	(blank)
3	0	"----" An optional line of minus signs may be inserted; this line will be ignored by the code.
	1	"`ELAStic and inelastic states`". Only the first four characters are necessary, others are optional. Units of excitation energy are eV unless specified anywhere on this line (after the first four characters) as "`in eV`", "`in keV`", or "`in MeV`".
	2,3,...	Center-of-mass excitation energy, spin, and parity for the *n*th target level (beginning with ground state). Format must be 3F10 (ten characters per number, three numbers on a line, decimal points must be included).
	Last	(blank)
4	0	"----" Optional.
	1,2,...	Key word = Value. Possible key words here are Key word — Meaning — Default `BINding energy` — neutron binding energy (MeV) — (none) `PAIring energy` — pairing energy (MeV) — (none) Only the letters in capitals are required; the values may be in any format. To override the default units, insert a phrase "`in eV`", "`in keV`", or "`in MeV`" after the key word and before the equal sign. Examples: `Binding Energy (in eV) = 6536000.` `Pairing energy in eV = 1610000.`
	Last	(blank)

Table VIII B.2 (continued)

Card set	Line No.	Description
5	0	"----" optional
	1	"`STReng del_s distnt del_d gamma width del_g bethed`" (Only first three characters are necessary. This line indicates that strength functions, distant-level parameters, etc., are coming next.)
	2	Strength function S_c, uncertainty, distant-level parameter R_c^{∞}, uncertainty, radiation width $< \Gamma_\gamma >$ in eV, uncertainty, mean level spacing D in eV for $l = 0$. F10 formats.
	3	Strength function, uncertainty, distant-level parameter, uncertainty, radiation width in eV, uncertainty, for $l = 1$
	4	Strength function, uncertainty, distant-level parameter, uncertainty, radiation width in eV, uncertainty, for $l = 2$
	5,6,...	As above, for higher l values as needed
	Last	(blank)
6	0	"----" optional line
	1	"`FISsion width fnu ethr wthr del_fission width`" (Only first three characters are necessary. This line indicates that fission parameters are coming next.)
	2	For the lowest J value for $l = 0$, Average fission width $\langle \Gamma_f \rangle$ (eV) Degree of freedom ν_f for fission width distribution Hill-Wheeler threshold energy E_{HW} Hill-Wheeler threshold width W_{HW} Uncertainty on the average fission width J, l The first line contains the lowest J value associated with $l = 0$. Formats are F10 for everything except the l-value, which is I5 (i.e., the right-most column is # 65). Inclusion of J and l in the input file is optional but recommended.
	3,4,…	Repeat line 2 for each possible value of J for $l = 0$.

Table VIII B.2 (continued)

Card set	Line No.	Description
6, cont.	5,6,…	Repeat lines 2–4 for each possible value of J for l = 1, 2, ... For a given spin J and parity (even or odd l), only one set of values is actually used for $<\Gamma_f>$ and the other parameters. Nevertheless, all J and l must be included in this list. Only the values associated with the lowest l value will be used for the calculations; the other values will be ignored. For example, the ground state of ^{235}U is $7/2^-$. For $l = 0$, J^π = $3^-, 4^-$. For $l = 1$, J^π = $2^+, 3^+, 4^+, 5^+$. For $l = 2$, J^π = $1^-, 2^-, 3^-, 4^-, 5^-, 6^-$. The 3^- and 4^- values used in the calculations will be those given for $l = 0$. The values given for $J^\pi = 3^-$ and 4^- with $l = 2$ will be ignored.
	Last	(blank)
7	0	"----" optional line
	1	Key word = Value. Only one possible keyword is permitted here: Key word — Meaning — Default `ENErgy maximum` — maximum energy in this region (eV) — (none) Only the letters in capitals are required; the values may be in any format. To override the units, insert a phrase "`in eV`", "`in keV`", or "`in MeV`" after the key word and before the equal sign. Example: `Energy maximum in MeV = 0.15`
4–7	all	Repeat card sets 4–7, once for each energy region, as many times as needed. Alternatively, repeat only line 1 of card set 7, in which case the starting parameter values are assumed to be identical to those in the previous energy region.
8		In either case, end with a line saying "`END of resonance parameter description`".

Table VIII B.2 (continued)

Card set	Line No.	Description
9	0	"----" optional line
	1	Type of cross-section data (`TOTAl`, `CAPTure`, `FISSion`, or `INELastic`). Card set 9 will be omitted from this file if the command "`EXPERIMENTAL DATA ARe in separate files`" appears in the INPut file.
	2	Uncertainties are `RELAtive` or `ABSOlute`. (Only "`RELA`" or "`ABSO`" is needed.)
	3	Energy (eV), cross section (barn), uncertainty (barn if ABSOlute, dimensionless if RELAtive) for first data point. Norm and unc (a and Δa) for this data set. Format is 3F10.
	4,5,...	Energy, cross section, uncertainty (Note: if `RELAtive`, then need specify only for first data point, rest are assumed to be the same.)
	Last	(blank)
9x	all	Repeat card set 9 as many times as needed, in any order
10	0	"----" optional line
	1	"`NORMalization`". [Card set 10 may be present only if INPut file specifies "`experimental data are in separate files`".]
	2	Type of cross section, normalization parameters a, Δa, b, Δb, c, Δc, where the normalization for this data set is given by $norm = a + b\,E^{c}$
	3,4,...	Repeat once for each data set. Note that normalizations must appear in the same order in which the data sets appear. SAMMY will check to be sure the data types are consistent.
	Last	(blank)
10a	0	"----" optional line
	1	"`EARLier normalization`". [Card set 10a, an alternative to card set 10, is to be used only if an earlier SAMMY run has produced a covariance file.]
	2	N1, N2, ... Nlast, in [40I2] format. Here N1 is the ordering of the first data set for this run, as it appeared in previous SAMMY runs; see test case tr145 for illustrative examples.
	Last	(blank)

Table VIII B.2 (continued)

Card set	Line No.	Description
11	0	"`----`" optional line
	1	"`DIRECT Inelastic contribution`", *or* "`DIRECT Capture contribution`". Note that eight characters (rather than the usual four) are required here.
	2	`Energy` = value, `Sigma` = value. Both key words (and both values) must be on the same line. <u>Key word</u> <u>Meaning</u> `Energy` Energy in (eV) `Sigma` Direct inelastic cross section (b) at that energy To use different units on energy, insert a phrase "`in eV`", "`in keV`", or "`in MeV`" after the key word "`Energy`".
	3,4,... etc.	Repeat line 2 as many times as required. Note that card set 11 may be omitted if the contribution of the direct inelastic cross section is negligible or unknown.

Table VIII B.3. Energy ranges encountered in the unresolved resonance region

EMIN and EMAX for this run –

- EMIN & EMAX refer to the min and max energies of the data to be fitted.
- EMIN & EMAX can be given in the INPut file.
  - "USE ENERGY LIMITS AS GIVEN IN THE INPUT FILE" must be specified (otherwise the values are ignored).
  - The same EMIN & EMAX apply to all data sets.
- If EMIN & EMAX are not given in the INPut file (or the command line is not used), then EMIN & EMAX are set to the min and max energies occurring in the data sets.

For each data set i –

- Actual range for which data exist = $Emin_i$ and $Emax_i$
  - never defined in the SAMMY input but seen in the data file
- Range to be used in this calculation
  - All data points (from $Emin_i$ to $Emax_i$) will be used unless EMIN & EMAX are specified in INPut file [and command line is there].
    - The same EMIN & EMAX are used for all data sets.

For the parameters, there are Numurr regions –

- Energy limits are specified in the PARameter file.
  - Engur0 is the "`MINImum energy`" for the first region.
    - If Engur0 is not given, then it will be set equal to EMIN.
  - Engurr(n) is the "`Energy Maximum`" for the nth region.
    - If a "`MINImum energy`" is specified for region n (n>1), the code will check whether it is equal to Engurr(n-1) and abort if it isn't.

Region number	**Energy at start of region**	**Energy at end of region**
1	Engur0	Engurr(1)
2	Engurr(1)	Engurr(2)
3	Engurr(2)	Engurr(3)
…		
Numurr	Engurr(Numurr-1)	Engurr(Numurr)

- If EMAX > Engurr(Numurr)
  - If data are to be used above Engurr(Numurr), the code will print an error message and abort, because parameters are not defined above Engurr(Numurr).

Table VIII B.3 (continued)

For the ENDF file –

- Provided energy limits are given elsewhere, it is NOT necessary to include any data sets for the run that generates the ENDF file.

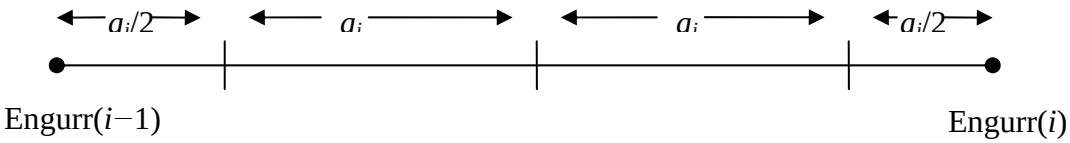
- If the *.ndf file contains the key word "`Energy=`", then
  - Only and exactly the energies given here are used in the ENDF file [tr133g, h, j].
  - Energies must be in monotonically increasing order.
  - The minimum and maximum energies to be printed in the ENDF file are the minimum and maximum energies from this list.
  - The command "`INCLUDE MIN & MAX Energies in endf file`" is ignored (test case tr133 runs h and j).

- If the *.ndf file contains key word "`NUmber` = *N*", then

  - This key word is ignored if "`Energy =`" key word is given.
  - The minimum and maximum energies to be printed in the ENDF file are Engur0 and Engurr(Numurr) for this run (defined above).

  - If $N = 1$, only the midpoint energy value for each parameter region will appear in the ENDF file (test case tr133 run b).

  - For $N > 1$, in each of the Numurr parameter regions, N equally-spaced points are used in the ENDF file. So $a_i = ((\text{Engurr}(i) - \text{Engurr}(i-1))/N$ in the figure below [tr133a].



  - If the command "`INCLUDE MIN & MAX Energies in endf file`" appears in the INPut file, then Engur0 & Engurr(Numurr) are also included in the ENDF listing (tr133 runs e and f, with `NU=`3 and 1, respectively).

VIII.C. OUTPUT FROM ANALYSIS IN UNRESOLVED RESONANCE REGION

As with the resolved resonance region, each SAMMY/URR run may produce several output files:

(1) The SAMMY.LPT file contains details of the calculations.

(2) For runs which involve the solution of Bayes' equations and hence the generation of updated parameter values (a "Bayes run" as opposed to a "no-Bayes run" which simply calculates cross sections), an output file SAMMY.PAR is provided in the annotated form described in Table VIII B.2. (This file, of course, is quite different from the file by the same name produced in a resolved resonance region run.)

(3) For Bayes runs, a COVariance file SAMMY.COV is produced, which contains (among other things) the final parameter covariance matrix; see below for more detail.

(4) Files SAMMY.NDF and SAMMY.N32 contain the URR portion of ENDF File 2 and 32, respectively; these files are produced when the appropriate command is in the INPut file.

(5) Files SAMMY.NDX and SAMMY.N3X contain the same information as in SAMMY.NDF and SAMMY.N32 respectively, but also include comment lines defining the parameters whose values are given. Only the uncertainty values are given in SAMMY.N3X; correlations are printed only in SAMMY.N32.

The binary COVariance file SAMMY.COV can be used as input to a subsequent SAMMY run that uses the same R-matrix parameters but different data sets and different normalizations, in a similar fashion to sequential runs in the RRR. There are slight differences, however, in the usage of this COVariance file; no auxiliary program comparable to SAMAMR is required here, as there is only one type of data-reduction parameter (the normalizations). The user must simply rename and modify the SAMMY.PAR file to contain the appropriate normalization parameters for the data sets about to be analyzed. The output PARameter file will contain card set 10a of Table VIII B.2; PARameter files to be used as input will use either card set 10 (for new data sets for which the normalizations have not yet been defined) or card set 10a (to re-use normalizations already defined for the current data sets). See test case tr145 for examples.

To use an output SAMMY.PAR file as input to a new run without the accompanying COV file, it is necessary to delete the first line of the file; this line reads as follows:

```
COVARIANCE MATRIX FRom old run is used
```

When the COV file is to be used (for sequential runs), keep this line in the PARameter file.

Test cases tr073, tr088, tr127, tr128, tr133, tr145, and others provide sample input and output for URR calculations.

VIII.D. CONVERTING SAMMY/URR PARAMETERS TO ENDF/B PARAMETERS

Parameters required by the ENDF formats [ENDF-102] are related to the SAMMY (FITACS) input parameters but are not identical. Likewise the cross sections calculated by ENDF processor codes such as NJOY [RM82] may have somewhat different values from those calculated by SAMMY [HD03] because the exact same formulae are not used. (Formulae in SAMMY and FITACS are more accurate than those supported by ENDF.)

The correspondence between the SAMMY and the ENDF parameter values is described below.

Channel radius

The R-matrix channel radius *a* used in SAMMY is related the ENDF scattering radius AP via

$$\mathrm{AP} = R' = a\left(1 - R_c^{\infty}\right) \qquad \text{(VIII D.1)}$$

Note that *a* is input to SAMMY in units of Fermi; AP is specified for ENDF in units of 10^{-12} cm.

Degrees of freedom

ENDF formats require that the number of degrees of freedom be explicitly stated for each channel), for each *l* and *J*. For SAMMY, only for fission channels is the number of degrees of freedom ν_f explicitly given in the input; for neutron channels, ν_n is calculated by the code to be either 1 or 2 (depending on the number of available channel spin values). For capture channels, ν_γ is infinite and therefore not given in the input. [See Eq. (VIII A.5) for use of ν_n .]

Level spacing

In SAMMY the mean level spacing *D* for *l* = 0 is specified in the input, and the energy- and *J*-dependent mean level spacing $D_J(E)$ is derived as described in Section VIII.A, Eqs. (VIII A.9–16). For ENDF, $D_J(E)$ is reported at particular energies.

Neutron widths

In SAMMY the strength function is used to generate the transmission coefficient for neutron channels, according to Eq. (VIII A.7) with the pole strength s_c defined in terms of the input strength function $\tilde{S}_c$. Using the analogous form from Eq. (VIII A.8) and equating to Eq. (VIII A.7), we find

$$2\pi\left\langle \Gamma_n \right\rangle / D_J = \frac{4\pi P_c s_c}{\left|1-\left\langle R_{cc}\right\rangle L_c\right|^2} \quad , \qquad \text{(VIII D.2)}$$

or

$$\left\langle \Gamma_n \right\rangle = \frac{2 P_c \tilde{S}_c \sqrt{E}/(2\rho)}{\left|1-\left(R_c^\infty + i\pi \tilde{S}_c \sqrt{E}/(2\rho)\right) L_c\right|^2} D_J \quad , \qquad \text{(VIII D.3)}$$

in which the expression for pole strength s_c in terms of strength function $\tilde{S}_c$, Eq. (VIII A.4), has been substituted. The ENDF manual [ENDF-102, page D18] specifies that it is the *reduced* neutron width which is to be reported. This width is related to the neutron width via

$$\left\langle \Gamma_n \right\rangle = \left\langle \Gamma_n^o \right\rangle \sqrt{E}\, P_n / \rho \qquad \text{(VIII D.4)}$$

or (with $c = n$)

$$\left\langle \Gamma_n^o \right\rangle = \frac{\tilde{S}_c}{\left|1-\left(R_c^\infty + i\pi S_c \sqrt{E}/(2\rho)\right) L_c\right|^2} D_J \quad , \qquad \text{(VIII D.5)}$$

which is the quantity reported in the ENDF file for a particular energy E.

Inelastic widths

The ENDF manual [ENDF-102] is exceedingly vague with regard to the inelastic widths. Two gross approximations are clearly required by the format: (1) Only a single inelastic width is permitted. (2) Only a single value of orbital angular momentum may be used. To work within these limitations, we have chosen to provide information only for the first inelastic channel, and to use the lowest value of orbital angular momentum l' consistent with the specified l (of the elastic channel) and J. The contribution from the other inelastic channels can be given in File 3. The contribution from higher l' must simply be ignored. No guarantee is made that SAMMY's implementation of ENDF's format is correct here.

Radiation widths

Radiation widths $\left\langle \Gamma_\gamma \right\rangle$ are input to SAMMY at $E = 0$. For ENDF, the widths are reported at particular energies as calculated by the giant dipole resonance model.

Fission widths

Fission widths $\left\langle \Gamma_f \right\rangle$ are likewise input into SAMMY at $E = 0$, and reported in ENDF at particular energies. The energy dependence is given by Eqs. (VIII A .17–18).

VIII.D.1. Relation of SAMMY/URR Radius to ENDF/B Radius

To understand the rationale for the choice of R' as the input radius for ENDF, we consider the value of the cross section in the limit in which the effect of resonances is negligible. From Eq. (VIII A.2), the average scattering matrix is given by

$$\left\langle S_{cc} \right\rangle = e^{-2i\varphi_c} \frac{1-\left\langle R_{cc} \right\rangle L_c^{0*}}{1-\left\langle R_{cc} \right\rangle L_c^{0}} \quad , \tag{VIII D1.1}$$

in which the average R-matrix is

$$\left\langle R_{cc} \right\rangle = R_c^{\infty} + \; i\pi s_c \quad . \tag{VIII D1.2}$$

Substituting iP for L, dropping subscripts for simplicity, and rearranging give

$$\begin{aligned}
\left\langle S_{cc} \right\rangle &= e^{-2i\varphi} \frac{\left[1-\left(R^{\infty}+i\pi s\right)\left(-iP\right)\right]}{\left[1-\left(R^{\infty}+i\pi s\right)\left(+iP\right)\right]} \;=\; e^{-2i\varphi} \frac{\left[1-\pi Ps+iPR^{\infty}\right]}{\left[1+\pi Ps-iPR^{\infty}\right]} \\
&= e^{-2i\varphi} \frac{\left[1-\pi Ps+iPR^{\infty}\right]}{\left[1+\pi Ps-iPR^{\infty}\right]} \frac{\left[1+\pi Ps+iPR^{\infty}\right]}{\left[1+\pi Ps+iPR^{\infty}\right]} \\
&= \left[\cos\left(2\varphi\right)-i\sin\left(2\varphi\right)\right] \frac{1-\pi^2P^2s^2-\left(PR^{\infty}\right)^2+2iPR^{\infty}}{\left(1+\pi Ps\right)^2+\left(PR^{\infty}\right)^2} \\
&= \frac{\begin{array}{l}\left[\left\{\cos\left(2\varphi\right)\left[1-\pi^2P^2s^2-\left(PR^{\infty}\right)^2\right]+\sin\left(2\varphi\right)2PR^{\infty}\right\}\right. \\ \left.\quad +\,i\left\{-\sin\left(2\varphi\right)\left[1-\pi^2P^2s^2-\left(PR^{\infty}\right)^2\right]+\sin\left(2\varphi\right)2PR^{\infty}\right\}\right]\end{array}}{\left(1+\pi Ps\right)^2+\left(PR^{\infty}\right)^2} \quad .
\end{aligned} \tag{VIII D1.3}$$

The cross section can then be expressed as

$$\begin{aligned}
\left\langle \sigma_c \right\rangle &= \frac{2\pi g}{k^2}\left(1-\mathrm{Re}\left\langle S_{cc} \right\rangle\right) \\
&= \frac{2\pi g}{k^2}\left(1-\frac{\cos\left(2\varphi\right)\left[1-\pi^2P^2s^2-\left(PR^{\infty}\right)^2\right]+\sin\left(2\varphi\right)2PR^{\infty}}{\left(1+\pi Ps\right)^2+\left(PR^{\infty}\right)^2}\right) \quad .
\end{aligned} \tag{VIII D1.4}$$

If we consider only s-waves ($l = 0$), both P and φ have the value $\rho = ka$. The expression for the cross section then becomes

$$\begin{aligned}
\langle \sigma_c \rangle &\approx \frac{2\pi g}{k^2}\left(1-\frac{\left(1-2\rho^2\right)\left[1-\pi^2\rho^2 s^2-\rho^2\left(R^\infty\right)^2\right]+4\rho^2 R^\infty}{\left(1+\pi\rho s\right)^2+\rho^2\left(R^\infty\right)^2}\right) \\
&= \frac{2\pi g}{k^2}\,\frac{\left(1+\pi\rho s\right)^2+\rho^2\left(R^\infty\right)^2-\left(1-2\rho^2\right)\left[1-\pi^2\rho^2 s^2-\rho^2\left(R^\infty\right)^2\right]-4\rho^2 R^\infty}{\left(1+\pi\rho s\right)^2+\rho^2\left(R^\infty\right)^2} \\
&\approx \frac{2\pi g}{k^2}\,\frac{1+2\pi\rho s+\pi^2\rho^2 s^2+\rho^2\left(R^\infty\right)^2-1+\pi^2\rho^2 s^2+\rho^2\left(R^\infty\right)^2+2\rho^2-4\rho^2 R^\infty}{\left(1+\pi\rho s\right)^2+\rho^2\left(R^\infty\right)^2} \quad ,
\end{aligned}$$

(VIII D1.5)

in which cos and sin have been expanded for small values of ρ, and terms $\sim\rho^4$ have been dropped in the numerator. Simplifying, we find

$$\begin{aligned}
\langle \sigma_c \rangle &\approx \frac{2\pi g}{k^2}\,\frac{\left[2\pi\rho s+2\pi^2\rho^2 s^2\right]+2\rho^2\left(R^\infty\right)^2+2\rho^2-4\rho^2 R^\infty}{\left(1+\pi\rho s\right)^2+\rho^2\left(R^\infty\right)^2} \\
&= \frac{4\pi g}{k^2}\,\frac{\pi\rho s+\pi^2\rho^2 s^2+\rho^2\left[1-\left(R^\infty\right)\right]^2}{\left(1+\pi\rho s\right)^2+\rho^2\left(R^\infty\right)^2} \quad .
\end{aligned}$$

(VIII D1.6)

In the limit in which all the resonances are considered to be distant resonances, the pole strength s is zero and the cross section becomes

$$\langle \sigma_c \rangle \approx \frac{4\pi g}{k^2}\,\frac{\rho^2\left[1-\left(R^\infty\right)\right]^2}{1+\rho^2\left(R^\infty\right)^2} \approx \frac{4\pi g}{k^2}k^2a^2\left[1-\left(R^\infty\right)\right]^2 = 4\pi g R'^2 \quad , \text{(VIII D1.7)}$$

in which R' is defined as $a\left(1-R^\infty\right)$. This is the customary low-energy formula, even in the resolved resonance region.

We now consider the more general case, for all energies. In Eq. (VIII D1.4), assume that the pole strength s is negligible but do not use the low-energy limit. The cross section can be shown to have the form

$$\langle \sigma_c \rangle \approx \frac{2\pi g}{k^2}\left(1-\frac{\cos(2\varphi)\left[1-\left(PR^\infty\right)^2\right]+\sin(2\varphi)\,2PR^\infty}{1+\left(PR^\infty\right)^2}\right) \qquad \text{(VIII D1.8)}$$

$$= \frac{2\pi g}{k^2}\sin^2(\varphi-\varepsilon) \quad ,$$

where the phase shift ε is given by

$$\varepsilon = \tan^{-1}\left(P\,R^\infty\right) \quad . \qquad \text{(VIII D1.9)}$$

To see this, note that

$$\begin{aligned}
\sin^2(\varphi-\varepsilon) &= \left(\sin\varphi\,\cos\varepsilon-\cos\varphi\,\sin\varepsilon\right)^2 \\
&= \sin^2\varphi\,\cos^2\varepsilon-2\sin\varphi\,\cos\varphi\,\cos\varepsilon\,\sin\varepsilon+\cos^2\varphi\,\sin^2\varepsilon \\
&= \tfrac{1}{2}\left[1-\cos(2\varphi)\right]\cos^2\varepsilon-2\left[\sin(2\varphi)/2\right]\cos\varepsilon\,\sin\varepsilon+\tfrac{1}{2}\left[1+\cos(2\varphi)\right]\sin^2\varepsilon \\
&= \tfrac{1}{2}\left\{1+\cos(2\varphi)\left[\sin^2\varepsilon-\cos^2\varepsilon\right]-\sin(2\varphi)\sin\varepsilon\,\cos\varepsilon\right\} \quad .
\end{aligned}$$

(VIII D1.10)

From Eq. (VIII D1.9) it can readily be seen that

$$\begin{aligned}
\tan\varepsilon &= PR^\infty \\
\sin\varepsilon &= \frac{PR^\infty}{\sqrt{1+\left(PR^\infty\right)^2}} \\
\cos\varepsilon &= \frac{1}{\sqrt{1+\left(PR^\infty\right)^2}} \\
\sin\varepsilon\,\cos\varepsilon &= \frac{PR^\infty}{1+\left(PR^\infty\right)^2} \\
\sin^2\varepsilon-\cos^2\varepsilon &= -\frac{1-\left(PR^\infty\right)^2}{1+\left(PR^\infty\right)^2} \quad .
\end{aligned}$$

(VIII D1.11)

Substituting these values into Eq. (VIII D1.10) reproduces (VIII D1.8) exactly.

IX. THE ENDF CONNECTION

Analyses accomplished with SAMMY often find their way into one or more of the evaluated nuclear data files [ENDF (United States), JEFF (European), CENDL (Chinese), JENDL (Japanese), BROND (Russian), FOND (Russian), ...]. Resonance parameters from the evaluated nuclear data files or experimental data from the EXFOR files are sometimes used as input for SAMMY analyses. Many options are available within SAMMY to expedite this information interchange. Some of these are described in various places throughout this document and summarized here. Others are described in more detail in this section. See also Section XI.C for miscellaneous comments regarding ENDF format conventions.

Command statements related to using ENDF formats as either input or output are summarized in Table VI A1.2 under the categories "ENDF as input" or "ENDF output." See also Sections VI.F.2 and VI.F.3 for other input requirements.

(In the following comments, "endf" in lowercase letters refers to "evaluated nuclear data files" in general, and "ENDF" in capital letters refers to the United States' Evaluated Nuclear Data Files as housed at the National Nuclear Data Center at Brookhaven National Laboratory.)

In 1998 the Cross Section Evaluation Working Group (CSEWG), an advisory group for the ENDF, appointed a "constants" task force subcommittee whose purpose was to ensure that each code contributing to or using data from the evaluated files would use the same values for mathematical and physical constants. The final report of that subcommittee is found in Section IX.A of this document. Also included there is Table IXA.1, which gives values for the physical constants used in the current version of SAMMY.

In the resolved resonance region (RRR), SAMMY can read resonance parameters directly from File 2 (extracted from an endf file), or from an entire endf file if the MAT (material) number is provided. Test cases tr049, tr050, tr086, tr102, and tr129 provide examples of this use of endf files. See Section VI.F.3 for details.

SAMMY can also write the R-matrix parameters into endf file 2 formats. For the RRR, see Section VI.F.2 for details. For the unresolved resonance region (URR), see Section VIII.D. Note that SAMMY can produce two output files corresponding to endf File 2, named SAMMY.NDF and SAMMY.NDX. The first of these is suitable for direct use within a complete endf file. The second (which is produced if the command "DEBUG" is included in the INPut file) contains the identical information but also includes comment lines (beginning with ####) that may be helpful in understanding the contents of the file.

When creating File 2, it is also possible to create File 32, which contains covariance information for the resonance parameters. The necessary command line is "`PUT COVARIANCE MATRIx into endf file 32`". The output file is named SAMMY.N32, and the corresponding annotated file (containing comment lines) is SAMMY.N3X. Test case tr126 has numerous examples with LCOMP = 0, 1, and 2. Test case tr128 gives examples in the URR.

When the input resonance parameters are in endf File 2 format (RRR), and the intent is to generate an estimated covariance matrix for endf File 32, SAMMY can automatically generate the input *.ndf file for that purpose. To invoke, include the command "`AUTOMATIC NDF FILE Creation`" in the INPut file. See test case tr137 (k and l) for examples. Note that other commands are also necessary:

```
AUTOMATIC NDF FILE Creation
INPUT IS ENDF/B FILE  MAT=9446
FLAG ALL RESONANCE Parameters
ENDF/B-VI FILE 2 IS wanted
NDF FILE IS IN KEY Word format (optional)
PUT COVARIANCE MATRIx into endf file 32
```

Point-wise cross sections can be printed in endf File 3 formats, in both the RRR and the URR. To invoke this option, include the phrase "`GENERATE FILE 3 POINt-wise cross section`", or "`FILE 3`", in the INPut file. An annotated "ndf" file, similar to that described in Section VI.F.2 for File 2, is also needed; see Table IX.1 for details. (Note that most entries in this table are optional.) The output file is named SAMMY.FL3, and the corresponding annotated file is SAMMY.FLX. For examples, see test case tr086 (w) in the RRR, and test case tr073 (n) in the URR.

It is possible to use ENDF File 3 as the "experimental data file". To do so, include one of these commands in the INPut file: "`DATA ARE ENDF/B FILE  MAT=1234`" or "`USE ENDF/B ENERGIES MAT=1234`", where the spacing before "MAT=" is not important (but there must be at least one space), and the endf MAT (material) number is used instead of "1234".

When calculating group averages, results can be reported in an endf-like format, similar to File 3, and the associated covariance matrix into a file with format similar to File 33. Include the command "`FILE 33 LB=1 COVARIAnce is wanted`" (or just "`FILE 33`") to write the average cross sections into file SAMMY.CRS and covariance information into file SAMMY.N33. See test case tr089 (h and i) for examples. (Historical note: SAMMY.N33 was once called SAMMY.NDF, but the name has been changed to avoid confusion with other files of the same name.) It is important to note that this is not the standard use for File 3 and 33; these files should not be used for inclusion in official ENDF files.

Legendre coefficients for angular distributions may be reported in endf File 4 format by including the command "`PREPARE LEGENDRE COEfficients in endf format`". The output file is called endf_legendre.dat. (File SAMJNK.DAT contains the same information in an expanded format, which some people may find useful.) The version of File 4 used here is that described in Section 4.2.2 of [ENDF-102], LTT = 1, LVT = 0, and LI = 0 (that is to say, the Legendre expansion coefficients Al(E) are given, no transformation matrix is given, and the angular distributions are not all isotropic). See test case tr112 for examples.

CAVEAT: As with all SAMMY options, it is the responsibility of the analyst (and not only of the SAMMY author) to ensure that these features are correct. In particular, when endf output files

are generated, SAMMY users are strongly encouraged to compare those files with the requirements of the endf formats. When endf files are used for input to SAMMY, users are urged to look carefully at all output to be sure that SAMMY is properly interpreting the input. When discrepancies are found, please notify the SAMMY author so that adjustments can be made.

Table IX.1. Key-word-based file needed for generating ENDF File 3 output

Card set	Key-word variable	Notes
1	`Z`	Z for target nucleus.
	`A`	Atomic mass number.
	`ZA`	If different from (1000 * Z + A), then value must be inserted directly.
	`AW`	Ratio of the mass of the sample nucleus to the neutron mass (if absent, will be calculated from the SAMMY input).
	`MAT`	ENDF MAT number (default = 9999).
	(blank)	
2	`NUclide` or `ISOtope`	No value need be given here; this word simply indicates that information for the next nuclide will follow. For the URR, card sets 2 and 3 are not used, as the present implementation of the URR in SAMMY permits only one nuclide at a time.
3	`Z`	Z for target nucleus (this isotope); not needed here if same as above.
	`A`	Atomic mass number (this isotope); not needed if same as above.
	`ZA`	If different from (1000 * Z + A), then value must be inserted directly.
	`AW`	Ratio of mass of sample nucleus (this isotope) to neutron mass.
	`ABN`	Abundance for this isotope, if different from unity.
	`SPIN`	Spin of this isotope.
	(blank)	

IX.A. CSEWG CONSTANTS

Recommendation of the CSEWG Constants Task Force
October 20, 1998

CSEWG participants: Mark Chadwick, Maurice Greene, Richard Hwang, Nancy Larson (chair), Robert MacFarlane, Vicki McLane, John White
Other participants: Dermott Cullen, Mick Moxon

In order to eliminate the use of different values for physical and mathematical constants as a source of discrepancy between calculations using different computer codes, CSEWG should take the following actions:

(1) Formally designate as official CSEWG constants the values reported in "1986 CODATA Internationally recommended values of the Fundamental Physical Constants" on the Web site *http://physics.nist.gov/cuu/Constants/*. This is the "NIST Reference on Constants, Units, and Uncertainty, one of the technical activities of the Fundamental Constants Data Center of the NIST Physics Laboratory. The contents of this site have been prepared by Barry N. Taylor of the Data Center in close collaboration with Peter J. Mohr of the Physics Laboratory's Atomic Physics Division."

a. Relevant numbers from the CODATA list will be published in ENDF-102.
b. Evaluators and code developers should use the values published in ENDF-102, updating only when that document is updated.

