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ORNL Controlled Fusion Atomic Data Center: Thirty Years Later

H. T. Hunter
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Physics Division

ORNL CONTROLLED FUSION ATOMIC DATA CENTER THIRTY YEARS LATER

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FOREWORD

The Controlled Fusion Atomic Data Center (CFADC) was founded informally at Oak Ridge National Laboratory by Clarence F. Barnett in 1959, and was officially established six years later. The continuing mission of the CFADC is to identify, compile, evaluate, and recommend data on atomic and molecular collision processes which are important in fusion energy research. "Barney" dedicated much of his professional career to the promotion of effective scientific communication between the atomic and fusion research communities, and was still actively engaged in this mission at the time of his death in 1989. His insights, guidance, and dedication to this mission will be sorely missed by the CFADC and the fusion research community. The *modus operandi* of the CFADC has changed considerably during these 31 years, as computers have evolved and assumed an ever-increasing role in scientific database management. This report documents some innovations of the CFADC in this area and is dedicated to Barney's memory.

ORNL CONTROLLED FUSION ATOMIC DATA CENTER THIRTY YEARS LATER

H. T. Hunter, R. A. Phaneuf, and M. I. Kirkpatrick

ABSTRACT

The ORNL Controlled Fusion Atomic Data Center (CFADC) handles requests for information and data on fusion processes, maintains a comprehensive bibliographical database, and publishes recommended atomic collision data in what have been popularly called "Redbooks," to support the fusion community's current atomic and molecular data needs. A recent improvement in the efficiency and operation of the data center has been the addition of a customized database management system implemented on a personal computer system in 1988, and a desktop publishing station in 1989. This paper will describe the present scheme for handling numerical and bibliographic data and emphasize how they facilitate the mission of the CFADC.

SUPPORT AND STAFF

Support for the CFADC comes from the Office of Fusion Energy of the U.S. Department of Energy (DOE). The staff involved in the CFADC efforts includes both on-site professionals and off-site consultants involved in searching and compiling data and bibliographic information from over 100 journals pertaining to atomic processes in controlled thermonuclear fusion research. One full-time data professional manages the databases, composes, and coordinates the CFADC's publications. The scientific support staff includes the part-time services of five ORNL staff members, and those of six consultants under contract, each an expert in a particular subfield of atomic and molecular physics.

SCOPE

The data compilation and evaluation activities of the CFADC staff are supported by comprehensive bibliographic database files. The bibliographic database is searchable by a personal computer (PC) data-handling code developed specifically for the CFADC's needs. Key topics that may be searched include atomic and molecular reaction processes, reactants, and authors. The searching for bibliographic references may be performed at any time on a network, allowing real time access in a time-sharing mode. Five searching stations are currently operational and are located in the ORNL Physics Division, Building 6003.

Other ongoing activities involve preparation of updates and additions to the "Redbook" series of data compilations. Since 1961, the data center has been producing compilations of recommended data for fusion. The atomic processes that are recommended are displayed in tabular and graphical form and distributed to the fusion community, at no charge, as part of the series entitled "Atomic Data for Fusion."

Several support services are currently available. Requests are received for bibliographic information or numerical data for specific atomic processes. These are generally handled and processed within 24 hours. The CFADC is a major contributor to the International Atomic Energy Agency (IAEA) Atomic and Molecular Data Unit as well as the Japan Atomic Energy Research Institute Data Center (JAERI) and the Data and Planning Center of the National Institute of Fusion Science, Nagoya, Japan. The CFADC communicates its updated database information on a regular basis to these centers. Specially developed CFADC fortran codes involving collisional rate coefficient generation from collision cross-section data and parametric fitting also have been exchanged with several international data centers. In a cooperative effort, the CFADC sends representatives to the IAEA and associated data centers to participate in a consolidated network of data centers supporting the interests of the DOE and the IAEA.

BIBLIOGRAPHIC DATA

The CFADC maintains, through searches of scientific journals, books, reports, and other publications, a comprehensive bibliographic database. Each entry includes the following information: entry number, reaction category, reactants involved, experiment or theory, energy range, authors, title, journal name, publication, and the year published. The current population of the database is 22,000 entries dating back to 1978. Efforts are in progress to restore the 1950-1977 bibliographies, which reside on tape backups, to the personal computer database.

A unique entry number accompanies each bibliographical entry. The reaction categories are coded to represent one or more of the following processes: heavy-particle collisions, charged particles penetrating into macroscopic matter, electron collisions with atomic particles, photon collisions with atomic particles, general theory, data compilation, general reviews, books, and bibliographies. A more comprehensive list of reactions paired with codes which are used for information retrieval, is attached as Appendix A1. The codes are used to represent the reactions, which saves database file space and increases the data retrieval rates.

Each bibliographic entry has a specific number and type of atomic or molecular species involved in the reaction. A list of the most common species is included in Appendix A2. If the entry is comprised of theory data, then 'TH' is noted or, if

experimental data is being published, then 'E' is coded. An energy range for the reaction is noted if it is available. All authors' names are stored which allows for a comprehensive author search. A full list of the journals currently searched appears in Appendix A3.

The new personal-computer-based bibliographic data handling system replaced a similar code that was used on the ORNL IBM mainframe. The PC-based system handles requests faster and more efficiently, with a hardware cost that was recovered in savings of main-frame computer charges within the first two years of operation.

The hardware used for the PC-based bibliographic storage and retrieval system consists of a Compaq 386 personal computer with a 130 megabyte hard disk, laser printer, and a Bernoulli backup drive. The hard disk is used in a 3Com network and stores all files pertaining to the bibliography. Currently, approximately 60 megabytes of storage are occupied by the database files and retrieval codes. All the system is backed up on 10 megabyte cartridges using the Bernoulli backup drive. The entire database and the retrieval code have been transported successfully to Germany, using an archival system to reduce the required storage space. Eight 1.2-megabyte diskettes were required to send the database.

The entire bibliographic database may be searched in a timesharing, network mode by up to five users. The file handling code is written in dBase III+ and compiled by using Clipper software. File and record locking are required to guarantee the integrity of the files as they are searched and updated on the network. An example of the most common search would proceed as follows:

1. Define an atomic process of interest (listed in Appendix A) and note the attached code (i.e., Heavy Particle Charge Exchange = A06).
2. Define species involved in the reaction, i.e., H (hydrogen projectile) and He (helium target).
3. The years to be searched (i.e., entire database from 1978 to present or a user-defined subset).

The program begins searching for the specified process and the reactants. Upon completion, a screen review and/or a printout of the comprehensive bibliographic list are available. In addition, a plot and printout of recommended numerical data for cross sections versus energy may be obtained if any recommended data are available for the reaction of interest. A sample of the bibliographic printout for the above search appears in Appendix A4.

Another common type of search performed is an author search. Any author who appears in the bibliographic entry of the database, whether second, third, or tenth author, may be specified, and all records with that author's name will appear.

Each journal article, report, conference abstract, book chapter, or book reference is defined as an entry and is assigned an entry number when that reference is added to the database. The on-line bibliographic database presently consists of 22,000 entries, dating back to 1978. Earlier CFADC references dating back to 1950 are stored on magnetic tape in a number of different formats, and will be added to the on-line system as manpower becomes available. To enhance the speed and efficiency of searches, the record structure of the bibliographic database is divided into three different, smaller databases. A category database stores the entry number, reaction process code, and a list of reactants. An author database stores the entry number and the authors' names. The third database stores the entry number and all associated information not accommodated within the first two databases, i.e., title, publication, journal reference, country of origin, etc. While editing or adding entries to the database, the three smaller databases are all opened and pulled together as a unit. This is accomplished by interactive screen query and input by the operator. In addition to access speed, the division into three separate databases allows the flexibility needed to store as many authors and/or categories and reactants as necessary for a complete bibliographic entry.

