

# **INDC International Nuclear Data Committee**

# A Survey of ENDF/B-VIII Resonance Parameters (MF=2)

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#### **ABSTRACT**

This report is a graphic survey of ENDF/B-VIII Resonance Parameters. The intent is to present the status of this data today (2020), compared to the development of ENDF/B over the last more than fifty years, and based on our experience to recommend how we can continue to improve in the future. Let me assure you that we have made enormous progress in our evaluated data compared to where we were 50 years ago, and this report is only intended to present what I hope will be constructive criticism, of our already excellent data.

#### **DEDICATION**

I dedicate this report to my dear friend of more than 50 years, Said Mughabghab, who throughout all these years devoted so much of his time and energy to Neutron Cross Sections, BNL-325. He contributed so much toward getting us to where we are today with resonance parameters. Said definitely left his mark and is greatly missed by all of us.

#### Acknowledgement

I thank Roberto Capote and Kira Nathani (Nuclear Data Section, IAEA, Vienna) for editing this report and making it available in a timely manner.

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# History 101

ENDF was started by Henry Honeck at Brookhaven National Laboratory (BNL) circa 1965; much of the design of ENDF was based on the earlier work on UKNDL (United Kingdom Nuclear Data Library). At the time one of our biggest problems was a lack of agreement of even the most basic of nuclear data definitions, e.g., each "standard" textbook could have its own definition of something as simple as single level Breit-Wigner resonance parameters. This made is virtually impossible to perform any benchmark or comparative studies, or to exchange data between computer codes or labs, with any degree of confidence that everyone would UNIQUELY interpret the data; without this confidence results could be not only useless, but even worse: misleading.

One of the most important things that has made ENDF such a big success is that Henry recognized this and attempted to standardize, as much as possible, the definitions and how to interpret nuclear data in the ENDF format; the result is ENDF-102 [1]. Henry had the foresight to understand that what was – and still is – most important is that the definitions and conventions need not be perfect or even necessarily the best or most widely accepted – **UNIQUE** – that is what is most important so that ALL ENDF users – data producers and users – we must ALL agree to use the UNIQUE ENDF definitions that are currently documented in what today I call the "ENDF Bible", ENDF-102.

Indeed, one of the biggest problems over the years has been due to new ENDF users who truly believe they have better ways to define evaluated data and they used different definitions in their evaluation. Here the intention was always good, but the results have been disastrous, because their data was not understood or uniquely interpreted by data users; this has many times resulted in inaccurate, and sometimes dangerous results in our applications [2, 3] and processing [4, 5, 6].

If you want to constructively contribute to the ENDF effort, PLEASE do not try to be independently creative and go rogue and misuse ENDF. Rather you can help improve ENDF by officially incorporating your ideas. Be aware that ENDF is not frozen in time; over the years it has evolved to meet current needs. These advances have always been accomplished and controlled through the governing body: The Cross Section Evaluation Working Group (CSEWG), that meets yearly, to among other things review proposed changes to ENDF formats and conventions. So, if you disagree with the current ENDF rules, PLEASE – it is so important – that you do not act individually to meet your personal ideas and needs. Instead please submit your ideas to CSEWG to allow our entire nuclear data community to review your suggestion, and to either accept your suggestion, that we will ALL then obey in the future. Alternatively, they can explain to you why your idea does not neatly "best" fit within ENDF system.

And very important: Remember that with ENDF what is most important is that the rules need not be perfect or even the best — **UNIQUE** is what is important. Ultimately the bottom line is that we MUST have UNIQUE rules that evaluators agree to follow when creating our evaluated data, and that users agree to follow in interpreting the evaluated data they receive in the ENDF format. Without this agreement by ALL parties involved we will not have a system, but rather CHAOS.

# A Survey of ENDF/B-VIII Resonance Parameters (MF=2)

#### **ENDF** Format

Here I assume readers are familiar with ENDF-102 definitions and conventions [1], and I will freely use ENDF terminology throughout this report. One of the prime reasons for the worldwide success of ENDF over more than the last 50 years, in the documentation included in ENDF-102 to uniquely define each and every parameter used in the ENDF format, and most important, the agreement of EVERYONE (both data producers and users) to strictly conform to these definitions. It is not the generality of ENDF, but rather the strict, unique definitions defined in the ENDF Bible (ENDF-102), that has made it such a success.