(2) Within the text of the next update of ENDF-102, remove numerical values for physical constants and replace by variable names; provide numerical values (and units) in a list in an appendix. This list should include (but is not limited to) the following:

a. m_n = mass of neutron in atomic mass units (u)
[Remove values from pages 0.18 and D.4 of the Nov. 1995 version of ENDF-102].
Recommended value from CODATA: m_n = 1.008 664 904 u

b. Boltzmann's constant k.
Recommended value from CODATA: $k = 8.617\,385 \times 10^{-5}$ eV K^{-1}

c. $\sqrt{2m_n}/\hbar$ = {sqrt (2 mass of neutron) / Plank's constant}. [Remove value from p. D.3.]
Recommended value based on information in CODATA:

$$\sqrt{2m_n}/\hbar = 0.002\,196\,807\,122\,623 / (10^{-12}\ \text{cm}\ \sqrt{\text{eV}}\ )$$

d. 2 (amu) / $\hbar^2$. [Remove value from Eq. (6.9).]
Recommended value based on information in CODATA:

$$2\ (\text{amu}) / \hbar^2 = 4.784\,504\,258\,066 \times 10^{-6} / (\ [10^{-12}\ \text{cm}]^2\ \ \text{eV}\ ).$$

e. $(e^2 / \hbar\ )^2$ amu. [Remove value from Eq. (6.10).]
Recommended value based on CODATA:

$$(e^2 / \hbar\ )^2\ \text{amu} = 2.480\,167\,060\,319 \times 10^4\ \text{eV}.$$

(3) Encourage code developers to locate any values for physical constants that may be currently buried deep within the coding, and replace by variables whose values are specified in one site only (e.g., in a block data statement). This ensures internal consistency, and expedites any necessary updates.

(4) Encourage code developers to double-check that numerical constants (e.g., π or e) are represented to a degree of accuracy consistent with the precision of the computers on which the codes are to be run.

(5) Encourage evaluators to use mass numbers, Q-values, etc., as specified on CODATA, for evaluations submitted for acceptance by ENDF. Values not found in CODATA should be obtained from G. Audi and A. H. Wapstra, *Nucl. Phys. A*, **595**, 409 (1995). The Web site for these values is maintained by the Atomic Mass Data Center, and located at *http://csnwww.in2p3.fr/massatom/masseval.html*.

(6) Encourage evaluators to specify values for "hidden" physical constants within the header text of the ENDF file, to prevent future confusion in the event of changes in the accepted values.

Submitted by the CSEWG Constants Task Force, N. M. Larson, Chair

---

Table IXA.1. Exact values of constants as used in the current version of SAMMY

Description	Value[a]	Units
mass of neutron	1.008 664 915 60	amu
mass of proton	1.007 276 466 88	amu
mass of deuteron	2.013 553 212 70	amu
mass of alpha	4.001 506 179 149	amu
mass of hellion (^{3}He)	3.014 932 243 4	amu
mass of triton (3H)[a]	3.016 049 268	amu
Boltzmann's constant	$8.617\ 343 \times 10^{-5}$	eV / K
$\hbar$ = Planck's constant / 2 π	$6.582\ 119\ 15 \times 10^{-16}$	eV s
atomic mass unit	$9.314\ 940\ 43 \times 10^{8}$	eV
speed of light	$2.997\ 924\ 58 \times 10^{8}$	m / s
α^{-1} = inverse fine-structure constant	$1.370\ 359\ 991\ 1 \times 10^{2}$	
amu	$1.660\ 538\ 86 \times 10^{-24}$	g (gram)
erg	$6.241\ 509\ 47 \times 10^{11}$	eV

[a]All values, except for the triton mass, are taken from the 2006 CODATA list. The triton mass was unavailable there and was instead taken from the ENDF-102 manual.

X. AUXILIARY PROGRAMS

A number of "auxiliary" programs, not an integral part of SAMMY itself, are designed to be used in conjunction with SAMMY. These programs manipulate SAMMY PARameter and/or COVariance files, aid in interpreting or illustrating SAMMY input or output, or offer a means of comparing SAMMY results with other calculations. The codes are listed in alphabetical order in Table X.1, which also provides a brief description of the purpose of the code, and the section number in which details can be found.

Table X.1. SAMMY auxiliary codes

Code name	Description	Section
ANGODF	Convert PLOT file from energy/angle to angle/energy	X.A
CONVRT	Convert from REFIT input to SAMMY or vice versa	X.B
LEVDEN	Fit the level-density formula	no longer supported
SAMAMR	Add, mix, or recover variables in COVariance file	X.C
SAMAMX	Alter the value of one non-varied parameter in the COVariance file after completion of an analysis	X.D
SAMCPR	Compare SAMMY calculations to those from other sources	X.E
SAMCNV	Convert to an ASCII covariance matrix	no longer supported
SAMDIS	Calculate statistical distributions for resonance parameters	X.F
SAMEST	Estimate array size for a particular configuration of resonances and experimental data	no longer supported
SAMFTZ	Modify the experimental energies with t_0 and L_0	X.G
SAMORT	Plot the ORR resolution function	X.H
SAMPLT	Alternative form for plot files	X.I
SAMQUA	Generate resonance quantum numbers for particle pairs	X.J
SAMRML	Read ENDF File 2; calculate cross sections and derivatives	X.Q
SAMRPT	Plot RPI resolution function	X.K
SAMRST	Plot Gaussian plus exponential resolution function	X.L
SAMSMC	Monte Carlo calculation of multiple scattering corrections	X.M
SAMSTA	Generate staircase plots of resonance widths	X.N
SAMTHN	Thin experimental data	X.O
SUGGEL	Estimate quantum numbers for resonances	X.P

When angular distribution data are analyzed, results are reported in an ODF file [JC78] from which plots of energy vs. cross section at a fixed angle can be made. To plot angle vs. cross section at fixed energy, it is necessary to reorganize the ODF file; this reorganization is accomplished with program ANGODF, discussed in Section X.A.

The task of converting from REFIT to SAMMY input can be eased by use of program CONVRT, discussed in Section X.B.

Program LEVDEN was developed years ago to fit the level-density formula of Gilbert and Cameron to the number of levels (as given in a SAMMY PARameter file) in a specified energy region. This program is no longer supported but may be revived if there is sufficient demand.

In Section X.C the program SAMAMR is described; this program is used to rearrange PARameter and COVariance files to facilitate analyses of disparate data sets with the same resonance parameter set. (Note that SAMAMR replaces the two codes SAMADD and SAMMIX described in early versions of this report.)

Program SAMAMX is used to alter the value of one non-varied parameter in the covariance file after completion of an analysis. See Section X.D.

The program SAMCNV was designed to read a SAMMY binary COVariance file and produce an ASCII file containing the complete covariance matrix for all resonance parameters. This program is no longer available.

For assistance in comparing results of calculations performed by different computer codes, use program SAMCPR; see Section X.E for details.

Program SAMDIS (elsewhere named SAMDIST) is used for calculating statistical distributions for R-matrix resonance parameters; see ref. [LL95]. Level spacing distributions are calculated according to the Wigner distribution law, distributions for widths are calculated via χ^2 distributions, and long-range correlations of the energies are tested via the Δ_3 statistic of Mehta-Dyson. A summary of features of this code is given in Section X.F, along with recent modifications of the input to the code.

The program SAMEST was created to estimate the storage requirements for SAMMY, based on information provided interactively by the user; this information included such items as the number of resonances, how many parameters are varied, and how many data points are to be included. With today's modern computing facilities, this capability is no longer crucial. Hence this program has not been maintained and is no longer available.

Program SAMFTZ is used to modify the experimental energies in a DATa file, in order to align them more accurately with other experimental data. See Section X.G for details.

Program SAMORT, described in Section X.H, is used for plotting the components of the Oak Ridge resolution function. Similar plots can be made for the RPI resolution function using program SAMRPT (Section X.K) and of the original Gaussian plus exponential resolution function (Section X.L).

Program SAMPLT, which provides an alternative methodology for generating plots, is discussed in Section X.I. (Note: This program has been renamed from SAMBIN.)

Quantum numbers can be generated using program SAMQUA, described in Section X.J. This program has recently been updated by Olivier Bouland et al. [OB03] to include more complicated cases.

Program SAMSMC may be used for Monte Carlo calculations of the self-shielding and multiple-scattering corrections to capture and fission yields. See Section X.M.

The program SAMSTA, described in Section X.N, is used to create a file from which "staircase plots" of the resonance from a SAMMY PARameter file can be generated.

Section X.O describes program SAMTHN, a simple program for averaging data files used as input to SAMMY runs.

Soo Youl Oh and Luiz Leal's SUGGEL code, used to provide initial estimates for the quantum numbers of resonances, is described in Section X.P.

Section X.Q describes SAMRML, a program designed as an aid for people wishing to implement the ENDF File 2 LRU=1 LRF=7 format. This code calculates cross sections and derivatives as SAMMY does but without the considerable overhead relating to comparisons to experimental data.

X.A. ANGODF: CONVERT FROM ENERGY/ANGLE TO ANGLE/ENERGY

When analyzing angular distribution data (differential elastic scattering), the results are reported in two ODF files. The first file, SAMMY.DAT, contains the experimental data and uncertainties for each angle, as a function of energy; contents of each section of this file are shown in Table X A.1. The second file, SAMMY.ODF, contains the results of the calculations; contents of this file are described in Table X A.2. Note that the angles themselves are not listed in these files; they are only in the user's INPut file, card set 8.

Table X A.1. Contents of the ODF file SAMMY.DAT

Sect. No.	Meaning
1	Energy in eV
2	Experimental cross section (barns) for the first angle
3	Absolute uncertainty on experimental cross section for the first angle
4	Experimental cross section (barns) for the second angle
5	Absolute uncertainty on cross section (barns) for the second angle
6,7, etc.	Repeat, two sections (data plus uncertainty) for each angle

Table X A.2. Contents of the ODF file SAMMY.ODF for angular distribution data

Sect. No.	Meaning
1	Energy in eV
2	Initial calculation of cross section (barns) for the first angle
3	Final calculation of cross section (barns) for the first angle
4	Initial calculation of cross section (barns) for the second angle
5	Final calculation of cross section (barns) for the second angle
6,7, etc.	Repeat, two sections (initial plus final calculation) for each angle

Using these two files, one can produce plots of the various cross sections (experimental vs calculated) at a given angle, with energy as the horizontal axis. Often, however, it is also useful to consider plots of cross sections at a given energy, with angle as the horizontal axis, which cannot be accomplished directly with forodf. Instead, the positions of energy and angle must be reversed in a new ODF file; this can be accomplished using the conversion program ANGODF.

To run program ANGODF, respond appropriately to the following questions:

- What is name of ODF file with experimental data? [SAMMY.DAT]
- What is name of ODF file with theoretical values? [SAMMY.ODF]
- What is name of new ODF file? [whatever name you choose]
- What is name of INPut file? [same as the INPut file that was used to generate SAMMY.DAT and SAMMY.ODF]
- Are all energies to be used? (default = NO)
- What energies? One per line, end with blank... [question is omitted if response to previous question was "yes"]

The program will generate an ODF file (with the name you chose), containing sections as described in Table X A.3.

Table X A.3. Contents of the ODF file created by program ANGODF

Sect. No.	Meaning
1	Angle in degrees
2	Experimental cross section (barns) for the first energy
3	Absolute uncertainty on the experimental cross section (barns)
4	Initial calculation of cross section (barns) for the first energy
5	Final calculation of cross section (barns) for the first energy
6,7, etc.	Repeat, four sections (data plus uncertainty, initial plus final calculation) for each energy requested

X.B. CONVRT: CONVERT FROM REFIT INPUT TO SAMMY OR VICE VERSA

During his 1996 visit to Oak Ridge, Mick Moxon and the SAMMY author made preliminary attempts to provide an interface between Moxon's code REFIT [MM89] and SAMMY. The result is a program CONVRT, which is intended to read the input files for one code and write the corresponding input files for the other code. Beginning from REFIT input files, program CONVRT is able to generate appropriate SAMMY-style INPut and PARameter files; similarly, beginning from SAMMY-style files, CONVRT can generate portions of the REFIT input files. In either case, the user will likely need to edit the new files to provide complete input. Note that CONVRT is not yet able to translate resolution parameters nor experimental data from one code to the other, because definitions are not completely compatible between SAMMY and REFIT.

Input to program CONVRT consists of one command line (either "sammy" if converting from SAMMY to REFIT, or "refit" if converting from REFIT to SAMMY), followed by names of input files.

When converting from SAMMY to REFIT, file names are given in the usual order (INPut, PARameter, and DATa file names). Output consists of a SAMMY.LPT file, plus files containing portions of the REFIT input files; these are named REFITx.DAT where "x" is a digit from 0 to 9. One file is given for each nuclide type; it is the user's responsibility to combine these properly into the REFIT input file.

When converting from REFIT to SAMMY, output consists of three files: SAMMY.LPT, SAMMY.INP, and SAMMY.PAR. The user should rename these files and check to be sure they are complete before using the INPut or PARameter file as input to SAMMY runs.

X.C. SAMAMR: ADD, MIX, OR RECOVER VARIABLES

Because the fitting procedure in SAMMY is Bayes' method (Section IV) rather than ordinary least squares, SAMMY may be used for general evaluation purposes, that is, for determining a set of parameters that simultaneously describe a large number of different types of experimental data taken at different times and/or at different laboratories.

Performing such evaluations with SAMMY originally required sequential analyses of the various data sets,* with the output parameter and covariance matrix from the first analyses used as input to the second, output from the second used as input to the third, and so forth. If none of the broadening parameters are varied during the analyses, and if no data-reduction parameters are included, this procedure poses no undue difficulty; the analyst simply changes the values of the thickness and/or of the broadening parameters in the INPut file to correspond to the data currently being analyzed. However, when any of the broadening parameters are varied, and/or when normalization or background is included in the analysis, the PARameter and COVariance files must also correspond to the current data set. The code SAMAMR performs the appropriate modifications to the PARameter and COVariance files.

For example, data may come from two or more samples of different thicknesses and at different temperatures. The initial PARameter file is set up to include thickness and temperature appropriate for the first sample; thickness and temperature for the other samples are simply omitted. After the analysis of the first data set, code SAMAMR is used to incorporate the second thickness (as yet uncorrelated to any other parameters) and to "mothball" the correlated but now-to-be-unused first thickness; a second run of SAMAMR introduces the new temperature parameter and mothballs the old. The resulting PARameter file can then be used as input for the SAMMY analysis of the second data set. If, for a subsequent SAMMY run, one of the "UNUSED" parameters must be used again, SAMAMR will interchange the current BROADening parameter with the appropriate UNUSED parameter.

To illustrate, suppose three data sets are available, taken from three samples at two different temperatures:

Data Set 1: Sample 1 (thickness n_1, Temperature T_1)
Data Set 2: Sample 2 (thickness n_2, Temperature T_2)
Data Set 3: Sample 3 (thickness n_3, Temperature T_1)

The sequence of commands required to properly analyze these data is shown in Table X C.1. The input PARameter file (t007a.par) is listed in Table X C.2. Output PARameter files are listed in Tables X C.3 through X C.12. (Data and analysis are courtesy of F. G. Perey [FP84].) Note that values (and covariances) of the unused parameters are updated in each

* This is still the "standard mode" of operation for SAMMY. However, it is also now possible to simultaneously analyze more than one data set (Section IV.E.1), so long as none of the data-specific parameters are varied. The uncertainties on the data-specific parameters can, however, be included in the data covariance matrix, via the PUP option as described in Section IV.D.2.

SAMMY run, even though the data have no direct effect on those parameters. Rather, the effect is indirect, via the parameter covariance matrix. Note also that values (and uncertainties) are never changed in a SAMAMR run. Complete listings of all INPut, PARameter, DATA, and LPT files for this example are given in Test Case tr007, which is available along with the SAMMY FORTRAN from the Radiation Safety Information Computational Center [RSICC].

SAMAMR was designed to be run interactively (though a command file can of course be created, once the user is sufficiently familiar with the input). The code will prompt the user with questions about the type of operation to be performed, the parameters involved, and values for any new parameters.

Type of operation. The first question asked by SAMAMR is "Do you want to Add, Mix, Remove, reCover, or Introduce variables?" The user will type the capitalized letter for the appropriate operation.

Add refers to (1) the removal of one parameter to the unused list and (2) the introduction of another parameter (of the same kind) into the active list. The user is asked to specify the particular parameter (from a list provided), to give the variable number for that parameter if it was varied in the run which produced this covariance file, and to give the value and uncertainty to be used for the new parameter. Mix refers to the interchange of one unused parameter with the corresponding parameter in the active variable set. The user must provide the location (variable number) within the unused parameter set.

The operations Remove, reCover, and Introduce are used to reorganize the attenuation or normalization-and-background parameters when the analysis involves both angle-differential data (such as the elastic angular distribution scattering data) and other data that are integrated over angle (such as transmission). The operation Remove moves normalization-and-background parameters for all angles, or attenuation parameters for all angles, from the active variable set to the unused variable set. The operation reCover performs the inverse, moving parameters from the unused to the active set. Introduce allows the introduction of new parameter values and uncertainties when switching from analysis of angle-integrated data to analysis of angular distribution data.

Type of parameter. The types of parameters to be treated by SAMAMR are different, depending on the operation to be performed.

For both Add and Mix, only one parameter is treated at a time; the example shown in Table XC.1 therefore requires two runs of SAMAMR between each run of SAMMY. The parameters that can be treated are taken from the following list, in which is also given the card set and line number from the PARameter file (see Table VI B.1):

(Broadening parameters)

TEMP , THICK, DEL-L, DEL-G, DEL-E	(card set 4, line 3)

(Normalization and background parameters)

NORML, BACKA, BACKB, BACKC, BACKD, BACKF	(card set 6, line 2)

(ORR resolution parameters)

BURST	(card set 9, line 2)
WATR0, WATR1, WATR2	(card set 9, line 3)
TANTA	(card set 9, line 3)
X1, X2, X3, X0	(card set 9, line 4)
WWW, ALPHA	(card set 9, line 6)
D, F, G	(card set 9, line 8)
DELTA	(card set 9, line 8)
CHANN	(card set 9, line 10)

(Miscellaneous parameters, with alternative names in square brackets)

DELTA, DELT2 [DELL1, DELL0]	(card set 11, line 2)
NU [ETA]	(card set 11, line 3)
ATTNI, ATTNO [FINIT, FINI2]	(card set 11, line 4)
TZERO, LZERO	(card set 11, line 6)
SIABN	(card set 11, line 7)
SITEM, SITHC [SELFI]	(card set 11, line 8)
EFFIC, FISEF [EFCAP, EFFIS]	(card set 11, line 9)
DELTE, DELE0, DELE2 [DELE1, DELE0, DELE2]	(card set 11, line 10)
CONCR, CONTR	(card set 11, line 11)

(RPI/GELINA/nTOF resolution function parameters)

BURST	(card set 14, line 2)
TAU	(card set 14, line 3)
LAMBD	(card set 14, line 5)
A1	(card set 14, line 7)
EXPON	(card set 14, line 9)
CHANN	(card set 14, line 11)

In addition to giving the parameter name, as given in the above list, the user will sometimes also need to specify which parameter of this type is to be used. The name is given in the first five columns (be sure to leave blanks if the name is fewer than five characters), and an integer number is then given. For the RPI resolution parameters, the second, third, etc., variables on the line (in the PARameter file) are specified by “2”, “3”, etc., in the SAMAMR input. See test case tr087 for examples of this.

For the operations Remove, reCover, and Introduce, only the parameters ATTEN and ALLNB may be specified. When ATTEN is specified, all attenuation parameters (both incident and outgoing, from card set 11, line 4 of the PARameter file) are involved. When ALLNB is specified, all normalization and background parameters are involved (see card set 6, line 2). Again, only one type can be treated during one run of SAMAMR.

When the operation Introduce is used, attenuation or normalization/background parameters are assumed to be given in a separate file in the same format as used in the PARameter file (either with or without the "MISCEllaneous parameters" or "NORMAlization and background" header lines of card sets 11 and 6; however, if they are included, the first five characters must be either all caps or all lowercase). SAMMY will ask for the file name instead of the parameter values. Test case tr036 shows examples of the use of this feature.

An additional restriction for operations Remove, reCover, and Introduce stems from the connection between the attenuation parameters and the number of angles: SAMAMR assumes that removal of attenuation parameters implies changing from angular-distribution data to angle-integrated data, and that recovery or introduction of attenuation parameters implies the reverse change. Removal of attenuation parameters, therefore, must be accomplished *after* removal of normalization and background parameters, and recovery or introduction of attenuation parameters must be accomplished *prior to* recovery or introduction of normalization and background parameters.

Test cases tr007, tr032, tr036, tr079, and tr087 all have examples of the use of program SAMAMR.

Table X C.1. Commands to analyze data from three samples of different thicknesses at two different temperatures

Interactive input	Description of what is being done

`sammy <<EOF`
`t007a.inp`
`t007a.par`
`t007a.dat`
 	
`EOF`
	analyze first data set using TEMP1 & THCK1

`mv -f SAMMY.LPT results/raa.lpt`
`mv –f SAMMY.ODF results/raa.odf`
`mv –f SAMMY.PAR results/raa.par`
`mv –f SAMMY.COV results/raa.cov`
	rename the output files

`samamr <<EOF`
`a`
`results/raa.par`
`results/raa.cov`
`results/rcc.par`
`results/rcc.cov`
`TEMP`
`TEMP1`
`181.0`
`10.0`
`EOF`
	mothball TEMP1; insert TEMP2

`samamr <<EOF`
`a`
`results/rcc.par`
`results/rcc.cov`
`results/rdd.par`
`results/rdd.cov`
`THICK`
`THCK1`
`0.01754`
`0.0001754`
`EOF`
	mothball THCK1; insert THCK2

`sammy <<EOF`
`t007d.inp`
`results/rdd.par`
`t007e.dat`
`results/rdd.cov`
 	
`EOF`
	analyze second data set with TEMP2 & THCK2; with UNUSED #1=TEMP1, #2=THCK1

`mv –f SAMMY.LPT results/ree.lpt`
`mv –f SAMMY.PAR results/ree.par`
`mv –f SAMMY.ODF results/ree.odf`
`mv –f SAMMY.COV results/ree.cov`	

Table X C.1 (continued)

Interactive input	Description of what is being done

`samamr <<EOF`
`m`
`results/ree.par`
`results/ree.cov`
`results/rff.par`
`results/rff.cov`
`TEMP`
`TEMP2`
`1`
`EOF`
	interchange so USED=TEMP1, UNUSED#1=TEMP2

`samamr <<EOF`
`a`
`results/rff.par`
`results/rff.cov`
`results/rgg.par`
`results/rgg.cov`
`THICK`
`THCK2`
`0.01319`
`0.0001319`
`EOF`
	mothball THCK2, insert THCK3

`sammy <<EOF  # tr7hhh`
`t007h.inp`
`results/rgg.par`
`t007h.dat`
`results/rgg.cov`
 	
`EOF`
	analyze third data set with TEMP1 & THCK3; with UNUSED #1=TEMP2, #2=THCK1, #3=THCK2

`mv SAMMY.LPT results/rhh.lpt`
`mv SAMMY.PAR results/rhh.par`
`mv SAMMY.ODF results/rhh.odf`
`mv SAMMY.COV results/rhh.cov`
	rename files

`samamr <<EOF`
`m`
`results/rhh.par`
`results/rhh.cov`
`results/rii.par`
`results/rii.cov`
`THICK`
`THCK3`
`2`
`EOF`
	interchange THICK and UNUSED#2 (so will use TEMP1 & THCK1)

Table X C.1 (continued)

Interactive input	Description of what is being done

`sammy <<EOF`
`t007j.inp`
`results/rii.par`
`t007a.dat`
`results/rii.cov`
 	
`EOF`
	generate cross section for first data set with TEMP1 & THCK1; with UNUSED #1=TEMP2, #2=THCK3, #3=THCK2

`mv SAMMY.LPT results/rjj.lpt` `mv SAMMY.ODF results/rjj.odf`	rename files

`samamr <<EOF`
`m`
`results/rii.par`
`results/rii.cov`
`results/rkk.par`
`results/rkk.cov`
`TEMP`
`TEMP1`
`1`
`EOF`
	interchange TEMP=TEMP1 with UNUSED#2=TEMP2

`samamr <<EOF`
`m`
`results/rkk.par`
`results/rkk.cov`
`results/rll.par`
`results/rll.cov`
`THICK`
`THCK1`
`3`
`EOF`
	interchange THICK=THCK1 with UNUSED#3=THCK2

`sammy <<EOF`
`t007m.inp`
`results/rll.par`
`t007e.dat`
`results/rll.cov`
 	
`EOF`
	generate cross section for second data set with TEMP2 & THCK2; with UNUSED #1=TEMP1, #2=THCK3, #3=THCK1

`mv SAMMY.LPT results/rmm.lpt` `mv SAMMY.ODF results/rmm.odf`	rename files

Table X C.2. The initial PARameter file t007a.par for the example of Section X.C

```
-2070.     1450.      186600.    0.         0.          0 0 0 0 0 1
27650.     1400.      1480000.   0.         0.          1 0 1 0 0 1
1151.07    600.       62.        0.         0.          1 1 1 0 0 2


BROADENING
6.00      329.00    0.2179    0.025     0.022     0.022      1 1 1 1 1 1

EXPLICIT
 2001              0.5
 2002              5.0
 2003              0.002179
 2004              0.005
 2005              0.005
 2006              0.005
    2    1         400.
    2    3         100000.
    3    1         5.
    3    2         300.
    3    3         15.
```

Table X C.3. Intermediate PARameter file raa.par

```
-2070.00000 1450.00000 186600.000                        0 0 0     1
27652.54913 1400.00000 1478023.10                        1 0 1     1
1151.115961 582.738578 58.8204626                        1 1 1     2

.100000000
BROADENING PARAMETERS FOLLOW
6.00413005 328.76010 .21794422 .02489528 .02195479 .02179978 1 1 1 1 1 1

COVARIANCE MATRIX IS IN BINARY FORM
```

Table X C.4. Intermediate PARameter file rcc.par

```
-2070.00000 1450.00000 186600.000                        0 0 0     1
27652.54913 1400.00000 1478023.10                        1 0 1     1
1151.115961 582.738578 58.8204616                        1 1 1     2

.100000000
BROADENING PARAMETERS FOLLOW
6.00413005 181.00000 .21794422 .02489528 .02195479 .02179978 1 1 1 1 1 1

UNUSED PARAMETERS FOLLOW
TEMP1
328.760096

COVARIANCE MATRIX IS IN BINARY FORM
```

Table X C.5. Intermediate PARameter file rdd.par

```
-2070.00000 1450.00000 186600.000                        0 0 0     1
27652.54913 1400.00000 1478023.10                        1 0 1     1
1151.115961 582.738578 58.8204626                        1 1 1     2

.100000000
BROADENING PARAMETERS FOLLOW
6.00413005 181.00000 .01754000 .02489528 .02195479 .02179978 1 1 1 1 1 1

UNUSED PARAMETERS FOLLOW
TEMP1     THCK1
328.760096 .21794422

COVARIANCE MATRIX IS IN BINARY FORM
```

Table X C.6. Intermediate PARameter file ree.par

```
-2070.00000 1450.00000 186600.000                        0 0 0     1
27650.53011 1400.00000 1486267.24                        1 0 1     1
1151.032862 571.778880 62.2006803                        1 1 1     2

.100000000
BROADENING PARAMETERS FOLLOW
6.02833418 175.89356 .01763260 .02454234 .02179889 .02349694 1 1 1 1 1 1

UNUSED PARAMETERS FOLLOW
TEMP1     THCK1
327.765105 .21676717

COVARIANCE MATRIX IS IN BINARY FORM
```

Table X C.7. Intermediate PARameter file rff.par

```
-2070.00000 1450.00000 186600.000                        0 0 0     1
27650.53011 1400.00000 1486267.24                        1 0 1     1
1151.032862 571.778880 62.2006803                        1 1 1     2

.100000000
BROADENING PARAMETERS FOLLOW
6.02833418 327.76511 .01763260 .02454234 .02179889 .02349694 1 1 1 1 1 1

UNUSED PARAMETERS FOLLOW
TEMP2     THCK1
175.893563 .21676717

COVARIANCE MATRIX IS IN BINARY FORM
```

Table X C.8. Intermediate PARameter file rgg.par

```
-2070.00000 1450.00000 186600.000                        0 0 0     1
27650.53011 1400.00000 1486267.24                        1 0 1     1
1151.032862 571.778880 62.2006803                        1 1 1     2

.100000000
BROADENING PARAMETERS FOLLOW
6.02833418 327.76511 .01319000 .02454234 .02179889 .02349694 1 1 1 1 1 1

UNUSED PARAMETERS FOLLOW
TEMP2     THCK1     THCK2
175.893563 .21676717 .01763260

COVARIANCE MATRIX IS IN BINARY FORM
```

Table X C.9. PARameter file rhh.par, containing final results for example of Section X.C

```
-2070.00000 1450.00000 186600.000                        0 0 0     1
27651.00483 1400.00000 1487173.71                        1 0 1     1
1151.033783 565.790617 61.6726510                        1 1 1     2

.100000000
BROADENING PARAMETERS FOLLOW
6.03414731 326.86586 .01317133 .02392383 .02155364 .02207008 1 1 1 1 1 1

UNUSED PARAMETERS FOLLOW
TEMP2     THCK1     THCK2
178.166780 .21674113 .01765984

COVARIANCE MATRIX IS IN BINARY FORM
```

Table X C.10. PARameter file rii.par, which is a permutation of the file rhh.par

```
-2070.00000 1450.00000 186600.000                        0 0 0     1
27651.00483 1400.00000 1487173.71                        1 0 1     1
1151.033783 565.790617 61.6726510                        1 1 1     2

.100000000
BROADENING PARAMETERS FOLLOW
6.03414731 326.86586 .21674113 .02392383 .02155364 .02207008 1 1 1 1 1 1

UNUSED PARAMETERS FOLLOW
TEMP2     THCK3     THCK2
178.166777 .01317133 .01765984

COVARIANCE MATRIX IS IN BINARY FORM
```

Table X C.11. PARameter file rkk.par, which is a permutation of the file rhh.par

```
-2070.00000 1450.00000 186600.000                        0 0 0     1
27651.00483 1400.00000 1487173.71                        1 0 1     1
1151.033783 565.790617 61.6726510                        1 1 1     2

.100000000
BROADENING PARAMETERS FOLLOW
6.03414731 178.16678 .21674113 .02392383 .02155364 .02207008 1 1 1 1 1 1

UNUSED PARAMETERS FOLLOW
TEMP1     THCK3     THCK2
326.865860 .01317133 .01765984

COVARIANCE MATRIX IS IN BINARY FORM
```

Table X C.12. The PARameter file rll.par, which is a permutation of the file rhh.par

```
-2070.00000 1450.00000 186600.000                        0 0 0     1
27651.00483 1400.00000 1487173.71                        1 0 1     1
1151.033783 565.790617 61.6726510                        1 1 1     2

.100000000
BROADENING PARAMETERS FOLLOW
6.03414731 178.16678 .01765984 .02392383 .02155364 .02207008 1 1 1 1 1 1

UNUSED PARAMETERS FOLLOW
TEMP1     THCK3     THCK1
326.865860 .01317133 .21674113

COVARIANCE MATRIX IS IN BINARY FORM
```

X.D. SAMAMX: MODIFY A SINGLE VALUE

Program SAMAMX is used to alter the value of one non-varied parameter in the covariance file after completion of an analysis.

Development of SAMAMX was prompted by the need to change the value of $\overline{\Gamma}_{\lambda\gamma}$ for a low-lying (negative-energy) resonance in order to obtain the correct thermal values but without having to reanalyze the higher-energy regions.

<u>The program is to be used only on rare occasions and with extreme caution!</u>

The program is designed to run interactively; SAMAMX will prompt you for the information that you need to provide to it.

For a sample run of SAMAMX, see test case tr007. Look near the end of the command file test007 for the SAMAMX run, which alters the value of $\overline{\Gamma}_{\lambda\gamma}$ in raa.cov for the second resonance, and puts the result in ryy.cov.

<u>BEWARE</u>: SAMAMX does *not* change resonance parameter values in the PAR file; changes in value occur only in the COV file. You may, if you wish, manually change them in the PAR file; however, it is not necessary to do so. SAMMY will use the values given in the COV file, not those in the PAR file; you can verify this by looking at the values given in the LPT file from the SAMMY run (file rzz.lpt in the example).

X.E. SAMCPR: COMPARE RESULTS

Program SAMCPR is an aide in comparing cross sections calculated by one computer code (e.g., NJOY [RM82] or REFIT [MM89]) with those calculated by SAMMY. First, a no-Bayes SAMMY run is made using the other code's calculations as the DATa file, and including the alphanumeric command "`COMPARE EXPERIMENT To theory`" in the INPut file. SAMMY generates a binary file SAM53.DAT, which can then be read by program SAMCPR to produce the ODF file SAMCPR.ODF.

