SAMMY Workshop Part 4.3a

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Part 4.3a, Comparison of different methods of treating the data covariance information during an R-matrix analysis

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Different methods for analysis

- **There are a variety of options for treatment of data covariance matrix**
- **Several seemingly-different methods are correct**
  - **These are all effectively equivalent**
- **Several seemingly reasonable methods are incorrect**
  - **Can lead to incorrect results**

How do we find parameter values?

Five-step process:

Step 1. Reduce the data
Step 2. Generate covariance matrix for data
Step 3. Choose prior values for parameters
Step 4. Find prior covariance matrix for parameters
Step 5. Analyze the data

Several different methods:

Method 1. The “conventional” approach
Method 2. A better approach
Method 3. The “usual” approach
Method 4. Another wrong method
Method 5. The hybrid approach
Method 6. Implicit data covariance method

The “conventional” approach

(Method 1)

Step 1. Reduce the data

$$r_i \rightarrow d_i$$

$$\text{raw data} \rightarrow \text{reduced data}$$

$$\text{counts per channel} \rightarrow \text{cross section}$$

Note that

$$d_i = D(r_i,\ r_{\tilde{i}},\ q_1,\ q_2,\ q_3, \ldots)$$

where q are data-reduction parameters

example: See Natural-Nickel Transmission paper

Step 2. Generate the data covariance matrix

Covariance matrix for *raw* data is diagonal:

$$\begin{pmatrix} \Delta^2 r_1 & 0 & 0 & 0 \\ 0 & \Delta^2 r_2 & 0 & 0 \\ 0 & 0 & \Delta^2 r_3 & 0 \\ 0 & 0 & 0 & \Delta^2 r_4 \end{pmatrix}$$

Simple case: $d_i = a\, r_i + b$

Covariance matrix for *reduced* data is **not** diagonal:

$$\begin{pmatrix} (a^2 \Delta^2 r_1 + r_1^2 \Delta^2 a + \Delta^2 b) & & & \\ (r_1 r_2 \Delta^2 a + \Delta^2 b) & (a^2 \Delta^2 r_2 + r_2^2 \Delta^2 a + \Delta^2 b) & & \\ (r_1 r_3 \Delta^2 a + \Delta^2 b) & (r_2 r_3 \Delta^2 a + \Delta^2 b) & (a^2 \Delta^2 r_3 + r_3^2 \Delta^2 a + \Delta^2 b) & \\ (r_1 r_4 \Delta^2 a + \Delta^2 b) & (r_2 r_4 \Delta^2 a + \Delta^2 b) & (r_3 r_4 \Delta^2 a + \Delta^2 b) & (a^2 \Delta^2 r_4 + r_4^2 \Delta^2 a + \Delta^2 b) \end{pmatrix}$$

General case:

$$d_i = D(r_i,\ r_{\tilde{i}},\ q_1,\ q_2,\ q_3, \ldots)$$

$$\delta d_i = \frac{\partial D_i}{\partial r_i}\,\delta r_i + \frac{\partial D_i}{\partial r_{\tilde{i}}}\,\delta r_{\tilde{i}} + \sum_k \frac{\partial D_i}{\partial q_k}\,\delta q_k$$

$$V_{ij} = \left\langle \delta d_i\, \delta d_j \right\rangle$$

$$= \delta_{ij}\left[\left(\frac{\partial D_i}{\partial r_i}\right)^2 \Delta^2 r_i + \left(\frac{\partial D_i}{\partial r_{\tilde{i}}}\right)^2 \Delta^2 r_{\tilde{i}}\right] + \sum_k \sum_l \frac{\partial D_i}{\partial q_k}\,\frac{\partial D_j}{\partial q_l}\,\left\langle \delta q_k\, \delta q_l \right\rangle$$

ALEX: Computer code to do the busy-work of generating V_{ij}

Natural Nickel: 30 parameters, 60,000 data points
1,800,030,000 elements in covariance matrix

Step 3. Find "prior" values for model parameters

- from the literature
- estimate by examining the data

Step 4. Set prior parameter covariance matrix

Note that conventional least squares implicitly assumes that prior uncertainties are infinite and correlations are zero.