# ENDF/B-VIII

ENDF/B-VIII [7] is the 8-th release of the ENDF/B library, first released over 50 years ago. There are a variety of combinations of types of resonance parameters (MF=2) data that may be included in any given ENDF formatted evaluation, as defined by ENDF parameters LRU & LRF [1]. These are combined with any tabulated "background" cross sections (MF=3), to define the cross sections that we actually use in our applications [2, 3], and processing [4, 5, 6]. For ENDF/B-VIII we find,

```
0 = No MF=2 (i.e., Every Evaluation includes MF=2)
64 = No Parameters (LRU = 0); only scattering radius given in MF=2; MF=3 defines cross sections.
143 = Only Resolved (LRU = 1)
31 = Only Unresolved (LRU = 2)
315 = Resolved & Unresolved (LRU= 1 & 2)
553 = Total Number of Evaluations in ENDF/B-VIII
```

The <u>resolved</u> resonance region (LRU=1), ENDF [1] includes seven (7) different types of resonance parameters as defined by the ENDF resolved parameter LRF [1]. For ENDF/B-VIII we find,

```
0 = LRF=1, single-level Breit-Wigner (SLBW)
399 = LRF=2, multilevel Breit-Wigner (MLBW)
49 = LRF=3, Reich-Moore (RM)
0 = LRF=4, Adler-Adler (AA)
0 = LRF=5, no longer available
0 = LRF=6, no longer available
10 = LRF=7, R-Matrix Limited (RML)
458 = Total having LRU=1 (Resolved Parameters)
```

Note in particular,

- 1) There are no LRF=1, single-level Breit-Wigner (SLBW)
- 2) There are no LRF=4, Adler-Adler (AA); LRF=5 and 6 are no longer allowed
- 3) There are only 10 LRF=7 R-Matrix Limited (RML) evaluations
- 4) Most are: 399 LRF=2, multi-level (MLBW) and 49 LRF=3, Reich-Moore (RM)

The unresolved resonance region (LRU=2), ENDF [1] only allows single-level (SLBW) resonances [1]; it includes two (2) different types of energy dependent resonance parameters based on ENDF unresolved parameter LRF. For ENDF/B-VIII we find,

```
4 = LRF=1, Energy Independent Unresolved Parameters 342 = LRF=2, Energy Dependent Unresolved Parameters 346 = Total having LRU=2 (Unresolved parameters)
```

# 

Unresolved/LRF

0 = Non = No Parameters 1 = Res = Resolved 2 = Unr = Unresolved

0 = None 2 = Multi-Level 1 = Energy Independent
2 = Energy Dependent

3 = Reich-Moore (RM)

7 = R-Matrix Limited (RML)