The contents of the various sections of the output file SAMCPR.ODF are as follows:

S1 = energy
S2 = X = "data," which may be a calculation from another code
S3 = S = "theory," which is the SAMMY calculation
S4 = $X - S$
S5 = $(X - S) / S$
S6 = $(X - S) / S \times 10^3$
S7 = $(X - S) / S \times 10^4$
S8 = $(X - S) / S \times 10^5$
S9 = $(X - S) / S \times 10^6$
S10 = S5 adjusted for small cross sections
S11 = S10 $\times 10^3$
S12 = S10 $\times 10^4$
S13 = S10 $\times 10^5$
S14 = S10 $\times 10^6$

For section 10, the quantity $(X - S) / S$ is replaced by 10^{-25} if both X and S are smaller than 0.0001. Thus the values in S10 through S14 will be sizeable only when the cross sections themselves are reasonably large.

Note that early versions of this program were called SAMCMP. However, "cmp" is a special word on Unix systems; hence, the name has been changed.

X.F. SAMDIS: STATISTICAL DISTRIBUTIONS

The code SAMDIS a slightly modified version of the code SAMDIST [LL95], which is used to verify the consistency of a resonance parameter set with the predicted theoretical statistical distribution. Three different tests can be performed:

1. Level spacing distributions are compared with the Wigner distribution law.
2. Neutron-, radiation-, and fission-width distributions are calculated and compared with the χ^2 distribution with the appropriate number of degrees of freedom ($\nu = 1$ for the Porter-Thomas distribution of neutron widths, $\nu = 2$ or 3 for fission, and ν = infinity for capture widths).
3. Long-range correlations of the energies are tested via the Δ_3 statistic of Mehta and Dyson.

Details of the three tests are given in the SAMDIST manual.

One modification to the code (and to the input; see Table XF.1) has been made subsequent to the publication of the SAMDIST manual: The calculation of distribution of neutron widths now includes penetrabilities. Hence it is necessary to define the orbital angular momentum and to give the atomic mass of the target nucleus.

Table X F.1. Input for program SAMDIS

Line number	SAMDIST prompt	Response	Notes
1	Type d (for spacing), w (for width), or d3 (for delta3)	"`d`", "`w`", or "`d3`"	Line 3 appears only for "`w`" in line 1
2	Parameter file name	name of file	30 characters or less
3 ("`w`" only)	Enter particle channel	"`neutron`", "`fission`", or "`gamma`"	only lowercase is permitted; note also that this line appears only for type 2 ("`w`" in line 1)
4	Spin group, initial and final energies	SAMMY spin group number, Emin and Emax	free format, separate by commas
5 ("`w`" and "`neutron`" only)	Enter *l* and awr	integer value of orbital angular momentum, mass of target nucleus	This line is absent unless line 1 is "`w`" and line 3 is "`neutron`"
6 ("`d`" or "`w`" only)	Bin width for sampling	in units of energy	This line is absent for "*d3*"
7 ("`w`" only)	Degrees of freedom	degrees of freedom for chi-squared distribution	This line is here for "w" only (not for "d" or "d3")

X.G. SAMFTZ: FIX TZERO

When the energy grids of two or more data sets are misaligned, SAMMY has an option to treat initial time t_0 and the flight-path length L as search parameters, in order to provide consistent energy grids; see Section III.E.8 for details.

Once appropriate values for t_0 and L are determined, it is often useful to adjust the experimental data set accordingly before proceeding with further analysis. This is accomplished using the auxiliary code SAMFTZ.

To run SAMFTZ, provide answers to the following questions:

What are tzero & Lzero? (default = 0.0 & 1.0)
What is the flight-path length in meters?
What is name of original data file?
What is name of new data file?
Are data in csisrs format? (default = yes)

Only CSISRS or TWENTY format is permitted for the "original data file;" answer "yes" to the final question if the original file is in CSISRS format and "no" if the file is TWENTY. The "new data file" will be in TWENTY format.

For an example of the use of SAMFTZ, see test case tr122.

X.H. SAMORT: PLOT THE OAK RIDGE RESOLUTION FUNCTION

When using the realistic resolution function (see Section III.C.2), it may be useful to plot both the individual components of the resolution function and the final composite function. This can be accomplished using program SAMORT, which requires only the PARameter file and three other numbers (energy, mass, and flight-path length) as input. Output consists of one ASCII file, as many as five plot (ODF) files, and as many as five additional ASCII files. The first ASCII file gives details of the case being run, including for example centroids for each component of the resolution function. Four plot files give time vs. resolution function for each component, and the fifth gives energy, resolution function, and time for the composite function (so that one can plot the resolution as a function of either energy or time). As with other plot files produced by SAMMY, these are in ODF format. For the benefit of SAMMY users who do not have the ORNL plotting package FORODF, the same information in the ODF files is also given in ASCII files with extension "PLT".

A sample interactive (Unix) run of program SAMORT is accomplished with the following lines of input:

```
samort
a.par
180000.,57.935,201.578
```

Here the energy at which the functions are to be evaluated is 180000 eV, the mass of the sample is 57.935 amu, and the flight-path length is 201.578 m.

The file a.par can be either the complete PARameter file or may contain only the ORRES portion thereof. The file may look similar to the following (see test case tr021, file t021tlo.par):

```
BURST 1        1.775    .5
TANTA 1        0.200       0.1
TANTA 1111     0.010     0.050     0.090     0.040
TANTA          0.005      .005     0.005     0.005
TANTA 11       0.079     1.000
TANTA          0.04      0.5
LITHI 111      5.000  0.392235     1.009
LITHI          2.000  0.200000     0.500
CHANN 1   200000.000     7.179     4.000
```

(See card set 9 of the PARameter file, Table VI B.2, for interpretation of these numbers.)

Output plot files are as follows: The file SAM_ORR.ODF contains energies in section 1, resolution function in section 2, and time of flight in section 3. File SAM_ORR_BURST.ODF contains time of flight in section 1, and the burst-width component of the resolution function in section 2. File SAM_ORR_TANTA.ODF contains time in section 1 and the tantalum target component of the resolution function in section 2. File SAM_ORR_CHANN.ODF contains time in section 1 and channel-width component in section 2. Finally, the file SAM_ORR_LITHI.ODF contains time in section 1 and the Lithium-glass detector resolution function in section 2.

If the water moderator or the NE110 detector had been used instead, the respective file names would be SAM_ORR_WATER.ODF and SAM_ORR_NE110.ODF.

For a description of the contents of the ASCII PLT files, substitute “column” for “section” in the above description.

What follows is the output ASCII file SAMMY.ORR produced by running the example described above:

```
p ----------------------------
            1.7750E-03
 a, w, x1, x2, x3, x0, alpha --
             1174.       463.6      1.7041E-06  8.5204E-06  1.5337E-05
            6.8163E-06   1.000
 c ----------------------------
            7.1790E-03
 d, f, g ----------------------
            5.0000E-03   392.2       1.009

 <t>, t1, t2, t3, t4 ----------
            1.0224E-02  8.8750E-04  1.5522E-03  3.5895E-03  4.1951E-03
 tlow, time, tup --------------
             34.252758       34.350628       34.360852
 eup , em  , elow -------------
             181030.09       180000.00       179892.89
 #########################
```

X.I. SAMPLT: ALTERNATIVE FORM FOR PLOT FILES

Plotting with SAMMY has traditionally been accomplished by means of a set of utility programs FORODF [JC78]. SAMMY produces "ODF" or "plot" files containing the information (such as energies and cross sections) from which plots may be made using FORODF. (See, for example, Section VII.C.) An alternative plotting program RSAP [RS03] is currently under development and will be made available at a future time.

Users on other systems may prefer to use other plotting packages. With version M5 (or earlier) of SAMMY, it was necessary for the "SAMMY manager" to choose between two alternatives when linking the program. To use the ODF option, file modfio.o (compiled form of modfio.f) would be included directly. To use the other option, file modfio.o was replaced with modf3.o (compiled form of modf3.f); this was most readily accomplished by simply renaming modf3.o to modfio.o prior to the link step. With this option, SAMMY-M5 would produce a "generic" binary file (also named SAMMY.ODF) that contained the same information normally stored in the ODF file, but in a form that could easily be read by a simple FORTRAN code.

With version M6 (including M6-Beta∗) of SAMMY, the procedure has changed. SAMMY now automatically produces both an ODF file and a "generic" binary file (which is now named SAMMY.PLT instead of SAMMY.ODF). Moreover, the SAMMY.PLT file is now in double precision while SAMMY.ODF remains in single precision.

A sample code SAMPLT (file mplt.f) is provided with the SAMMY FORTRAN. SAMPLT reads the binary file and produces an ASCII file (ASCII.PLT), which contains the same information as the ODF file (see Section VII.C for details). The local SAMMY manager may wish to modify the file mplt.f to accommodate his or her system's needs; mplt.f contains extensive comment cards to aid in making the needed modifications.

Note that versions of this program (SAMPLT) prior to SAMMY-M5 were named "sambin" instead of "samplt". However, the word "bin" has special meaning on Unix systems; hence, the name has been changed to avoid potential conflict with system routines.

Caution: There may be problems associated with the creation of PLT files for certain configurations of SAMMY runs, notably those for which more than one PLT file is produced by an individual run (and possibly in other situations). Generally such problems should be immediately obvious to the user; when in doubt, cross sections can be printed in the LPT file for comparison with the PLT file. (See "options for printing into SAMMY.LPT" in Table VI A1.2 to learn how this can be done.) Users are encouraged to contact the SAMMY author at LarsonNM@ornl.gov if they encounter difficulties with these files.

∗ Users of version M6-Beta should be aware that a modification is needed in file mend1.f, in which the line reading

```
      CALL Oldopn (61, 'SAMMY.PLT', 1)
```

should be replaced with

```
      CALL Oldopn (61, 'SAMMY.PLT ', 1)
```

That is, a blank must be added after SAMMY.PLT, before the quote. Similar changes are needed in file mplt.f.

X.J. SAMQUA: RESONANCE QUANTUM NUMBERS

The code SAMQUA can serve as an aide to generating the correct (and complete) set of resonance spin quantum numbers for any given set of incident and exit channels. The original version of this program was quite limited, assuming a neutron incident on a single nuclide, and including only elastic channels. In 2003 Bouland and Babut of Cadarache, in collaboration with the SAMMY author, developed a more general version of this code [OB03]. This version of SAMQUA treats the general case of elastic, inelastic, reaction, and fission channels, including charged particles as needed.

Two distinct modes of input are available for SAMQUA. The first (the Cadarache input mode) uses free-format values interspersed with descriptive information, and is described in detail in the SAMQUA documentation [OB03]. The second (the Particle-Pair mode) uses essentially the particle-pair information from SAMMY's card set 4 of Table VI.A.1. In both cases, the output consists of portions of the SAMMY INPut file: Output file "quantum2.dat" contains card sets 4 and 10.2, as well as the necessary commands (to be included in card set 3 of the INPut file) for use of those input options. Output file "quanpar.dat" may be used (perhaps with modifications) for card set 7 (radius parameters) and card set 10 (isotopic abundances) of the SAMMY PARameter file. Another output file, "table.dat", gives the spin group information in tabular form.

One additional output file, "quantum.dat", contains card set 10.1 (for SAMMY's INPut file) plus command lines. However, use of this option in SAMMY runs is discouraged as the format is crowded, awkward, and non-intuitive and will eventually be disallowed. SAMMY users are encouraged to convert to card set 10.2 (as given in quantum2.dat of SAMQUA output).

Subsequent to publication of the SAMQUA manual [OB03], the code has again been upgraded [OB04] with options to provide additional information to the user, and to reorganize the output. For each run, another output file ("quantum3.dat") is created. This file contains the same information as quantum2.dat, with extra lines following each channel descriptor in card set 10.2; the extra lines give penetrability and hard-sphere cross section at specified energies. (The hard-sphere cross section is that cross section that would be calculated if there were no resonances.) By default these energies are 1.0 eV, 500 keV, and 1 MeV, but (for the particle-pair input mode) there are other options:

(1) The user can specify values Emin and Emax, and SAMQUA will calculate penetrabilities and cross sections at Emin, (Emin+Emax)/2, and Emax.

(2) A list of energies can be given in a separate file; this can be a SAMMY PARameter file or a simple list of energies.

Because the calculation of penetrabilities and cross sections requires knowledge of radii, and the radii used in an evaluation may differ from SAMQUA's default values, the user may also provide radii values.

Finally, a single input command will alter the ordering of the spin groups from $\{J, \pi\}$ as in the 2003 version to $\{L, J\}$ (where L here indicates the orbital angular momentum of the first entrance channel for any given spin group, and J and π indicate the total angular momentum and parity for the spin group).

Table X J.1 summarizes the input options for the particle-pair mode.

Test case tr143 gives numerous examples of the use of this code. Cases whose names end in "a" use the Cadarache mode of SAMQUA input, and cases whose names end in "b" use the particle-pair mode. Cases labeled with "c" include the option to read channel radii from a separate file, and cases labeled with "d" provide reordered output. Cases labeled "e" read from a parameter file to learn energies on which to calculate penetrabilities and hard-sphere cross sections.

Table X J.1. Input options for SAMQUA in particle-pair mode

Line	Contents	Notes	Required?
1	Title	1. Alphanumeric title, will be printed but not used.	Yes
2,3, …	Blank, or containing # in first column.	1. Blank or # lines may be inserted almost anywhere into the file.	No
4, 5	"`EMIN =`" *or* "`EMAX =`", followed by the real value.	1. The penetrability and hard-sphere cross section will be calculated at Emin, (Emin+Emax)/2, and Emax. 2. If either Emin or Emax is unspecified, the default values (1 eV, 1 MeV respectively) will be used. 3. The equal sign *must* be included.	No
Alt. 4 (no 5)	"`ENERgy file =`", followed by name of file in which energies are stored	1. Energies are listed one per line, in the first eleven columns. 2. A SAMMY-style resonance PARameter file can be used here (in which case negative energies and continuation lines will be ignored).	No
6	"`RADius file =`", followed by the name of the file in which the radii are stored	1. The "radius file" defines values for the channel radii, which are needed for calculating the penetrabilities and hard-sphere cross sections. The format for the radius file is the same as card set 7a of the PARameter file, with the caveat that only particle-pair and orbital angular momentum information can be given, and not spin group and channels (since these will be determined by the samqua run).	No

Table X J.1 (continued)

Line	Contents	Notes	Required?
6, cont.		2. If channel radii are not specified (i.e., if this line is absent and no "radius file" exists), the SAMQUA default values are used. 3. Only the first three characters of "radius file" are needed; however, the equal sign *must* be included. 4. This line may be interchanged with line 7.	
7	"`REOrder according to LJ not Jpi`" or "`ORDer by LJ`".	1. If this line is present, the spin groups will be listed in the output files in order of increasing *L*, where *L* here refers to the orbital angular momentum of the first (incident) channel for each spin group. If two spin groups have the same value of *L*, the one with the smaller value of *J* will be listed first. 2. If this line is absent, the spin groups are ordered by increasing *J*, with negative-parity spin groups listed before those with positive parity. 3. This line may be interchanged with line 6.	No
8	"`NUclide, Lmax=`" or "`First nuclide, Lmax=`", followed by integer value for Lmax. Line may also contain "`Number of fission channels =`", followed by integer value	1. Indicates the beginning of information for the first nuclide. Only the first two characters (NU) and the first equal sign are required. 2. Lmax is the maximum value of the orbital angular momentum. 3. If a second equal sign is present, the integer value following that equal sign is the number of fission channels to be included.	Yes
9	"`Abundance =`", followed by real value	1. Indicates the abundance of this isotope. Printed in file quanpar.dat for use in card set 10 of the SAMMY PARameter file. 2. No blank line (or # line) is permitted between Line 8 and Line 9.	Yes
10, etc.		1. These lines give the particle-pair information, exactly as in card set 4 of the INPut file. 2. End with a blank line (*not* a # line)	Yes

Table X J.1 (continued)

Line	Contents	Notes	Required?
11	"`NUCLide, Lmax=`" or "`NEXT nuclide, Lmax=`" or "`NEW nuclide, Lmax=`" Line may also contain "`Number of fission channels =`", followed by integer value	Like line 8 for another nuclide: 1. Indicates the beginning of information for the new nuclide. Only the first four characters and the first equal sign (plus the value of Lmax for this nuclide) are required. 2. Lmax is the maximum value of the orbital angular momentum. 3. If a second equal sign is present, the integer value following that equal sign is the number of fission channels to be included.	No
12,13		Repeat lines 9 and 10 for this nuclide	
14 …		Repeat lines 11 through 14 as needed	

X.K. SAMRPT: PLOT RPI RESOLUTION FUNCTION

To plot the components and the total RPI resolution function (see Section III.C.3) at a given energy, use program SAMRPT. Input to SAMRPT consists of two lines of information: The first is the name of the PARameter file. Alternatively, it could be the name of a file containing the RPI portion of the PARameter file; the header line ("RPI Resolution function") may or may not be present. The second line contains the energy in eV, mass in atomic mass units (amu), and flight-path length in meters (m), in 3F format (separated by commas or spaces); alternatively, the same information may be given as the first line in the RPI file. (Default values for these three quantities are 150.0, 183.85, and 25.604, respectively.)

Output from a run of SAMRPT consists of one ASCII file, SAMMY.RPI, which gives derived quantities such as the time-width associated with each component of the resolution function, as many as four plot (ODF) files plus four additional ASCII files:

SAM_RPI.ODF	- S1 = energy, S2 = (total) resolution function, S3 = time
SAM_RPI_BURST.ODF	- S1 = time, S2 = burst-width component
SAM_RPI_TDXXX.ODF	- S1 = time, S2 = target-plus-detector component
SAM_RPI_CHANN.ODF	- S1 = time, S2 = channel-width component

The four ASCII files have similar names to the four ODF files, with extension "ODF" replaced by "PLT". The same information from the various sections of the ODF files is given in the corresponding columns of the PLT files.

Test case tr053 gives numerous examples (not all of which make physical sense!) for the use of this program.

X.L. SAMRST: PLOT RESOLUTION FUNCTION

Even though program SAMRST is actually a module of SAMMY, it is covered in this section because comparable programs (SAMORT and SAMRPT) are also presented here.

To generate a plot file containing the Gaussian plus exponential resolution function (see Section III.C.1) at specific energies, insert the command line

```
PLOT RESOLUTION FUNCtion
```

in the INPut file. Also in the INPut file, directly after the blank line signifying the end of the alphanumeric commands (card set 3), insert one line specifying the energies (in 8F10.1 format) at which the resolution function is to be reported; a maximum of eight such energies are allowed. This line is card set 4.5 of the INPut file.

Program SAMRST will generate one plot file (ODF file) per energy; these files are named SAMRSx.ODF, where “x” is a digit from 1 to 8; these files contain energy in S1 and resolution function in S2. In the event that there are too few points to resolution broaden at the specified energy, an error message is printed and the plot file is not generated.

An example using SAMRST is given in test case tr018.

X.M. SAMSMC: MONTE CARLO MULTIPLE SCATTERING

In Section III.D, SAMMY's method of calculating the multiple-scattering corrections to the capture and fission yields is presented. Because these calculations involve complicated expressions as well as approximations whose legitimacy can be questioned, it is desirable to have an independent means of testing the calculations. Monte Carlo is suitable for this task, as the method is completely different from the analytic-with-approximations approach taken in Section III.D.

The precursor to the code SAMSMC was written during the 1980's by Gerard de Saussure [GD80] and subsequently modified by Francis Perey. More recently, the SAMMY author has modified this code to include anisotropic scattering (non-s-waves) and more than one nuclide. In addition, an interface was developed with the SAMMY code, in order for SAMSMC to read and use the same Doppler-broadened cross sections and energies that are used in SAMMY.

Use of the SAMSMC code is a multi-step process, described below.

1. Run SAMMY with a line in the alphanumeric section of the INPut file which says

   ```
   PREPARE INPUT FOR MONte carlo simulation
   ```

   This command causes the code to stop at the point where it would otherwise begin execution of segment SAMSSM. Two or three files are produced that are needed for the Monte Carlo simulation: File SAM54.DAT contains the unbroadened cross sections and SAM51.DAT contains Doppler-broadened cross sections (assuming the INPut file specified that Doppler broadening was to be done). Rename these file for use in later steps.

   The third file is SAMMY.MCR, which contains most of the information to be given to SAMSMC (as specified in # 2 below). Some of this information you will use as is; other values may be modified.

2. Run program SAMSMC (SAM-Ssm-Monte-Carlo), with the following lines of input:
   a. Title (whatever you wish)
   b. Energy-mesh information (Emin, Emax, 0.)
   c. Name of file with energy mesh (here only if Emin = 0 in part a)
   d. THSAMP, XSAMP, YSAMP, XBEAM, YBEAM (like card set 11 in INPut file for the regular SAMMY run)
   e. Thickness (in atoms/barn), Mass (in amu)
   f. Maximum number of histories
   g. Number of scatterings to include
   h. Name of the file generated by SAMMY run of step 1 (renamed from SAM51.DAT)
   i. Maximum *L*-value in that file (where *L* is the vector sum of the orbital angular momentum for the individual levels); number of nuclides
   j. Normalize as yield (Y) or cross section (C) or other (O)

k. If more than one nuclide, give masses of each

l. If more than one nuclide, give abundance for each

Two output files are produced by the SAMSMC run. MC_1.DAT holds the various cross sections, and MC_2.DAT contains results from 0 scattering, 1 scattering, two-or-more scatterings, and the sum of those three. Rename these, if desired.

3. Run program SAMSMX (SAMSMc-fiX), with the following input:

   a. Name of the cross section file produced by SAMSMC (MC_1.DAT)

   b. Name of the second file produced by SAMSMC (MC_2.DAT)

   Four output files are produced by this run. Three are ASCII files name MC_Y0.DAT, MC_Y1.DAT, and MC_Y2.DAT; these contain the self-shielded yield, the self-shielded plus single-scattering-corrected yield, and the full multiple-scattering-corrected yield, respectively. These files are in a form suitable for use as SAMMY DATa files, in the TWENTY format (see Section VI.C.1).

   The other output file produced by this procedure is named MC.ODF. This file is an ODF file (see Section VII.C) with the following sections:

   S1. energy in eV

   S2. 0 scattering (self-shielding) only

   S3. 1 scattering

   S4. 2 scatterings

   S5. 0 + 1

   S6. 0 + 1 + 2

   S7. capture cross section

   S8. total cross section

   S9. (1-exp(-thickness $\times$ total cross section)) $\times$ capture / total

   Sections of this file can be compared to output in section 4 of the ODF file produced by the corresponding SAMMY runs. For example, output from a SAMMY run that includes single scattering (finite disk) but not double scattering would be compared to Section 5 in MC.ODF.

X.N. SAMSTA: STAIRCASE PLOTS

To produce an ODF file from which can be made staircase plots of SAMMY resonances for specified spin groups, use the program SAMSTA. Input to SAMSTA is shown in Table X N.1. Output consists of a single file in ORELA Data FORMAT (ODF) (or binary, depending on the system); Section 1 of that file contains resonance energies, and Section 2 contains the number of resonances (from the specified spin groups) at or below the corresponding energy.

Note that the SAMMY INPut file is not read by SAMSTA; the only information required from that file is the *l*-value associated with the given spin groups, and that information is provided directly to SAMSTA. The user should therefore take care to provide correct input, since SAMSTA cannot make consistency checks (*l*-value vs. spin group number, for example).

Table X N.1 Input for Program SAMSTA

	Question	Response
1.	What is name of parameter file?	Name of SAMMY PARameter file
2.	What is spin (*l*)? What are spin group numbers?	Orbital angular momentum for channel 1, as specified by the variable LSPIN in card set 10 of the INPut file; spin group numbers for those groups have this *l*-value. Format is “6I3”
3.	What is name for ODF file?	Name for the output ODF file to be produced by SAMSTA
Questions 2 and 3 are repeated until the user enters “0” for spin and group numbers.		

X.O. SAMTHN: THINNING DATA

Often a data file will contain more points than are needed to define the measurement (e.g., data appear to be very dense in energy regions where there is little structure in the data). SAMMY runs will therefore require far more computer time than is actually needed. For these reasons, it is often deemed reasonable to "thin" the data, at least for preliminary runs. A program SAMTHN has been written for this purpose; it has not, however, been studied extensively, so use with caution! Please note, also, that any results obtained with thinned data should ultimately be tested against the complete dense data set, to ensure that no important features were missed.

In running SAMTHN, the user provides two files, plus the name for the new thinned data file. The first user-provided file gives instructions on how the thinning should be done; the second is the dense data file. The first line of the thinning file contains three numbers (*N*,*Emin*,*Emax*) in I5, 2F10.1 format. The integer *N* tells how many data points are to be averaged together in the energy range from *Emin* to *Emax*. Second and subsequent lines contain two numbers (*N*,*Emax*); *Emin* is assumed to be equal to the previous *Emax*. Note that energies must be given from low to high, no matter what the ordering of data points in the original dense data file.

The fourth line of input (after the three file names) contains one character, which describes the type of input data in the dense file: `O` = Original (three energy-points per line, as in the original MULTI-style data format), `C` = CSISRS data, `T` = Twenty format, and `D` = Differential elastic data (ASCII format only). For differential elastic data, there is one additional line of input, an integer equal to the number of angles.

For `O`, `C`, or `T`, the format for the output thinned data file is always (3F20.10); in using this data file for SAMMY runs, the INPut file must contain the line "`USE TWENTY SIGNIFICANT DIGITS FOR EXPERImental data`". For `D`, the output format is (F10.2,7F10.5); if this format is inappropriate, for this simple code the author assumes the user can make the necessary changes him/herself.

The algorithms used by SAMTHN to average the data are as follows:

$$\bar{E} = \left(\frac{1}{N} \sum_{i=1}^{N} \frac{1}{\sqrt{E_i}} \right)^{-2} \qquad \text{(X O.1)}$$

and

$$\bar{D} = \frac{1}{\bar{V}} \sum_{i=1}^{N} \frac{D_i}{V_i} \quad , \qquad \text{(X O.2)}$$

with

$$\bar{V} = \left(\sum_{i=1}^{N} V_i^{-1} \right)^{-1} \quad , \tag{X O.3}$$

in which E represents the energy, D the data, and V the variance (i.e., the square of the uncertainty). Quantities with subscripts are from the original dense data set, and quantities with bars represent the averaged values.

Test case tr072 has two examples for thinning data.

X.P. SUGGEL: ESTIMATING *L* AND *J*

Often when beginning an analysis, the SAMMY user will start from spin assignments and resonance parameters already available in the literature or in the ENDF files. Sometimes, however, such information is either nonexistent, inadequate, or unavailable through the entire energy range. In such situations, the analyst must use alternative methods to obtain starting parameter values.

The computer program SUGGEL [SO01], written by S. Y. Oh and L. C. Leal, provides one such method. The following description is taken from the abstract to that document:

"The SUGGEL computer code has been developed to suggest a value for the orbital angular momentum of a neutron resonance that is consistent with the magnitude of its neutron width. The suggestion is based on the probability that a resonance having a certain value of $g\Gamma_n$ is an *l*-wave resonance. The probability is calculated by using Bayes' theorem on the conditional probability. The probability density functions (pdf's) of $g\Gamma_n$ for up to d-wave ($l = 2$) have been derived from the χ^2 distribution of Porter and Thomas. The pdf's take two possible channel spins into account."

"This code is a tool which evaluators will use to construct resonance parameters and help to assign resonance spin. The use of this tool is expected to reduce time and effort in the evaluation procedure, since the number of repeated runs of the fitting code (e.g., SAMMY) may be reduced."

SAMMY test case tr141 gives three examples of SUGGEL runs.

Readers are referred to the documentation [SO01] for details concerning the use of this code. That document's description of the input to the code is repeated here (below the line, and in Table X P.1). Note that the second of the two input files is the resonance-parameter portion of a SAMMY-style PARameter file, and the name for this file is provided in the suggel.inp file discussed below.

The program requires two input files and generates two output files. The basic data, as well as some control options, for the calculation are included in a file named "suggel.inp", while sets of resonance energy and neutron width are provided in the other input file. One of the output files shows calculation results, and the other file contains resonance parameters in SAMMY.PAR format.

<u>Input Description</u>

The file "suggel.inp" is prepared in the name-list type of input. This file consists of:

The first line: "&indata" from column 2 to 8,

In the second to the (last-1) lines: data section with the name-list key words (each line shall have the first column blank), and

The last line: "&end" from column 2 to 5. Some notes can be added after this line for user's convenience.

Table X P.1. Variables appearing in the "suggel.inp" file

Key word	Units	Description
Parin		Input resonance parameter data file name. In the file, the resonance energy is given in eV and Γ_n (or $g\Gamma_n$) in meV.
Partyp		Type of neutron width in 'parin' file. If partyp = 0, the parin file is in SAMMY.PAR file format and Γ_n's are given; otherwise, the file is in rsap.gamma format and $g\Gamma_n$'s are given. Concerning the rsap.gamma file, see following this table.
Fout		Output list file name.
Parout		File name of the output resonance parameter file, which is in SAMMY.PAR format.
Awri		Atomic mass of target nuclide divided by the neutron mass.
Spin		Spin of the target nuclide (I).
Scattr	fermi	Scattering radius (R'). If scattr = 0.0, the program calculates it as $R' = 0.123\ (awri)^{1/3} + 0.08\ [10^{-12}\ \text{cm}]$
Disp		Spin dispersion parameter (s). If disp = 0.0, the program calculates the value. Very large 'disp' value (e.g., 999.) implies to use ($2J$+1) law, with which the level density is proportional to $2J$+1. See further discussion following the table.
Bn	MeV	Neutron separation energy of (A+1) nuclide
Pair	MeV	Pairing energy
Denpar	MeV^{-1}	Level density parameter
Eini	eV	Lower energy boundary under the analysis
Efin	eV	Upper energy boundary under the analysis
Pcut		Probability cutoff. The suggested orbital angular momentum is adopted for a resonance for which the probability is higher than this value. If it is not the case, the l value is not altered from its original assignment as given in 'parin' file. It is not effective with the input rsap.gamma file.

Table X P.1 (continued)

Key word	Units	Description
Optj		Method of *J* assignment. If optj = 0, the most probable *J* value is adopted; otherwise, the *J* value is assigned randomly. Regardless of this option, the original *J* value is maintained if the original *l* value is maintained due to the probability cutoff. See Section 2.6 of [SO01].
Stn(*i*), *i*=1,2,3	10^{-4}	Neutron strength functions for *s*-, *p*-, and *d*-waves, respectively
Dzero	eV	Average level spacing of s-wave resonance. Level spacings of *p*- and *d*-waves are calculated in the program.
Frac(*i*), *i*=1,2,3		*A priori* probability correction factors for *s*-, *p*-, and *d*-waves, respectively. See Section 2.2 of [SO01].
Sam(*i*), *i*=1~max.18		*l* value of spin group *i* in 'parin' file. This definition shall be kept in subsequent SAMMY run. The number of spin groups can be more than 18 in SAMMY run (e.g., in case of the analysis of a natural element), and it is also possible to define the spin group not to begin with 1 in SAMMY. However, the SUGGEL assumes that the spin group starts at 1.
Ajsam(*i*), *i*=1~max.18		*J* value of spin group *i* in 'parin' file. This definition shall be kept in subsequent SAMMY run.

Note from SAMMY author: This program does not run under the VMS operating systems. In general, portability of SUGGEL is not guaranteed.

X.Q. SAMRML: CALCULATE CROSS SECTIONS FROM ENDF FILE 2

The program SAMRML was created as an aid for persons wishing to implement the ENDF File 2 LRF=7 (R-Matrix Limited) Format. SAMRML can be used in at least two ways: This coding may be inserted directly into a processor code (after appropriate re-writes). When independent coding is developed, SAMRML can be used to test the results.

The stand-alone code SAMRML was derived from the cross-section-calculation portion of SAMMY, with the following changes: Experiment-related pieces were removed from this code; only one nuclide is considered at a time, and no corrections are made for any measurement-related effects. All cross section types are generated in a single SAMRML run.

SAMRML calculates energy-differential (angle-integrated) elastic, absorption, and reaction cross sections. If requested, SAMRML will also calculate elastic angular distributions. In addition, an option exists for generating partial derivatives of the angle-integrated cross sections with respect to the resonance parameters.

The code will calculate one of two versions of the partial derivatives: In the default mode, derivatives are with respect to the resonance widths $\Gamma_{\lambda x}$ and energies E_λ, as they appear in the ENDF files. Alternatively, the derivatives can be given with respect to SAMMY's *u*-parameters as defined in Section II of this report; this option is useful for ensuring that SAMRML is indeed working properly. The default option is currently the more useful one for processor codes that make more direct use of the ENDF files than does SAMMY.

Two input files are needed for SAMRML. The first contains a list of energies (one per line, ending with a blank line) and angles (one per line, ending with a blank line) at which the calculation is to be performed. If no angles are given, no angular distributions will be calculated.

The second file is an ENDF file in which File 2 uses LRF=1 (single-level Breit Wigner), 2 (multilevel Breit Wigner), 3 (the so-called Reich-Moore format), or 7 (the R-matrix limited format).