Bayes' method (generalized least squares) requires explicit numbers:

- When uncertainties are known, they should be used. Correlations should also be included.
- When nothing is known use "non-informative prior" (i.e. infinite uncertainty). In SAMMY use ~ 10% of the parameter value, which is effectively infinite.

Step 5. Analyze the data

I.e. find values for parameters that give "best fit" to data
I.e. run SAMMY (or REFIT, or ... ?)

Output includes parameter values and parameter covariance matrix.

The end of conventional approach.

A better approach (Method 2)

Fit the raw data directly

Step 1. Do not reduce the data
but do figure out exactly what would need to be done to convert to cross sections

Step 2. Do not generate data covariance matrix (raw data has diagonal covariance matrix)

Step 3. Find prior values for model parameters, *including data-reduction parameters*

Step 4. Set prior parameter covariance matrix, *including uncertainties and covariances for data-reduction parameters*

Step 5. Analyze the data
Analysis code must convert from cross-section to whatever function was actually measured.

The "usual" approach (Method 3)

Just like the "conventional" approach except pretend that the covariance matrix for the reduced data is diagonal:

Simple case:

$$\begin{pmatrix} (a^2\,\Delta^2 r_1 + r_1^2\,\Delta^2 a + \Delta^2 b) & & & \\ 0 & (a^2\,\Delta^2 r_2 + r_2^2\,\Delta^2 a + \Delta^2 b) & & \\ 0 & 0 & (a^2\,\Delta^2 r_3 + r_3^2\,\Delta^2 a + \Delta^2 b) & \\ 0 & 0 & 0 & (a^2\,\Delta^2 r_4 \;\; r_4^2\,\Delta^2 a + \Delta^2 b) \end{pmatrix}$$

General Case:

$$V_{ij} \approx \delta_{ij} \left[\left(\frac{\partial D_i}{\partial r_i} \right)^2 \Delta^2 r_i + \left(\frac{\partial D_i}{\partial r_{\tilde{i}}} \right)^2 \Delta^2 r_{\tilde{i}} + \sum_k \sum_l \frac{\partial D_i}{\partial q_k} \frac{\partial D_i}{\partial q_l} \left\langle \delta q_k \, \delta q_l \right\rangle \right]$$

<u>Question</u>: What's wrong with this?

<u>Answer</u>: It can

- distort results
- hide inconsistencies

Which method to use?

The data-covariance approach is OK, *but often cumbersome*:

- Experimentalists don't like to generate covariance matrices
- There are too many numbers!
- Mistakes may be hidden from evaluators

The fit-to-raw-data approach is best, *but is usually neither practical nor probable*:

- Analysis codes must include all the data-reduction procedures
- Experimentalists are not happy with publishing "counts per channel" rather than "cross section"

The "drop-the-off-diagonal-elements" approach is just plain wrong!

Fortunately, there are alternatives...

Possible Analysis Methods

Method 1. Fit reduced data using true off-diagonal covariance matrix -- "the conventional approach"

Method 2. Fit to raw data, using data-reduction operations (in reverse) on the theory instead of on the data -- "a better approach"

Method 3. Fit reduced data using diagonal part of covariance matrix (both statistical and systematic errors) -- "the usual approach"

Method 4. Fit reduced data using only statistical errors (diagonal)

Method 5. Fit reduced data with pseudo data-reduction parameters included (hybrid method)

Method 6. Adjust the reduced data using parameter values obtained in Method 5, then fit using implicit data covariance

Note that Method 2 is exact, Methods 1, 5, and 6 are correct, Methods 3 & 4 are wrong!