A flow chart outlining the organization of the databases and the sequence of steps involved in a search is presented in Fig. 1. A search procedure begins by matching the key information to be searched upon, such as the author or a reaction process, to a previously indexed file containing pointers which specify which records match the request. This is a faster data retrieval method than a simple sequential data search. For every match to the searcher's request, such as a specific author, the code stores the unique entry number for that match. The entry number then serves as the key relationship of the three databases, which allows a complete record regeneration (see Fig. 1).

The bibliographical database retrieval code is accessible by five PC work stations linked to the file server via a 3Com Ethernet PC network. All the bibliographic records searched by a user are locked until the records are retrieved, and then become unlocked for the next user. The file and record locking is built into the retrieval code to ensure a file's or a record's integrity by removing the possibility of more than one user accessing the same record at the same time. The file and record locking is supported by the Clipper compiler software, which also speeds up the runtime of the dBase III+ database handling code.

The final part of the search for a reaction process looks for recommended data associated with the reaction of interest. If recommended data are found, a Basic program, which plots and prints the information, is loaded and executed within the runtime environment. The recommended data, usually reaction cross sections versus energy, may be plotted or printed, after which the program returns to the main menu to begin another search.

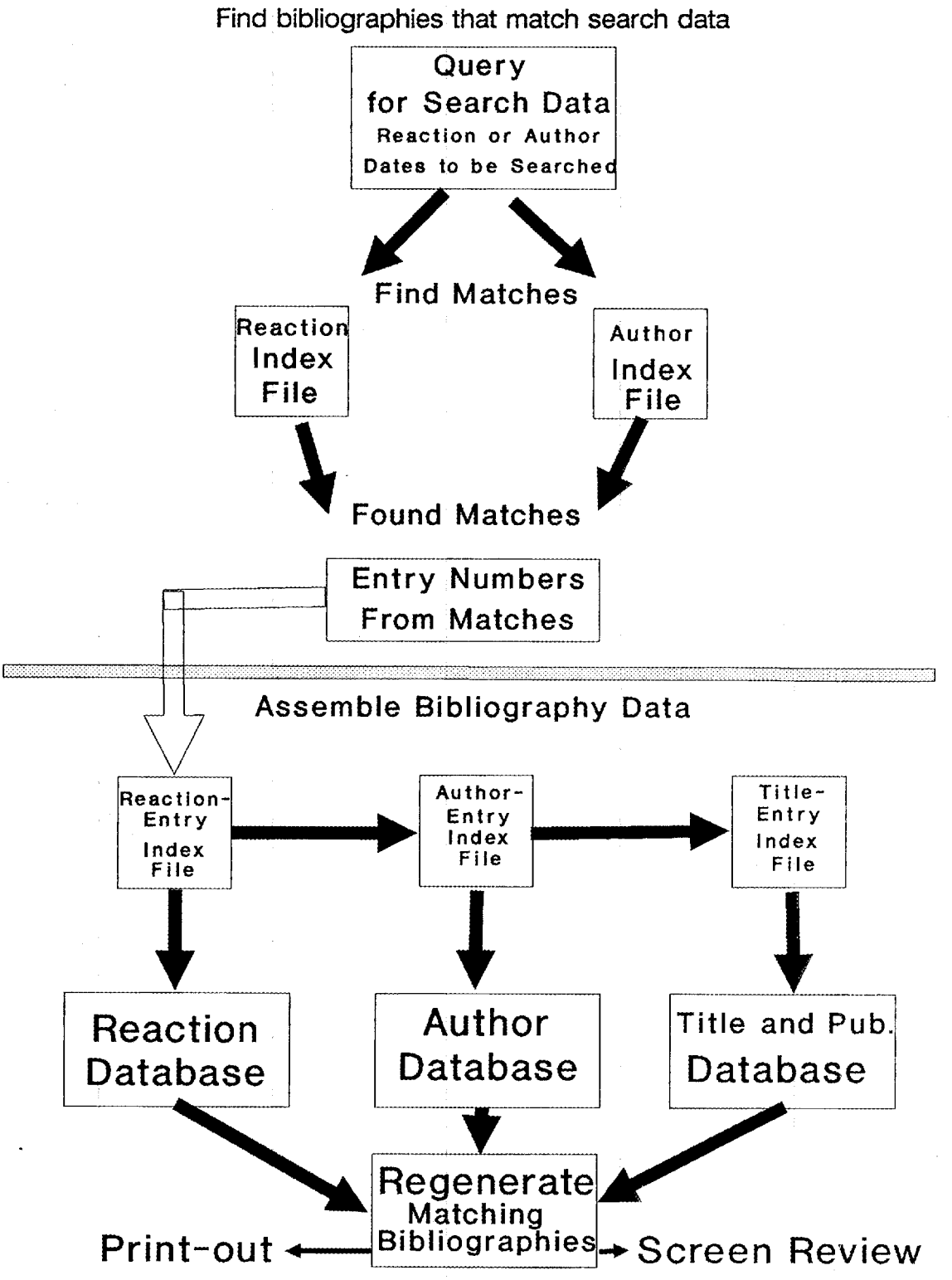


Fig. 1. Flow chart of data retrieval for a typical search.

The network hardware consists of five personal computers, network cards, and monitors. Each station is connected, via BNC cables that are daisy-chained together, and are separated by 20 to 30 feet. The Compaq 386 personal computer was purchased as the main file server because of its fast processing speed. The 130 megabyte hard disk stores all the files for the database and has a 20 millisecond access time, facilitating exceptionally fast data retrieval and storage.

Copies of the codes and file structure for the database and the database searches are available upon request from the authors.

NUMERICAL DATA COMPILATIONS

While a significant fraction of the time of the research staff and consultants is used to update the comprehensive CFADC database, significant amounts of time of a few staff have been periodically dedicated to producing recommended numerical data for fusion as new reactions are needed or as new information appears in the literature. A listing of the "Atomic Data For Fusion" compilations appears in Appendix B1.

Most of the recommended data produced by the CFADC is in the form of atomic collision cross sections versus collision energy. An efficient procedure for producing the recommended data for publication has emerged after years of effort and experience. The steps are as follows.

1. Define reaction types and reactants involved that are to be reviewed.
2. Search the CFADC bibliographic database for all relevant references.
3. Collect the references of interest from on-site sources, i.e., ORNL Central Research Library.
4. Make photocopies of all pertinent information, such as the abstract, notes, and the data results.
5. Define an accuracy and energy range of data to be used from each reference.
6. Use the CFADC digitizing station to extract data from graphs (see below for further description).
7. Plot all data sets for a particular reaction onto a single graph with each data set represented by a different color.
8. Judging from relative accuracies, experimental or theoretical method used, data scatter, etc., a "best fit curve" is hand drawn onto the graph.
9. The recommended curve is then redigitized and stored as a recommended data table (usually cross section vs. energy).
10. Plots of the single recommended curve are fitted using a Chebyshev polynomial curve-fitting routine.
11. A reaction rate-coefficient program generates rates, plots, and tabular data from recommended cross sections.

12. A local laser printer is used to produce publication-ready graphs of data and a local word processing station produces publication-ready data tables with accuracies, references, and any explanatory notes.

Since the recommendation process often involves reviewing hundreds of graphs of datasets from various experimental and theoretical sources, a digitizing station was developed in 1984 to quickly and accurately move data from published graphs to a local personal computer. The digitizing station consists of a digitizer pad, personal computer, and a color printer. A FORTRAN program that captures *x,y* points from the digitizer pad was developed by the CFADC.