Four lines of input are needed following the "samrml" run command:

1. name of energy/angle file
2. name of ENDF File 2 file
3. the ENDF material number (MATNUM); if MATNUM is zero, only the File 2 portion of the ENDF file is to be included in the file specified in the previous line.
4. two characters, in the first two columns of this line. If the first character is "y" or "Y" (for "yes"), then partial derivatives will be generated. If the second character is "s" or "S", then those derivatives will be with respect to the SAMMY *u*-parameters.

XI. HELPFUL HINTS FOR RUNNING SAMMY

This section covers a multitude of topics, all designed to facilitate the smooth operation of SAMMY. Careful attention to the ideas covered here should make your job (and the author's!) a lot easier.

Section XI.A describes an agenda for performing a SAMMY evaluation. Even experienced SAMMY users might benefit from reading this section, as it includes mention of useful features of the SAMMY code which might be unfamiliar to them.

Section XI.B offers suggestions for solving common problems encountered by SAMMY users. The procedure to be used in obtaining the author's help is also discussed.

Section XI.C contains discussions on a variety of topics related to running the SAMMY code. Included are such topics as Bayes' method, spin-group definitions, negative reduced-width amplitudes, and transmission vs total cross section.

XI.A. STRATEGY FOR DATA EVALUATION WITH SAMMY

In the "best of all possible worlds," data analysis with SAMMY (or any other analysis code) would follow a "cookbook procedure" and produce perfect results on the first attempt. However, the real world is far too complicated for that. Nevertheless, an outline is presented here, as a guide to the user in designing his/her own stratagem for data analysis. The discussion below applies primarily to analyses in the resolved resonance region.

(The author is greatly indebted first to Claire Perey for drafting the original version of this guide, during the early days of SAMMY development, based on her extensive experience using SAMMY to analyze transmission data, and also to current members of the ORNL Nuclear Data Group for their advice and improvements to the 2006 version.)

Step 1. Preparation of DATa files

For guidance in choice and preparation of experimental data to be used in the SAMMY analysis, the reader is referred to the many papers describing particular evaluations. Examples can be found in [LL99, RS00, and others]. In general, one should include all available data that is considered to be reliable and consistent. Ideally, many different types of data should be included (transmission, capture, fission, differential elastic, etc.).

Whenever possible, transmission data should be used rather than total cross section, because analyses of total cross section data often incur numerical problems due to blacking-out resonances. In addition, experimental resolution applies to transmission, not to total cross section; for this reason, cross sections derived by taking the logarithm of experimental transmissions are considered "effective total cross sections" and are highly dependent on the thickness of the sample. For best results, always fit transmission data rather than total cross section.

The formats for experimental data in SAMMY are discussed in Section VI.C.

Care must be taken to determine the conditions under which the experimental data were measured. Effective temperature (for Doppler broadening), components of the resolution function (burst width, channel width, flight-path length, etc.), background, and normalization information should be noted, as should nuclide abundances within the sample(s). Uncertainties should be determined or estimated for all parameters. When information is not available for older data, reasonable assumptions should be made; values for these parameters can be adjusted (fitted) during the analysis process.

Step 2. Preparation of INPut and PARameter files

Before the INPut and PARameter files (Sections VI.A and VI.B, respectively) can be created, quantum number information (spin groups and channels) must be established; see Section II.C.1 for details. For help in determining the appropriate spin group quantum numbers, use program SAMQUA [OB03, OB04] as described in Section X.J.

In many cases, results of earlier evaluations for some of the relevant nuclides are available in the evaluated nuclear data files (ENDF). ENDF File 2 (which contains resonance parameters) can be used as input to SAMMY, greatly simplifying the SAMMY setup procedure. (See Section IX of this manual for details concerning the use of ENDF files as input to SAMMY.) Do not, however, rely entirely on the information in the ENDF files, for the following reasons:

- Older files sometimes did not give proper descriptions of the spin groups and channels.
- Except for the new LRF = 7 format, ENDF formats do not have provision for defining parity. *Do not assume that the spins and parities extracted from ENDF files are correct.*
- Many older files used one of the Breit-Wigner approximations, which should <u>not</u> be used for new evaluations. (When reading an ENDF file, SAMMY produces a comparable SAMMY-style INPut file called SAMNDF.INP; be sure to remove any command lines referring to Breit-Wigner from this file before using it as input to future SAMMY runs.)
- Small resonances observable in new measurements may not have been seen in the early measurements.
- New measurements may permit extension of the resolved resonance region to higher energies, requiring the use of higher *l*-values.

Therefore, even when preliminary information is available from ENDF File 2, it is recommended that SAMQUA be used to ensure that all possible spin groups and channels are considered for inclusion in the analysis.

If R-matrix parameters are not available from ENDF, results from resonance parameter analyses may be found in the EXFOR files [EXFOR]. Users should be aware that these are not full evaluations but are closely tied to individual measurements.

Information concerning individual resonances may be available in the literature. See, for example, the Mughabghab compilation [SM06].

Information from data bases or the literature will probably need to be augmented with information available only in the new data you are preparing to analyze. Program SUGGEL (Section X.P) was designed to provide guidance in making spin-group assignments for resonances. Program RSAP [RS03] also has features that aid in PARameter-file preparation. One such feature is a peak search procedure that “finds” resonances in new data and generates starting PARameter-file entries. A certain amount of trial and error on the analyst’s part will also be needed but will pay dividends in the future.

The R-matrix is a complicated function, involving long-range interference. At any given energy, the "background" R-matrix has contributions from nearby small resonances, from large resonances within the region being analyzed, and from resonances outside the region of analysis. The effect of the outside resonances is approximated either by fictitious or "dummy" resonances or by a parameterized external R-function. (For more on this topic, see Section II.B.1.d and references [LL99] and [FF01].) Be sure to include either dummy resonances or another description of the external levels in your PARameter file, as it will not be possible to fit the data without this.

Step 3. Initial SAMMY calculations

Once preliminary INPut and PARameter files have been created, and DATa files are available, it is time to make preliminary SAMMY runs. Begin with the "best" data, which generally means the highest-resolution (longest flight path, lowest temperature, etc.) transmission data.

The first runs will be "no-Bayes" runs, which means that no fitting of theory to data is to be attempted. Instead, the purpose is to debug your input, that is, to determine whether the input is sensible and to make any necessary adjustments. For these initial runs, the following commands should be included in the INPut file:

```
DO NOT SOLVE BAYES Equations
GENERATE PLOT FILE AUtomatically
PRINT ALL INPUT PARAmeters
```

and possibly

```
PRINT INPUT DATA
```

Only statements that are not defaults are listed above; to see exactly what these commands will accomplish, see Table VI A1.2. Depending on the particular experiment being calculated, other commands may be needed as well.

When the initial run is completed, look carefully at the results. Probably you will wish to start with a plot, to visually compare the measured data with the calculated cross section. (See Section VII.C for a discussion of plotting options.) Next, especially if the calculated curve is very different from what you expected, carefully compare parameter values listed in the SAMMY.LPT file (Section VII.A) with those from the PARameter and INPut files; this will help you locate input mistakes such as misplaced decimal points, typographical errors, misunderstood units, and other mishaps.

You will also want to look over the experimental cross sections (or transmissions) and uncertainties carefully (either from the plot file or as printed in the LPT file, if you chose to print that information). This will help you discover and correct/discard/adjust any oddities. Among the possibilities here are the following:

- Uncertainties that are unreasonably small; often these are associated with very small cross section values. One way to spot these is to look at the weighted residuals (using the `PRINT WEIGHTED RESIDUALS` command) for values that are orders of magnitude higher than most.

- Large discontinuities, which may indicate a formatting problem.
- For total cross section data (which you will use only if absolutely necessary), the peaks of large resonances may appear "chopped off" (because the cross section values were taken from blacking-out resonances in transmission experiments). The uncertainties on these data points will need to be increased significantly.

Corrections for experimental conditions can have major effects on the calculated cross sections, so reasonable estimates for Doppler- and resolution-broadening parameters will probably need to be included even at this early stage. Unless you have other information about the conditions under which these data were measured, initial attempts should assume room temperature (300 K) for the Doppler broadening (Section III.B.1), and the simple Gaussian resolution function with reasonable parameter values (Section III.C.1.a).

By performing a few successive no-Bayes runs, you will eventually reach the stage where the calculated cross sections are roughly consistent with the measured data. That is, you will find

- good approximations for the values of the energy parameters for the large resonances seen in the region you are planning to analyze and
- a combination of parameters for your external R-function (or outside dummy resonances) and for the widths of the large resonances in your energy range to give reasonable estimates of the effect of outside resonances.

For some of the data sets, you may also discover energy-scale misalignments and/or normalization or background problems. Energy re-alignment of all the experimental data sets should be performed at this stage, using the transmission experiment with the longest flight path as the standard. See Section III.E.8 for guidance for correcting the energy scale, and Section III.E.3 for normalization and background options.

Step 4. Preliminary analysis: gross features

Perform a preliminary analysis on each individual data set (again beginning with the "best" data set), using Bayes' theorem to adjust the most relevant parameters. At this stage it is recommended that you assign

- small but realistic uncertainties on the energy parameters of the large resonances inside your energy range and
- fairly large uncertainties on the widths of these resonances and on the parameters outside your range of analysis.

Table VI B.2 provides many options for input of prior uncertainties on resonance and other parameters.

In a few runs you will have generated a theoretical cross section that roughly agrees with your data. (In earlier years, when computation time was prohibitive, these runs were often made

using severely averaged data sets to speed up the calculation. With today's high-speed computers, averaging is almost never necessary.)

For these runs, you will need to modify your INPut files by disabling the command that prohibits fitting. This command line can either be removed, or it can be commented-out with a pound sign (#) in the first column, as shown here:

```
#DO NOT SOLVE BAYES Equations
```

One default command should be noted:

```
DO NOT SUPPRESS ANY intermediate printout
```

When things go wrong, the additional printout (in the SAMMY.LPT file, as described in Section VII.A) provided by this command is helpful in detecting where, and possibly why, the trouble started. If everything goes right, use of this option allows you to follow the path of the parameters' adjustments.

Step 5. Further analysis: small energy regions

Small regions should now be studied individually, with all the necessary details, progressively including narrow resonances. At this stage you will want to refine the resolution function for each data set, and include other corrections (multiple scattering, background, etc.); see Section III for details.

Care should be taken to include enough points in the auxiliary energy grid to properly describe the unbroadened cross section, in order to perform the Doppler and resolution integrations accurately. (See the discussion in Section III.A.1 regarding the density of points in the auxiliary grid.) One simple test you can make to see whether your grid is sufficiently dense is to double the number of points used (i.e., set NXTRA = 1 in card set 2 of the INPut file). If values for the Doppler- and resolution-broadened cross sections change appreciably, then the grid is not sufficiently dense. If values remain approximately the same, then the original grid is acceptable. Remember that it is the analyst's responsibility (not the SAMMY author's) to ensure that the auxiliary grid is adequate for your purposes.

Step 6. Final fitting runs

At the end of this final step you will obtain the complete and consistent parameter and covariance files for all data sets included in the analysis. Therefore, none of the input parameter values or their uncertainties, nor the data points or their uncertainties, should be manually changed at any time during this final step. If changes are needed, the entire process should begin anew.

All relevant parameters should be varied in this step: set the flag = 1 in the PARameter file.

Some parameters may be held fixed: (1) Values for some parameters are well determined from other experiments but have little effect for the current data; these should be held fixed or perhaps PUPped (see Section IV.D.2) so that their uncertainty contributes to the data covariance matrix. (2) If necessary to conserve computer resources, some parameters may be held fixed at the values found in earlier steps. Care should be taken to hold fixed only those parameters whose effect is short range. (3) In some cases, a parameter may be essentially irrelevant for the data being analyzed and therefore need not be flagged.

All measurement uncertainties should be included at this stage. Statistical uncertainties are defined in the DATa file, but systematic uncertainties require different treatments. The simplest way for the user to take care of systematic measurement uncertainties is to PUP the data-reduction parameters (normalization, background, sample thickness, etc.) by setting the flag = 3 in either the PARameter or (more likely) the INPut file. When additional systematic uncertainties are available, these should be included via the user-supplied implicit data covariance option (see Section IV.D.3 for a discussion and VI.C.3.b for input details).

Two options are now available in SAMMY for analyzing several data sets together. The first (SAMMY's original) method involves sequential analyses, one data set after another, using the output parameter covariance matrix (PCM) from one run as input to the next run. The other is to analyze all data sets simultaneously. There are advantages and disadvantages to each.

<u>Sequential analyses</u>: Final results from sequential analyses would be exactly equivalent to final results from simultaneous analysis, provided the theory were linear with respect to the varied parameters. Since R-matrix theory is exceedingly non-linear, exact equivalence is not possible. Further, the ordering of the data sets in the sequence can be important. Generally, one would include the best data sets first, to firmly establish values for the most important parameters, before moving on to less reliable data.

Often the analyst will take the final PARameter and COVariance file from the entire sequence of runs, and repeat the sequence using those files as initial input. This process may be repeated several times, until convergence is reached. Generally, the criterion for convergence is that parameter values (and hence chi-squared values) no longer change very much. (Caution: When this kind of repetition is used a total of N times through the sequence, the final parameter covariance matrix is diminished by a factor of N. That is, the uncertainty on any parameter must be multiplied by $\sqrt{N}$ to obtain the "true" uncertainty as determined by this sequential analysis.)

A major advantage of sequential analysis is the ability to locate data sets which are inconsistent with the other data. When such a data set is encountered in the sequence, parameter values will always be modified, so it is unlikely that convergence will be reached. By studying the sequence of runs, the analyst will be able to determine which data set is causing the problem, and make adjustments as needed.

Simultaneous analysis: It is now possible, although still a bit awkward, for SAMMY to do simultaneous analysis of even very large data sets. (Details are presented in Section IV.E.1.) A series of runs is made, one for each data set. The contributions to the *Y* and *W* matrices (needed for Bayes' equations) are generated in those runs and saved in binary files. An additional SAMMY run then reads those files and solves Bayes' Equations to determine the updated parameter values and associated parameter covariance matrix.

Iteration for non-linearities is also possible with simultaneous analysis, although each iteration requires another complete series of K+1 runs (where K is the number of data sets). Details are given in Section IV.E.1.

With simultaneous analyses, it is possible to calculate the true least-squares solution, in which the prior parameter covariance matrix is assumed to be diagonal and infinite. (See Section IV.E.3 for details.) This feature was added primarily to facilitate comparison with other codes, most of which use least squares rather than the more general Bayes' equations used in SAMMY.

Step 7. Obtaining the parameter covariance matrix

The procedure described in step 6 produces both a "good" set of parameter values and the associated parameter covariance matrix (PCM). Ideally, this is the PCM which would be included in the analyst's final report. In practice, this PCM is widely regarded as too small, which means that the uncertainties (the square root of the diagonal of the covariance matrix) are deemed to be smaller than expected. In reality, not all sources of uncertainty are included in the analysis, even when the analyst goes to great pains to include all known sources of experimental uncertainty. (See Section IV.E.6 for further discussion.)

Analysts therefore usually wish to adjust (increase) the SAMMY-produced PCM in some fashion, to better conform to their expectations regarding the correct PCM. A variety of techniques have been developed to assist in this process; these are described in Section IV.E.6.

Given the recent surge in perception of the importance of uncertainty information in all aspects of nuclear data, it is important that anyone reporting the results of data analysis should include information about the PCM. Do not neglect this aspect of your analysis.

Step 8. Statistical studies

Most reports regarding resonance parameters also include discussion of statistical properties of those parameters. See, for example, references [HD90], [OB97], [LL99], [RS06]. The code SAMDIS (Section X.F) can be used for some of those studies.

Step 9. Reporting results

To create a table of resonance parameters, including uncertainties, use SAMMY's command

```
PUBLISH, or
CREATE PUBLISHABLE List of parameters
```

which creates a file called SAMMY.PUB. This file can be ported to a spreadsheet to be formatted as needed for publication. See Section VII.F for details.

To write the resonance parameters and covariance matrix into an ENDF file, see Section IX.

The SAMMY author would appreciate receiving preprints or reprints of any publications describing work using the SAMMY code. Kindly e-mail these to LarsonNM@ornl.gov.

XI.B. PROCEDURES TO FOLLOW WHEN YOU HAVE PROBLEMS

(Most of this section is taken almost directly from the SAMMY workshop material. The procedure described here has proven to be useful in helping users debug their input and in helping the author debug the code when that is needed.)

What to do when SAMMY does not work?!

1. Do not panic – this happens to **everyone**.

2. Is this run *really* the same as the one that worked last week? Think carefully — *exactly* what did you change?

3. Look at the SAMMY.LPT file in **detail**:
   a. Did SAMMY understand all of your instructions? *Maybe you had a typographical error.*
   b. Is SAMMY using the same parameter values that you intended? *Maybe you had a typo. Look for factors of ten, for example.*
   c. Would additional information help? *Maybe you need to ask SAMMY to print out more initial values, or more intermediate steps.*
   d. Did SAMMY give you an error message? *Look at the very end of the file.*

4. Can you simplify and/or isolate the problem?
   a. Use a smaller energy range.
   b. Vary fewer parameters.
   c. Drop normalization & background options.
   d. Do no broadening.
   e. Find the smallest case for which the error occurs, and try to understand what is unique about that case.

5. See Table XIB.1 for additional suggestions.

6. If the problem persists, ask for help. (See the next page.)

Help is available

1. Talk to your office-mate or the person next door. *Perhaps you have simply been looking at it for too long, and someone else can see immediately what you can no longer see.*

2. Talk to the most experienced SAMMY user in the neighborhood. *It does get easier with practice.*

3. Send an e-mail to the author at LarsonNM@ornl.gov.

   a. First, send information but not files. Describe the problem in some detail:
      i. What version of SAMMY are you using? (If you are not using the most recent release, your bug may already be fixed.)
      ii. What features are in use?
      iii. Did the code bomb or "merely" give wrong answers?
      iv. How do you know that the answers are wrong?
      v. In which module did the bomb occur?
         - For example, SAMMY-RSL might be the last thing in the LPT file.
         - Or M6-SAMMY-SSM might appear on the screen right before the bomb.
      vi. What error message did SAMMY give you?
      vii. Does a minor perturbation of this case work properly?

   b. When requested, send very small files from the simplest case that illustrates the problem: command file, INPut file, PARameter file, DATa file, and any other necessary input files.
      i. Send these files as attachments if possible, otherwise as separate e-mail messages.
      ii. See item # 4 on the previous page for suggestions on how to simplify the run.

NOTE: If you should find an error in your version of SAMMY (either the code or the manual), please tell the author about it so that it can be corrected in the "official" version.

ALSO: When you encounter a SAMMY error message that does not convey appropriate information, can you suggest a more informative message? If so, please contact the author with your suggestion.

Table XI B.1. Possible solutions to some common problems

	Problems that may occur during a SAMMY run	Possible solutions
1	SAMMY tells you that the matrix is nearly singular	* Initial values are very far from "true" values. * Initial parameter uncertainties are too large. Modify by using one or more of the uncertainty options described in Table VI B.2 for the PARameter file. * Too many parameters are being varied (this is unlikely). * Too few data points are used. * Sometimes this message can be ignored! But do so at your own risk.
2	A "divide check" or "floating overflow" or similar error message occurs	* Your INPut or PARameter or DATa file has a zero (or a number which SAMMY reads as nearly zero) where none is permitted. Look over the LPT file carefully to be sure your input is correct. * SAMMY has a bug?
3	Cryptic messages occur before SAMMY bombs	* You are trying to analyze too many data points at one time. Use fewer points, or vary only the parameters of interest. * You have mistyped a file name. * The computer has had a bad day. Try again tomorrow.
4	Results "run away" from your "reasonable" input values.	* Your input did not properly describe the "background" R-matrix. Try adding more dummy resonances, check if spin groups are properly assigned, etc. * Data uncertainties are unrealistic. Zeros are never allowed, and very small values should be increased. (Or, use VMIN, in card set 7 of the INPut file, Table VIA.1.) * Total cross sections may look funny at large resonances (due to "blacking out" of transmission dips), so increase the uncertainties. Better yet, use transmission data and increase uncertainties for low T. * Systematic errors in data should be handled with off-diagonal data covariances, or by varying or PUPing data reduction parameters such as normalization or background. (See Section IV.D.2 for information regarding PUPs.) * "DIVIDE DATA INTO REGions" landed in the middle of a resonance. Change the number of data points, choose the regions yourself, or (ideally) analyze all data at once. * The number of iterations is too small. (This is rarely true, experience has shown.) * Your input contained errors such as misplaced decimal points. Check the LPT file to be sure. * Try analyzing any "sensitive" energy regions first and/or last. Or analyze all data at once. * Initial parameter uncertainties are too large. This is especially likely to be a problem for resonance energies.

XI.C. MISCELLANEOUS COMMENTS AND SUGGESTIONS

Bayes' method

Users should bear in mind that there is a fundamental difference between SAMMY and most other data analysis programs with which they might be familiar: SAMMY was designed to use Bayes' equations rather than least-squares equations to update parameter values. The approach taken to data analysis can be quite different from that taken with least squares. Some of these differences are indicated here.

SAMMY can be used sequentially* to obtain results valid over extremely large energy regions or over many different data sets. One need not do a series of independent analyses followed by much labor to provide consistency over all the data; consistency is a by-product of Bayes' equations. Parameters relevant to all data sets being analyzed should be flagged for fitting.

Parameters irrelevant to the data currently being analyzed (e.g., energies or widths for far-away resonances) may be varied (flagged for fitting) without ill effect. These parameter values will not be changed significantly, nor will their uncertainties. (This feature, in particular, is quite different from many implementations of the least-squares method, in which significant computation time is often consumed looking for the "best" value of parameters about which the current data have no information.)

During the initial stages of an analysis, when starting values are poorly known, ** SAMMY may be used much like least-squares programs are used, analyzing the same data with different starting values, varying different parameters, etc., until reasonable parameter values are found for the data being studied. The user should bear in mind that those values are accurate only under the assumption that all the fixed parameters remain fixed; hence, it is necessary to later do a global fitting of all parameters.

Occasionally a user may find it convenient to include a data set more than once during a sequential fit. However, in this case, the parameter covariance matrix (PCM) produced by the sequential analyses must not be considered to be accurate: This is equivalent to including the same data twice in a simultaneous fit, that is, to reducing the uncertainty on each data point by the square root of 2. Sometimes this can be used to advantage: For example, to obtain extremely accurate parameter values, one might run sequentially through all data sets 100 times. Upon completion, the final PCM must be multiplied by 100 (the uncertainties multiplied by 10) to give the actual PCM.

---

* A "sequential fit" is one in which the output PARameter and COVariance file from one run (analyzing one energy region or one of the data sets) are used as input to the next run (using another energy range or another data set), analyzing each and every data point once and only once.

** When starting values are far from true values, the assumption of linearity (implicit in both Bayes' equations and the least-squares equations) is not even approximately true. Hence the blind use of even the iterative form of either set of equations will often not produce a good fit of theory to data.

It is possible to use an output PARameter file as input to a future run without using the COVariance file. To do this, the user may either (i) edit the PARameter file, deleting the final line which states "COVariance matrix is in binary form" and using instead an initial (prior) large uncertainty on each parameter, (ii) include in the input file a card that says "`IGNORE INPUT BINARY covariance matrix file`", which will cause the default prior uncertainties to be used, or (iii) answer "`IGNORE`" when SAMMY requests the name of the binary file.

Prior (initial) uncertainties for each varied parameter are required as input to SAMMY (although they will be assigned default values if not stated explicitly). In the case where it may be assumed that we have no prior knowledge about the value of a certain parameter (i.e., usually), the value for the uncertainty should ideally be infinite. (Recall that Bayes' equations, in the limit of infinite prior uncertainty, reduce to the familiar least-squares equations.) Computers, however, require finite numbers. Moreover, it has not been possible to program SAMMY to operate via least squares for some parameters and via Bayes' equations for others. Compromise is therefore necessary. A convenient and practical compromise is that formulated in SAMMY's default values for prior uncertainties (see Section V1.B). As far as Bayes' equations are concerned, these default uncertainties are effectively infinite, yet they are usually not so large as to cause singularity problems in inverting the matrix.∗ A major exception is the default uncertainty on resonance energy, which may be much too large, especially for large s-wave resonances.

The ratio of the output uncertainty for a given parameter to its initial (prior) uncertainty is a measure of the effect the data have on that parameter. An unchanged or slightly changed uncertainty implies that the data have little or no effect on the parameter. A drastic reduction in the uncertainty (i.e., a ratio which is, say, less than 0.05 or 0.10) implies that this is an important parameter for these data, and, further, that the prior value was effectively infinite. An increase (a ratio > 1.0) perhaps indicates that numerical problems exist.

Occasionally there are significant changes in values of parameters which should be unaffected in the region being analyzed. This might be the case, for example, for the width of a large s-wave resonance. If, however, the uncertainty on that parameter remains large and the correlations between it and other parameters are also large, possibly the value of that parameter will resume its expected magnitude once data directly affecting it are analyzed. Values of correlated parameters will be altered to ensure that the fit to the data analyzed earlier is not degraded. On the other hand, it may happen that SAMMY is unable to recover from major changes in parameter values. In this case, the analyst should carefully consider whether some data are inconsistent with the others and make appropriate changes. If all data are deemed to be good, it will likely be necessary to alter the sequential order in which data are analyzed or to decrease prior uncertainties on parameters. Alternatively, one could do simultaneous runs, as described in Section IV.E.1.

∗ Experience has shown that the choice of prior uncertainties can, in fact, make some difference in the final results, both for parameter values and for parameter uncertainties. This has often been stated as a deficiency in Bayes' method, since the output depends upon the input. The analyst should keep in mind, however, that output from least-squares analyses also depends upon the input, but with least squares the user has no choices regarding that particular piece of input – the prior uncertainties are always infinite.

Spin group definitions

It is legitimate to specify a spin group in the INPut file without giving any resonance for that spin group in the PARameter file. Potential scattering (via hard-sphere phase shifts) will be calculated for that spin group. It is not permitted, however, to request a spin group or channel in the PARameter file without specifying that group in the INPut file.∗

The ENDF so-called "Reich Moore" format (LRF=3), however, does not allow spin groups to be defined without at least one resonance in the spin group. (See the next paragraph for the exception to this rule.) Evaluators who require an "empty" spin group are encouraged to use the new, less restrictive "R Matrix Limited" format (LRF=7).

The original ENDF LRF=3 format made the implicit but unwarranted assumption that all resonances having a given l and J would have the same s. Because this assumption is not always valid, the format was modified in 1999 to specify which channel spin would be used; see Section VI.F.2 for details. The format also requires that "the other" channel spin be added if it is absent, in order to obtain the correct hard-sphere-phase-shift cross section.

A critic has suggested that SAMMY should *require* that all analyses always use all possible spin groups and channels (up to a user-determined value of l, presumably); the critic is recalling an early ENDF evaluation for which "the other channel spin" was omitted during the analysis, causing great consternation when processor codes reconstructed a cross section which differed from the original. Nevertheless, the SAMMY author has chosen not to hamstring the SAMMY user in this fashion, relying instead on the expertise of today's evaluators to avoid repetition of a single 25-year-old mistake.

There are legitimate reasons for giving the analyst the ability to define spin groups as s/he chooses: (1) Only the analyst understands all aspects of the evaluation, so only he or she should be responsible for including all relevant information. (2) Forcing the inclusion of spin groups or channels with negligible contribution will add nothing of value to the calculation, and only increase the CPU time used for calculating zero. (3) It is often useful for the analyst to consider the effect of an individual spin group without including the others.

To be sure that your final evaluation includes the "complete" set of spin groups and channels (and to justify the SAMMY author's faith in the thoroughness of today's evaluators), users are strongly encouraged to make use of program SAMQUA for assistance in determining spin groups.

∗ When the command "`QUANTUM NUMBERS ARE in parameter file`" is given and the spin-group definitions are at the beginning of the PARameter file rather than in the INPut file, the same arguments hold. A channel or spin group cannot be used in the resonance-parameter list if it is not first defined in the spin-group list.

Negative reduced-width amplitudes

In Section II.B.1, in the paragraph following Eq. (II B1.7), it is stated that reduced-width amplitudes can be either positive or negative. However, the reduced-width amplitude itself is not printed in either SAMMY or ENDF files. Instead, the partial width (related to the square of the reduced-width amplitude) is printed; if the value in the file is given as negative, the sign is assumed to belong to the amplitude rather than to the partial width. (This potentially confusing convention is standard practice, is unambiguous, and soon becomes second-nature to experienced R-matrix practitioners.)

In light of the previous paragraph, one might ask why so few negative signs are observed in SAMMY or ENDF files. There are several reasons:

- The "natural" thing to do is to use positive signs until and unless the need for a negative sign becomes apparent. Because it is the easy thing to do, we assign all the amplitudes as positive unless there is evidence to the contrary.

- The sign is irrelevant for widely spaced resonances of the same spin groups (and for resonances of different spin groups). Even for neighboring resonances of the same spin group, only the relative sign is sometimes observable.

- Interferences between neutron widths are often effectively invisible under experimental conditions, lost in the noise and the Doppler and the resolution broadening, etc.

- Negative signs are most often observed for fission widths, when two or more fission widths are specified for each resonance. These signs appear naturally as needed during the course of an analysis – but again, they only appear when needed, and they are not needed very often.

- Rather than starting with all positive amplitudes, a more realistic approach would be to assign the signs randomly for the starting parameters. This is rarely done, most often with fission widths.

- A basic assumption underlying the Reich-Moore approximation is that the signs of the gamma-width amplitudes are randomly distributed. This randomness plus the sheer number of capture channels allow us to treat the gamma width as an average, non-interfering, positive quantity.

Transmission vs. total cross section

Analysts will want to make use of transmission data rather than total cross section data whenever possible. Total cross section data are typically derived from transmission data, which cannot reliably be translated to cross section data for all resonances for any given sample thickness. Ideally, transmission data from several different-thickness samples should be included in the evaluation, in order to determine the peaks for resonances of widely differing widths.

ENDF files

Anyone creating or using ENDF files for the resolved resonance region should be aware of idiosyncrasies in the ENDF formats:

- The ENDF multilevel Breit-Wigner format (LRF = 2) is "multi" only for elastic scattering. Other cross sections are single level.

- The so-called Reich-Moore format (LRF = 3) permits only a limited subset of options available in Reich-Moore. Use the new "R-Matrix Limited format" (LRF = 7) for situations that do not fit the LRF = 3 format. That is, use LRF = 7 for more than one entrance channel, for more than two fission channels, for other reaction channels (inelastic, proton, alpha, etc.), for combinations of orbital angular momenta and/or channel spins, and for other generalizations.

- The so-called Reich-Moore format (LRF = 3) requires that, for a given l and J, any non-identified (i.e., missing) channel spin s must be added to the configuration as a new spin group. With this format, it is not possible to explicitly define a spin group or channel for which there are no resonances. Hence, missing channels are implicitly assumed to be present so that the hard-sphere phase shift contributed will be added to the cross sections.

- In contrast, the R-Matrix Limited format (LRF = 7) requires that each and every spin group and channel be explicitly defined. It is the evaluator's responsibility to be sure that all non-negligible spin groups and channels are included.

- Except for the new LRF = 7 format, no ENDF formats have provision for defining parity explicitly. Hence, for example, the ENDF file for ^{235}U suggests that the ground state is $7/2^+$ when it is in fact $7/2^-$.

- The ENDF formats, like the SAMMY PARameter file format, use $G = A\Gamma = A\left(2P\gamma^2\right)$, where A is the sign of γ, for the input quantity.

- Unlike SAMMY, ENDF resonance parameter covariance matrices (RPCM) are written in terms of the input quantity G rather than of the more physical quantity Γ. (As of this writing, this topic has not been discussed by CSEWG and is not addressed in the ENDF-102 manual. The convention that ENDF RPCM be written in terms of G is used in SAMMY to create ENDF File 32, is used in the two processor codes ERRORJ [GC04] and AMPX [MD02], and is being recommended to CSEWG. In contrast, the RPCM printed in the SAMMY.LPT file has always been expressed in terms of Γ rather than G.)

XII. EXAMPLES

Three quite different types of examples are provided with the SAMMY code.

The first is a series of tutorial exercises, designed as a learning aid for novice users. These were originally designed for use in the SAMMY workshops but have been successfully used for independent study as well. For a description of the tutorial exercises, see Section XII.A.

The second type, described in Section XII.B, is a series of test cases that are designed to test the various features of the code to ensure consistent behavior over time and across computer platforms. A second, equally useful, function of these test cases is to provide users with examples of input for the different features available in the code. Prior to release of the code, all these test cases are run on a variety of platforms. Users who are having difficulty with particular features of the code are strongly encouraged to run the relevant test cases prior to contacting the author for assistance.

Some of the examples that previously were part of the test cases of Section XII.B have now been moved* into a category called "simulations," described in Section XII.C. These are Monte Carlo simulations of the multiple-scattering corrections for capture or fission data.

---

* The move was prompted by the author's propensity to absentmindedly rerun the simulations, even when nothing was changed with respect to the simulations. Putting these very long runs into a separate category ensured that they will be rerun only when necessary.