Example: ^{241}Am (see test case tr74 and exercise ex018; neither is exactly like this example, but both are similar)

Data – based on measured values but modified for this example

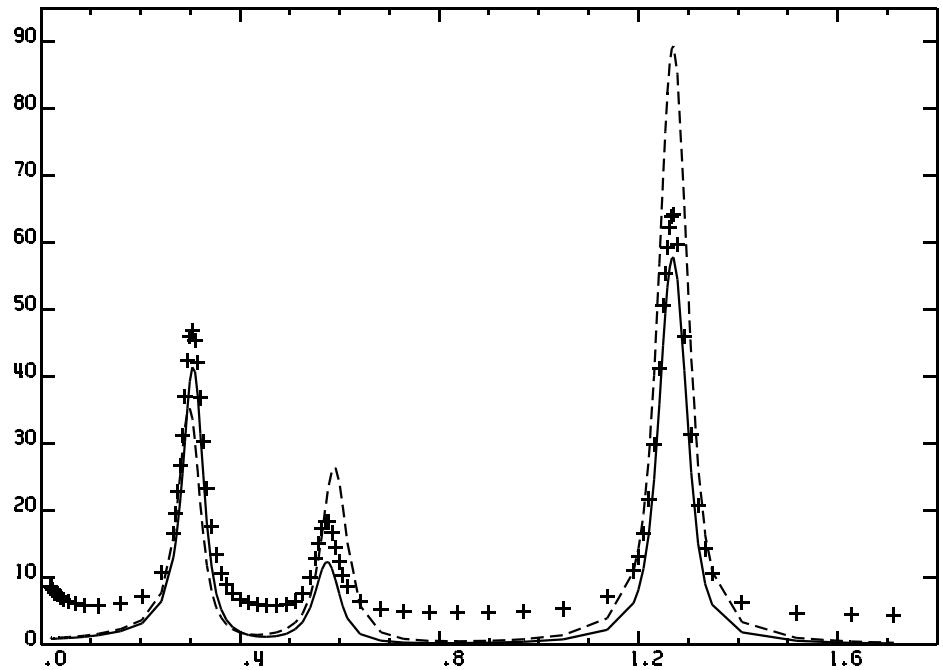
- Assume the "raw data" are related to the experimental fission cross section as r_i = (1031 × σ_i + 4970) counts.

- Assume the uncertainty on r_i is given by $\Delta r_i = \sqrt{r_i}$

- The reduced data should then be of the form $d_i = a\, r_i + b$
  where normalization a is ~ 1/1031 ~ 0.00097
  and background b is ~ - 4970/1031 ~ - 4.82

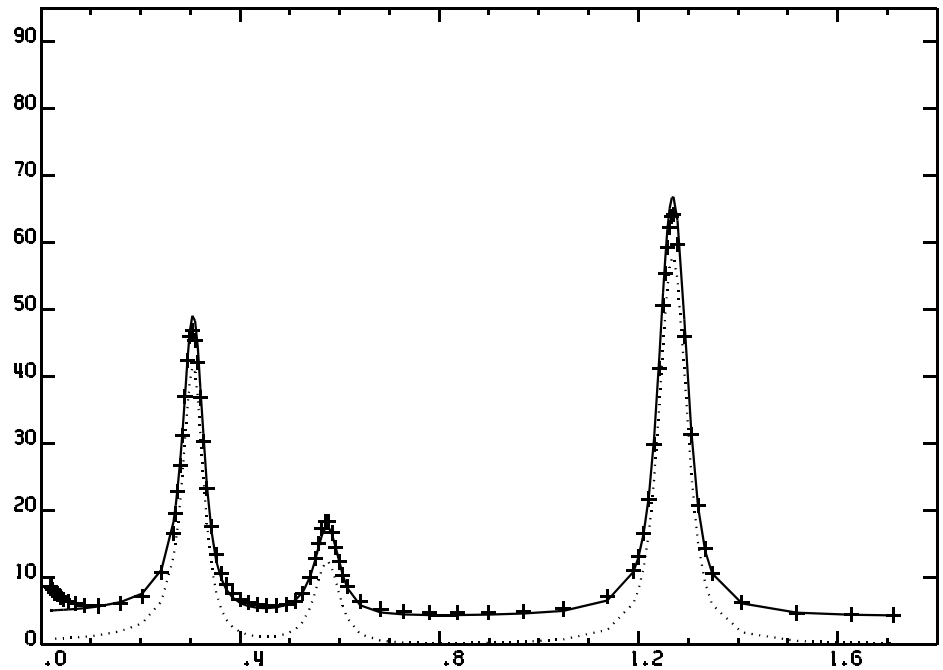
- Assume the experimenter measured the normalization and background (erroneously) as a = 0.00105 ± 0.00007 and b = -1.05 ± 1.05