The procedure for operating the digitizing station follows. First, the plot in the publication that contains the reaction cross section versus energy of interest is photocopied. The photocopy is taped to the active surface (11 in. × 11 in.) of the digitizer pad so it does not move. A device called the puck or pen is attached to the digitizer pad and is used to touch points on the graph axes to calibrate the scale and then the individual data points or curve of interest. The personal computer receives the *x,y* coordinates from the digitizer pad puck and translates them into a cross section and corresponding energy. Enough points on each curve of a plot are digitized to ensure an accurate representation of the original curve. A digitizing accuracy of 1 to 2% is routinely obtainable with this system.

A new plot is produced with all of the different digitized datasets for a particular reaction of interest. Each dataset is represented by a different color to discriminate easily between them. The recommendation is made by hand drawing a curve through the data. This requires full knowledge of the reaction type and only highly qualified scientists perform this task. The hand drawn curve is then digitized and stored on diskette for later publication.

The final recommended cross sections versus energy, along with the parametric curve fit coefficients, are shown in Appendix B2. The recommended curves are fitted using a least-squares Chebyshev polynomial fitting routine. The fitting coefficients (usually 7), the fit accuracy, and the energy range of the fit accompany each recommended cross section data set (Appendix B3). A plot of the recommended cross section is generated so that the user may quickly review the quality of the fit to the recommended cross section data. The Chebyshev fits allow a convenient general representation of recommended cross sections or rate coefficients, and means of readily reconstructing the data or creating a numerical database.

Notes are attached to the tabular data describing the recommendation and any limitations of the resulting data set or other cautions. References and accuracies are included for each reaction, all of which enable the user to properly apply the recommended data.

In the further interest of fusion engineering applications, reaction rate coefficients have been calculated using a special code developed at the CFADC during 1982 through 1986. Many different temperature regions exist in current magnetic fusion devices such as stellerators and tokamaks. These temperatures have been used along with the recommended cross sections in the rate generation program to calculate the reaction rates of interest to the fusion research community.

Most of the recommended cross sections have accompanying reaction rate coefficients. A typical set of reaction rate curves and their Chebyshev polynomial curve fits are included in Appendix B4. Eight different curves with their tabular data are shown. Each curve represents a specific set of temperatures assigned to each of the two reactants. In the example given above, charge exchange reaction involving H + He, each reactant was assigned a Maxwellian temperature distribution. The target atom or ion has its temperature displayed across the top of the tabular data sheet as headings for the columns. The projectile atom or ion has its temperature displayed down the side of the page and usually spans the range from 1 eV to 20000 eV, which are typical plasma temperatures. A plot of the eight curves is shown with their Chebyshev fits in Appendix B5.

Another type of velocity distribution is used to calculate reaction rates in addition to the above Maxwellian reaction rates. One reactant ion or atom is at a constant velocity (e.g., a "beam") impacting the Maxwellian velocity distribution which characterizes the other ion or atom reactant. This reaction rate coefficient calculation is of primary importance to neutral or ion beam injection, which is used either to heat or to diagnose most current fusion plasma devices.

As the graphic and tabular data are stored, methods and means of producing the final publication-ready plots and tables locally and cost-effectively have emerged. The final tables are produced on a desktop publishing station, which consists of a laser printer, a personal computer, and WordPerfect 5.0 software. A local laser printer connected to a VAX computer in the Physics Division is used with the VAX version of DISSPLA to produce the final plots. This method of local production saves time and reduces the cost of production.

NUMERICAL DATA STORAGE AND RETRIEVAL

The CFADC has been involved with other data centers and the fusion plasma physics community in a cooperative effort to develop and implement a universal data storage and retrieval format and code. The ALADDIN code written by R. A. Hulse[1] has provided the flexibility to store most, if not all, types of atomic and molecular experimental, theoretical, and recommended data. The code was developed at Princeton Plasma Physics Laboratory[1] and tested and implemented here at the CFADC. It has been approved and recommended for use by the International

Atomic Energy Agency's Atomic and Molecular Data Center Network. The ALADDIN code has been written in Fortran-77 to support the widest possible user community, the broadest range of scientific computers, and to facilitate interfacing with other computer codes.

ALADDIN provides a uniform format and vehicle for storing and exchanging atomic and molecular physics data. This is a major step in improving the collaborative efforts of the major atomic and molecular data centers, and provides a means to begin an accurate collection of previous work done in experimental and theoretical atomic physics. ALADDIN provides an organized storage and retrieval system for data which will help eliminate future overlap of data center efforts.

SUMMARY

The CFADC has upgraded its bibliographic data storage capabilities by moving from mainframe computers and cumbersome magnetic tapes to sophisticated personal computer hard disks and software. This change has not only reduced operating costs but improved the data accessibility. The bibliographic data retrieval handling codes were rewritten to be used in a local area personal computer network. This has in turn decreased the database access time and increased the ability to upgrade and customize the retrieval software at a lower cost.

The use of a digitizing station has improved the accuracy of data collection from the literature and has streamlined procedures for producing atomic collision cross section recommendations. Personal computer storage of the digitized data allows a quick, low cost, and accurate way for future retrieval and display.

The generation of compilations of recommended cross sections and reaction rates has increased the overlap between the CFADC and the needs of the fusion community. The use of the Chebyshev fits to store and represent the recommended data has proven to be efficient, accurate, flexible, and provides a convenient means of generating ALADDIN-formatted data files.

REFERENCE

1. R. A. Hulse, "The ALADDIN Atomic Physics Database System," Proceedings, 7th Topical Conference on Atomic Processes in Plasmas, Gaithersburg, Maryland, Oct. 2-5, 1989 (to be published).