XII.A. TUTORIAL

A series of computer exercises has been developed as an aide to persons wishing to learn how to run SAMMY. Novice users are urged to work their way through the entire series of exercises in numerical order; experienced SAMMY users may find particular exercises helpful when beginning to use an unfamiliar feature.

Files for each exercise are located in a separate subdirectory; instructions for the exercise are given in the text file README.FIRST, located in that subdirectory. The author's results from running the exercise are in subdirectory "answers".

Table XII A.1 explains which SAMMY features are addressed in the examples. Note that each example assumes that the user has knowledge of features described in earlier examples. Also note that the first example (ex000) teaches the use of the ORNL plotting packages FORODF [JC78] and RSAP [RS03]. (The RSAP code is not yet available for public release.) For users at facilities not using these plotting packages, this example should be modified.

Table XII A.1. Computer exercises for the student

No.	Description of feature emphasized in this example
000	Use of plotting package FORODF
001	Simple one-resonance nonfissile nucleus; capture experiment
002	Fissile nucleus, several resonances; capture experiment
003	Different kinds of cross sections
004	$l > 0$ (s, p, d waves); $I > 0$
005	Doppler broadening
006	Resolution broadening (Gaussian)
007	Resolution broadening (ORR)
008	Resolution broadening (RPI)
009	Normalization
010	Backgrounds
011	More than one channel radius
012	Multiple nuclides within a single sample
013	Uncertainties on parameters
014	Angular distributions
015	Sequential vs. simultaneous fitting of data
016	Sequential fitting of three data sets; parameter covariance matrix as input
017	Several data sets; varying data-reduction parameters
018	Data covariances (implicit and explicit)
019	Self-shielding and multiple-scattering corrections to capture yields
020	Integral quantities
021	Almost real data: W transmission with many complications
022	Almost real data: ^{235}U. How to do an evaluation
023	Finding input errors
024	Run program LADDER
025	Run program SAMDIS
026	Create ENDF File 2
027	Running SAMMY with ENDF files for input

XII.B. TEST CASES

The SAMMY quality assurance program involves a series of "test cases," each of which is designed to test a particular feature of the code. Whenever a new feature is added to SAMMY or a major bug exterminated, a new test case is developed. Prior to the release of a new version of the code, all test cases are run on several computer platforms, to ensure that recent changes have not adversely affected the behavior of older features. These test cases, both input and output, are released, along with the source codes (e.g., from RSICC); anyone wishing to port SAMMY to his or her own computer is advised to run a significant number of test cases, compare output, and resolve major differences before beginning new analyses. In particular, a user should run the test cases which contain those features that are used in her/his own research.

Table XII B.1 gives a brief description of the test cases, which are numbered in arbitrary order. Cases 1 through 174 are labeled "tr001" through "tr174" where "tr" denotes "trial" number.

Each test case is contained in a separate subdirectory named .../samtry/trxyz, where xyz represents the three-digit case number. The Unix command file for each test case is denoted "testxyz"; the comparable command file for Windows is named "test.bat". Running this file will cause several SAMMY (or auxiliary code) runs to be made with results written into subdirectory .../samtry/trxyz/results. A second additional command file, named "check", is provided for each test case; this file can be used to compare new results (those run on the user's computer) to the standard results (found in subdirectory .../samtry/trxyz/answers). A third command file, named "t", runs both "testxyz" and "check". The command file "zzauto" (found in subdirectory …/samtry) can be used to run all test cases automatically.

For version 7.0.0 of SAMMY, the test cases have been somewhat reorganized from previous versions. Certain of the old test cases (e.g., tr038) were incomplete or used non-portable input; these cases have been eliminated and the numbers reassigned to newer examples. Test cases involving Monte Carlo simulations of multiple-scattering corrections have been relocated into "samsim" instead of "samtry"; see Section XII.C for details.

<u>Note</u>: All experimental data used in the test cases are to be treated as "dummy" data, not to be used for any purpose other than to verify the accuracy of the SAMMY calculations. The same is true of resonance parameters used in the test cases. *Neither data nor parameters should ever be assumed to have any physical validity*.

In addition to providing the basis for SAMMY's quality assurance program, the test cases fill another role: They serve as examples of input for the various features of the code. Persons wishing to begin using an unfamiliar feature of the code may consult the test cases for guidance in preparing input.

Table XII B.1. SAMMY test cases

No.	Module tested	Main feature being tested	Data type	Nuclide
001	dat	Correlated data (DCV file)	Elastic	^{60}Ni
002	ipq, npv	Comparison of different solution methods for Bayes' equations	Trans-mission	dummy
003	par	R-external	Trans	^{60}Ni
004	fin, old	Simultaneous vs sequential solution of Bayes' equations	Trans	^{60}Ni
005	dat	Use ODF file as input	Fission	^{241}Am
006		Resonance parameters only	Trans	^{60}Ni
007	amr	Rearranging "active" data-reduction parameters	Trans	^{56}Fe
008	dat	Comparing alternative auxiliary grids	Trans	^{58}Ni
009		Simultaneous vs sequential solution of Bayes' Equations; explicit input of prior uncertainties	Fission	^{239}Pu
010	inp	New spin group format	Trans	^{93}Zr
011		R-external	Trans	^{54}Fe
012		Varying channel radius, normalization, and/or background	Trans	^{58}Ni
013	xct	Channel radius	Trans	^{58}Ni
014	avg	Averaging experimental and theoretical data	Fissi	^{239}Pu
015	new	"Relative uncertainties" vs "explicit uncertainties" in PARameter file	Trans	^{58}Ni
016		Radius	Trans	^{58}Ni
017		Long run	Fission	^{239}Pu
018		Different cross sections	(All)	^{235}U
019	old	Read and use "old" par covariance file	Trans	^{235}U
020	fgm, dbd, dop	Different versions of Doppler broadening	Fission	^{235}U
021	orr	Oak Ridge Resolution function; vary radius	Trans	^{58}Ni
022	rsl	Shift exponential tail on resolution function	Trans	^{56}Fe
023	ndf	Make ENDF File 2	Trans	^{204}P, ^{58}Ni
024		Vary radii	Trans	Natural Fe

Table XII B.1 (continued)

No.	Module tested	Main feature being tested	Data type	Nuclide
025	mlb	MLBW vs RM	Trans	^{56}Fe
026	fgm	Compare different Doppler broadening methods	Fission	^{241}Am
027		Generate partial derivatives	Fission	^{235}U
028	dbd	No low-energy Doppler broadening	Total	^{241}Pu
029		Abundance as a variable	Trans	^{58}Ni
030		Remove resonances using negative group number in PARameter file	Trans	^{58}Ni
031	dop	Leal-Huang vs. no broadening vs. free-gas model at thermal energy	Fission	^{235}U
032	amr	Vary radii, convert "active" data-reduction parameters	Trans	^{56}Fe
033	ang	Differential elastic (no Coulomb)	diff el	~ ^{14}N
034	orr	ORR resolution function at thermal energies	Trans	^{65}Cu
035		Γ_γ as miscellaneous parameter	Capture	^{235}U
036	amr	Sequential data sets; converting data-reduction parameters	diff el, trans	~ ^{14}N
037	rec	Reconstruct point-wise cross sections from resonance parameters	All	lots
038	many	Broadening parameters as PUPs (Propagated Uncertainty Parameters); see tr007	Trans	^{56}Fe
039	ssm	Self-shielding and multiple-scattering corrections to capture yields	Capture	^{58}Ni
040	xct	External R-matrix parameters as PUPs (Propagated Uncertainty Parameters); see tr011	Trans	^{54}Fe
041	many	Normalization and background as PUPs (Propagated-Uncertainty Parameters); see tr012. Also see tr138 for non-PUP like tr041	Trans	^{58}Ni
042	mxw	Maxwellian (stellar) averages	Capture	^{58}Ni
043	ang	Differential elastic angular distributions	angular distribution	^{58}Ni,^{52}Cr,...
044	xct	Resonance parameters as PUPs; see tr009	Fission	^{239}Pu

Table XII B.1 (continued)

No.	Module tested	Main feature being tested	Data type	Nuclide
045	ssm	Multiple-scattering corrections with more than one nuclide in sample	Capture	Natural Fe
046	ssm	Ditto, making plots with and without corrections	Capture	Natural Fe
047		Vary t_0 and L_0	Trans	^{56}Fe
048	rsl	Channel resolution varies with energy	Fission	^{239}Pu
049	rec, mxw	Reconstruct point-wise cross sections; use results to calculate stellar averages	Capture	^{54}Fe
050	mas	Use ENDF File2 for input to SAMMY	Trans	^{59}Co
051	mxw	Various ways to generate stellar averages	Capture	^{136}Ba
052	ssm	Self-shielding and multiple-scattering corrections	Capture	^{134}Ba
053	rpt	Generate RPI resolution function	none	none
054	rpi	Use RPI resolution function	Trans	W
055	xct	Paramagnetic cross section (including PUPs)	Total	Dummy
056		Background function	Dummy	Dummy
057	ssm	Self-indication data	Self-indication	Dummy
058	dop, fgm	Very-low-energy Doppler broadening	Capture	Dummy
059	xct	Channel radii as PUPs; see tr093	Reaction	^{16}O
060	ssm	Self-shielding and multiple-scattering corrections	Capture	^{136}Ba
061	ref	Convert REFIT input to SAMMY and vice versa		
062		Abundances as PUPs	Trans	^{58}Ni
063		Constant cross section		Dummy
064		Fission yields, polar coordinates	Fission	^{235}U
066	many	Miscellaneous parameters as PUPs	many	many
067	dat	Twenty significant digits for data		Dummy
068	orr	ORR parameters as PUPs. See tr117 for related unPUP case.	Trans	^{58}Ni
069	ntg	Integral quantities	All	^{235}U

Table XII B.1 (continued)

No.	Module tested	Main feature being tested	Data type	Nuclide
070	idc, fdc	Implicit data covariances		^{235}U
071		Write covariance matrix in compact ASCII format		^{235}U
072	thn	Thinning data		
073	fff	Unresolved resonance region	many	^{235}U
074	idc	Various ways to use data covariance information		^{241}Am
075	avg	Generate group-average cross sections with and without covariances	fission	^{235}U
076		Uncorrected tr039; include direct capture	Capture	^{58}Ni
077	xct, ntg	Comparison with other codes	(All)	^{235}U
078	xct	Spin-group-dependent detector efficiencies	Capture	^{136}Ba
079	rsl	Energy-dependent exponential broadening	Capture	^{136}Ba
080	rsl	Exponential folding width	Total	^{235}U
081	rsl	Energy-dependent exponential folding width	Total	^{235}U
082	ywy, wyw	Retroactive covariance	many	^{235}U
083	old, grp	Compact covariance format; Bondarenko multi-group cross sections	many	^{235}U
084	old	Compact covariance format	Capture	^{235}U
085	grp	Bondarenko averaging	Capture, Total	^{235}U, ^{27}Al
086	ndf	Generate and/or read-and-use ENDF file 2	Trans, Capture	^{27}Al
087	amr	Background functions and RPI resolution function	Trans	^{183}W
088	fff, acs	Unresolved resonance region with many data sets, each with its own normalization	many	^{244}Cm
089	ywy, wyw	Retroactive covariance matrix; covariance for multigroup cross sections	Total	^{29}Si
090	rpi	RPI resolution function	Capture	nat Sm
091	xct	Coulomb	(n,α)	^{16}O
092	dis	Luiz Leal's samdis (samdist) program		

Table XII B.1 (continued)

No.	Module tested	Main feature being tested	Data type	Nuclide
093	xct	Exit channels specified separately	Reaction	^{16}O
094	rpi, rpt	RPI resolution function	Trans	^{99}Tc
095	rpt	RPI resolution function		Tc
096	rpi	RPI resolution function parameters as PUPs; see tr054	Trans	^{183}W
097	many	Background functions as PUPs; see tr066. Also see tr121 for non-PUP runs like tr097.	Total	nat Fe
098	clm	Crystal-lattice model for Doppler broadening	Trans	^{238}U
099	orr, fgm	General	Capture	^{192}Pt
100	xct	Coulomb	(α,n)	$^{17}O(\alpha,n)^{20}Ne$
101	inp, xct	Two-channel interactions	Total	dummy
102	xct	Very small cross sections; numerical stability	many	^{28}Si, ^{60}Ni
103	rsl, orr	Combination of resolution functions	Trans	^{58}Ni
104	rpi	RPI Resolution function mod for Geel & nTOF	Trans	^{99}Tc
105	dex	Square resolution function	several	^{16}O, ^{17}F
106	mlb	Compare MLBW to SLBW	Elastic	^{56}Fe
107	rpi, clq	Dirac on RPI Res function		^{99}Tc
108	rpi, clq	Gunsing's values for Geel- and nTOF-RPI resolution function		dummy
109	ang	Differential elastic with charged particles; Rutherford scattering	Angular distrib	F + p
110	xct	Level-level interference in capture	Capture	dummy
111	xct	Like tr059 but channel radii not PUPed.		
112	ang	Angular distributions (artificial data)	Reactions	$^{12}C(\alpha,n)$
113	par	Interchangeable channels	Artificial	^{16}O
114	udr	User-defined resolution function (not working well yet -- user beware!)	Total	^{235}U
115	clq, rpi	Constant, linear, quadratic, Dirac delta function, or 1/v for "cross section" RPI resolution function with and without shift		^{235}U

Table XII B.1 (continued)

No.	Module tested	Main feature being tested	Data type	Nuclide
116	ang	Rutherford scattering, with non-elastic channels	Differential elastic	^{13}C
117	orr	Like tr068 but ORR parameters not PUPed	Trans	^{58}Ni
118	idc	Norm + background + RPI background	Capture	Tc
119	xct	*Many* channels	Reaction	$^{18}O(\alpha,n)^{21}Ne$
121	many	Like tr097 but background functions not PUPed	Total	nat Fe
122	ftz	Fix t-zero	Trans	^{56}Fe
123	ang	Angle average	Diff elas	$^{17}F+p$
124	clm	Crystal lattice model for Doppler broadening (DOPUSH)	several	dummy ^{238}U
125	xct, ang	Running as pseudo R-matrix (no Reich-Moore approximation); Coulomb; many channels	many	^{16}O
126	ndf	Prepare compact covariance file in ENDF File 32 format	Fission, Total	^{235}U, ^{27}Al, ^{23}Na, ^{242}Pu, ^{240}Pu, ^{241}Am
127	lru	Create File 2 for unresolved resonance region	all	^{235}U, ^{244}Cm
128	fff	Use several energy regions in URR calculation	all	^{235}U
129	mas	Read all of ENDF file, not just File 2		^{242}Pu, ^{23}Na, ^{240}Pu, ^{241}Am
130	new	Read ENDF File 32 as generated in tr126		
131	ndf	Write compact covariance matrix in ENDF format		^{152}Gd
132	ndf, new	Create PAR & COV file, generate ENDF File 2 and File 32, read them back		dummy like ^{27}Al
133	lru	Write ENDF File 2 and File 32 for URR	all	^{235}U
134	lru	Write ENDF File 2 for URR; options for energies in ENDF file		^{238}U
135	inp, par	More than fifty spin groups	Total	dummy (Si)
136	rpi	Derivatives with respect to RPI resolution function parameters	Trans	Gd
137	ndf	Create File 32 original ENDF formats (LCOMP = 0 or 1)		^{242}Pu, ^{23}Na, ^{240}Pu, ^{241}Am

Table XII B.1 (continued)

No.	Module tested	Main feature being tested	Data type	Nuclide
138	many	Like tr041 but normalization and background are not PUPs	Trans	^{58}Ni
139	xct, xxx	Calculate hard-sphere phase shift at high energy	Reaction	^{9}Be(α,n)^{12}C
140	idc	User-supplied implicit data covariance matrix	Trans	^{129}I
141	suggel	Estimate quantum numbers for resonances		
142	fit, fff	Sequential runs in URR	all	^{233}U
143	qua	Prepare spin group quantum number information in SAMMY input format		^{58}Ni, ^{99}Tc, ^{26}Fe, ^{241}Am, ^{235}U, ^{16}O, ^{17}O, ^{13}C
144	inp, par	Treat channels properly: 10 spin groups vs. 18; 2 or 3 channels vs. 1	Trans	^{27}Al
145	fff, acs	Covariances, normalizations in URR	Total, Fission	^{235}U
146	avg, grp, fin	"Compact" format for ENDF	Capture	^{235}U
147	rml	Read and use LRF=7 ENDF format; test SAMRML program (see tr147a for SAMRML runs with no SAMMY runs)	Elastic, Absorp-tion, Fission	^{27}Al, ^{16}O, ^{235}U
148	rml	Test SAMRML program, including derivatives and angular distributions (see tr148a for only SAMRML runs, no SAMMY runs)	many	^{52}Cr
149	many	Create retroactive covariance matrix for ENDF File 32	many	^{233}U
150	rml	Extension of tr147 with fewer resonances and parameters but more features (see tr150a for SAMRML without SAMMY)	Angular distribs, derivatvs	^{16}O
151	par	Additional possibilities for input of prior uncertainty on resonance parameters	input	^{58}Ni
152	par, xct	Exclude channels from entire calculation	Trans	^{19}F
153	inp, par	Input data-related parameters via the INPut file rather than PARameter file	Trans	^{19}F

Table XII B.1 (continued)

No.	Module tested	Main feature being tested	Data type	Nuclide
154	ndf	Prepare covariance file in ENDF File 32 format. Like tr126 but use default uncertainty option ("def = value" in *.ndf file; see Section VI.F.2 for details). All resonances appear in File 32.		^{235}U, ^{27}Al, ^{23}Na, ^{242}Pu, ^{240}Pu, ^{241}Am
155	ang	Angular distribution of reaction cross sections	Differential reaction	^{9}Be
156	grp	Bondarenko averaging with Doppler broadening and resolution broadening	Capture	^{238}U
157	inp, par	Broadening parameters in INPut file	Trans	^{238}U
158	ndf	Write ENDF File 2 in LRF = 7 format		^{19}F
159	inp	Use particle-pair input format to define reaction channels	Reaction	^{16}O
160		Varying resonance energy might require modifications to auxiliary grid	Capture	^{232}Th
161	ndf, new, avg	Reading ENDF File 2 and File 32, creating multigroup averages and covariances	Total	Several
162	many	Derivatives with respect to t_0 and L_0	Total	Dummy
163	many	Least squares and other extensions	(n,t) and total	^{6}Li
164	inp, par	Broadening parameters with uncertainties in the INPut file or PARameter file	Trans	Dummy
165	ndf	Prepare compact covariance file in ENDF File 32 format		Pseudo ^{27}Al
166	ndf	Creating ENDF File 32 with LCOMP=2 and Ndigit > 2	Trans	^{27}Al
167	ndf	Prepare covariance file in ENDF File 32 format. Like tr154 but only resonances with flagged parameters are listed in File 32 (except for LCOMP = 2, which must include all resonance parameters)		^{27}Al, ^{23}Na, ^{242}Pu, ^{240}Pu
168	several	Creating and then using PUP covariance file	Trans	^{56}Fe
169	ndf	Short-range sections in LCOMP=1 for ENDF File 32	Fission	^{235}U

Table XII B.1 (continued)

No.	Module tested	Main feature being tested	Data type	Nuclide
170	mlb	Artificial energy grid with multilevel Breit Wigner	Fission	^{241}Am
171	ssm	Neutron sensitivities	Capture	^{55}Mn
172	ang	Elastic angular distributions with charged particles	Elastic	^{7}Be+p
173	old, ndf	Read a COVariance file created by version M6, create ENDF File 2 and 32 when there are two or more nuclides in the PARameter file		Natural LiCl
174	ndf, avg	Read ENDF File 2 and 32 as generated in tr167; calculate average cross sections		^{27}Al, ^{23}Na, ^{242}Pu, ^{240}Pu

XII.C. MONTE CARLO SIMULATIONS OF MULTIPLE-SCATTERING CORRECTIONS

One aspect of the SAMMY quality assurance program is the use of any and all available methods for double-checking the implementation of the various features in the code. For the multiple-scattering corrections for capture or fission data described in Section III.D, the most reliable checking method is Monte Carlo simulation of those corrections. The code SAMSMC (Section X.M) is used for these simulations. Sample simulations are stored in subdirectories samsim/sim001 through samsim/sim008; details are shown in Table XII C.1. The command file in each subdirectory is called sim*xyz*, where *xyz* is the three-digit simulation number.

Table XII C.1. Sample Monte Carlo simulations

Simulation Number	Sample composition	Related test case number
sim001	^{58}Ni	tr039
sim002	natural Sm plus heavy water	
sim003	^{137}Ba	tr060
sim004	natural Si	
sim005	^{28}Si; artificial data	
sim006	Natural Li Cl	
sim007	^{35}Cl with proton channel	
sim008	W	

XIII. DESCRIPTION OF THE COMPUTER CODE SAMMY

The computer code SAMMY was originally developed to run efficiently on the DECSystem-10 (PDP-10) at the Oak Ridge Electron Linear Accelerator (ORELA). Because memory rather than CPU time was the limiting factor on the PDP10, a number of techniques were used to conserve memory, occasionally at the expense of run time. These techniques include dynamic allocation of array storage (Section XIII.A), use of temporary data files to store intermediate results (Section XIII.B), and division of the program into substantially independent segments (Section XIII.C).

In 1985 ORELA replaced its PDP10 with a VAX785, and SAMMY migrated to the system. Since the mid 1990's, the primarily operating system for SAMMY development has been UNIX or LINUX. Currently the author maintains the code under UNIX (f77 on IBM and VAX-Alpha workstations) and LINUX operating systems; the same version also works on Windows under Compaq FORTRAN. Portability to VMS operating systems is no longer maintained.

Prior to release M5 of the code in 2000, the "division of the program into substantially independent segments" was significantly altered; see Section XIII.C for details. Future plans call for continued modernization of the coding, including conversion to FORTRAN 90; this will eliminate the rather archaic (but nevertheless useful) "dynamic allocation of array storage" currently in use (Section XIII.B).

For the 2006 release 7.0.0 of SAMMY, the use of temporary data files has been significantly lessened but not yet completely eliminated.

For the benefit of persons wishing to port SAMMY to a new computer system, a brief discussion is included in Section XIII.D regarding routines and statements specific to a given computer. The discussion is not expected to cover all conversion problems but merely to point out a few problems of which the author is aware.

The ODF (ORELA Data Format) plotting package in use at Oak Ridge is not easily portable to most machines. See Section XIII.E for a discussion of this topic, and Section X.I for a discussion of alternatives.

In 2005 a modern configuration and distribution system was designed by ORNL researcher Dorothea Wiarda. This system, described in Section XIII.F, makes it significantly simpler for a user to install SAMMY.

XIII.A. DYNAMIC ALLOCATION OF ARRAY STORAGE

Because SAMMY was developed prior to the advent of FORTRAN 90, which supports dynamic storage allocation, SAMMY uses its own scheme for dynamic allocation of array storage. This scheme should be effectively invisible to the most SAMMY users. On porting the code to a new machine, minor modification may be needed: If the total memory on your machine is larger or smaller than the default value, you may need to change the total array size during the "configure" part of the installation process. See Section XIII.F to learn how this is done.

Historically there have been many advantages to using dynamic allocation of array storage. First, core requirements are kept to a minimum, since only the array length actually needed is allocated and temporary arrays are released when no longer needed. Secondly, because allocation is made during the execution of a program, substantial changes in the dimensions for a specific case do not require recompilation of the program. Finally, when recompilation is needed (when the maximum array space requirement must be changed), only a few routines need to be recompiled.

The SAMMY scheme for dynamic allocation of array storage is best illustrated with a simple example. Let us suppose that two vectors V1 and V2, both of length N, are to be initialized, added, and stored in V1, after which V2 is no longer required. A program to perform these operations is given in Table XIII A.1. Mnemonic names can be used in the usual manner in all subroutines, provided arrays are input to the subroutines through argument listings.

Table XIII A.1. Illustration of dynamic allocation of array storage

```
PROGRAM MAIN
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
DIMENSION A(-12345:12345)
NSIZE = 12345
N = 50
IV1 = IDIMEN (N, 1, 'V1  N, 1')        #Allocate storage for V1
IV2 = IDIMEN (N, 1, 'V2  N, 1')        #Allocate storage for V1
CALL SET (A(IV1), A(IV2), N)           #Initialize V1 and V2
CALL ADD (A(IV1), A(IV2), N)           #Add V1 = V1 + V2
I = IDIMEN (IV2, -1, 'I   I, -1')      #Release storage for V2
...
I = IDIMEN (0, 0, 'I    0, 0')         #Request that IDIMEN print out the
STOP                                   #           maximum length used
END
```

```
SUBROUTINE SET (V1, V2, N)
DIMENSION V1(N), V2(N)
READ (11) V1
READ (11) V2
RETURN
END
```

```
SUBROUTINE ADD (V1, V2, N)
DIMENSION V1(*), V2(*)
DO I=1,N
    V1(I) = V1(I) + V2(I)
END DO
RETURN
END
```

What follows is a brief description of the scheme currently in use in SAMMY for dynamic allocation of array storage. Most users of the code will not need to be concerned with the remainder of this section. The information is included here for completeness' sake, and for the benefit of anyone who may need to modify the code.

The current scheme is essentially the same as in previous releases of the SAMMY code, though different in detail. All arrays required by the computer program are stored in one array A, dimensioned A(-*n*:*n*) where *n* is a large number. [Use of this form, rather than the more common A(*n*), makes use of the negative integers and thus effectively doubles the maximum size of the array available with the largest possible 8-byte (32-bit) integer (2^{31}-1 = 2 147 483 647, since the 32nd bit is used for the sign). For a very few applications, this large size is needed and can be accommodated on computers with sufficient memory.] The precise value to be used for *n* is machine dependent. The SAMMY default is 65 million, but this can be overwritten when the code is configured for a specific machine, as described in Section XIII.F.

As shown in Table XIII A.1, allocation of space in this array is accomplished via a call to FUNCTION IDIMEN, which keeps track of the last location allocated, and appends the new array to that position. When an array is no longer needed, its space is released via another call to IDIMEN. At the end of each segment, IDIMEN is called one more time to report the maximum size actually used in that segment. IDIMEN also issues a warning if more than 2*n* words are required in the array A(-*n*:*n*), and then aborts the run.

Three arguments are used for IDIMEN (m1, m2, a3): The third, a3, is an arbitrary alphanumeric phrase used by the author for debugging. The second, m2, tells IDIMEN what to do with the first, m1. If m2 > 0, an array of size m1 is allocated. If m2 < 0, everything in A(-*n*:*n*) beyond position A(m1) is released for reuse. If m2 = 0, the total amount of storage used since the previous such call is reported (written into the SAMMY.LPT file).

Users familiar with the array storage system in earlier versions of SAMMY will note some differences in the 7.0.0 release of the code, especially with respect to the array sizes printed in the SAMMY.LPT file.

First, the storage requirement for segment XCT will generally be twice the size for the same segment in previous versions of the code; nevertheless, the largest requirement (for all segments) remains approximately the same. At the beginning of segment XCT, the new array-storage system allots all of the storage (for theory and derivatives, original and Doppler broadened, for example) needed to store intermediate results. SAMMY reuses those same storage locations as it goes from segment to segment. For a typical run including both Doppler and resolution broadening, after completion of segment FGM (Doppler), the "original" array positions will be re-used to hold the resolution-broadened values.

In the old version of the code, only the arrays needed in segment XCT were defined in XCT; these were then written to a temporary file and the space released. Then in FGM, space was allocated for the original arrays and for the Doppler-broadened arrays; the original values were read in from the temporary file. When the FGM calculations finished, the Doppler-broadened values

were written to a temporary file and the space (for all these arrays) was released. This process was repeated in every module of the code.

Hence, the new system uses essentially the same total storage space but eliminates the reads and writes to the temporary files. Total time for a SAMMY run is therefore decreased. (Future development will likely eliminate nearly all of the temporary files. For more on the use of temporary files, see Section XIII.B.)

As indicated above, SAMMY allocates the array space for *storing* the values and derivatives at the beginning of segment XCT. However, it does not allocate all array space needed for all of the processes involved in *calculating* those values and derivatives. Thus, for example, the SSM segment (which calculates self-shielding and multiple-scattering corrections) requires many auxiliary calculations, for which it needs extra array space.

XIII.B. USE OF TEMPORARY DATA FILES TO STORE INTERMEDIATE RESULTS

Output to and input from temporary files is a time-honored method of saving memory at the expense of run time. In versions of SAMMY prior to M5, the use of temporary files also provided the necessary linkage from one module to another; I/O for this purpose has now been eliminated, since the segments of the code are now united into one large code. Nevertheless there are still many temporary files created by a SAMMY run; these are being phased out as modernization of the code proceeds. For now, upon successful completion of a SAMMY run, the temporary files may be deleted.

It is still occasionally possible for the author to debug the code in a piece-wise fashion, one segment at a time. However, it now requires a bit more planning. First, a SAMMY run is made that includes the alphanumeric line

`STOP` *xyz* *n*

in the INPut file, where *n* is a one-digit integer preceded by <u>two</u> spaces, and *xyz* is the name of the segment for which debugging is needed. This line is a command to SAMMY to cease execution just prior to the beginning of the *n*th pass through segment *xyz* and generate the temporary files that permit restart of that segment alone. After this run finishes, those temporary files can, in principle, be used as input for debugging on segment sam*xyz*. However, with modern high-speed computers, it is now generally more trouble to ensure that the one segment runs properly than to run the entire program. This capability is gradually being eliminated, and the additional routines necessary for reading the temporary files and starting a run in the middle are no longer distributed with the code.

The temporary files generated by SAMMY are listed in Table XIII B.1. "Standard" names referenced in the third column of the table are "SAMxx.DAT," where "xx" is replaced by the unit number. Caution: The list in Table XIII B.1 may not be completely accurate.

Input and output files are also included in Table XIII B.1, without detailed explanation. For a more comprehensive list of input files, see Table VI.1. For a list of output files, see Table VII.1.

Table XIII B.1. Files used by SAMMY. The letter A, B, or O in the second column indicates whether the file is written as ASCII, binary, or ODF file. Only SAMMY files (not those for auxiliary codes) are listed here.