Query: Can the analysis process nevertheless give the correct cross section (i.e. the correct resonance parameters) ?



Fission cross section for ^{241}Am using Method 1
(fit reduced data using covariance matrix)

- crosses = reduced data
- dashed curve = *a priori* parameter values
- solid curve = SAMMY fit

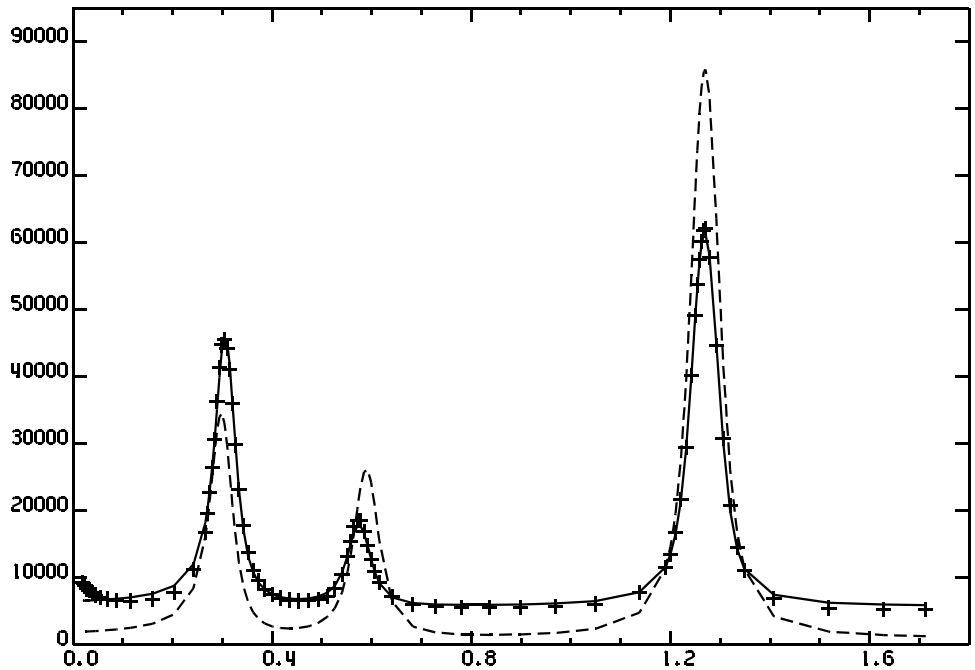


Fission cross section for ^{241} Am

Using Method 1, revised plot

(fit reduced data using covariance matrix)

- crosses = reduced data
- dotted curve = SAMMY fit (as shown in solid curve on previous plot)
- solid curve = SAMMY fit adjusted by data-reduction parameters (1.08421×dotted+4.17895)