APPENDICES

Appendix A1

REACTION CATEGORIES WITH CODES

Code	Reaction Description
A01	Heavy Particle - Heavy Particle: GENERAL
A02	Heavy Particle - Heavy Particle: ELASTIC SCATTERING COLLISIONS
A03	Heavy Particle - Heavy Particle: EXCITATION
A04	Heavy Particle - Heavy Particle: DISSOCIATION
A05	Heavy Particle - Heavy Particle: FLUORESCENCE
A06	Heavy Particle - Heavy Particle: ELECTRON CAPTURE
A07	Heavy Particle - Heavy Particle: IONIZATION
A08	Heavy Particle - Heavy Particle: STRIPPING
A09	Heavy Particle - Heavy Particle: RECOMBINATION OR MUTUAL NEUTRALIZATION LEADING TO NEUTRAL PRODUCTS (ION-ION)
A10	Heavy Particle - Heavy Particle: ENERGY TRANSFER - VIB, ROTATIONAL, ELECTRONIC
A11	Heavy Particle - Heavy Particle: COLLISIONAL DE-EXCITATION
A12	Heavy Particle - Heavy Particle: COLLISIONAL LINE BROADENING
A14	Heavy Particle - Heavy Particle: INTERCHANGE INVOLVING H OR He
A15	Heavy Particle - Heavy Particle: ASSOCIATIVE REACTIONS
A16	Heavy Particle - Heavy Particle: ELECTRON DETACHMENT FROM NEG IONS ->CONTINUUM
A17	Heavy Particle - Heavy Particle: INTERACTION POTENTIALS
A18	Heavy Particle - Heavy Particle: ANGULAR SCATTERING
A20	Heavy Particle - Heavy Particle: ATTENUATION
B01	INTERACTION OF INDIVIDUAL ATOMS OR MOLECULES WITH EXTERNAL FIELDS
B07	COLLISIONS IN PRESENCE OF STATIC OR TIME VARYING FIELDS
C01	Particle Penetration in Macroscopic Matter: GENERAL
C02	Particle Penetration in Macroscopic Matter: ENERGY LOSS AND STOPPING POWER
C04	Particle Penetration in Macroscopic Matter: PARTICLE RANGE
C05	Particle Penetration in Macroscopic Matter: MULTIPLE SCATTERING
C06	Particle Penetration in Macroscopic Matter: CHARGE STATE POPULATION
C07	Particle Penetration in Macroscopic Matter: EXCITED STATE POPULATION
D01	Particle Interactions with Solid Surfaces: GENERAL
D02	Particle Interactions with Solid Surfaces: SPUTTERING BY ELECTRONS, NEUTRONS, H
D03	Particle Interactions with Solid Surfaces: SPUT PART CHARGE AND QUANTUM DIST
D04	Particle Interactions with Solid Surfaces: SEC ELECTRON EJECTION BY HEAVY PARTICLE AND ELECTRONS
D05	Particle Interactions with Solid Surfaces: PHOTOELECTRIC EJECTION OF ELECTRONS
D06	Particle Interactions with Solid Surfaces: REFLECTION OF ELECTRONS FROM SURFACE
D07	Particle Interactions with Solid Surfaces: REFLECTION OF HEAVY PARTICLES FROM SURFACES
D08	Particle Interactions with Solid Surfaces: CHARGE AND QUANTUM STATE DISTRIBUTION OF REFLECTED HEAVY PARTICLES
D09	Part Inter w/ Solid Surf: DE-EXCITATION, NEUTRALIZATION, IONIZATION, OR DISSOCIATION OF PARTICLES INTERACTING WITH SURFACES
D11	Part Inter w/ Solid Surf: STICKING COEFF, THERMAL ENERGIES AND ADSORPTION

Appendix A1 (Continued)

Code	Reaction Description
D12	Part Inter w/ Solid Surf: ELECTMAGNETIC RADIATION INDUCED BY ELECTRON OR HEAVY PARTICAL IMPACT ON SURFACES
D13	Part Inter w/ Solid Surf: DESORPTION OF GASES FROM SURFACES
D17	Part Inter w/ Solid Surf: ELECTRON, ION AND PHOTON INDUCED CHEMICAL CHANGES TO SURFACES
D18	Part Inter w/ Solid Surf: TRAPPING AND REEMISSION OF HYDROGEN AND HELIUM
E01	Electron - Particle Interaction: GENERAL
E02	Electron - Particle Interaction: ELASTIC COLLISIONS
E03	Electron - Particle Interaction: EXCITATION
E04	Electron - Particle Interaction: DISSOCIATION
E05	Electron - Particle Interaction: IONIZATION
E06	Electron - Particle Interaction: RECOMBINATION (ELECTRON-ION)
E07	Electron - Particle Interaction: COLLISIONAL DE-EXCITATION
E08	Electron - Particle Interaction: COLLISIONAL LINE BROADENING
E09	Electron - Particle Interaction: NEGATIVE ION FORMATION
E11	Electron - Particle Interaction: FREE-FREE TRANSITIONS (BREMSSTRAHLUNG)
E13	Electron - Particle Interaction: ELECTRON DETACHMENT FROM NEGATIVE IONS
E16	Electron - Particle Interaction: FLUORESCENCE
E17	Electron - Particle Interaction: ANGULAR SCATTERING
E19	Electron - Particle Interaction: MOMENTUM TRANSFER
H01	Photon Collisions w/H.P. and Elec: GENERAL
H02	Photon Collisions w/H.P. and Elec: TOTAL ABSORPTION
H03	Photon Collisions w/H.P. and Elec: ELASTIC SCATTERING
H04	Photon Collisions w/H.P. and Elec: EXCITATION
H05	Photon Collisions w/H.P. and Elec: DISSOCIATION
H06	Photon Collisions w/H.P. and Elec: IONIZATION
H07	Photon Collisions w/H.P. and Elec: PHOTODETACHMENT
H08	Photon Collisions w/H.P. and Elec: FLUORESCENCE
H11	Photon Collisions w/H.P. and Elec: FREE-FREE ABSORPTION OR INVERSE BREMSSTRAHLUNG
J01	Data Compilation: HEAVY PARTICLE
J02	Data Compilation: ELECTRONS
J03	Data Compilation: PHOTONS
J04	Data Compilation: PARTICLES ON SURFACES AND SOLIDS
J05	Data Compilation: TRANSPORT
J06	Data Compilation: STRUCTURE
K01	Reviews and Books: HEAVY PARTICLE
K02	Reviews and Books: ELECTRONS
K03	Reviews and Books: PHOTONS
K04	Reviews and Books: PARTICLES ON SURFACES AND SOLIDS
K05	Reviews and Books: TRANSPORT
K06	Reviews and Books: STRUCTURE
K07	Reviews and Books: GENERAL
K08	Reviews and Books: USE OF ATOMIC DATE FOR PLASMA STUDIES
L01	Bibliographies: HEAVY PARTICLE
L02	Bibliographies: ELECTRONS
L03	Bibliographies: PHOTONS
L04	Bibliographies: PARTICLES ON SURFACES AND SOLIDS
L05	Bibliographies: TRANSPORT
L06	Bibliographies: STRUCTURE

Appendix A2

MOST COMMON REACTANTS APPEARING IN BIBLIOGRAPHIC ENTRIES

Atoms and Ions

H, deuterium, tritium, and their ions

He, Li, Be, C, O, and their ions

Al, Ar, Ti, Cr, Fe, Ni, and their ions

Cu, Zn, and their ions

Kr, Mo, and their ions

Xe, Ta, W, and their ions

Electrons

Molecules

H_2, H_3, HeH, N_2, O_2, CO, CO_2, and their ions

OH, H_2O, CH, CH_2, CH_3, CH_4, and their ions

*Note: All elements of the periodic table exist in the bibliography; only the most common are listed above.