Unit No.	A, B, O	File name if not standard	Subdirectory: subroutines in which this file is written	Subdirectory: subroutines in which this file is read	Content
5	A	Interactive input		mas: many places	See Table VI E.1
6	A	Log file	[Many places]		
10	A	CLM file		clm: Readclm_0, Find_Osc, Readclm	Crystal lattice information; see Section III.B.4
10	A	ENDF/B-VI file 2		mas: Rcontx, Rcont, Rtab1, Rlist, Read_Pp7, Endf7	Resonance parameters in ENDF formats
10	A	ENDF/B file 3		rec: Read3, Rdndf3	File 3 contribution to cross section
10	A	MXW file		mxw: Rktxxx, Readkt	See Section V.D and VI.F.4
10	A	NDF file		ndf: Rdndf7, Read_ndf, Rdndf	See Section VI.F.2
10	A	NTG file		ntg: Rdntgq_0, Rdntgq	Integral data; see Sections V.B and VI.D
11	A	INPut file		mas: Finpx, Finp, New_Input_File, Newinp	See Tables VI A.1 and VI A1.2
12, 32	A	Initial PARameter file		mas: Fpar_If_Cov inp: many places par: many places fdc: Paramf	See Table VI B.2
12	A	SAMNDF. PAR	mas: several		SAMMY-style PAR file generated from ENDF/B file 2

Table XIII B.1 (continued)

Unit No.	A, B, O	File name if not standard	Subdirectory: subroutines in which this file is written	Subdirectory: subroutines in which this file is read	Content
13	A	SAMNDF. INP	mas: several		SAMMY-style INPut file generated from ENDF/B file 2
13, 14	A or O	DATa file		mas: Ascidt, Ascxdt odf: many dat: many fdc: Rddat0_Fdc, Rddat1_Fdc	See Table VIC.1
14	A		mas: odfdat		ASCII version of ODF data file
14	A	SAMNDF. PAR *or* SAMMY. PAR		mas: Rewrite_12	Rewriting output PARameter file
15	A	SAMMY. FFF		fff: many	FITACS input file, see Section VIII
16	A		mas: Sumstr, Wrt16x, Writ16, File2x,	inp: Saminp_0, Files, Filesx, Qcova old: Addup fff: Pass	Controls for passes 1 and 2 through SAMMY
17					
18	A		mas: finp, writ19, file2x odf: chck18	odf: Chck18, Read18	Controls for running ODF segment
19	A		mas: Writ19	inp: Saminp_0, Files, Filesx, Qcova old: Addup fff: Pass	Controls for pass 3 through SAMMY
20					
21	A	SAMMY. LPT	many places	never	“Line Printer” output giving details for this SAMMY run

Table XIII B.1 (continued)

Unit No.	A, B, O	File name if not standard	Subdirectory: subroutines in which this file is written	Subdirectory: subroutines in which this file is read	Content
22	A	INPUT. NEW	inp: Rdspnx		Error message when using obsolete input
22	A		mas: New_Input_File, Sett, Set, Write_Alpha	inp: many places fff: Pass	Copy of INPut file, with appropriate modifications for first pass through SAMMY
23, 24	A				Like 22, for passes 2 and 3
25	B	SAMMY. SSM	inp: Qqqwrt	ssm: Qqqxxx, Qqqget	Edge effects for single-scattering corrections to capture or fission yields
25	B	REMORI. PAR	wyw: Getywy	wyw: Getywy ywy: Get_Dminth_ Gppn	Original parameter covariance matrix for retroactive method
26, 27	A		inp: Saminp_0, Rdspno fin: Find_More_Data avg: Again	fin: Find_More_Data avg: Tryrng, Test_If_Data, Again mxw:Rktxxx ndf: Endfb6	Similar to SAM16.DAT
28	A	AVG file		avg: Tryrng, Qrange	See Section VI.F.1
29					
30	B		acs: Wrt30	mpw: Readwx	Arrays *W* and *Y* for M+W inversion scheme (see Section IV.B.3)

Table XIII B.1 (continued)

Unit No.	A, B, O	File name if not standard	Subdirectory: subroutines in which this file is written	Subdirectory: subroutines in which this file is read	Content
30	A	(user-supplied)	idc: Wrt30_Idc	ipq: Estx, estipq, findxx npv: Get_Idc_1, Findxx, Read_Cov_Idc	Implicit data covariance information
30	B		ntg: Wrntgq, Wrntgx	npv: Rdntg1, Prepare_Storage ywy: Rdntg1_Ywy	Integral data information
31					
32	A		mas: Datcov	wyw: Getywy	File names for Y_i and W_i for data set i; see Section IV.E.1
32	A	SAMMY. PAR	fit: Writep		Updated PAR file for the URR (unresolved resonance region); see Section VIII.C
33	A	SAMMY. PA2	fdc: Paramf		Modified PAR file; see Section VI.C.3.c
34	A	SAMMY. IDC	fdc: Paramf	idc: many places	See Section VI.C.3.c
33-35	A				Debug printout
36					
37	B		npv: Get_W_Idc old: Rdcov_Pup	inp: Reorg_Cov old: Rparfl_Pup end: Outvs	Covariance matrix for Propagated-Uncertainty Parameters

Table XIII B.1 (continued)

Unit No.	A, B, O	File name if not standard	Subdirectory: subroutines in which this file is written	Subdirectory: subroutines in which this file is read	Content
38	A		mas: Endf2, Endf7 fin: Oldord	mas: Rewrite_12	Temporary site for storing parameters prior to rewriting
39	A		mas: Read_Pp7	mas: Rewrite_12	SAMMY-style input file created from ENDF File 2
40					
41	B		old: Set41	fin: Compare_Values	Original parameter uncertainties
42	B		new: Rparf_Retro, Reorg_Cov, Rparfx old: Rdcov, Rdcovx fin: Gnalvr, Gncrfn, Gnradi	old: Set41, Addup fin: Wrcov, Compare_Values end: Outvs, User_Output	Temporary storage for covariance matrices, etc.
43	B		dat: Stndrd	npv: Read_Data_Red_Par	Partial derivatives with respect to data-reduction parameters
44	B		dat: Wr44 the: Uset	int: Pdwrit npv: Get_Exp_Data ref: Read44	Data and data uncertainties
45	B		npv: Setvdt	fin: Vodf	Theoretical uncertainties

Table XIII B.1 (continued)

Unit No.	A, B, O	File name if not standard	Subdirectory: subroutines in which this file is written	Subdirectory: subroutines in which this file is read	Content
46	B		new: many places old: Rdcov, Rdcovx, Addup fff: Parin ipq: Chngc2 mpw:Newpar_Mpw npv: Chngcv wyw:Newpar_Wyw	new: Reorg_Cov, Set41 old: Set41 squ: Square npv: Test_Eig ywy: Setywy_Diag, Setywy_Off_Diag, Rdntg1_Ywy wyw:Getywy fin: Gnalvr, Wrcov, Compare_Values fit: Parnew, Csunc, Fintab, Write_C acs: Begin_Iteration lru: Read_Covar (several): Outvs	Covariance matrix for *u*-parameters in triangular form
47	B		squ: Square mpw:Newpar_Mpw fff: Parin new: Reorg_Cov	avg: Thefix ccm: Create_Cov ipq: Newpar_Ipq npv: Setemg mpw: Newpar_Mpw mxw: Fixcov_Mxw ntg: Fixcov	Covariance matrix for *u*-parameters in full square form
48	B		xct: Write_W_48	dbd: Read_W_48	Partial derivatives
49	B		fff: Wrt_49 new: Write_49, Write_49_No_U old: Rdcov, Rdcovx ipq: Samipq_0, Writeu npv: Samnpv_0 mpw:Sammpw_0	int: Finished, Leal_Hwang squ: Samsqu_0 npv: Get_Organized mpv: Sammpw_0 fin: Samfin_0, Convrt, Wrcov fit: Parnew, Write_C	Dimensions, etc., as needed by matrix manipulator routines
50	B		dat: Wr44	npv: Compar, Findxx, Make_File_3	Experimental energies
51, 54	B		xct: Write_Cross_ Sections	dbd: Read_Cross_ Sections	Cross sections and derivatives

Table XIII B.1 (continued)

Unit No.	A, B, O	File name if not standard	Subdirectory: subroutines in which this file is written	Subdirectory: subroutines in which this file is read	Content
52					
53	B		npv: Compar, Set_Dminth		Energy, data, theory for code-comparison studies
54	B		xct: Write_Cross_ Sections	dbd: Read_Cross_ Sections	Cross sections and derivatives
55	A	SAMMY. CRS	grp: Rewrite_3		Averaged cross sections in ENDF format
55	A	SAMMY. N33	grp: Rewrite_33		ENDF File 33 (covariance) for averaged cross sections
55	A	SAMMY. NDF, SAMMY. N32, SAMMY. FL3	ndf: Rewrite_Ndf and others lru: Write_Cmpc_ Cov_2		ENDF files
56	A	SAMMY. NDX, SAMMY. N3X, SAMMY. FLX	ndf: Rewrite_Ndf and others lru: Write_Cmpc_ Cov_2		Annotated ENDF files
57	A		grp: File 33	grp: Rewrite_33, Rewrite_3	Intermediate ENDF files
57, 58	A		lru: several ndf: several npv: Make_File_3		Intermediate ENDF files
59					
60	B	SAMMY. 001	mas: Sammas_0	odf: odfio	

Table XIII B.1 (continued)

Unit No.	A, B, O	File name if not standard	Subdirectory: subroutines in which this file is written	Subdirectory: subroutines in which this file is read	Content
60	A		mas: Writ16x, Writ16	acs: Make_File_3_Urr clm: Readclm_0 npv: Make_File_3 ntg: Rdntgq_0	Name of special-purpose input files
61	A		mxw: Mxwell		Maxwellian-averaged capture cross sections in legible format
62	B		fin: Gnalvr	fin: several old: many	Binary covariance matrix for P-parameters
63	A	DCV file		dat: Qdatcv	Explicit data covariance matrix
64	B	SAMMY.COV	fin: Wrcov		Output binary covariance matrix for P-parameters
65					
66	A	fort.66	ssm: Ssssds		Debug printout of corrections to capture yield
67-69					
70	A	SAMMY.IO	end: Outpar		Like SAMMY.LPT (unit 21), except contains only input and output

Table XIII B.1 (continued)

Unit No.	A, B, O	File name if not standard	Subdirectory: subroutines in which this file is written	Subdirectory: subroutines in which this file is read	Content
71	A	SAMMY. PDS	new: Opnpds int: Pdwrit		Partial derivatives, for use in generating parameter covariance matrix
72	O or B	SAMMY. ODF	odf: several int: Thodf fin: Vodf	int: Thodf fin: Vodf	ODF file containing broadened cross sections, from which plots can be made
73	O or B	SAMMXW. ODF	grp: Mxwodf		ODF file containing stellar-averaged cross sections
77	A	SAMMY. CCV	old:Covnd3		Covariance matrix in ENDF compact format (LCOMP = 2)

XIII.C. DIVISION OF THE PROGRAM INTO AUTONOMOUS SEGMENTS

Prior to version M5 of SAMMY (in the year 2000), the code SAMMY was actually a system of ~50 semi-autonomous codes that executed sequentially and that communicated with each other via I/O from/to temporary files. This structure was originally necessary when computer memory was small and virtual memory nonexistent, and it also had the great virtue of permitting the author to debug each segment independently of the others.

With the advent of modern computers, this independent nature of the segments became obsolete and has therefore been eliminated. The various pieces have been assembled into one code. Many (but not yet all) of the read and write operations have also been eliminated. Users will notice two immediate benefits from this modernization of the code:.

(1) Porting SAMMY to a new platform is considerably easier than in the past. Subroutine execv, the C-language (or system) routine which permitted one FORTRAN routine to initiate execution of another, was a major source of difficulty in porting the program; execv is no longer used. Also, the location (path name) of the executable files must no longer be specified within the code prior to compilation.

(2) Execution time is shortened. The author has noted improvement by as much as 70% on the test cases, though more modest gains are likely on routine runs.

The basic structure of the code has not changed, however: SAMMY still consists of semi-independent segments that are now called sequentially by a main routine. There are approximately fifty segments (or modules), not all of which are used for every SAMMY run. Table XIII C.1 describes the functions of each segment and indicates the calling sequence. The order of the segments in the table is alphabetical.

A flow chart (Figure XIII C.1) shows the order in which the most commonly used modules are invoked. The path shown across the top of the table is used for unresolved resonance region runs, and the downward path is for resolved resonance runs. Dotted boxes on the flow chart indicate modules that may be omitted in some runs; multiple entries inside a box indicate that only one of those modules is used in a particular run.

By convention, the segment name is "sam*abc*" where *abc* is replaced by the three characters listed in the table. For most of the segments, relevant files are contained within a subdirectory of the same three-character name (in lowercase, on UNIX operating systems). (Most segments also make use of subroutines in files stored in other subdirectories.) The name and location conventions are not, however, rigidly followed. Some subdirectories store files used in many segments but do not themselves constitute a segment. Other subdirectories hold coding for several segments.

In addition to the segments that operate within a SAMMY run, a number of auxiliary programs are available to be used in conjunction with SAMMY. These programs are described in Section X; most are also included in Table XIII C.1.

Table XIII C .1. Segments of the code SAMMY

Segment; Site	Alter-native	Primary functions	Control passes to which segment?	Control comes from which segment?
ACS VIII		Calculate cross sections, etc., for unresolved resonance region	MPW	FFF, FIT
AMR X.C		Reorganize covariance file when changing data-reduction parameters	(Stand-alone code SAMAMR)	
AMX X.D		Reorganize final covariance file to modify a single non-relevant parameter	(Stand-alone code SAMAMX)	
ANF X.A		Interchange energy and angle in ODF file for plotting purposes	(Stand-alone code ANGODF)	
ANG II.B.1.b		Generate angular distribution	INT, ORR, RPI, or RSL	INT, DBD, DOP, FGM, or XCT
AVG V.C	GRP	Generate "multigroup cross sections" (averages of theoretical and experimental cross sections)	DAT or END	SQU
BIN	PLT	(Renamed to PLT because BIN is a reserved name on some systems)		
BLK		(Subdirectory stores common blocks)		
CCM		Generate covariance matrix for point-wise cross sections	(quit)	SQU
CLM III.B.4	FGM, DOP, DBD	Crystal-lattice model of Doppler broadening	ANG, INT, ORR, RPI, RSL, or SSM	CRO, INT, MLB, or XCT
CLQ V.E	CRO, MLB, XCT	Generate pseudo cross sections for use in testing Doppler- and resolution-broadening techniques	DBD, DOP, FGM, INT, MXW, NTG, ORR, RPI, RSL, or SQU	THE
COU	XXX	Subdirectory contains routines used to generate Coulomb penetrabilities, shift factors, and hard-sphere phase shifts		

Table XIII C .1 (continued)

Segment; Site	Alter-native	Primary functions	Control passes to which segment?	Control comes from which segment?
CONVRT X.B		Main program for converting from REFIT format to SAMMY or v.v. Stored in subdirectory /ref/	INP, refsam	
CPR X.E		Read binary file SAM53.DAT (which was generated by samnpv or samipq) and create plot file	(Stand-alone program SAMCPR)	
CRO II.A	MLB, XCT	Generate theoretical cross sections using Reich-Moore approximation to multilevel R-matrix theory (obsolete)	DBD, DOP, FGM, INT, MXW, NTG, ORR, RPI, RSL, or SQU	THE
DAT		Read the DATa file; generate the auxiliary energy grid used for broadening	IDC, REF, or THE	AVG, FIN, NEW, or OLD
DBD III.B.3	DOP, FGM, CLM	Doppler broaden the theoretical cross section using the high-energy Gaussian approximation	ANG, DEX, INT, ORR, RPI, RSL, SSM, or UDR	CLQ, CRO, INT, MLB, or XCT
DEX III.C.4	ORR, RPI, RSL, UDR	Resolution broaden the cross sections using square function in energy	INT, ORR, RPI, or UDR	ANG, CLM, CLQ, CRO, DBD, DOP, FGM, RSL, or SSM
DIS X.F		Calculate statistical properties	(Stand-alone program SAMDIS)	
DOP III.B.2	DBD, FGM, CLM	Doppler broaden theoretical cross section using Leal-Hwang method	ANG, DEX, INT, ORR, RPI, RSL, SSM, or UDR	CLQ, CRO, INT, MLB, or XCT
END		Reorganize files for another pass, or delete temporary files at end of run. Subdirectory also contains files with output subroutines	INP or quit	AVG, FIN, GRP, MAS, MXW, NDF, ODF, or REC, RST, YWY

Table XIII C .1 (continued)

Segment; Site	Alter-native	Primary functions	Control passes to which segment?	Control comes from which segment?
FDC VI.C.3.c		Update data file with implicit data covariance information	(quit)	INP
FFF VIII		Read input for analysis of unresolved resonance region	ACS	MAS
FGM III.B.1	CLM, DBD, DOP	Doppler-broaden via the free-gas model	ANG, DEX, INT, NTG, ORR, RPI, RSL, SQU, SSM, or UDR	CLQ, CRO, MLB, or XCT
FIN		Convert results from *u*-parameters to physical parameters; print results	DAT, END, or THE	IPQ, MPW, or NPV
FIT VIII		Print results for unresolved resonance region	ACS	MPW
FNC		(Subdirectory contains coding for frequently used mathematical functions)		
FTZ X.G		Modify data by adjusting t_zero and L_zero	(Stand-alone code SAMFTZ)	
GRP V.C.2 V.C.3	AVG	Generate multigroup cross sections using Bondarenko narrow-resonance weighting scheme, also for unweighted average	END	SQU
IDC VI.C.3. c		Read and sort implicit data covariance information	REF, RST, THE	DAT
INP		Read INPut file for control commands and for information about the data set; read through PARameter file to set array sizes	FDC, PAR	END or MAS

Table XIII C .1 (continued)

Segment; Site	Alter-native	Primary functions	Control passes to which segment?	Control comes from which segment?
INT		Print theoretical cross sections and/or partial derivatives; put values into parts of plot file	ANG, CLM, DBD, DOP, FGM, MXW, NPV, NTG, ORR, RPI, RSL, SQU, SSM, WYW, or YWY	ANG, CRO, CLM, CLQ, DBD, DOP, FGM, MLB, ORR, RPI, RSL, SSM, or XCT
IPQ IV.B.2	MPW, NPV	Solve I+Q form of Bayes' equations	FIN	SQU
LRU VIII		Write ENDF File2 for Unresolved Resonance Region	(end)	FFF
MAS		Read input commands and file names; read portions of INPut and other files; organize the manner in which SAMMY runs	END, FFF, INP, or ODF	SAMMY
MLB II.B.3	CLQ, CRO, XCT	Generate theoretical cross sections using the single or multilevel Breit-Wigner theory	CLM, DBD, DEX, DOP, FGM, INT, MXW, NTG, ORR, RPI, RSL, SQU, or UDR	THE
MPW IV.B.3	IPQ, NPV	Solve Bayes' equations via the M+W method	FIN, FIT	ACS, SQU, WYW
MXW V.D		Generate stellar (Maxwellian) average capture cross section	END	CLQ, CRO, MLB, REC, SQU, XCT
NDF VI.F.2		Write resolved resonance parameters into ENDF-6 file 2 format	END	NEW or OLD
NEW	OLD	Generate the initial covariance matrix for the parameters	DAT, NDF, REC, REF, WYW	PAR
NPV IV.B.1	IPQ, MPW	Solve N+V form of Bayes' equations	FIN	INT, NTG, or SQU

Table XIII C .1 (continued)

Segment; Site	Alter-native	Primary functions	Control passes to which segment?	Control comes from which segment?
NTG V.B		Calculate integral quantities	NPV	CRO, FGM, MLB, REC, SQU, XCT
ODF VII.C		Initialize the plot (ODF) output file by writing energies into section 1, data into sections 2 and 6, and uncertainties into sections 3 and 7. See Section VII.C of this document for a description of ODF "sections."	END	MAS
OLD VII.B	NEW	Read the initial parameter covariance matrix from binary file generated by an earlier SAMMY run	DAT, NDF, or REC, WYW	PAR
ORR III.C.2	DEX, RPI, RSL, UDR	Resolution broaden the theoretical cross section using Oak Ridge resolution function	INT	ANG, CLM, CRO, DBD, DEX, DOP, FGM, INT, MLB, RSL, SSM, or XCT
ORT X.H		Study ORR resolution function	(Stand-alone code SAMORT)	
PAR VI.B		Read parameters from PARameter file	NEW or OLD	INP
PLT X.I		Convert from binary plot file to another option	(Stand-alone code SAMPLT)	
QUA X.J		Generate spin group information for given particle-pair quantum numbers and orbital angular momenta	(Stand-alone program SAMQUA)	
REC V.A		Reconstruct point-wise cross section from resonance parameters	END, MXW, or NTG	NEW or OLD

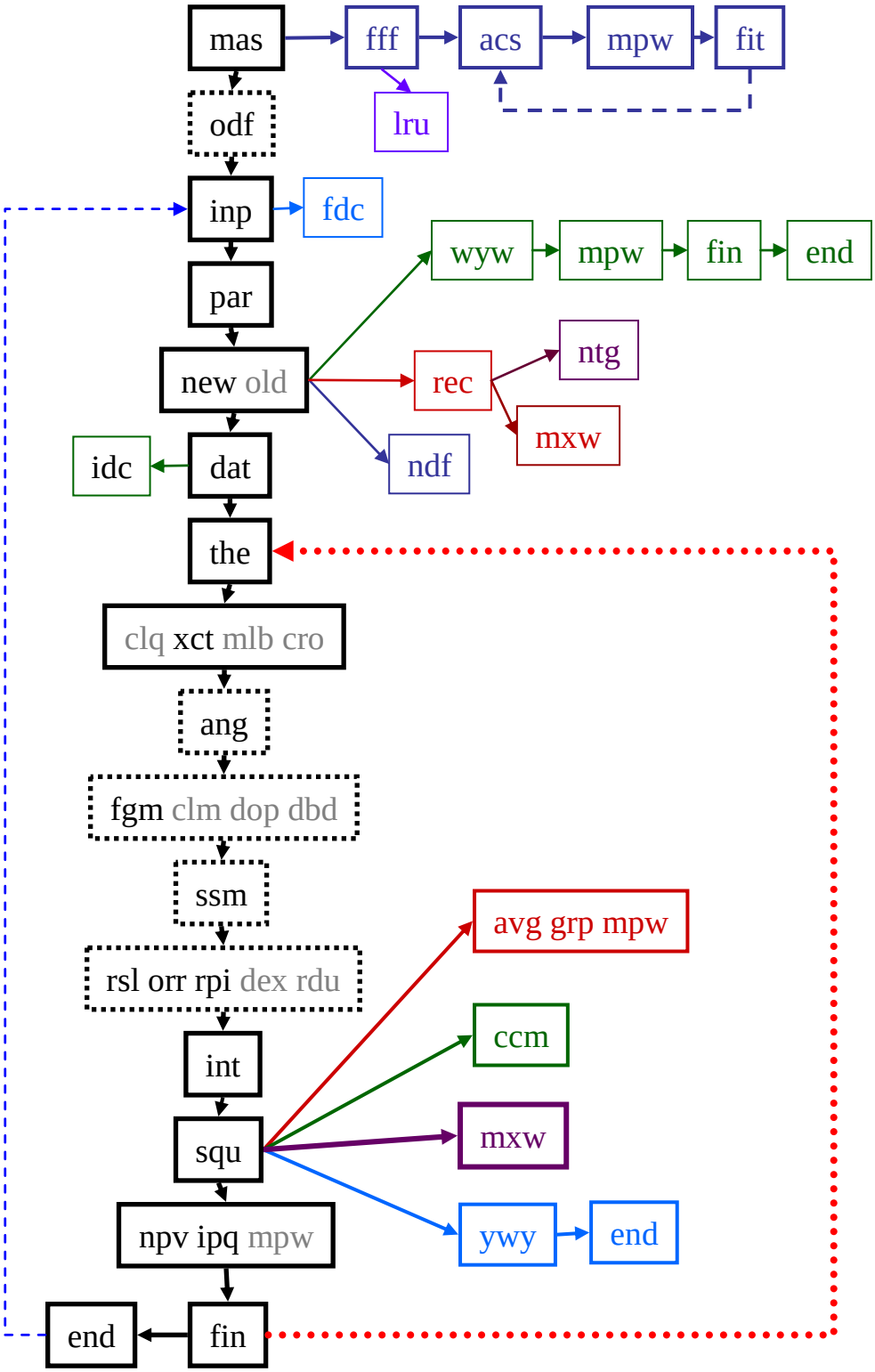
Table XIII C .1 (continued)

Segment; Site	Alter-native	Primary functions	Control passes to which segment?	Control comes from which segment?
REF X.B		Convert resonance parameters from SAMMY to REFIT format; a part of program CONVRT, not program SAMMY		DAT, IDC
REFSAM X.B		Convert resonance parameters from REFIT to SAMMY format; a part of program convrt; files in subdirectory /ref/		CONVRT
RML X.Q		Calculate R-matrix cross sections and derivatives	(Stand-alone code SAMRML)	
RPI III.C.3	DEX,ORR, RSL,UDR	Resolution-broaden the theoretical cross section using the RPI resolution function	INT	ANG, CLM, CLQ, CRO, DBD, DOP, FGM, INT, MLB, SSM, or XCT
RPT X.K		Study RPI resolution function	(Stand-alone code SAMRPT)	
RSL III.C.1	DEX,ORR, RPI, UDR	Resolution-broaden theoretical cross section using the original method	INT	ANG, CLM, CLQ, CRO, DBD, DOP, FGM, INT, MLB, SSM, or XCT
RST X.L		Study RSL resolution function	(Stand-alone code SAMRST)	
SAMMY		Begin, get organized	MAS	
SMC III.D, X.M		Generate multiple-scattering correction to capture or fission yields via Monte Carlo method	(Stand-alone program SAMSMC)	
SQU		Expand the triangular storage of the covariance matrix to full square form	AVG, IPQ, MPW, MXW, NTG, or NPV	CLM, CLQ, CRO, INT, MLB, or XCT

Table XIII C .1 (continued)

Segment; Site	Alter-native	Primary functions	Control passes to which segment?	Control comes from which segment?
SSM III.D		Perform self-shielding and multiple-scattering calculation for capture yields	INT, ORR, RPI, or RSL	CLM, CLQ, DBD, DOP, FGM, INT, or XCT
STA X.N		Generate staircase plots	(Stand-alone code SAMSTA)	
THE		Perform bookkeeping related to cross-section calculations	CLQ, CRO, MLB, or XCT	DAT, FIN, IDC
THN X.O		Thin dense data	(Stand-alone code SAMTHN)	
UDR III.C.5	DEX, ORR, RPI, RSL	User-defined numerical resolution function	INT	ANG, CLM, CLQ, CRO, DBD, DOP, FGM, INT, MLB, SSM, or XCT
WYW IV.B.3		Read Y_i and W_i and add, for use in segment MPW	MPW	NEW, OLD
XCT II.B.1	CLQ, CRO, MLB	Generate theoretical cross sections using accurate formulation of Reich-Moore	ANG, DBD, DOP, FGM, INT, MXW, NTG, ORR, RPI, RSL, SQU, or SSM	THE
XXX II.A	COU	Generate penetrabilities, shift factors, and hard-sphere phase shifts for non-Coulomb interactions (subroutines only, not complete segment)		
YWY IV.B.3		Generate Y_i and W_i, for use in segment MPW	END	INT, NTG, SQU

Figure XIII C .1. Flow chart for commonly used SAMMY modules



XIII.D. COMPUTER-SPECIFIC FEATURES

The current version of SAMMY is compatible with most UNIX operating systems, with LINUX, and with Compaq Visual Fortran under Windows. Details about specific machines on which the code has been tested are available from the Radiation Safety Information Computational Center [RSICC].

Input/Output statements are the most likely sources of incompatibility from one computer platform to another. To mitigate problems associated with portability, most of SAMMY's file-OPEN statements are localized in one file, end/msamxx.f, which can be modified as necessary to suit the particular platform.

SAMMY is designed to provide CPU timing information as it passes through the various segments during a run. However, because the routine which generates this information is computer-dependent, function jstime in file end/jstime.c is not guaranteed to provide correct results on all platforms. (Function jstime is the only the C-language routine used in SAMMY.)

The output file SAMMY.LPT is written (added to) in numerous subroutines in nearly every segment of the code. Many of the WRITE statements for SAMMY.LPT (unit number 21) and for SAMMY.IO (unit 70) occur in subroutines whose names begin with the characters "OUT". The output file SAMMY.IO contains only Input and Output values of the parameters. Originally these files were designed to be sent to the line-printer for printing and examination by the analyst. Over the years, as work habits have evolved to include less hard-copy printing and more on-line viewing, the format for these files has also evolved to become compatible with an eighty-character screen. Portability should not be a problem with these files.

See the next section (Section XIII.E) for a discussion of plot files, for which portability may be a problem.

XIII.E. ORELA DATA FORMAT

Plotting of results in SAMMY may be accomplished by first generating a "plot file," named SAMMY.ODF, and using program FORODF [JC78] to produce plots. The code FORODF has both advantages and disadvantages for the user; advantages include data-manipulation capabilities not readily available in other plotting packages. The major disadvantages are the age, the lack of routine maintenance, the use of single precision, and the difficulties in porting this program. Because of these disadvantages, FORODF is no longer distributed along with the SAMMY code.

For information on alternative plotting packages, see Sections VII.C and X.I.

Calls to three different ODF routines occur in the coding for SAMMY. Names and arguments for these routines are

```
Odfio (Iu,File,Ifb,New,Ins,Incmx,Mode,Ndstrt,Iener,Irun)
Outodf(Iu,Ifb,Ins,Isn,Mode,Ndstrt,Isc,Inc,Array(J),N)
Inodf (Iu,Ifb,Ins,Isn,Mode,Ndstrt,Isc,Inc,Array(J),N)
```

The first subroutine (ODFIO) is used to open or create the plot file; the second (OUTODF), to write INC elements of ARRAY into section number ISN of the file; and the last (INODF), to read from the file. Access to the plot file is random rather than sequential.

Meanings for the arguments of these subroutines are given in Table XIII E.1. Note that many of the arguments are irrelevant to SAMMY, either because they are unused or because only one value is used. These are marked as "irrelevant" in the table.

Table XIII E.1. Arguments for ODF subroutines

Argument name	Included in which routine	Meaning of argument
IU	All three: ODFIO, OUTODF, and INODF	FORTRAN unit number
FILE	ODFIO	File name for plot file
IFB	All three	Irrelevant to SAMMY
NEW	ODFIO	Irrelevant
INS	All	Number of sections in the file (see Table VII C.1)
ISN	OUTODF, INODF	Which section is being written or read now
INCMAX	ODFIO	Total number of data points for this plot file
MODE	All	Irrelevant
NDSTRT	All	Irrelevant (equal to zero)
IENER	ODFIO	Irrelevant
IRUN	ODFIO	Irrelevant
ISC	OUTODF, INODF	This “write” or “read” begins with the ISCth data point
INC	OUTODF, INODF	This “write” or “read” includes a total of INC data points
ARRAY(j)	OUTODF, INODF	This subroutine will write from or read into the array elements ARRAY(j) through ARRAY(j+INC-1)
N	OUTODF, INODF	Irrelevant

XIII.F. CONFIGURATION AND DISTRIBUTION SYSTEM

In 2005, ORNL researcher Dorothea Wiarda created a modern configuration and distribution system for SAMMY. This system makes it significantly easier for a user to install SAMMY on another computer.

SAMMY is distributed as a set of four *.gz files. The primary file, sammy-7.0.0.tar.gz, contains the FORTRAN plus installation commands. To unpack this file, type the command

```
gunzip -c sammy-7.0.0.tar.gz|tar xvf -
```

This command will create a subdirectory named sammy-7.0.0/, which contains a number of command and comment files, plus three subdirectories doc/, obj/, and src/. Subdirectory doc/ contains this document (the SAMMY users' manual) in pdf format. Subdirectory src/ contains 68 subdirectories, each of which hold several FORTRAN files. Subdirectory obj/ contains only two files initially but after compilation holds the object files (compiled version of the FORTRAN files).

Before creating the SAMMY executables, decide where you want to store them; you must have write privileges for that directory. To create the executables, type the following commands (substituting, of course, your chosen location for the directory name):

```
cd sammy-7.0.0
./configure --bindir=/xxx/sammydir --with-array=32500000
make
```

In this example, we have arbitrarily chosen "/xxx/sammydir" to represent the directory name. The absolute path name must be used. The number 32500000 represents one-half of the array size and may need to be modified (increased* or decreased) for your particular installation; see Section XIII.A for more information. If no change is needed in this value, the second line above can be shortened by dropping "`--with-array=32500000`".

The "make" command will compile the FORTRAN files and place the results as *.o into the `sammy-7.0.0/obj` directory. It will also create executable files, placing them in the same directory. After this step is successfully completed, type the command

```
make install
```

which copies the executables to subdirectory `/xxx/sammydir`. The executable files are as follows:

angodf	sam012	samcpr	sammy	samplx	samrpt	samsta
convrt	samamr	samdis	samort	samqua	samsmc	samthn
dopushx	samamx	samftz	samplt	samrml	samsmx	suggel

* The maximum possible value for this number is 2^{31}-1 = 2147483647 on a 32-bit machine. It is recommended to use smaller values than these unless absolutely necessary. If the number is too big for your compiler, compilation may fail. Alternatively, installation may appear to be complete, but the program will not run. In either case, try a smaller value.

If errors occur during the “make” stage, you will want to first verify that you have properly completed all earlier commands (gunzip …, cd …, and ./configure…). If it becomes necessary to contact the author for assistance, you should provide the following information: (1) the config.log file, created during the “configure” step, and (2) the fatal error messages from the “make” command. The latter may be retrieved by repeating the “make” command and sending a screen dump (including system error messages) to a separate file. (On some systems, the command “make >& makelog” will accomplish this task, sending the screen dump to a file named “makelog”.)

In directory sammy-7.0.0 is a file named INSTALL. This file contains complete installation instructions; a portion of this file is printed as Table XIII F.1 below.

Three other *.gz files are included in the SAMMY package. The file `samexm-7.0.0.tar.gz` contains the tutorial exercises, `samtry-7.0.0.tar.gz` contains the test cases, and `samsim-7.0.0.tar.gz` contains the Monte Carlo simulations. To unpack these files, type the commands

```
gunzip -c samexm-7.0.0.tar.gz|tar xvf -
gunzip -c samtry-7.0.0.tar.gz|tar xvf -
gunzip -c samsim-7.0.0.tar.gz|tar xvf -
```

With the first of these commands, a subdirectory samexm-7.0.0/samexm will be created, which contains other subdirectories with the specific exercises. Similarly, samtry-7.0.0/samtry and samsim-7.0.0/samsim subdirectories are created for the test cases and simulations using the second and third commands. The reader is referred to Section XII for details on the use of the tutorial exercises, test cases, and simulations.