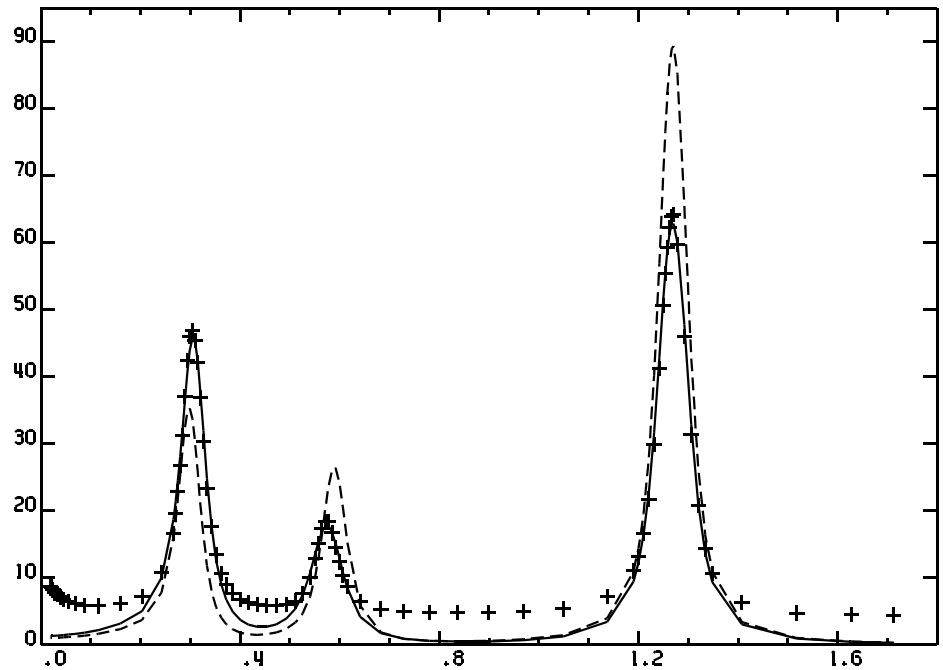


Fission cross section for ^{241} Am

Using Method 2, "a better approach"

(fit raw data using data-reduction operations in reverse)

- crosses = raw data
- dashed curve = with *a priori* parameter values
- solid curve = SAMMY fit

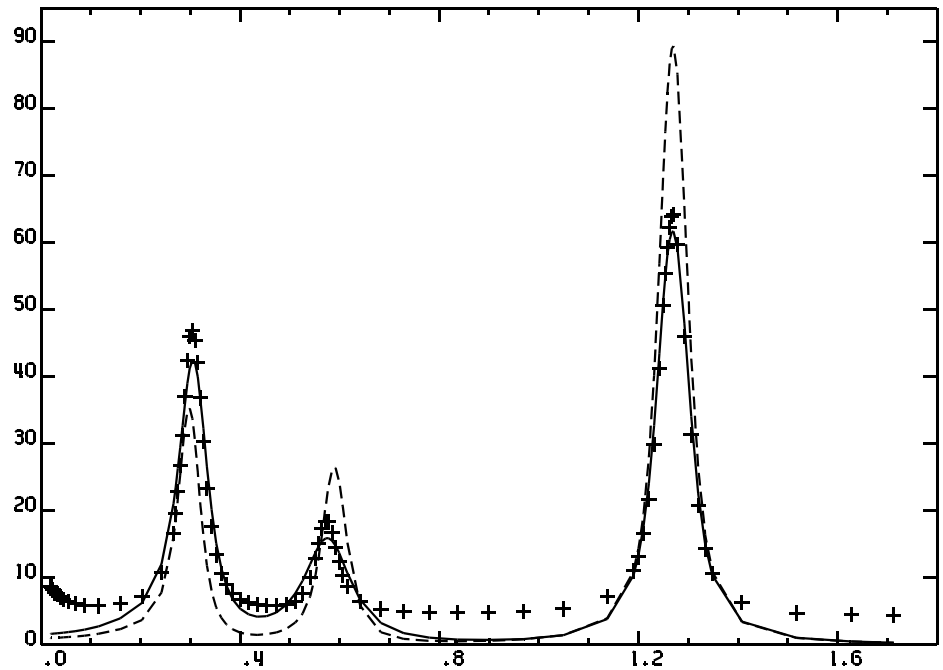


Fission cross section for ^{241} Am

Using Method 3, “the usual approach”