Appendix A3

JOURNALS SEARCHED WITH ACCOMPANYING CODES

Code	Journal
3	Ann. Geophys.
4	Appl. Phys. Lett.
6	Appl. Spectrosc. Rev.
7	Astrophys. J. Pt. 1
8	Aust. J. Phys.
10	Bull. Acad. Sci. USSR Phys. Ser.
11	Can. J. Chem.
12	Can. J. Phys.
13	Compt. Rend. Ser. II
14	J. Chem. Soc. Faraday Trans. Pt. I
15	Indian J. Phys. A
16	J. Chem. Soc. Faraday Trans. Pt. II
17	J. Am. Chem. Soc.
18	J. Appl. Phys.
19	J. Atmos. Terr. Phys.
20	J. Chem. Phys.
21	Europhys. Lett.
24	J. Phys. Chem.
25	J. Quant. Spectrosc. Radiat. Transfer
26	J. Opt. Soc. Am. A
27	J. Phys. Soc. Jpn.
28	Mol. Phys.
29	Mon. Not. R. Astron. Soc.
30	Nucl. Fusion
31	Nucl. Instrum. Methods Phys. Res. A
32	Phys. Status Solidi B
33	Opt. Spectrosc.
34	Physica B
35	Physica A
36	Phys. Status Solidi A
37	Phys. Rev. A
38	Phys. Rev. Lett.
39	Phys. Lett. A
40	Phys. Fluids B
41	J. Phys. B
42	Proc. R. Soc. London Ser. A
43	J. Phys.: Condens. Matter
44	J. Phys. D
45	Rev. Mod. Phys.
46	Sov. Astron.-AJ
47	Sov. Phys.-Dokl.
48	Sov. Phys.-JETP
49	Sov. Phys.-Solid State
50	Sov. Phys.-Tech. Phys.
51	Sov. Phys.-Usp.
54	Z. Naturforsch. A
55	Z. Phys. D
58	Z. Phys. B
59	J. Phys. E
62	Helv. Phys. Acta
63	J. Mol. Spectrosc.
65	Vacuum
67	Phys. Rev. B
95	Planet. Space Sci.
116	Sov. Phys.-JETP Lett.
123	Appl. Opt.
126	J. Phys. [Paris]
132	Nuovo Cimento B
134	Nuovo Cimento D
136	Nuovo Cimento Lett.
139	Jpn. J. Appl. Phys. Pt. 1
142	Acta Phys. Acad. Sci. Hung.
145	Acta Phys. Austriaca
150	Indian J. Phys. B
160	Fortschr. Phys.
180	Solar Phys.
185	Acta Phys. Pol. A
197	Surf. Sci.
201	Astrophys. J. Suppl. Ser.
208	Astrophys. Space Sci.
216	Rep. Prog. Phys.
235	J. Vac. Sci. Technol. A
250	High Temp.
252	High Temp. Sci.
260	J. Opt. Soc. Am. B
278	Mass Spectrom. Rev.
281	Indian J. Pure Appl. Phys.
289	J. Appl. Spectrosc.
291	Space Sci. Rev.
309	Adv. Chem. Phys.
310	Adv. Phys.
311	Nucl. Instrum. Methods Phys. Res. B
312	Ber. Bunsenges. Phys. Chem.
354	Rev. Phys. Appl. (Paris)
355	Sov. Phys. J.
376	Int. J. Quantum Chem.
377	Chem. Phys. Lett.
379	Czech. J. Phys. B
380	IEEE J. Quantum Electron.
381	Int. J. Mass Spectrom. Ion Phys.
385	Ann. Phys. (Germany)
386	Ann. Phys. [Paris]
387	Astron. Astrophys.
389	Int. J. Chem. Kinet.
393	At. Data Nucl. Data Tables
396	Comments At. Mol. Phys.

Appendix A3 (Continued)

Code	Journal
397	Radiat. Eff.
398	Radiat. Eff. Express
399	Chin. J. Phys.
400	Astron. Astrophys. Suppl. Ser.
401	Chem. Phys.
402	Contemp. Phys.
403	IEEE Trans. Plasma Sci.
404	J. Electron. Spectrosc. Relat. Phenom.
405	J. Nucl. Mater.
406	J. Plasma Phys.
407	J. Phys. Chem. Ref. Data
410	Opt. Commun.
411	Phys. Scr.
412	Phys. Rep.
413	Rev. Geophys. Space Phys.
414	Sov. Astron. Lett.
415	Sov. At. Energy
416	Sov. J. Plasma Phys.
417	Sov. J. Quantum Electron.
418	Sov. Tech. Phys. Lett.
420	Appl. Phys. [Germany] A
422	Appl. Phys. [Germany] B
426	J. Res. Nat. Bur. Stand. Sect. A
427	J. Phys. [Paris] Lett.
430	Thin Solid Films
432	Opt. Lett.
500	Prog. Surf. Sci.
502	Astrophys. J. Pt. 2
503	High Energy Chem.
504	Appl. Surf. Sci.
505	J. Phys. [Paris] Colloq.
506	IEEE Trans. Nucl. Sci.
507	Jpn. J. Appl. Phys. Pt. 2
508	J. Vac. Sci. Technol. B
509	Comput. Phys. Commun.
601	XV ICPEAC, Brighton, Abstracts

Appendix A4

EXAMPLE OF A TYPICAL BIBLIOGRAPHIC SEARCH RESULT

SEARCH CATEGORY = Heavy Particle - Heavy Particle: ELECTRON CAPTURE : REACTANTS = H + He:

REF. NO. = 4165
(A06)ELECTRON CAPTURE: H + H_2; H + He; H + N_2
(A06)ELECTRON CAPTURE: H + O_2; H + Ne; H + Ar
(A06)ELECTRON CAPTURE: H + Kr; H + Xe; H + CO
(A06)ELECTRON CAPTURE: H + NO; H + HI; H + Mg
(A06)ELECTRON CAPTURE: H + Cs; H + Pb; H^+ + H_2
(A06)ELECTRON CAPTURE: H^+ + He; H^+ + N_2; H^+ + O_2
(A06)ELECTRON CAPTURE: H^+ + Ne; H^+ + Ar; H^+ + Kr
(A06)ELECTRON CAPTURE: H^+ + Xe; H^+ + CH_4; H^+ + NH_3
(A06)ELECTRON CAPTURE: H^+ + H_2O; H^+ + CO; H^+ + CO_2
(A06)ELECTRON CAPTURE: H^+ + C_4H_{10}; H^+ + Li; H^+ + Na
(A06)ELECTRON CAPTURE: H^+ + Mg; H^+ + K; H^+ + Rb
(A06)ELECTRON CAPTURE: H^+ + Cs; H^+ + Pb;
(A08)STRIPPING: H + H_2; H + He; H + N_2
(A08)STRIPPING: H + O_2; H + Ne; H + Ar
(A08)STRIPPING: H + Kr; H + Xe; H + CH_4
(A08)STRIPPING: H + NH_3; H + H_2O; H + CO
(A08)STRIPPING: H + NO; H + CO_2; H + HI
(A08)STRIPPING: H + Mg; H + Cs; H + Pb
(A08)STRIPPING: H^- + H_2; H^- + He; H^- + N_2
(A08)STRIPPING: H^- + O_2; H^- + Ne; H^- + Ar
(A08)STRIPPING: H^- + Kr; H^- + Xe; H^- + CO
(A08)STRIPPING: H^- + NO; H^- + Mg; H^- + Cs
EXPERIMENTAL ENERGY RANGE: 10-10000 eV
Tawara, H.; ;
Cross sections for charge transfer of hydrogen beams in gases and vapors in the energy range 10 eV-10 keV.
Atomic Data and Nuclear Data Tables **22**, 491 (1978) Japan