Table XIII F.1. Installation instructions for SAMMY, as given in the INSTALL file

```
##########################################################################
# Here is the super-short installation guide.  Be sure to change “somedir”
#    to your directory location.  For details or alternatives, read the
#    remainder of this file.  Additional information is available in
#    Section XIII.F of SAMMY users’ manual, found in sammy-7.0.0/doc.
##########################################################################
     gunzip -c samtry-7.0.0.tar.gz|tar xvf -
     gunzip -c samexm-7.0.0.tar.gz|tar xvf -
     gunzip -c samsim-7.0.0.tar.gz|tar xvf -
     gunzip -c sammy-7.0.0.tar.gz|tar xvf -
     cd sammy-7.0.0
     ./configure --bindir=/somedir/sammy/bin
     make
     make install
##########################################################################
```

Table XIII F.1 (continued)

```
===================
SYSTEM REQUIREMENTS
===================

  (1) tar  -- unix tape utility, needed to unpack the software and examples
  (2) gzip -- the gnu unzip utility (http://directory.fsf.org/gzip.html)
                 to unpack the software package
  (3) F77 compiler
  (4) C compiler – needed only for timing routines, if used
  (5) make – the unix make utility



=========
UNPACKING
=========

  The SAMMY code is distributed as four gzipped tar files --
       sammy-7.0.0.tar.gz contains the code;
       samtry-7.0.0.tar.gz contains the test cases;
       samexm-7.0.0.tar.gz contains the tutorial exercises;
       samsim-7.0.0.tar.gz contains the simulations.
  “7.0.0” is the version number.

  In your main directory, type one of the following sets of commands
     to unpack the file sammy-7.0.0.tar.gz:

     (1) tar xzf sammy-7.0.0.tar.gz
     (2) gunzip -c sammy-7.0.0.tar.gz|tar xvf -

  or (3) gunzip sammy-7.0.0.tar.gz (which must be followed by)
    (3a) tar xf sammy-7.0.0.tar

     This will create a subdirectory sammy-7.0.0 which contains the
     FORTRAN code plus command files.

  Similar commands can be used to unpack the other three files.
  Test cases will then be found in subdirectory samtry-7.0.0/samtry
                          tutorial exercises in samexm-7.0.0/samexm
                             and simulations in samsim-7.0.0/samsim



============
INSTALLATION
============

  If you have system privileges, you may now install executable files for
     sammy and the auxiliary programs into /usr/local/bin by typing the
     following commands:

     cd sammy-7.0.0
     ./configure
     make
     make install
```

Table XIII F.1 (continued)

```
=====================
A DIFFERENT DIRECTORY
=====================

  Alternatively, you may wish to install the executables into another
     directory, for example /somedir/sammy/bin.  To do this, first
     be certain you have write authority for the subdirectory.  Then
     execute the following commands, being sure to use the correct
     complete path name for the subdirectory:

     ./configure --bindir=/somedir/sammy/bin
     make
     make install

  These commands would install sammy and auxiliary-code executable files
     into /somedir/sammy/bin.


========================
CHANGING THE ARRAY SIZE
========================

  Dynamic dimensioning is achieved in SAMMY by assigning and de-assigning
     space in a large container array, designated as A(-N:N).  The default
     value for N is 32500000.  To use a different value, modify the
     configure line as shown here, substituting the appropriate value for
     your computer system:

     ./configure --with-array=100000000
or   ./configure --bindir=/somedir/sammy/bin --with-array=210000000



=======================
COMPILER OPTIONS, ETC.
=======================

  If you want to use a different FORTRAN compiler, for example f90,
  then set the environment variable F77=f90
     in bash: export F77=f90
     in csh:  setenv F77 f90
  and then do the above install sequence.

  If you want to set compiler flags, for example -Wall, then use
     in bash: export FFLAGS=-Wall
     in csh:  setenv FFLAGS -Wall
  and then do the above install sequence.


=====================
Other useful commands
=====================

     make clean      <- removes all generated object and source files
     make distclean  <- cleans the tree for a new invocation of configure
     make dist       <- creates a new *.gz file which includes any updates
                        that you may have made to the FORTRAN files
```

Table XIII F.1 (continued)

```
========================
PC (WINDOWS) EXECUTABLES
========================

  For those who wish to run SAMMY in a Windows environment on a pc,
  executable files for SAMMY and the auxiliary programs are provided in
  subdirectory sammy-7.0.0/Windows/ and can be copied from there to the pc.


======================
RUNNING THE TEST CASES
======================

  -------------
  Unix or Linux
  -------------

  The command file “zzauto” (found in samtry-7.0.0/samtry) can be used
  to run all of the test cases on a Unix or Linux system.  Command file
  “zzauto_short” runs a representative sample of thirteen test cases.
  Individual test cases can be run by using the command file “t” or
  “test???” in the subdirectory for that test case.  See Section XII.B
  of the SAMMY manual for details.

  -------
  Windows
  -------
  Command file “test.bat” in the subdirectory tr??? can be used to run
  the individual test case under Windows.


================
THE SAMMY MANUAL
================

  The SAMMY manual is found in subdirectory sammy-7.0.0/doc in pdf format.
  Two versions are given there.  SAMMY7.pdf is the version to use on screen.
  SAMM7_print.pdf is the version to use if you wish to print a double-sided
  listing of the manual; it contains extra blank pages as needed to make
  the pagination come out correctly.
```

REFERENCES

AB82 A. R. Barnett, *Comp. Phys. Comm.* **27**, 147 (1982); *Comp. Phys. Comm.* **21**, 297 (1981).

AB05 A. Borella, *Determination of the neutron resonance parameters for ^{206}Pb and of the thermal neuton capture cross section for ^{206}Pb and ^{209}Bi*, PhD Thesis, Universiteit Gent, 2004–2005.

AC05 A. D. Carlson, S. A. Badikov, Chen Z. P., E. Gai, G. M. Hale, F.-J. Hambsch, H. M. Hofmann, N. M. Larson, S. Y. Oh, V. G. Pronyaev, D. L. Smith, S. Tagesen, H. Vonach, "An International Evaluation of the Neutron Cross Section Standards," *12th International Symposium on Reactor Dosimetry*, May 8–13, 2005, Gatlinburg, TN.

AF71 A. Foderaro, *The Elements of Neutron Interaction Theory*, MIT Press, 1971.

AG65 A. Gilbert and A. G. W. Cameron, *Can. J. Phys.* **43**, 1446 (1965).

AG73 A. Gandini, *Nuclear Data and Integral Measurements Correlations for Fast Reactors*, Part I and II, Comitato Nazionale Energia Nucleare, Casaccia, Italy, 1973, RT/FI(73)5 and 22 (1973).

AL58 A. M. Lane and R. G. Thomas, *Rev. Mod. Phys.* **30**, 257 (1958).

AM94 A. Meister, *Calculations on lattice vibration effects in the Doppler broadening of the 0.18eV Cd neutron resonance cross section*, CE/R/VG/78/94 (January 1994).

BM96 B. E. Moretti, *Molybdenum Neutron Transmission Measurements and the Development of an Enhanced Resolution Neutron Target*, Ph.D. Thesis in Nuclear Engineering and Science, Rensselaer Polytechnic Institute, Troy, NY, August 1996.

CC83 C. Coceva, R. Simonini, and D. K. Olsen, "Calculaton of the ORELA Neutron Moderator Spectrum and Resolution Function," *Nucl. Inst. Meth.* **211**, 459 (1983).

CR58 C. W. Reich and M. S. Moore, *Phys. Rev.* **111**, 929 (1958).

CZ95 Chen Z. P., "Reduced R-Matrix Analysis for ^{17}O system," *Atomic Energy Science and Technology* **29** (4), 366-371 (1995).

DC04 D. Cullen, PREPRO 2004, IAEA-NDS-39**,** Rev. 12, Nov. 22, 2004. Also see http://www-nds.iaea.org/ndspub/endf/prepro/.

DH53 D. L. Hill and J. A. Wheeler, *Phys. Rev.* **89**, 1102 (1953).

DL83 D. C. Larson, N. M. Larson, J. A. Harvey, N. W. Hill, and C. H. Johnson, *Application of New Techniques to ORELA Neutron Transmission Measurements and their Uncertainty Analysis: the Case of Natural Nickel from 2 keV to 20 MeV*, ORNL/TM-8203, ENDF-333, Oak Ridge National Laboratory, October 1983.

DL84 D. C. Larson, N. M. Larson, and J. A. Harvey, *ORELA Flight Path 1: Determinations of Its Effective Length vs Energy, Experimental Energies, and Energy Resolution Function and Their Uncertainties*, ORNL/TM-8880, Oak Ridge National Laboratory, June 1984.

DN99 D. G. Naberejnev, "Etude de L'Influence des Liaisons Chimiques sur L'Absorption et la Diffusion de Neutrons aux Energies de Resonance," Ph.D. Thesis, ISSN 0429-3460, CEA-N-2840 (Fevrier 1999).

DN99a D. G. Naberejnev, C. Mounier, and R. Sanchez, "The Influence of Crystalline Binding on Resonant Absorption and Reaction Rates," *Nucl. Sci. Eng.* **131**, 222–220 (1999).

ENDF-102 *ENDF-102, Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF-6*, written by the Members of the Cross Section Evaluation Working Group, ed. V. McLane, C. L. Dunford, P. F. Rose, BNL-NCS-4495, Brookhaven National Laboratory, April 2001. Updated BNL-NCS-4495/04-Rev, ed. M. Herman, June 2005.

ENDF99 *Summary of the 48th Cross Section Evaluation Working Group Meeting*, Brookhaven National Laboratory, November 1999, Attachment 3–5.

EV58 E. Vogt, *Phys. Rev.* **112**, 203 (1958).

EXFOR Experimental Nuclear Reaction Data Files at Brookhaven National Laboratory (EXFOR/CSISRS), http://www.nndc.bnl.gov/exfor3/exfor00.htm.

FF80 F. H. Fröhner, *Applied Neutron Resonance Theory*, reprinted from *Nuclear Theory for Applications*, p. 59 ff., International Centre for Theoretical Physics, Trieste (1980). Available as KFK 2669 (1978). See also "Applied Theory of Resolved and Unresolved Resonances," *Applied Nuclear Theory and Nuclear Model Calculations for Nuclear Technology Applications*, M. K. Mehta and J. J. Schmidt, eds., World Scientific, Singapore, 1989, p. 170.

FF83 F. H. Fröhner, B. Goel, and U. Fischer, "Calculation of Average on Capture Cross Sections for Actinides — Level-Statistical vs Global Approach," *Proc. Mtg. Fast Neutron Capture Cross Sections*, Argonne, Illinois, April 20–23, 1982, ANL-83-4, p. 116, Argonne National Laboratory (1983).

FF89 F. H. Fröhner, "Evaluation of the Unresolved Resonance Range of ^{238}U," *Nucl. Sci. Eng.* **103**, 119–128 (1989).

FF99 F. H. Fröhner, Kernforschungszentrum Karlsruhe, Germany, private communication, 1999.

FF00 F. H. Fröhner, *Evaluation and Analysis of Nuclear Resonance Data*, JEFF Report 18, NEA/OECD (2000).

FF01 F. H. Fröhner and O. Bouland, "Treatment of External Levels in Neutron Resonance Fitting: Application to the Nonfissile Nuclide 52Cr," *Nucl. Sci. Eng.* **137**, 70–88 (2001).

FF02 F. H. Fröhner, lecture notes on R-Matrix theory, presented at the SAMMY workshop of February 18–22, 2002, at the NEA Headquarters in Paris, France (2002).

FG98 F. Gunsing, CEA Saclay, France, private communication, 1998.

FG05 F. Gunsing, CEA Saclay, France, private communication, 2005.

FP84 F. G. Perey, Oak Ridge National Laboratory, private communication, 1984.

FP89 F. G. Perey, Oak Ridge National Laboratory, private communication, 1989.

FP89a F. G. Perey, *RFUNC — A Code to Analyze Differential Elastic-Scattering Data*, ORNL/TM-11112, Oak Ridge National Laboratory, March 1989.

FP92 F. G. Perey, Oak Ridge National Laboratory, private communication, 1992.

GA74 G. F. Auchampaugh, *MULTI, A FORTRAN Code for Least-Squares Shape Fitting of Neutron Cross-Section Data Using the Reich-Moore Multilevel Formalism*, LA-5473-MS, Los Alamos Scientific Laboratory, l974.

GB36 G. Breit and E. Wigner, "Capture of Slow Neutrons," *Phys. Rev.* **49**, 519 (1936).

GC04 G. Chiba, *ERRORJ–Covariance Processing Code System for JENDL, Version 2*, JNC TN9520 2003-008; also G. Chiba and M. Ishikawa, *Revision and Application of Covariance Data Processing Code, ERRORJ*, ND2004, Sept. 26–Oct. 1, 2004, Santa Fe, New Mexico.

GD78 G. deSaussure, D. K. Olsen, and R. B. Perez, *SIOB: A FORTRAN Code for Least-Squares Shape Fitting Several Neutron Transmission Measurements Using the Breit-Wigner Multilevel Formula*, ORNL/TM-6286, ENDF-261, Oak Ridge National Laboratory, 1978.

GD80 G. deSaussure and F. G. Perey, Oak Ridge National Laboratory, private communication, 1980.

GH75 G. M. Hale, D. C. Dodder, and K. Witte, Los Alamos National Laboratory, Los Alamos, New Mexico, USA, private communication, 1975.

GH02 G. M. Hale, Los Alamos National Laboratory, Los Alamos, New Mexico, USA, private communication, 2002.

HD90 H. Derrien, G. de Saussure, and R. B. Perez, "R Matrix Analysis of the ^{239}Pu Neutron Cross Sections in the Energy Range Up to 1000 eV," *Nucl. Sci. Eng.* **106**, 434–51 (1990).

HD97 H. Derrien, N. M. Larson, and L. C. Leal, *Covariance Matrices for Use in Criticality Safety Predictability Studies*, ORNL/TM-13492, Oak Ridge National Laboratory, September 1997.

HD00 H. Derrien, J. A. Harvey, N. M. Larson, L. C. Leal, and R.Q. Wright, *Neutron Total Cross Sections of ^{235}U from Transmission Measurements in the Energy Range 2 keV to 300 keV and Statistical Model Analysis of the Data*, ORNL/TM-2000/129, May 2000.

HD00a H. Derrien, Oak Ridge National Laboratory, private communication, 2000.

HD02 H. Derrien, L. C. Leal, K. H. Guber, T. Valentine, N. M. Larson, and T. Rauscher, *Evaluation of Silicon Neutron Resonance Parameters in the Energy Range Thermal to 1800 keV*, ORNL/TM-2001/271, August 2002.

HD03 H. Derrien, Oak Ridge National Laboratory, private communication, 2003.

HJ61 H. Jeffreys, *Theory of Probability*, Third Edition, Oxford University Press, London, 1961.

IB64 I. I. Bondarenko, ed., *Group Constants for Nuclear Reactor Calculations*, Consultant Bureau, New York, 1964.

INDC02 *Summary Report of the First Research Co-ordination Meeting on Improvement of the Standard Cross Sections for Light Elements*, 23–27 Sept. 2002, IAEA Nuclear Data Section, Vienna, Austria, ed. A. D. Carlson, G. M. Hale and V. G. Pronyaev, INDC(NDS)-438, January 2003.

INDC03 *Summary Report of the Second Research Co-ordination Meeting on Improvement of the Standard Cross Sections for Light Elements*, 13–17 Oct. 2003, IAEA Nuclear Data Section, Vienna, Austria, ed. A. D. Carlson, G.M. Hale and V.G. Pronyaev, INDC(NDS)-438, March 2004.

INDC04 *Summary Report of the Third Research Co-ordination Meeting on Improvement of the Standard Cross Sections for Light Elements*, 18–22 Oct., 2004, IAEA Nuclear Data Section, Vienna, Austria, ed. A. D. Carlson, G. M. Hale and V. G. Pronyaev, INDC(NDS)-453, November 2004.

JB52 J. M. Blatt and L. C. Biedenharn, "The Angular Distribution of Scattering and Reaction Cross Sections," *Rev. Mod. Phy.* **24**, 258 (1952).

JC78 J. G. Craven, *OPRODF, A DECsystem-10 Data Manipulation Program for ORELA Data Formatted Files*, ORNL/CSD/TM-45, Oak Ridge National Laboratory, May 1978.

JD79 J. J. Dongarra, C. B. Moler, J. R. Bunch, G. W. Stewart, *LINPACK User's Guide*, SIAM (1979).

JL58 J. E. Lynn, *The Theory of Neutron Resonance Reactions*, Clarendon Press, Oxford (1958).

JM80 J. H. Marable, C. R. Weisbin, and G. deSaussure, "Combination of Differential and Integral Data" in *Sensitivity and Uncertainty Analysis of Reactor Performance Parameters, Adv. Nucl. Sci. and Technology*, Plenum Press, New York, ed. Martin Becker, 1980.

KC53 K. M. Case, F. de Hoffman, and G. Placzek, *Introduction to the Theory of Neutron Diffusion*, Los Alamos Scientific Laboratory, 1953.

KW84 K. Wisshak, F. Kappeler, G. Reffo, and F. Fabbri, "Neutron Capture in *s*-Wave Resonances of Iron-56, Nickel-58, and Nickel-60," *Nucl. Sci. Eng.* **86**, 168 (1984).

LL85 L. C. Leal, Oak Ridge National Laboratory, private communication, 1985.

LL95 L. C. Leal and N. M. Larson, *SAMDIST, A Computer Code for Calculating Statistical Distributions for R-Matrix Resonance Parameters*, ORNL/TM-13092, Oak Ridge National Laboratory, September 1995.

LL98 L. C. Leal, R. O. Sayer, N. M. Larson, and R. R. Spencer, "R-Matrix Evaluation of ^{16}O Neutron Cross Sections up to 6.3 MeV," ANS Winter Meeting, Washington, D.C., Nov. 16–20, 1998.

LL99 L. C. Leal, H. Derrien, N. M. Larson, and R. Q. Wright, "R-Matrix Analysis of ^{235}U Neutron Transmission and Cross Sections in the Energy Range 0 to 2.25 keV," *Nucl. Sci. Eng.* **131,** 230 (February 1999) also published as ORNL/TM-13516 (November 1997).

MD02 M. E. Dunn and N. M. Greene, "AMPX-2000: A Cross-Section Processing System for Generating Nuclear Data for Criticality Safety Applications," *Trans. Am. Nucl. Soc.* (2002).

MM64 M. D. Mintz and D. P. Jordan, *A 'Progressive' Interpolation Scheme for Hand and Digital Computer Analysis of Tabulated Data*, Report UCRL-7681, Lawrence Livermore Laboratory, 1964.

MM89 M. C. Moxon, *REFIT2: A Least Squares Fitting Program for Resonance Analysis of Neutron Transmission and Capture Data*, NEA-0914/02, July 1989.

NAG Numerical Algorithms Group (USA) Inc., Suite 220,1431 Opus Place, Downers Grove, IL 60515-1362, USA; http://www.techexpo.com/firms/numeralg.html. Modified versions of NAG subroutines from ~1980 are used in SAMMY.

NL80 N. M. Larson and F. G. Perey, *User's Guide for SAMMY: A Computer Model for Multilevel R-matrix Fits to Neutron Data Using Bayes' Equations*, ORNL/TM-7485, ENDF-297, Oak Ridge National Laboratory, November 1980.

NL82 N. M. Larson, *User's Guide for BAYES: A General-Purpose Computer Code for Fitting a Functional Form to Experimental Data*, ORNL/TM-8185, ENDF-323, Oak Ridge National Laboratory, August 1982.

NL84 N. M. Larson, *User's Guide for ALEX: Uncertainty Propagation from Raw Data to Final Results for ORELA Transmission Measurements*, ORNL/TM-8676, ENDF-332, Oak Ridge National Laboratory, February 1984.

NL92 N. M. Larson, "Cross Section Parameterization in the Resolved Resonance Region," invited paper presented October 12–16, 1992, at Brookhaven National Laboratory and published in *International Symposium on Nuclear Data Evaluation Methodology*, ed. Charles L. Dunford, pp. 285–294, 1993.

NL97 N. M. Larson, L. C. Leal, and H. Derrien, *Integral Data Analysis for Resonance Parameters Determination*, ORNL/TM-13495, Oak Ridge National Laboratory, September 1997. Also *Nucl. Sci. and Eng.* **131,** 254 (February 1999).

NL98 N. M. Larson, M. C. Moxon, L. C. Leal, and H. Derrien, *Doppler Broadening Revisited*, ORNL/TM-13525, Oak Ridge National Laboratory, 1998.

NL98a N. M. Larson, "Introduction to the Theory and Analysis of Resolved (and Unresolved) Neutron Resonances via SAMMY," in *Proceedings of the IAEA Workshop on "Nuclear Reaction Data and Nuclear Reactors: Physics, Design and Safety*, held at the International Centre for Theoretical Physics, Trieste, Italy, 23 February–27 March 1998, published by World Scientific, 1999. Also published as ORNL/M-6576, July 1998.

NL02 N. M. Larson and K. N. Volev, "Validation of Multiple-Scattering Corrections in the Analysis Code SAMMY," Paper A0203 of the *International Conference on the New Frontiers of Nuclear Technology: Reactor Physics, Safety and High- Performance Computing* (Physor 2002), October 2002 in Seoul, South Korea. Published on CD rom.

NL04a N. M. Larson,"Treatment of Data Uncertainties," *ND2004 (International Conference on Nuclear Data for Science and Technology)*, Sept. 26–Oct. 1, 2004.

NL04b N. M. Larson, "On the Efficient Treatment of Data Covariance Matrices," *71st Annual Meeting of the Southeastern Section of the APS*, Oak Ridge, TN, November 11–13, 2004.

NNDC The National Nuclear Data Center at Brookhaven National Laboratory, http://www.nndc.bnl.gov/.

OB97 O. Bouland, H. Derrien, N. M. Larson, and L. C. Leal, "R-Matrix Analysis of the ^{240}Pu neutron Cross Sections in the Thermal to 5700-eV Energy Range," *Nuclear Science and Engineering* **127,** 105–129 (1997). Also published as ORNL/TM-13450 (August 1997).

OB03 O. Bouland, R. Babut, and N. M. Larson, *SAMQUA – A Program for Generating All Possible Combinations of Quantum Numbers Leading to the Same Compound Nucleus State in the Framework of the R-Matrix Code SAMMY*, JEF-DOC 929 OECD/NEA Publications (2003) and ENDF-363 (October 2003).

OB04 O. H. Bouland, R. Babut, N. M. Larson, "SAMQUA - A Program for Generating All Possible Combinations of Quantum Numbers Leading to the Same Compound Nucleus State in the Framework of the R-Matrix Code SAMMY," *ND2004 (International Conference on Nuclear Data for Science and Technology*, Sept. 26–Oct. 1, 2004) page 414 *ff*.

PM80 P. A. Moldauer, *Nucl. Phys.* **A344**, 185 (1980).

PS06 P. Schillebeeckx, Institute for Reference Materials and Measurements, Geel, Belgium, private communication, 2006.

RH87 R. Hwang, *Nucl. Sci. Eng.* **96**, 192 (1987).

RM82 R. E. MacFarlane, D. W. Muir, and R. M. Boicourt, *The NJOY Nuclear Data Processing System, Volume II: The NJOY, RECONR, BROADR, HEATR, and THERMR Modules*, LA-9303-M, Vol. II (ENDF-324) (May 1982). Also R. E. MacFarlane, *Introducing NJOY 89*, LA-UR 89-2057, June 1989.

RM98 R. E. MacFarlane, Los Alamos National Laboratory, Los Alamos, New Mexico, private communication, 1998.

RP87 R. W. Peelle, Oak Ridge National Laboratory, private communication, 1987.

RS00 R. O. Sayer, L. C. Leal, N. M. Larson, R. R. Spencer, and R. Q. Wright, *R-Matrix Evaluation of ^{16}O Neutron Cross Sections up to 6.3 MeV*, ORNL/TM-2000/212, Oak Ridge National Laboratory, Oak Ridge, TN, August 2000.

RS03 R. O. Sayer, *Updated Users' Guide for RSAP—A Code for Display and Manipulation of Neutron Cross Section Data and SAMMY Fit Results*, ORNL/TM-2003/133, Oak Ridge National Laboratory, Oak Ridge, TN.

RS06 R. O. Sayer, K. H. Guber, L. C. Leal, N. M. Larson, and T. Rauscher, "R-Matrix Analysis of Cl neutron cross sections up to 1.2 MeV," *Phys. Rev.* C **73**, 044603 (2006).

RS06a R. O. Sayer and D. Wiarda, Oak Ridge National Laboratory, private communication, 2006.

RSICC Radiation Safety Information Computational Center (formerly the Radiation Shielding Information Center), Oak Ridge National Laboratory, Bldg 6025, MS-6362, P.O. Box 2008, Oak Ridge, TN 37831-6362. See also http://www-rsicc.ornl.gov/.

SC92 S. N. Cramer and F. G. Perey, "Time-Dependent Monte Carlo Calculations of the Oak Ridge Electron Linear Accelerator Target Neutron Spectrum," *Nucl. Sci. Eng.* **111**, 102–111 (1992).

SC94 S. Chiba and D. L. Smith, *Some Comments on Peelle's Pertinent Puzzle*," AERI-M 94-068, 1994.

SO01 S. Y. Oh and L. C. Leal, *SUGGEL: A Program Suggesting the Orbital Angular Momentum of a Neutron Resonance from the Magnitude of its Neutron Width*, ORNL/TM-2000/314, Oak Ridge National Laboratory, February 2001.

SM06 S. F. Mughabghab, *Atlas of Neutron Resonances*, 5th edition, published by Elsevier, Amsterdam, The Netherlands, 2006.

VP04 V. G Pronyaev (IAEA, Austria), S. A. Badikov (IPPE, Russia), Chen Zhenpeng (Tsinghua University, China), A. D. Carlson (NIST, USA), E.V. Gai (IPPE, Russia), G. M. Hale (LANL, USA), F.-J. Hambsch (IRMM, Belgium), H. M. Hofmann (ITP III, Erlangen-Nürnberg University, Germany), N. M. Larson (ORNL, USA), D. L. Smith (ANL, USA), Soo Youl Oh (KAERI, Republic of Korea), S. Tagesen (IIK, Wien University, Austria), H. Vonach (IIK, Wien University, Austria), "Status of the International Neutron Cross Section Standards File," *International Conference on Nuclear Data for Science and Technology*, Sept. 26–Oct. 1, 2004.

WV12 W. Voigt, *Sitz-Ber. Bayer. Akad. Wiss*. (1912), p. 603.

YD98 Y. Danon et al., "Neutron Total Cross Section Measurements and Resonance Parameter Analysis of Ho, Tm, and Er from 0.001 eV to 20 eV," *Nucl. Sci. Eng.* **128**, 61–69 (1998).

ZZ92 Z. Zhao and F. G. Perey, *The Covariance Matrix of Derived Quantities and Their Combination*, ORNL/TM-12106, Oak Ridge National Laboratory,1992.

APPENDIX A. VERSIONS OF THIS MANUAL

(This page is taken from the Introduction to the original document ORNL/TM-9179, published in 1984, with ~~strikeouts and~~ {inserts} to clarify topics that might otherwise cause confusion.)

In 1980 the multilevel multichannel R-matrix code SAMMY [NL80] was released for use in analysis of neutron data at the Oak Ridge Electron Linear Accelerator (ORELA). At its inception, SAMMY was a severely altered version of George Auchampaugh's multilevel R-matrix code MULTI [GA74], the fundamental difference being that SAMMY uses Bayes' method while MULTI uses a least-squares method to update parameter values. Since that time, significant modifications and improvements have been incorporated into SAMMY: (1) User-friendly options have been introduced to streamline common operations and to protect a run from common user errors. (2) The Reich-Moore formalism has been extended to include an optional logarithmic parameterization of the external R-matrix, for which any or all parameters may be varied. (3) The ability to vary sample thickness, effective temperature, matching radius, and/or resolution-broadening parameters has been incorporated. (4) To avoid loss of information (i.e., computer round-off errors) between runs, the "covariance file" now includes precise values for all variables. (5) Unused but correlated variables may be included in the analysis.

Because of these and earlier changes, the 1980 SAMMY manual is now hopelessly obsolete. This report is intended to be complete documentation for the current version of SAMMY. Its publication in ~~loose-leaf form~~ {pdf format} will permit updates to the manual to be made concurrently with updates to the code itself, thus eliminating most of the time lag between update and documentation.

Because Bayes' method is a new concept to many users, its derivation and implementation are described in some detail in Section ~~II~~ {IV} of this report. Though a similar discussion is included in both the earlier SAMMY report [NL80] and the BAYES report [NL82], it is repeated here for completeness sake.

The evaluation of theoretical cross sections is described in Section ~~III~~ {II}. Doppler- and resolution-broadening are discussed in Section ~~IV~~ {III}. ~~Special data types (such as transmission or combinations) are discussed in Section V.~~

Section VI describes the input to SAMMY, with tables detailing each file the user must create. A discussion of the output is given in Section VII.

In Section ~~VIII~~ {X.C} the auxiliary codes ~~SAMADD and SAMMIX are~~ {SAMAMR is} described: ~~these codes are~~ {this code is} to be used in conjunction with SAMMY when multiple experiments are analyzed sequentially.

~~Two examples of SAMMY runs are presented in Section IX; these runs are typical of runs required for analysis of transmission and fission data.~~

"Helpful hints for running SAMMY" are given in Section ~~X~~ {XI}. ~~It is hoped that this section can be considerably expanded in the future: ideas from users would be appreciated here.~~ {This section was completely rewritten for Revision 7.}

Section ~~XI~~ {XIII} gives a general description of the computer code, more for the benefit of someone wishing to convert SAMMY to another computer than for a physicist wishing to use SAMMY to perform data analyses.

~~A FORTRAN listing of the code is provided in the appendix in microfiche form. Input and output for several test cases are also given there.~~

Appendix A.1. MODIFICATIONS AND ADDITIONS IN REVISION 1

(This page is taken from the Introduction to Revision 1 of this manual, with ~~strikeouts and~~ {inserts} to clarify topics that might otherwise cause confusion.)

Changes documented in this revision are as follows:

1. An alternative matrix-manipulation method, the (I+Q) inversion scheme, has been devised (see Sect. ~~II~~ {IV}). Use of this scheme requires that the data covariance matrix be diagonal, and that the number of data points be much larger than the number of varied parameters. When these two requirements are met, the (I+Q) inversion scheme uses significantly less computer core than does the original method, the (N+V) inversion scheme.
2. Cross-section calculations and broadening operations are now performed in two separate stand-alone segments of the computer code, since they are in fact two distinct operations. Within the broadening segment, the various broadening procedures have been sufficiently disentangled that one can, e.g., Doppler-broaden but not resolution-broaden.
3. The multilevel Breit-Wigner approximation may be used to generate cross sections; see ~~Sect. III.C~~ {Section II.B.3}.
4. New input options are explained in the tables of Section VI. NOTE: No input has been changed; a user need not fear that his or her old INP or PAR tiles are obsolete.
5. All temporary files are now called SAM??.DAT with the question marks replaced by FORTRAN unit numbers. Thus if a run bombs or is aborted, all SAMMY files may be deleted with the single command "DEL SAM??.DAT" {or the equivalent command on modern computer systems}. ~~CAUTION: If you wish to discuss with the author why your job bombed, it would be best *not* to delete these files first.~~ See Sect. ~~X.B~~ {XI.B}.
6. It is now sometimes possible to analyze very large data sets, of a thousand or more points, in one shot. This is due to the invention of a sophisticated "bookkeeping" system to use temporary files rather than in-core storage for larger arrays. ~~To decide whether your particular case will fit into the PDP10, run the code SAMEST; i.e., type 'R SAMEST' interactively and answer the questions asked. Caveat: array sizes given are estimates only, not to be trusted absolutely.~~
7. The internal FORTRAN coding of SAMMY, version O, is considerably different from version P. (While users of the code will not notice these changes, anyone wishing to implement SAMMY on his or her own computer is warned to use one version or the other and not intermix them.) A consistent nomenclature for the several types of varied parameters has been developed. Subroutines have been subdivided so that each routine deals with a single well-defined operation. Attempts have been made to standardize FORTRAN usage, to minimize necessary changes when converting to another computer. Many of these changes were designed in preparation for future revisions, including (a) more correct treatment of resolution broadening, (b) inclusion of data parameters (such as normalization or background subtraction) as varied parameters, and (c) proper treatment of multiple isotopes.

Appendix A.2. MODIFICATIONS AND ADDITIONS IN REVISION 2

(This page is taken from the Introduction to Revision 2 of this manual, with ~~strikeouts and~~ {inserts} to clarify topics that might otherwise cause confusion.)

Version C of SAMMY, documented in this Revision, is currently operational on the VAX computer, on the FPS (Floating Point Systems, Inc.) AP (Array Processor) computer, and on the IBM computer. Version C incorporates all features of earlier versions of SAMMY, as documented in previous reports. Additional features of version C include:

1. Internal structural changes in the coding to accommodate VAX, FPS, and IBM computers (and hopefully to ease the transition to other computer systems).
2. Streamlining of portions of the coding to increase computation speed and decrease array storage.
3. Separation of broadening segments into logical components; e.g., Doppler broadening is now performed in a separate segment from resolution broadening.
4. A more careful choice of "auxiliary grid" for use in Doppler broadening. This new choice of grid alleviates many of the problems encountered when the experimental grid was not sufficiently dense; for such data, earlier versions of SAMMY did not include enough points in the auxiliary grid to correctly evaluate the integrals required for generating the Doppler-broadened cross section. For details, the reader is referred to ~~Section IV~~ {Section III.A}.
5. Additional user-defined options in choosing the auxiliary grid; that is, the user may inform SAMMY that the experimental grid is not dense and thus require introduction of extra points between each experimental point, or he may require even more points added near small resonances. For details, see ~~Section IV~~ {Section III} on broadening and Section VI.A for input.
6. An option to use an entirely different scheme for Doppler broadening, based on work by Luiz Leal and Richard Hwang. Details are given in Section ~~IV.D~~ {III.B.2}.
7. An option to generate averaged theoretical cross sections (or transmissions) using parameters determined from previous SAMMY runs. Details are given in Section V.C.
8. The possibility to omit one or more spin groups from a particular calculation, while retaining parameters associated with the excluded spin groups in the set of varied parameters. Thus one can analyze two disparate experimental situations and obtain one parameter set appropriate for both. See Section ~~V.D~~ {III.E.2} for details.
9. An option to suppress output of small correlation coefficients, to minimize line-printer output; see Section VI.A for input.
10. An option to input resonance energy uncertainties at the end of the line in the PARameter file; see Table ~~VI B.1~~ {VI B.2}, card set 1, for input.