(fit reduced data using diagonal portion of covariance matrix)

- crosses = reduced data
- dashed curve = with *a priori* parameter values
- solid curve = SAMMY fit

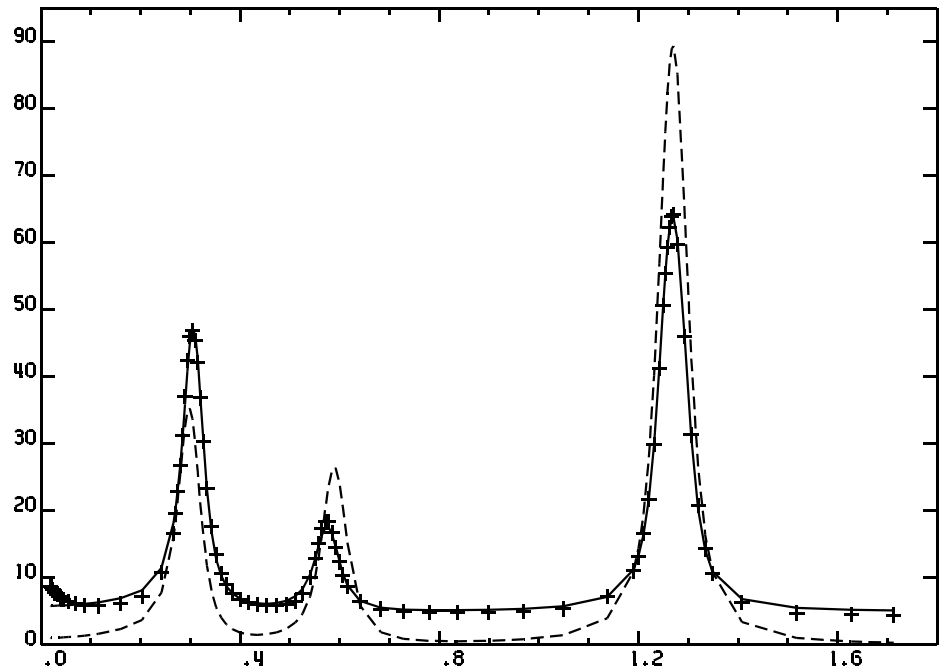


Fission cross section for ^{241} Am

Using Method 4

(fit reduced data with statistical errors only)

- crosses = reduced data
- dashed curve = with *a priori* parameter values
- solid curve = SAMMY fit