REF. NO. = 6989
(A06)ELECTRON CAPTURE: H + He; H + Ne; H + Ar
(A06)ELECTRON CAPTURE: H + Kr; H + Xe; H + Li
(A06)ELECTRON CAPTURE: H + Na; H + K; H + Rb
(A06)ELECTRON CAPTURE: H + Cs; D + Ne; D + Ar
(A06)ELECTRON CAPTURE: D + Xe; ;
(A08)STRIPPING: H^- + He; H^- + Ne; H^- + Ar
(A08)STRIPPING: H^- + Kr; H^- + Xe; H^- + Li
(A08)STRIPPING: H^- + Na; H^- + K; H^- + Rb
(A08)STRIPPING: H^- + Cs; D^- + Ne; D^- + Ar
(A08)STRIPPING: D^- + Xe; H + He; H + Ne
(A08)STRIPPING: H + Ar; H + Kr; H + Xe
(A08)STRIPPING: H + Li; H + Na; H + K
(A08)STRIPPING: H + Rb; H + Cs; D + Ne
(A08)STRIPPING: D + Ar; D + Xe;
(A16)ELECTRON DETACHMENT FROM NEG IONS -> CONTINUUM: H^- + He; H^- + Ne; H^- + Ar
(A16)ELECTRON DETACHMENT FROM NEG IONS -> CONTINUUM: H^- + Kr; H^- + Xe; H^- + Li
(A16)ELECTRON DETACHMENT FROM NEG IONS -> CONTINUUM: H^- + Na; H^- + K; H^- + Rb
(A16)ELECTRON DETACHMENT FROM NEG IONS -> CONTINUUM: H^- + Cs; D^- + Ne; D^- + Ar
(A16)ELECTRON DETACHMENT FROM NEG IONS -> CONTINUUM: D^- + Xe; ;
(C06)Particle Penetration in Macroscopic Matter: CHARGE STATE POPULATION: H^- + H_2; H^- + D_2; H^- + He
(C06)Particle Penetration in Macroscopic Matter: CHARGE STATE POPULATION: H^- + Ne; H^- + Ar; H^- + Kr
(C06)Particle Penetration in Macroscopic Matter: CHARGE STATE POPULATION: H^- + Xe; H^- + Li; H^- + Na
(C06)Particle Penetration in Macroscopic Matter: CHARGE STATE POPULATION: H^- + K; H^- + Rb; H^- + Cs
(C06)Particle Penetration in Macroscopic Matter: CHARGE STATE POPULATION: H^- + N_2; H^- + O_2; H^- + CO_2
(C06)Particle Penetration in Macroscopic Matter: CHARGE STATE POPULATION: H^- + SF_6; H^- + C_4; H^- + H_{10}
(C06)Particle Penetration in Macroscopic Matter: CHARGE STATE POPULATION: H^- + C_5; H^- + H_{12}; H^- + Br_2
(C06)Particle Penetration in Macroscopic Matter: CHARGE STATE POPULATION: H^- + I_2; H^- + CF_4; H^- + CHF_3
(C06)Particle Penetration in Macroscopic Matter: CHARGE STATE POPULATION: H^- + $CBrF_3$; H^- + H_20;
EXPERIMENTAL ENERGY RANGE: 30-200 keV
Anderson, C. J.; Girnius, R. J.; Howald, A. M.
Anderson, L. W.; ;
Production of fast H^0 atoms by stripping H^- ions in gas and vapor targets.
Phys. Rev. A **22**, 822 (1980) United States

REF. NO. = 8128
(A06)ELECTRON CAPTURE: H + H_2; H + He;
(A07)IONIZATION: H + H_2; H + He;
(A08)STRIPPING: H + H_2; H + He;
EXPERIMENTAL ENERGY RANGE: 50-3000 eV
van Zyl, B.; Lee, T. Q.; Ammc, R. C.
Charged-particle production in low-energy H + H_2 and H + He collisions.
J. Chem. Phys. **74**, 314 (1981) United States

Appendix B1

MAJOR CFADC NUMERICAL AND BIBLIOGRAPHIC DATA PUBLICATIONS

CFADC Redbook Numerical Compilations	Date
Atomic and Molecular Collision Cross Sections of Interest in Controlled Thermonuclear Research (C. F. Barnett, W. B. Gauster, J. A. Ray) ORNL-3113	1961
Atomic and Molecular Collision Cross Sections of Interest in Controlled Thermonuclear Research (C. F. Barnett, J. A. Ray, J. C. Thompson) ORNL-3113, Revised	1964
Atomic Data for Controlled Fusion Research Vol. I (C. F. Barnett, J. A. Ray, E. Ricci, M. I. Wilker, E. W. McDaniel, E. W. Thomas, H. B. Gilbody) ORNL-5206	1977
Atomic Data for Controlled Fusion Research, Revisions and Additions to Sections D.1 Sputtering, D.5 Ion Reflection from Surfaces, and D.6 Trapping (E. W. Thomas, Georgia Institute of Technology) ORNL-5207/R1	1979
Atomic Data for Controlled Fusion Research Vol. II (C. F. Barnett, J. A. Ray, E. Ricci, M. I. Kirkpatrick, E. W. McDaniel, E. W. Thomas, H. B. Gilbody) ORNL-5207	1980
Atomic and Ionic Spectrum Lines Below 2000 Angstroms (Raymond L. Kelly, Naval Postgraduate School) ORNL-5922	1982
Particle Interactions with Surfaces (E. W. Thomas, Georgia Institute of Technology) ORNL-6088	1985
Spectroscopic Data for Iron (W. L. Wiese, National Bureau of Standards) ORNL-6089	1985
Collisions of Carbon and Oxygen Ions with Electrons, H, H_2, and He (R. A. Phaneuf, R. K. Janev, and M. S. Pindzola) ORNL-6090	1987
Spectroscopic Data for Titanium, Chromium, and Nickel (W. L. Wiese and A. Musgrove, NIST) ORNL-6551	1989
Collisions of H, H_2, He, and Li Atoms and Ions with Atoms and Molecules (C. F. Barnett) ORNL-6086 (currently in final draft)	1990
Collisions of Electrons with Atoms and Molecules (J. W. Gallagher and D. C. Gregory) (to be completed)	1991

Appendix B1 (Continued)

Major CFADC Bibliographic Publications	Date
Bibliography of Molecular Dissociation in Heavy Particle Collisions 1950-1975 (S. W. Hawthorn et al.) ORNL-5500	1979
Bibliography of Atomic and Molecular Excitation in Heavy Particle Collisions 1950-1975 (S. W. Hawthorn et al.) ORNL-5501	1979
Bibliography of Electron Transfer in Heavy Particle Collisions 1950-1975 (S. W. Hawthorn et al.) ORNL-5502	1979
Bibliography of Ionization and Stripping in Heavy Particle Collisions 1950-1975 (S. W. Hawthorn et al.) ORNL-5503	1979
Bibliography of Atomic and Molecular Processes Vol. I, 1978-1981 (C. F. Barnett et al.) ORNL-5921/V1	1982
Bibliography of Atomic and Molecular Processes Vol. II, 1978-1981 (C. F. Barnett et al.) ORNL-5921/V2	1982
Bibliography of Atomic and Molecular Processes 1982 (C. F. Barnett et al.) ORNL-6052	1984
Bibliography of Atomic and Molecular Processes 1983 (C. F. Barnett et al.) ORNL-6095	1984
Bibliography of Atomic and Molecular Processes 1984 (C. F. Barnett et al.) ORNL-6157	1985
Bibliography of Atomic and Molecular Processes 1985 (C. F. Barnett et al.) ORNL-6287	1986

Appendix B2

TYPICAL RECOMMENDED CROSS SECTION DATA FORMAT
(Taken from Redbook Vol. V, ORNL-6090, 1987)

Total Electron Capture Cross Sections for
$C^{3+} + He \rightarrow C^{2+} + He^{+}$

Energy (eV/amu)	Velocity (cm/s)	Cross Section (cm^2)
1.0E+00	1.39E+06	1.56E-16
2.0E+00	1.96E+06	3.16E-16
4.0E+00	2.78E+06	4.94E-16
7.0E+00	3.68E+06	6.88E-16
1.0E+01	4.39E+06	8.33E-16
2.0E+01	6.21E+06	1.13E-15
4.0E+01	8.79E+06	1.37E-15
7.0E+01	1.16E+07	1.56E-15
1.0E+02	1.39E+07	1.65E-15
2.0E+02	1.96E+07	1.78E-15
4.0E+02	2.78E+07	1.79E-15
7.0E+02	3.68E+07	1.76E-15
1.0E+03	4.39E+07	1.69E-15
1.7E+03	5.66E+07	1.61E-15
2.0E+03	6.21E+07	1.56E-15
4.0E+03	8.79E+07	1.33E-15
7.0E+03	1.16E+08	1.11E-15
1.0E+04	1.39E+08	9.63E-16
2.0E+04	1.96E+08	6.74E-16
4.0E+04	2.78E+08	4.50E-16
7.0E+04	3.68E+08	2.68E-16
1.0E+05	4.39E+08	1.88E-16
2.0E+05	6.21E+08	6.72E-17
4.0E+05	8.78E+08	1.22E-17
7.0E+05	1.16E+09	7.77E-19

References: E.22, E.24, E.25, E.26, T.9, T.32

Accuracy: 30% for $2x10^2 \leq E(eV/amu) \leq 1x10^4$; 40% for $1x10^4 \leq E(eV/amu) \leq 4x10^5$; 100% for $1 \leq E(eV/amu) < 2x10^2$; 100% for $4x10^5 < E(eV/amu) < 1x10^6$

Notes: (1) According to two-state Landau-Zener calculations [T.32] (having an accuracy of 100%), the cross section for $E < 1$ eV/amu continues to decrease, reaching values of $6x10^{-18}$ cm^2 at $E = 0.1$ eV/amu, and $7x10^{-19}$ cm^2 at $2x10^{-2}$ eV/amu.