E	Terrolination IDII	E1tion IDII	Elustics IDII	Elustics IDII
Evaluation LRU	Evaluation LRU	Evaluation LRU N R U	Evaluation LRU	Evaluation LRU
NRU	NRU	_	NRU	N R U o e n
o e n	oen	o e n	o e n	
nsr	nsr	nsr	nsr	nsr
Neutron 0	20-Ca-45 2 2	33-As-74 2 2	43-Tc-99 2 2	50-Sn-118 2 2
1-н -1 0	20-Ca-46 0	33-As-75 2 2	44-Ru-96 2	50-Sn-119 2 2
1-н -2 0	20-Ca-47 2 2	34-Se-74 2 2	44-Ru-97 2 2	50-Sn-120 2 2
1-н -3 0	20-Ca-48 2	34-Se-75 2 2	44-Ru-98 2	50-Sn-121m 2 2
2-не-3 0	21-Sc-45 2	34-Se-76 2 2	44-Ru-99 2 2	50-Sn-122 2
2-He-4 0	22-Ti-46 2	34-Se-77 2 2	44-Ru-100 2 2	50-Sn-123 2
3-Li-6 0	22-Ti-47 2	34-Se-78 2 2	44-Ru-101 2 2	50-Sn-124 2
3-Li-7 0	22-Ti-48 3	34-Se-79 2	44-Ru-102 2 2	50-Sn-125 2 2
4-Be-7 0	22-Ti-49 2	34-Se-80 2 2	44-Ru-103 2 2	50-Sn-126 2
4-Be-9 0	22-Ti-50 2	34-Se-81 2	44-Ru-104 2 2	51-Sb-121 2 2
5-B -10 0	23-V -49 2 2	34-Se-82 2 2	44-Ru-105 0	51-Sb-122 2
5-B -11 0	23-V -50 2	35-Br-79 2 2	44-Ru-106 2	51-Sb-123 2 2
6-C -12 0	23-V -51 3	35-Br-80 2	45-Rh-103 2 2	51-Sb-124 2
6-C -13 0	24-Cr-50 3	35-Br-81 2 2	45-Rh-104 2	51-Sb-125 2
7-N -14 0	24-Cr-51 2 2	36-Kr-78 2 2	45-Rh-105 2 2	51-Sb-126 2 2
7-N -15 0	24-Cr-52 3	36-Kr-79 2	46-Pd-102 2	52-Te-120 2
8-0 -16 0	24-Cr-53 3	36-Kr-80 2 2	46-Pd-103 2 2	52-Te-121 2
8-0 -17 0	24-Cr-54 3	36-Kr-81 2 2	46-Pd-104 2	52-Te-121m 2
8-0 -18 2	25-Mn-54 2 2	36-Kr-82 2 2	46-Pd-105 2 2	52-Te-122 2 2
9-F -19 0	25-Mn-55 3 2	36-Kr-83 2 2	46-Pd-106 2	52-Te-123 2 2
10-Ne-20 2	26-Fe-54 7	36-Kr-84 2	46-Pd-107 2 2	52-Te-124 2 2
10-Ne-21 2 2	26-Fe-55 2 2	36-Kr-85 2 2	46-Pd-108 2	52-Te-125 2 2
10-Ne-22 2 2	26-Fe-56 3	36-Kr-86 2	46-Pd-109 2	52-Te-126 2 2
11-Na-22 2 2	26-Fe-57 7	37-Rb-85 2 2	46-Pd-110 2	52-Te-127m 2
11-Na-23 2	26-Fe-58 3 1	37-Rb-86 2 2	47-Ag-107 2 2	52-Te-128 2 2
12-Mg-24 2	27-Co-58 2 2	37-Rb-87 2 2	47-Ag-108 2	52-Te-129m 2
12-Mg-25 2	27-Co-58m 2	38-Sr-84 2 2	47-Ag-109 2 2	52-Te-130 2 2
12-Mg-26 2	27-Co-59 3	38-Sr-85 2	47-Ag-110m 2 2	52-Te-131 2
13-A1-26m 2	28-Ni-58 3	38-Sr-86 2 2	47-Ag-111 2 2	52-Te-131m 2
13-A1-27 3	28-Ni-59 2 2	38-Sr-87 2 2	47-Ag-112 2	52-Te-132 2 2
14-Si-28 3	28-Ni-60 3	38-sr-88 2	47-Ag-113 2	53-I -127 2
14-Si-29 3	28-Ni-61 2	38-Sr-89 2	47-Ag-114 2	53-I -128 2
14-Si-30 3	28-Ni-62 2 2	38-Sr-90 2	47-Ag-115 2	53-I -129 2 2
14-Si-31 2	28-Ni-63 2 2	39-Y -89 2	47-Ag-116 2	53-I -130 2 2
14-Si-32 2	28-Ni-64 2	39-Y -90 2 2	47-Ag-117 2	53-I -131 2
15-P -31 0	29-Cu-63 7	39-Y -91 2	47-Ag-117 2 47-Ag-118m 2 2	53-I -131 2 53-I -132 2
16-S -32 2	29-Cu-64 2	40-Zr-90 2 2	48-Cd-106 3 2	53-I -132m 2
16-S -33 2	29-Cu-65 7	40-Zr-91 2 2	48-Cd-107 2	53-I -133 2
16-S -34 2	30-Zn-64 2 2	40-Zr-91 2 2 40-Zr-92 2 2	48-Cd-107 2 48-Cd-108 3 2	53-I -133 2 53-I -134 2
16-S -35 2 2	30-Zn-65 2	40-Zr-93 2 2	48-Cd-109 2 2	53-I -134 2 53-I -135 0
17-C1-35 7	30-Zn-66 2 2	40-Zr-94 2 2	48-Cd-110 3 2	54-Xe-123 0
17-C1-35 7 17-C1-36 2 2	30-Zn-66 2 2 30-Zn-67 2 2	40-Zr-94 2 2 40-Zr-95 2	48-Cd-110 3 2 48-Cd-111 3 2	54-Xe-123 0 54-Xe-124 2 2
17-C1-36 2 2 17-C1-37 3	30-Zn-68 2 2	40-Zr-95 2 40-Zr-96 2 2	48-Cd-111 3 2 48-Cd-112 3 2	54-Xe-125 2
18-Ar-36 2 2	30-Zn-69 2 2	41-Nb-93 2 2	48-Cd-112 3 2 48-Cd-113 2 2	54-Xe-126 2 2
18-Ar-36 2 2 18-Ar-37 2 2	30-Zn-69 2 30-Zn-70 2 2			
		41-Nb-94 2 2 41-Nb-95 2		
			48-Cd-115m 2 2	
18-Ar-39 2	31-Ga-70 2	42-Mo-92 2 2	48-Cd-116 3 2	54-Xe-129 2 2
18-Ar-40 3	31-Ga-71 2	42-Mo-93 2 2	49-In-113 2 2	54-Xe-130 2
18-Ar-41 2 2	32-Ge-70 2 2	42-Mo-94 2 2	49-In-114 2	54-Xe-131 2 2
19-к -39 3	32-Ge-71 2 2	42-Mo-95 2 2	49-In-115 2 2	54-Xe-132 2 2
19-K -41 3	32-Ge-72 2 2	42-Mo-96 2 2	50-Sn-112 2 2	54-Xe-133 2
20-Ca-40 7	32-Ge-73 2 2	42-Mo-97 2 2	50-Sn-113 2 2	54-Xe-134 2 2
20-Ca-41 2	32-Ge-74 2 2	42-Mo-98 2 2	50-Sn-114 2 2	54-Xe-135 2 2
20-Ca-42 2	32-Ge-75 2	42-Mo-99 2	50-Sn-115 2 2	54-Xe-136 2
20-Ca-43 2	32-Ge-76 2 2	42-Mo-100 2 2	50-Sn-116 2 2	55-Cs-133 2 2
20-Ca-44 2	33-As-73 3	43-Tc-98 2 2	50-Sn-117 2 2	55-Cs-134 2 2