11. An option to use energy-independent normalization and/or any of five different energy-dependent backgrounds; normalization and background parameters may be varied, if desired. Details are given in Section ~~V.E.1~~ {III.E.3.a}.

12. The ability to include data reduction parameters (such as numerically-defined backgrounds or dead-time correction parameters) among the set of varied parameters. Details may be found in Section ~~V.E.2~~ {III.E.3.a}.

13. The possibility of using separate radii for potential scattering vs. penetrability and shift factor; also, the possibility of using different radii for different spin groups. Any or all of the radii may be varied. Details are given in Section ~~V.D~~ {III.E.2} and VI.B.

14. A more realistic resolution broadening function, designed especially for ORELA data but hopefully useful for analysis of data from other facilities as well; see Section ~~IV.E~~ {III.C.2}

15. An option to vary the isotopic abundances within an analysis; see Section ~~V.D~~ {III.E.2}

16. The ability to output resonance parameters to ENDF/B-VI File 2 format; see Section ~~VI.F~~ {VI.F.2}.

~~One major item remaining on the "wish list" for future work is the incorporation of multiple-scattering effects for capture cross sections.~~ {This was accomplished by Revision 3.)

Appendix A.3. MODIFICATIONS AND ADDITIONS IN REVISION 3

(This page is taken from the Introduction to Revision 3 of this manual, with ~~strikeouts and~~ {inserts} to clarify topics that might otherwise cause confusion.)

Major modifications and improvements to SAMMY have been incorporated subsequent to the publication of Revision 2 of this manual; these changes are documented in Revision 3.

Chief among the improvements is the incorporation of self-shielding and multiple-scattering corrections in the calculation of capture yields. Self-shielding is included exactly. Single-scattering is included exactly for specific geometries (a disk or flat rectangular sample inserted perpendicular to the neutron beam), or may be approximated (by pretending the radius of the disk or dimensions of the rectangle are infinite) in order to shorten computer run time. ~~(Double-scattering in approximate form is "on the drawing board" still.)~~ See Section ~~III.F~~ {III.D}for a more complete description of these corrections.

The ability to calculate angular distributions (double differential elastic cross sections) was initially a by-product of the single-scattering correction, but is also useful in its own right. SAMMY can now be used to analyze angular distributions of elastic cross sections for samples of any spin. Separate normalizations, backgrounds, and attenuation factors can be applied to each angle. A formal description of differential elastic scattering {and other angular distributions} is given in ~~Section III.E~~ {Section II.B.1.b}, and input is described in Section VI.

Mixtures of different isotopes or even nuclei with different Z can now be treated properly in SAMMY; thus data from oxides or other chemical combinations, with impurities, and/or samples with natural isotopic abundances can all be analyzed properly. Spins, abundances, masses, and scattering radii are individually given for each separate nucleus. Abundances and radii may be varied if desired. See Section VI for input information and Section ~~V.D~~ {III.E.2} for a description of the options.

"Simultaneous analyses" (i.e., sequential analyses connected via the parameter covariance matrix) of different data sets is often hindered because of slightly offset energy scales for the two data sets. To compensate for this, SAMMY now permits the user to vary t_0 and L. See Section ~~III.A.2.c~~ {III.E.8} for details and Table ~~VIB.1~~ {VI B.2}, card set 11, for input.

Reconstruction of point-wise cross sections from resonance parameters can now be done automatically in SAMMY, without the user having to provide an energy grid. Details are in Section ~~V.G~~ {V.A}.

SAMMY can now accept ENDF/B File 2 as input, replacing part of the usual SAMMY INPut file and all of the PARameter file. Details are given in Section ~~VI.G~~ {VI.F.3}.

An alternative method for calculating the Reich-Moore R-matrix cross sections is described in ~~Section III.D~~ {Section II.B}. This method was programmed for two reasons: First, accurate calculation of low-energy absorption or capture cross sections required revisions of the coding, since the original method produced numerical instabilities. Secondly, restructuring of the coding was required in order to facilitate incorporation of some of the other new features (multiple-scattering, angular distributions, reconstruction of point-wise cross sections).

Maxwellian (or stellar) averages of capture cross sections may be calculated from resonance parameters alone, or with resonance parameters plus point-wise cross sections for the unresolved region. See Section ~~V.F~~ {V.D} for details and ~~VI.H~~ {VI.F.4} for input.

The Oak Ridge Resolution function was available at the printing Revision 2 of this manual; documentation, however, was not, but is provided here (see Section ~~IV.E~~ {III.C.2}). The implementation of the ORR function within SAMMY has been modified somewhat, notably in changing all input parameters to consistent units, and introducing energy-dependence into the mean free path for the water moderator. In addition, the auxiliary program SAMORT (Section ~~VIII.C~~ {X.H}) was created to view individual components as well as the complete Oak Ridge Resolution function.

The data-reading segment in SAMMY has been modified to (1) take the "even grid for broadening at end points" as the default in designing the auxiliary grid, and (2) streamline the coding. ~~The user retains the option to use the original version should the need arise; however this "original version" (segment DAX) is not being carefully maintained, so is useful only in simple cases.~~ {Segment DAX is no longer available.}

Auxiliary program SAMAMR replaces SAMADD and SAMMIX (see Section ~~VIII.A~~ {X.C}). In addition to those features contained in SAMADD and SAMMIX, SAMAMR also facilitates simultaneous analysis of angular distributions with angle-integrated data by Adding, Mixing, or Removing data-set-dependent varied parameters from the "active" list.

Computer systems which choose not to use the ORELA "ODF" plotting package are encouraged to make use of SAMMY's alternative, which is to write the information into a "generic" binary file and process this file via a modification of the program ~~SAMBIN~~ {SAMPLT}. Details are given in Section ~~VIII.F~~ {X.I}

Finally, the input/output protocols for temporary storage within SAMMY have been extensively altered as a means of improving run time. This is possible because memory on modern computers has vastly increased; it is no longer necessary, e.g., to read derivatives at only one energy while keeping all others in temporary files. This change should be invisible to most users, except as manifested in increased speed of computation.

Appendix A.4. MODIFICATIONS AND ADDITIONS IN REVISION 4

(This page is taken from the Introduction to Revision 4 of this manual, with ~~strikeouts and~~ {inserts} to clarify topics that might otherwise cause confusion.)

Modifications and improvements to SAMMY subsequent to the publication of Revision 3 of this manual are documented here. These changes fall into several categories: (1) Significant additions to the code were requested (and funded) to ensure compatibility with experimental conditions of the linac at Renssaelar Polytechnic Institute (RPI). (2) Other features were designed to facilitate interaction between differential and integral data analysis; this work was funded primarily by the Nuclear Criticality Predictability Program (NCPP). (3) Miscellaneous new features and/or new descriptions of old features. (4) Modifications that fall under the general heading of "routine maintenance." (5) Planned future modifications and improvements. Even though the features are itemized in this section under these categories, the reader is encouraged to read the entire introduction, because features developed for one purpose are often suitable for use for another.

1. <u>RPI Options</u>

Further options have been added for background functions. See Section ~~V.E.1, page 98g~~ {III.E.3.a}.

A resolution function has been added which was designed specifically for use with data taken at the Gaerttner LINAC at RPI, but is presumably useful for data taken on other machines as well. See Section ~~IV.G, page 92s~~ {III.C.3}. Note that this resolution function is not necessarily the "final word" for RPI data, but may be updated for the next revision of SAMMY.

The ability to analyze self-indication experiments has been implemented; composition and temperature of the transmission and capture samples need not be identical. See Section ~~III.G~~ {III.E.6}.

A truly *multiple* multiple-scattering correction has been developed for capture and fission yields, and implemented in the code; see Section ~~III.F~~ {III.D}. Detailed documentation is being prepared, to describe precisely what approximations are used for this important correction factor.

An option has been added to use *l*-dependent detector efficiencies for capture or fission yields or for self-indication experiments. See Section ~~V.K~~ {III.E.5}.

An option has been added to include paramagnetic cross section in addition to the total cross section calculated from the resonance parameters. See Section ~~V.H~~ {III.E.4}.

2. <u>Integral/differential features</u>

Average theoretical cross sections can now be calculated accurately, using SAMMY's auxiliary energy grid, without generating experimental corrections (Doppler and resolution broadening, etc.) on the theoretical values. The inability to do so was a shortcoming overlooked

until recently and therefore not included in earlier versions of the code. Use the command "MAKE NO CORRECTIONS To theoretical values" in the INPut file (see Section VI.A., Table VIA.2), and do include some broadening parameters (which will not be used, but will force SAMMY to generate and use the dense auxiliary grid).

In addition to the energy-differential (and angle-differential) data that SAMMY was designed to analyze, some types of integral data can now be fitted directly with SAMMY. These are described in Section ~~VI.I, page 130m~~ {V.B}, and in greater detail in a separate document [NL97]. (Note that two additional types of integral data have been added to SAMMY subsequent to the release of that document.)

Most experimental data have both statistical errors (for which the covariance matrix is diagonal) and systematic errors (for which the covariance matrix is decidedly off-diagonal). Often analyses include only the statistical errors, or only the diagonal portion of the systematic errors, even though this practice is known to give inaccurate results. To make it easier for SAMMY users to use the correct covariance matrix, SAMMY now contains an option to include Implicit Data Covariance (IDC) information, for which the user must provide only minimal input; see Section VI.C.3. For an application of this technique, see ref. [HD97].

In an effort to improve communication with data processing codes, and to encourage such codes to make use of covariance information for resonance parameters, SAMMY can now provide output of the resonance parameter covariance matrix in a format that may be efficient for transmittal to those codes. See Section ~~V.K (page 98u)~~ {VII.E}.

3. Miscellaneous New Features

Values for fundamental physical and mathematical constants have been sited at one location only within the code, to ensure that the exact same values are used consistently throughout the code. Default values have been modified to conform to the current ENDF standards; see ~~Appendix E, page 241~~ {Section IX}, for the Cross Section Evaluation Working Group recommendations regarding values of constants.

Test cases (both input and output) have always been available for quality control with SAMMY and can also be useful in learning to use a new feature. A table describing the various test cases has been added to this manual (see Section ~~XI.D, Table XID.1~~ {XII.B}), and many sections now include references to the appropriate test cases.

For the *Workshop on Nuclear Reaction Data and Nuclear Reactors—Physics, Design and Safety* (held February 23 through March 27, 1998, at the International Centre for Theoretical Physics, Trieste, Italy), a series of exercises was developed as an aid in learning how to run SAMMY. These exercises are now included in the standard SAMMY package when the code is requested from the Radiation Safety Information Computational Center (RSICC) (formerly the Radiation Shielding Information Center) or other data centers. See Section ~~X.D (page 206a)~~

{XII.A} for information about these exercises. The companion lecture notes are available as [NL98a].

Generating the appropriate set of spin groups for the nuclide of interest can be a confusing task. See Section ~~VIII.I (page 150o)~~ {X.J} for guidance.

Converting from REFIT input [MM89] to SAMMY input (or vice versa) is discussed in Section ~~VIII.J (page 150w)~~ {X.B}.

Direct comparison of theoretical cross sections calculated by SAMMY with those calculated by other codes is facilitated by the use of program SAMCMP. See Section ~~VIII.K, page 150y~~ {X.E}.

SAMMY now automatically calculates average resonance widths and uncertainties thereon. These widths and uncertainties are reported in the LPT file, along with the updated resonance parameters, after data are fitted.

For guidance on the analysis of experimental data for which the sample contains more than one nuclide (multiple isotopes, chemical compounds, contaminants), see Section ~~V.D on page 98c~~ {III.E.2}.

Previously, when varying channel radii, SAMMY has implicitly assumed that reduced width amplitudes are held constant; hence the various partial widths (neutron widths, in particular) would be modified even if they were not explicitly varied. The user now has an option to override this assumption by specifying "DO NOT MODIFY UNVARied widths" in the INPut file; see Table VIA.2~~, page 114c~~.

4. Routine Maintenance

The entire code has been converted to double precision; previously, only those pieces deemed critical utilized double precision.

Output in the LPT file has been modified to (usually) fit 80 columns rather than 120; this change was driven by the current habit of viewing files on a screen rather than making hard (paper) copy of each file.

A few of the defaults have been changed:

USE 1999 ENDF-102 CONSTANT VALUES now replaces USE PRECISE VALUES OF CONSTANTS. This change ensures that SAMMY results are consistent both with ENDF conventions and with results obtained from other Reich-Moore codes such as NJOY [RM82], {PREPRO [DC04]} MULTIPOLE [RH87], and REFIT [MM89]. Internally, values for the constants are now sited in only one location in the coding, to ensure self-consistency and to facilitate future

changes. See ~~Appendix E~~ {Section IX.A} for the CSEWG recommendations regarding values for physical constants and Table {VI A1.2} ~~VIA.2 (page 114)~~ for description of how "older" values of the constants may be obtained.

The free-gas model (FGM) of Doppler broadening has been shown [NL98] to be a better choice for **all** energies, rather than the high-energy Gaussian approximation to the free-gas model. FGM is now the default option for Doppler broadening.

The "new" spin group format is more versatile and contains more information than the original format, and is now the default. Users whose INPut files do not use this format will receive error messages from SAMMY, along with suggestions about the necessary changes. [Note: The obsolete spin group format has been found to produce erroneous results when used in conjunction with angle-differential calculations (e.g., multiple-scattering corrections for capture or fission yields). Use of the obsolete spin group option is therefore not permitted in cases where it would produce errors.]

Minor bugs have been fixed; a partial list is given here:

The ASCII option for reading differential elastic scattering data now works consistently.

Integration limits for Doppler broadening have been extended somewhat to ensure more accurate results in those situations where the end of the integration region falls in the middle of a resonance. In addition, the algorithm for choosing the auxiliary grid near small resonances has been improved.

Errors in the documentation of the differential elastic cross section (Section ~~III.E~~ {II.B.1.b}) have been corrected. These errors were only in the documentation, not in the coding.

A correction has been made for programming error affecting only reaction (inelastic or fission) cross sections, in the case when there are more than two reaction channels.

5. Future Plans

Among the features planned for addition to SAMMY in the near future are: (1) More integral quantities, particularly those appropriate for intermediate energies. (2) Charge-dependent penetrabilities, to more accurately describe outgoing fission channels and to extend the capability of the code from neutron-induced reactions to charged-particle-induced reactions. {See Section II.C.4.} (3) Interface with other codes for use of covariance matrix. (4) Resolution function appropriate for use with Geel data (in collaboration with Saclay and Cadarache). {See Section III.C.3.} (5) Restructuring of the code to permit truly simultaneous analysis of any and all data sets~~; see Appendix F for details.~~

Appendix A.5. MODIFICATIONS AND ADDITIONS IN REVISION 5

(This page is taken from the Introduction to Revision 5 of this manual, with ~~strikeouts and~~ {inserts} to clarify topics that might otherwise cause confusion.)

Modifications and improvements to SAMMY subsequent to the publication of Revision 4 of this manual are summarized here.

(1) The ability to calculate Coulomb penetrabilities, shift factors, and phase shifts will extend the applicability of SAMMY to other types of data such as (n,α), (n,p), (p,n), (α,n). Section ~~III.H~~ {II.C.4} provides details on the Coulomb implementation in SAMMY.

(2) One change which is essentially invisible to the SAMMY user is the combination of the various segments into one large program. In addition to easing portability problems, this change has resulted in increased computation speed; SAMMY runs with Version M5 will require less CPU time than the same runs with earlier versions. Details are found in Section ~~XI~~ {XIII.C}.

(3) From the equations for Doppler broadening (~~Sect. IV.A.1 and IV.F~~ {Section III.B}), it is clear that the Doppler width is mass dependent, and therefore changes from nuclide to nuclide. Unfortunately this detail was overlooked in prior versions of SAMMY (M2a and earlier). That oversight has been corrected for Version M5. For most experimental conditions, this will be a small effect. For cases in which two nuclides, both with large abundances, have vastly different masses, the effect will be more pronounced. SAMMY users will want to be aware of this error and consider what impact it might have on their evaluations.

(4) It is now possible to calculate individual reaction types or individual fission channels. For example, one might wish to know the (n,α) cross section separately from (n,p) or (n,n`). [In prior versions of SAMMY, all "exit channels" were automatically included in the outgoing final state whenever the data was specified as inelastic, fission, or reaction.] Details on how this is accomplished are given in ~~Sect. V.L, page 98w~~ {Section II.B.1.c}.

(5) A bug was discovered (and exterminated) in the derivatives with respect to resonance parameters. This bug was found while the author was playing with artificial data, and occurred only when the penetrability was very small, that is, for low energies and non-zero angular momentum. Hence it is highly unlikely to have affected calculations relating to physical data.

(6) Errors in implementation of the RPI resolution function have been corrected, and the form of the function generalized. Preliminary values of resolution parameters suitable for use with Geel data are provided. See ~~Sect. IV.G.~~ {Section III.C.3}.

(7) Values of parameters for either the RPI resolution function or the ORR resolution function can now be given in either the INPut file or the PARameter file. If any parameter is to be varied, the PARameter file must be used.

(8) Improvements in the treatment of the unresolved-resonance region include more exact calculation of partial derivatives, normalization options for the experimental data, and increased flexibility for input of experimental data. Details are given in Section ~~V.J (page 98s)~~ {VIII }.

(9) Derivatives with respect to the matching radius (channel radius) are now generated in a self-consistent and logical manner. When the matching radius is varied but the neutron width is held fixed, the width Γ_n and not the partial-width amplitude γ_n remains unchanged. This is true also for other widths with non-unit penetrabilities (including Coulomb penetrabilities).

(10) It is now possible to utilize the ~~MPW~~ {M+W} solution for Bayes' equations in the resolved resonance region in a limited fashion. Individual SAMMY runs can generate W_i and Y_i for several data sets, and an additional SAMMY run will read those arrays, add them appropriately, and update the parameter values and covariance matrix (i.e., solve Bayes' equations via ~~MPW~~ {M+W} method). See ~~Sect. II.B.1.c (page 20c)~~ {Section IV.B.3} for more details. This scheme was initially devised for retroactively generating an approximate covariance matrix for a pre-existing set of resonance parameters {Section IV.E.2}.

(11) Bondarenko averaging is now available for the generation of multigroup cross sections; see Section V.C.2 for details.

(12) Output covariance matrices for the resonance parameters can now be provided in an abbreviated ~~"concise"~~ {"compact"} ASCII file, which the author intends to propose for adoption as an ENDF format. Details are given in Section VII.E.

(13) SAMMY can utilize ENDF File 2 (LRU=1, LRF=3, i.e. the Reich-Moore format) for input of resonance parameters (see ~~Sect. VI.G~~ {Section VI.F.3}), and can also provide output in ENDF File 2 format (see ~~Sect. VI.F~~ {Section VI.F.2}). The format change approved at the November 1999 CSEWG meeting is included; this format change permits specification of channel spin as well as resonance spin and orbital angular momentum for each resonance.

(14) Additional output files, in legible (ASCII) format, are now provided by the auxiliary programs SAMORT (~~Sect. VIII.C~~ {Section X.H}) and SAMRPT (~~Sect. VIII.M~~ {Section X.K}). These new files, with extensions PLT, are intended for use where the ORNL plotting package FORODF is replaced by another package.

(15) Auxiliary code SAMSMC can be used to generate Monte Carlo simulations of the multiple-scattering corrections to capture and/or fission yields. See ~~Sect. VIII.O page 150z.7~~ {Section X.M}.

Appendix A.6. MODIFICATIONS AND ADDITIONS IN REVISION 6

(This section is modified slightly from Appendix A.6 in Revision 6 of this manual, with ~~strikeouts~~ and {inserts} to clarify topics that might otherwise cause confusion.)

Modifications, additions, and improvements to SAMMY subsequent to the publication of Revision 5 of this manual are summarized here.

<u>New Input Options</u>

1. The "obsolete spin group format" is no longer supported. Current formats are described in Table VI.A.1, card sets 10.1 and 10.2. (For help in converting to one of those formats, users can attempt to make a SAMMY run with the obsolete INPut file and then follow the instructions which SAMMY provides.)

2. Key-word-based input is now available as an alternative to the sometimes-confusing earlier possibilities: particle-pair and spin group definitions (See Section VI.A, Table VI A.1, card set ~~4.1~~ {4}), information needed when writing an ENDF File 2 output file (~~VI.F~~ {VI.F.2}), and input to unresolved resonance calculations (VIII).

3. Input for R-matrix parameters has traditionally been provided in two locations, with spin-group definitions in the INPut file and resonance parameters in the PARameter file. Eventually the intent is to have one file for each nuclide, and that file would give all R-matrix information for only that one nuclide. As an intermediate step in that direction, version M6 of SAMMY includes the possibility to store all R-matrix information (for all nuclides) in the PARameter file rather than splitting it between INPut and PARameter files. SAMMY can also provide guidance for making the conversion. See Section VI on input.

4. Mistakes in command lines in the INPut file are now reported "live" as well as in the LPT file. (By "live" is meant "on screen", or "in the file to which the on-screen information is printed.") Command lines may be "commented out" (so that SAMMY ignores them) by inserting a pound sign (#) in the first column. See Table ~~VI.A.2~~ {VI A1.2}.

5. Previous versions of SAMMY permitted at most 50 spin groups, due to restrictions in the input format. An alternate format now makes it possible to use up to 500 spin groups. See Table VI A .1 and ~~VI B.1~~ {VI B.2} for details.

6. When using an ENDF file to obtain resonance parameters for SAMMY, it is no longer necessary to edit and extract File 2; instead, the complete ENDF file may be used as input to SAMMY. See Sections IX ("the ENDF Connection") and ~~VI.G~~ {VI.F.3} (input).

7. Units may be specified by the user for the energies in the plot file (SAMMY.PLT or SAMMY.ODF). See Table ~~VI.A.2~~ {VI A1.2}. A flag indicating which units are used is

reported in both versions of the plot file (see the FORTRAN file plt/mplt.f), and can be used for printing column headings for example.

Output Changes

1. An effort has been made to eliminate inconsistencies in output in the SAMMY.LPT file. Users are requested to report any remaining inconsistencies to the author.

2. The formulae used to generate chi-squared values printed in the LPT file have been modified somewhat: When off-diagonal data covariances are given (either explicitly or implicitly), they are now included in the calculation of χ^2.

3. To ease your publication efforts, an option exists for generating a listing of resonance parameters and uncertainties in a format suitable for porting to a spreadsheet program, which can then be used to arrange the information in publishable form. See Table VIA.2 for details.

4. ENDF files can be created for analyses in the unresolved resonance region (URR) as well as in the resolved. See Sections VIII (URR) and IX (ENDF) for details.

New Features

1. Angular distributions for reaction cross sections can be generated; previously, only elastic angular distributions were permitted. See Section ~~III.E~~ {II.B.1.c}.

2. Angular distributions can be angle-averaged; see Section ~~III.E.3~~ {III.E.7}.

3. A crystal-lattice model (CLM) of Doppler broadening has been added, based on the DOPUSH model of Naberejnev [DN99]; see Section ~~IV.B.4~~ {III.B.4}.

4. For testing purposes, fictitious cross sections can be generated (in lieu of actual Reich-Moore cross sections) in the form of constant, linear, quadratic, Dirac-delta, or 1/v functions. Along with these, specific types of energy grids (uniform in energy, time, or velocity) may be used. See Section V.E for details.

5. Enhancements have been made to the RPI resolution function, Section ~~IV.C.3~~ {III.C.3}.

6. A straight-line energy-average resolution function “DEX” has been added; see Section ~~IV.C.4~~ {III.C.4}for details.

7. The resolution function can now be specified numerically; see Section ~~IV.C.5~~ {III.C.5} for a description of this UDR resolution function. (Use with extreme caution, as this is a preliminary implementation and is known to be flawed.)

8. More than one type of resolution function may be used during a single SAMMY run. For details, see Section ~~IV.C~~ {III.C}.

9. Numerous enhancements have been made in the unresolved resonance region, described in Section VIII. "Annotated" input files may be used to increase the legibility and reduce the risk of input errors; output parameter files are given in annotated format. Output parameters and covariance matrix can be used as input to another run, in similar fashion to that used for sequential runs in the RRR. Parameters and covariance matrix, or point-wise cross sections, can be written in ENDF format.

10. Experience has shown that it is possible to use SAMMY's Reich-Moore approximation in a manner which mimics full (unapproximated) R-matrix behavior. See Section ~~III.I~~ {II.B.2} for details.

11. When appropriate, covariance matrices are now tested to ensure that they are positive-definite. Error messages are written if they are not. (Note: For virtually all the SAMMY test cases, the parameter covariance matrices are positive definite. The notable exceptions are those involving approximate covariance matrices.)

Debugging the Code

1. Bugs were uncovered and resolved in the calculation of the partial derivatives with respect to the resolution parameters, for both the ORR and RPI resolution functions. Attempts to include these parameters in the fitting procedure should now meet with far more success than previously.

2. Other less-obvious bugs have also been corrected; these will not be itemized here. Users are encouraged to contact the author when they suspect their problems to be due to a bug in the code. See Section XI.B for suggested procedures for resolving problems and for contacting the author.

Modifications to the Manual

1. Irrelevant and outdated material from the earlier releases has been eliminated:

   APPENDIX A. FORTRAN LISTING OF SAMMY. A listing of the coding for SAMMY, currently ~ ~~120,000~~ {140,000} lines, is no longer provided in the manual. See Table XIII.C.1 for a description of the various segments of the code.

   APPENDIX B. EXAMPLES. Please see Section XII for a description of the SAMMY tutorial exercises and test cases, which provide examples of input and output for most features of the code.

APPENDIX C. POSSIBLE JCL FOR IBM VERSION OF SAMMY. This information is no longer relevant.

APPENDIX D. ANALYSES USING SAMMY. Revision 5 (and earlier versions) of this manual contained a listing of publications describing SAMMY analyses. Because it is impossible to maintain an accurate and complete listing, this appendix is discontinued with Revision 6.

Information from the old "APPENDIX E. CONSTANTS" is now included in a new section (Section IX. THE ENDF CONNECTION), which summarizes SAMMY features related to the Evaluated Nuclear Data Files.

APPENDIX F, detailing future plans for restructuring of the SAMMY code and input, ~~has been repositioned to Appendix B~~ {removed}.

2. The structure of much of the manual has been reorganized in a more logical fashion. (~~Sections II and III will be reorganized at a later date.~~ {Sections II, III, and IV are reorganized for Revision 7.})

3. Tables in Section VI (Input) have been redesigned.

4. The page numbering system ~~(for Section IV through the appendix)~~ has been revised to use sequential integer numbers. Some numbers are skipped, to ease future expansion efforts. References to page numbers are generally omitted throughout the manual; instead, the references are to section numbers.

5. The manual is no longer published on paper, but only as a pdf file. Readers wishing to have hard copy of the manual can print from the pdf file.

APPENDIX B. ACKNOWLEDGMENTS FROM EARLIER VERSIONS

Acknowledgments from earlier versions of this manual are repeated in this appendix.

ACKNOWLEDGMENTS FOR ORIGINAL VERSION

Impetus for the development of a comprehensive users' guide for SAMMY was provided by those brave souls who struggled through a SAMMY analysis without benefit of such a guide. Foremost on this list of data analysts are Claire Perey, Bob Carlton, and Berger Folgelberg, whose comments, suggestions, and error-detection abilities have greatly enhanced both the user-friendly aspects and the accuracy of SAMMY. Other users, too numerous to mention, have also contributed to the continuing process of maintaining and upgrading the code.

Programming help from Jack Craven and Connie Malarkey is gratefully acknowledged: Jack, for devising a method of automatically increasing array sizes as needed, and Connie, for converting SAMMY to the ORIC VAX computer, and in the process discovering a few obscure bugs.

The assistance of Francis Perey in interpreting results and understanding subtleties of Bayes' method has proven invaluable. Francis has also contributed ideas for extension of the code, some of which have already been incorporated into the present version and others of which are being studied for incorporation into the next version of SAMMY.

Thanks to Claire Perey, Francis Perey, and Gerard de Saussure for permitting the use of their preliminary analyses as examples of SAMMY runs. Special thanks to Claire Perey for a careful review of this report. Her efforts have resulted in elimination of a number of obscurities, ambiguities, and just plain errors.

Lastly, the author wishes to thank Bobbie Roth for her patient efforts in typing this manuscript and especially for producing the complicated tables presented in the later sections of this report.

ACKNOWLEDGMENTS FOR REVISION 1

Special thanks go to Sue Damewood for typing and assembling this document, and to Gerard de Saussure, without whose patient insistence many of the improvements described in this report would not have been made.

ACKNOWLEDGMENTS FOR REVISION 2

The scientists and researchers who collectively constitute the SAMMY users group provide the author with a seemingly unending source of inspiration and (at times) frustration. Without the persistent encouragement of Claire Perey, Gerard de Saussure, Mike Moore, Herve Derrien, Ron Winters, Francis Perey, and Duane Larson (among others), this code would never have reached its current state. Special thanks go to Claire Perey and Ron Winters for carefully reviewing the pages of this revision.

Encouragement and financial support for implementation of an IBM version of SAMMY were provided by the Linac group at the Central Bureau for Nuclear Measurements (GELINA) in Geel, Belgium.

Once again the author gratefully acknowledges the able assistance of Sue Damewood in the preparation of the many tables and pages of text for this manual.

ACKNOWLEDGMENTS FOR REVISION 3

SAMMY users throughout the world continue to provide inspiration, encouragement, and support for the author's endeavors to improve and extend the code; the author is grateful for their interest. Among these are Luiz Leal of ORNL and the research staff of ORELA. In addition the author wishes to thank Ann McCoy, who patiently typed the first drafts of most pages in this revision.

ACKNOWLEDGMENTS FOR REVISION 4

Encouragement from and collaboration with the research staff at Renssaelar Polytechnic Institute are gratefully acknowledged. The continued support from colleagues here at Oak Ridge National Laboratory (notably Luiz Leal and Herve Derrien) and around the world is also appreciated. Thanks to SAMMY users who report problems with coding or documentation (John Burke, Olivier Bouland, Klaus Guber, Bob Spencer, Albert Popov). Thanks to Luiz Leal and Royce Sayer for careful proofreading of equations, and to Cecil Lubitz and Norm Francis for thorough reading of this and other documents. Finally, the author wishes to thank M. C. Moxon for numerous interesting conversations relevant to the further development of data analysis tools such as SAMMY and Moxon's code REFIT.

This work was sponsored by the U.S. Department of Energy (DOE), under contract DE-AC05-96OR22464 with Lockheed Martin Energy Research Corporation. The author is particularly indebted to D. Cabrilla, Environmental Management, U.S. Department of Energy, Washington, D.C., for his support.

ACKNOWLEDGMENTS FOR REVISION 5

The encouragement and support of SAMMY users is gratefully acknowledged. I am indebted first to ORNL researchers (Luiz Leal, Herve Derrien, Royce Sayer, Klaus Guber, Paul Koehler) and then to outside users (Frank Gunsing, Olivier Bouland, Soo Youl Oh, Kun Joong Yoo, Greg Leinweber, Yaron Danon) for their helpful suggestions and for their skill in uncovering my programming errors. Royce Sayer's work was invaluable in adding the Coulomb capability to the code. Special thanks must go to Ali Nouri of NEA, Paris, for organizing the SAMMY workshop held in September of 1999 and for maintaining the Web site at http://www.nea.fr/html/dbdata/sammy.htm. Finally, my apologies to the many SAMMY users whose names are not mentioned here, but whose contributions are important to the development and maintenance of this code.

ACKNOWLEDGMENTS FOR REVISION 6

As always, the development of SAMMY is heavily influenced by the many SAMMY users throughout the world who provide their suggestions, comments, criticisms, and even occasional praise for the code and the manual. In addition to those persons mentioned in earlier acknowledgments (most of whom are still contributing but whose names will not be repeated here), several newcomers have recently made important contributions: among these are Dan Bardayan, Jeff Blackmon, Michael Heil, Gilles Noguere, and Arjan Plompen. Again my apologies for inadvertent omissions from this list.

Special thanks must also go to (1) Olivier Bouland and Richard Babut from Cadarache, for development of an update to the auxiliary code SAMQUA, (2) the research staff at Rensselaer Polytechnic Institute for their strong encouragement in eradicating errors in SAMMY's ORR and RPI resolution functions, and to (3) Peter Siegler et al. at Geel for financial support for incorporation into SAMMY of the DOPUSH crystal-lattice model of Doppler broadening.

This work was sponsored by the Office of Environmental Management, U. S. Department of Energy, under contract DE-AC05-00OR22725 with UT-Battelle, LLC.