(2) In the region below $E = 1.0x10^4$ eV/amu, the $C^{2+}(2s2p)\,^1P^0$ final (metastable) state is dominantly populated, while for energies above ~ $2x10^4$ eV/amu a significant contribution to σ comes also from capture to $(2s2p)\,^3P^0$, and $(2p^2)$ ^3P, ^1D excited states of C^{2+}, [E.24], [E.27].

For Chebychev fits of the above cross sections it is necessary to use the following parameters.
E_{min} = 1.0E+00 eV/amu, E_{max} = 7.0E+05 eV/amu

Chebychev Fitting Parameters for Cross Sections

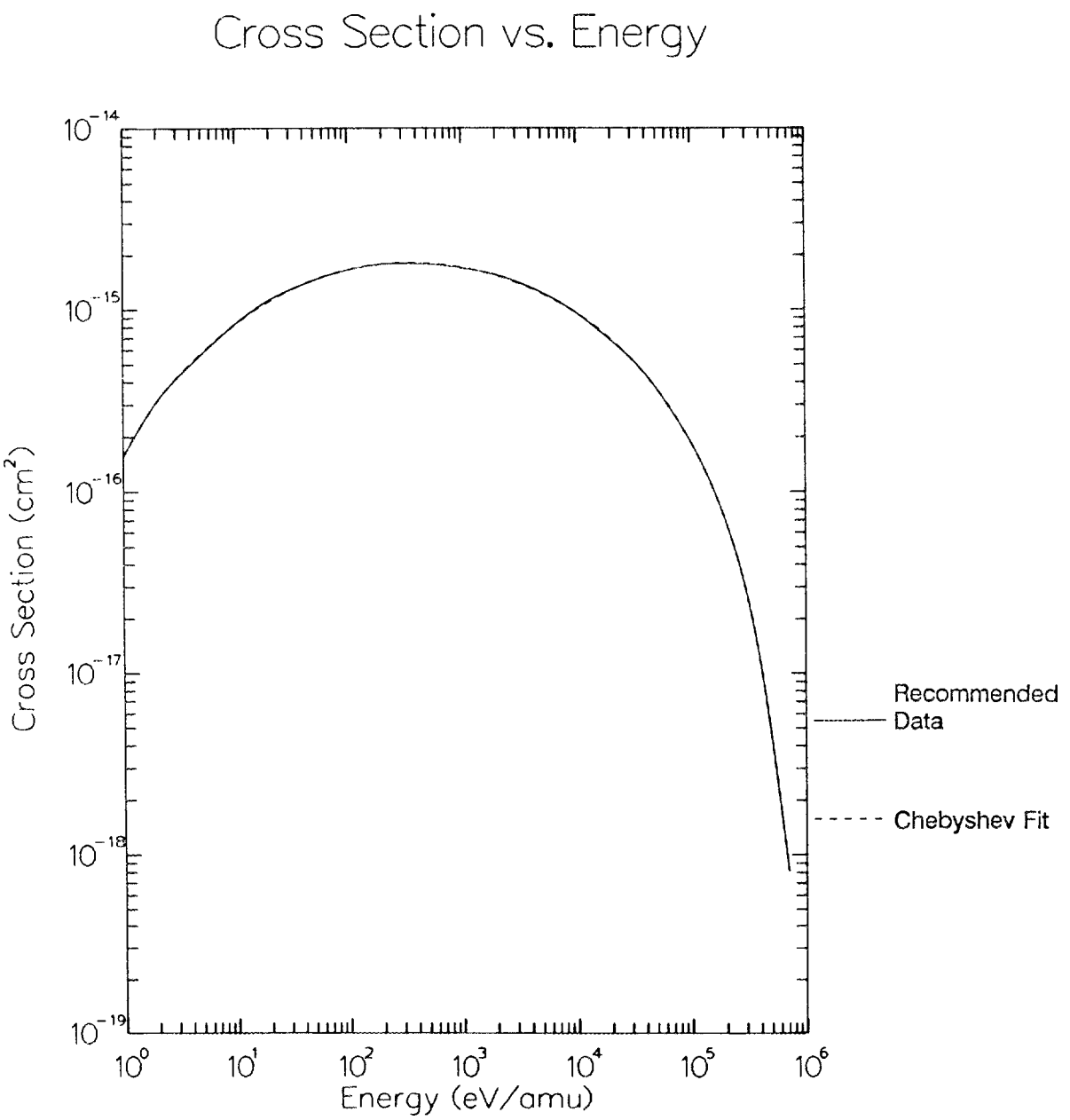
C1	C2	C3	C4	C5	C6	C7	C8	C9
1.363E-15	-2.279E-16	-8.005E-16	1.862E-16	2.321E-16	-4.510E-17	-3.149E-17	9.203E-18	-3.221E-18

The fit represents the above cross sections with an rms deviation of 1.1%.
The maximum deviation is 2.3% at 2.0E+04 eV/amu.
See appendix for Chebychev fit details.

Appendix B3

GRAPHIC REPRESENTATION OF DATA IN APPENDIX B2
(Taken from Redbook Vol. V, ORNL-6090, 1987)

$$C^{3+} + He \rightarrow C^{2+} + He^{+}$$



Appendix B4

TYPICAL RECOMMENDED RECTION RATE DATA FORMAT
(Taken from Redbook Vol. V, ORNL-6090, 1987)

Total Electron Capture Rate Coefficients for
$C^{3+} + He \rightarrow C^{2+} + He^{+}$

Maxwellian - Maxwellian Rate Coefficients (cm^3/s)