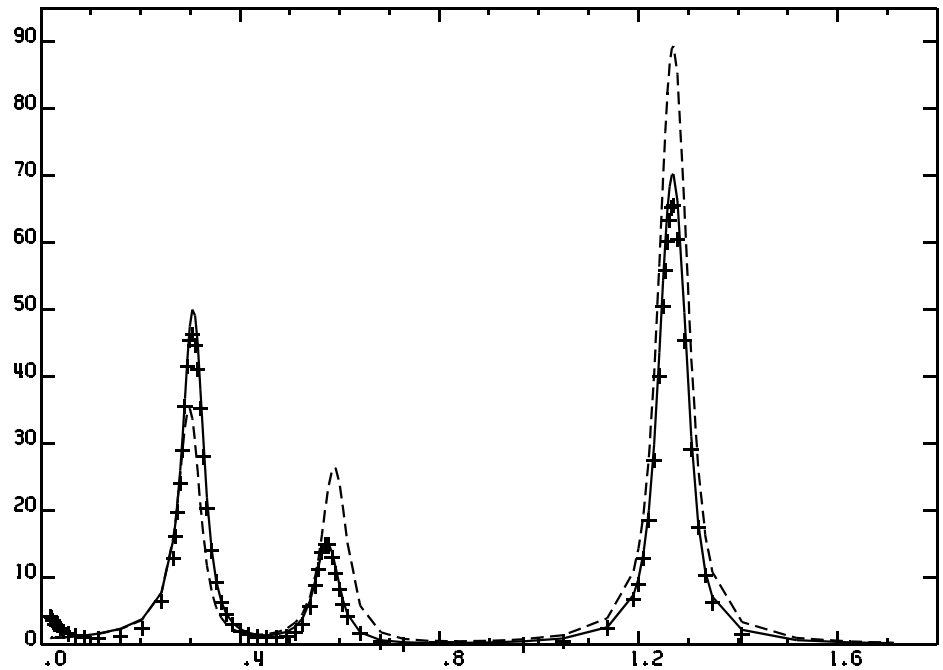


Fission cross section for ^{241}Am

Using Method 5

(fit reduced data but include data-reduction operations)

- crosses = reduced data
- dashed curve = with *a priori* parameter values
- solid curve = SAMMY fit



Fission cross section for ^{241} Am

Using Method 6, implicit data covariance
(fit *adjusted* reduced data)

- crosses = adjusted reduced data
- dashed curve = with *a priori* parameter values
- solid curve = SAMMY fit

Comparison of parameter values

	prior	1 explicit	2 raw	3 diagonal	4 statistical	5 hybrid	6 implicit
E_1	.3000 ±.0294	.3073 ±.0001	.3071 ±.0001	.3081 ±.0001	.3086 ±.0001	.3072 ±.0001	.3073 ±.0001
Γ_1	47.39 ± 4.70	43.60 ± 0.20	43.41 ± .20	62.09 ± 0.26	67.85 ± 0.22	43.12 ± 0.20	43.57 ± 0.20
Γ_{1f}	.3200 ±.0233	.3237 ±.0198	.3277 ±.0204	.4116 ±.0219	.4782 ±.0226	.3205 ±.0201	.3234 ±.0198
E_2	.5900 ±.0321	.5765 ±.0001	.5758 ±.0002	.5776 ±.0002	.5781 ±.0002	.5763 ±.0002	.5765 ±.0002
Γ_2	48.15 ± 4.75	46.50 ± 0.49	43.77 ± 0.52	108.73 ± 0.85	117.09 ± 0.63	44.81 ± 0.50	46.41 ± 0.49
Γ_{2f}	.6000 ±.0447	.4455 ±.0335	.4417 ±.0337	.8667 ±.0464	.9810 ±0.050	.4398 ±.0336	.4450 ±.0335
E_3	1.270 ± .356	1.2696 ±.0001	1.2695 ±.0001	1.2695 ±.0008	1.2693 ±.0001	1.2695 ±.0001	1.2695 ±.0001
Γ_3	47.69 ± 4.67	42.91 ± 0.33	42.33 ± 0.34	57.21 ± 0.42	59.77 ± 0.42	42.41 ± 0.33	42.88 ± 0.33
Γ_{3f}	.8001 ±.0800	.5674 ±.0474	.5772 ±.0488	.7389 ±.0542	.7627 ±.0481	.5627 ±.0481	.5671 ±.0474

Note that there are actually five parameters for each resonance: energy E_λ, widths $\Gamma_{\lambda\gamma}$, $\Gamma_{\lambda n}$, $\Gamma_{\lambda f1}$, and $\Gamma_{\lambda f2}$. However, the combinations which are relevant to fission cross sections for isolated resonances are included in the table. These are E_λ, $\Gamma_\lambda = \Gamma_{\lambda\gamma} + \Gamma_{\lambda n} + |\Gamma_{\lambda f1}| + |\Gamma_{\lambda f2}|$, and $\Gamma_{\lambda f} = |\Gamma_{\lambda f1}| + |\Gamma_{\lambda f2}|$.

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