C^{3+} Temp. (eV)	Equal Temp.	He Temp. (eV) 1.	10.	100.	1000.	5000.	10000.	20000.
1.0E+00	9.08E-11	9.07E-11	1.33E-09	1.05E-08	4.31E-08	8.41E-08	1.03E-07	1.17E-07
1.2E+00	1.20E-10	9.78E-11	1.34E-09	1.05E-08	4.31E-08	8.41E-08	1.03E-07	1.17E-07
2.4E+00	3.26E-10	1.44E-10	1.40E-09	1.06E-08	4.31E-08	8.41E-08	1.03E-07	1.17E-07
4.8E+00	7.74E-10	2.45E-10	1.51E-09	1.06E-08	4.32E-08	8.41E-08	1.03E-07	1.17E-07
8.4E+00	1.45E-09	4.08E-10	1.67E-09	1.07E-08	4.32E-08	8.41E-08	1.03E-07	1.17E-07
1.2E+01	2.11E-09	5.76E-10	1.84E-09	1.08E-08	4.32E-08	8.41E-08	1.03E-07	1.17E-07
2.4E+01	4.12E-09	1.14E-09	2.38E-09	1.11E-08	4.33E-08	8.42E-08	1.03E-07	1.17E-07
4.8E+01	7.44E-09	2.24E-09	3.40E-09	1.17E-08	4.35E-08	8.42E-08	1.03E-07	1.17E-07
8.4E+01	1.14E-08	3.76E-09	4.80E-09	1.26E-08	4.37E-08	8.43E-08	1.03E-07	1.17E-07
1.2E+02	1.47E-08	5.13E-09	6.08E-09	1.34E-08	4.40E-08	8.43E-08	1.03E-07	1.17E-07
2.4E+02	2.31E-08	8.95E-09	9.70E-09	1.59E-08	4.48E-08	8.46E-08	1.03E-07	1.17E-07
4.8E+02	3.43E-08	1.48E-08	1.53E-08	2.03E-08	4.63E-08	8.50E-08	1.03E-07	1.17E-07
8.4E+02	4.56E-08	2.13E-08	2.17E-08	2.56E-08	4.85E-08	8.56E-08	1.03E-07	1.17E-07
1.2E+03	5.38E-08	2.64E-08	2.67E-08	3.00E-08	5.06E-08	8.63E-08	1.04E-07	1.18E-07
2.4E+03	7.17E-08	3.86E-08	3.88E-08	4.09E-08	5.67E-08	8.82E-08	1.05E-07	1.18E-07
4.8E+03	9.09E-08	5.38E-08	5.39E-08	5.53E-08	6.61E-08	9.18E-08	1.06E-07	1.18E-07
8.4E+03	1.05E-07	6.81E-08	6.82E-08	6.91E-08	7.65E-08	9.63E-08	1.08E-07	1.19E-07
1.2E+04	1.13E-07	7.79E-08	7.80E-08	7.86E-08	8.41E-08	1.00E-07	1.10E-07	1.20E-07
2.0E+04	1.21E-07	9.19E-08	9.20E-08	9.24E-08	9.57E-08	1.06E-07	1.14E-07	1.21E-07

Notes: For Chebychev fits of the above rate coefficients it is necessary to use the following parameters.
E_{min} = 1.0E+00 eV, E_{max} = 2.0E+04 eV

Chebychev Fitting Parameters for Rate Coefficients

He Temp. (eV)	C1	C2	C3	C4	C5	C6	C7
1.	5.269E-08	4.175E-08	2.030E-08	4.953E-09	-2.819E-10	-5.462E-10	-1.174E-10
10.	5.415E-08	4.103E-08	2.014E-08	5.024E-09	-3.186E-10	-6.452E-10	-1.617E-10
100.	6.528E-08	3.606E-08	1.908E-08	5.645E-09	1.992E-11	-7.424E-10	-2.695E-10
1000.	1.113E-07	2.123E-08	1.302E-08	5.433E-09	1.173E-09	-2.174E-10	-3.061E-10
5000.	1.777E-07	8.254E-09	5.472E-09	2.721E-09	9.535E-10	1.753E-10	-5.166E-11
10000.	2.100E-07	4.075E-09	2.757E-09	1.432E-09	5.510E-10	1.357E-10	-5.782E-12
20000.	2.360E-07	1.462E-09	1.003E-09	5.376E-10	2.217E-10	6.535E-11	7.578E-12
Equal Temp.	8.387E-08	6.190E-08	2.244E-08	2.481E-10	-3.237E-09	-1.281E-09	-1.829E-10

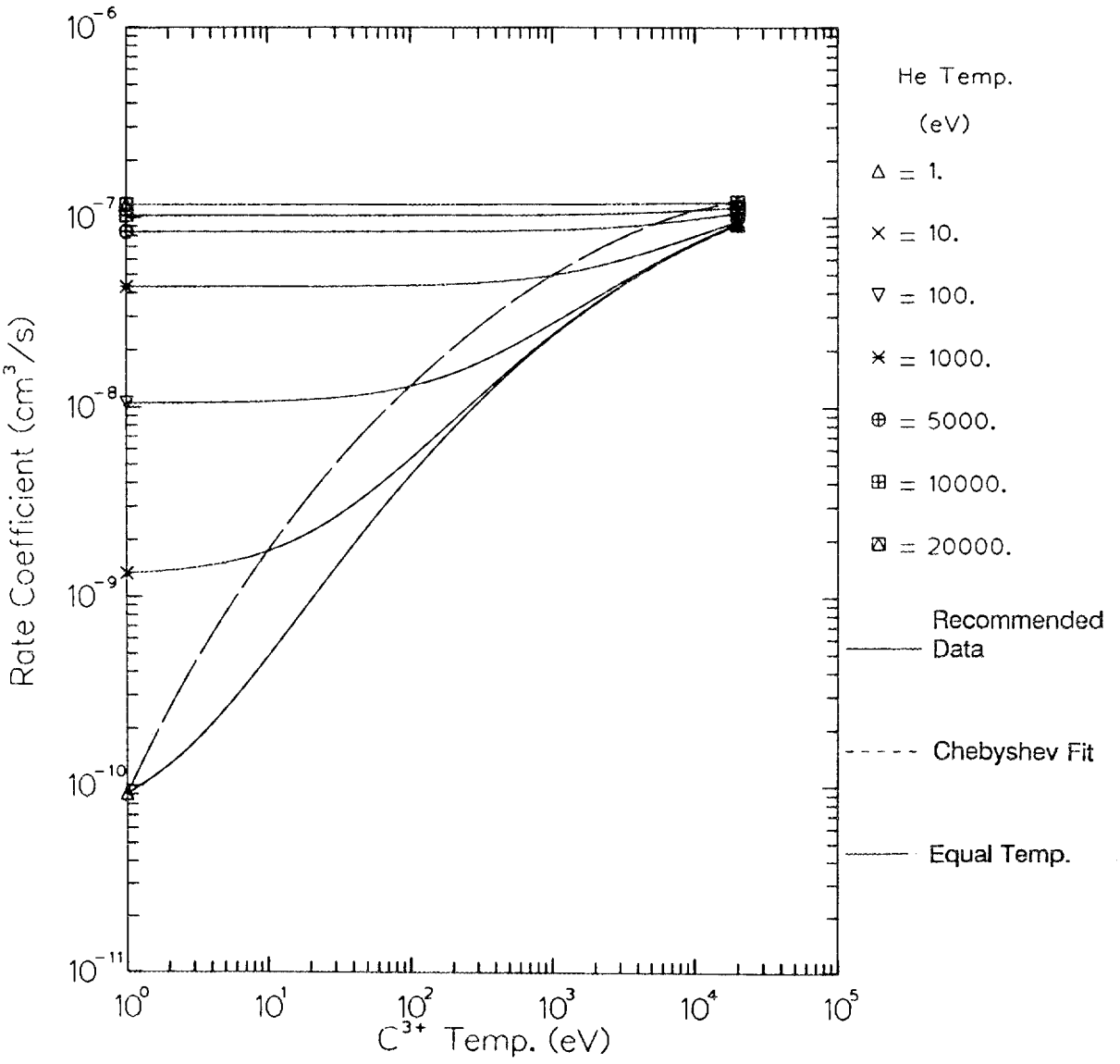
See appendix for Chebychev fit details.

Appendix B5

GRAPHIC REPRESENTATION OF DATA IN APPENDIX B4
(Taken from Redbook Vol. V, ORNL-6090, 1987)

$C^{3+} + He \rightarrow C^{2+} + He^{+}$

Maxwellian – Maxwellian



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