0 = Non = No Parameters 0 = None 1 = Energy Independent 1 = Res = Resolved 2 = Unr = Unresolved 2 = Multi-Level 2 = Energy Dependent

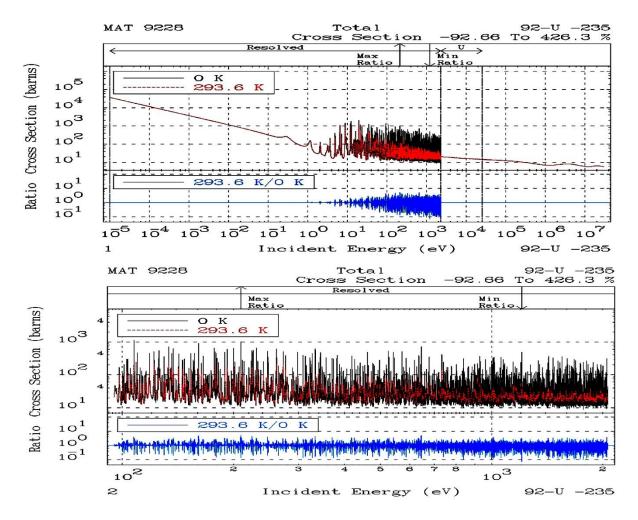
3 = Reich-Moore (RM) 7 = R-Matrix Limited (RML)

Evaluation LRU	Evaluation LRU	Evaluation LRU	Evaluation LRU	Evaluation LRU
NRU	NRU	NRU	NRU	NRU
o e n	o e n	oen	oen	o e n
nsr	nsr	nsr	nsr	nsr
55-Cs-135 2 2	62-Sm-151 2 2	70-Yb-174 2 2	80-Hg-201 2	94-Pu-236 2 2
55-Cs-136 2	62-Sm-152 2 2	70-Yb-175 2 2	80-Hg-202 2	94-Pu-237 0
55-Cs-137 2	62-Sm-153 2 2	70-Yb-176 2 2	80-Hg-203 2 2	94-Pu-238 2 2
56-Ba-130 2 2	62-Sm-154 2 2	71-Lu-175 2 2	80-Hg-204 0	94-Pu-239 3 2
56-Ba-131 2	63-Eu-151 2 2	71-Lu-176 2 2	81-T1-203 2 2	94-Pu-240 3 1
56-Ba-132 2 2	63-Eu-152 2 2	72-Hf-174 2 2	81-T1-204 2 2	94-Pu-241 3 2
56-Ba-133 2 2	63-Eu-153 2 2	72-Hf-175 2	81-T1-205 2 2	94-Pu-242 2 2
56-Ba-134 2 2	63-Eu-154 2 2	72-Hf-176 2 2	82-Pb-204 2	94-Pu-243 2 2
56-Ba-135 2 2	63-Eu-155 2 2	72-Hf-177 2 2	82-Pb-205 2 2	94-Pu-244 2 2
56-Ba-136 2 2	63-Eu-156 2	72-Hf-178 2 2	82-Pb-206 3	94-Pu-245 2
56-Ba-137 2 2	63-Eu-157 2 2	72-Hf-179 2 2	82-Pb-207 3	94-Pu-246 0
56-Ba-138 2	64-Gd-152 3 2	72-Hf-180 2 2	82-Pb-208 3	95-Am-240 0
56-Ba-139 2	64-Gd-153 3 2	72-Hf-181 2	83-Bi-209 2	95-Am-241 2 2
56-Ba-140 2 1	64-Gd-154 3 2	72-Hf-182 2	83-Bi-210m 2 2	95-Am-242 2 2
57-La-138 2 2	64-Gd-155 3 2	73-Ta-180 0	84-Po-208 2 2	95-Am-242m 2 2
57-La-139 2 2	64-Gd-156 3 2	73-Ta-181 2 2	84-Po-209 2 2	95-Am-243 2 2
57-La-140 2 2	64-Gd-157 3 2	73-Ta-182 2 2	84-Po-210 2 2	96-Cm-240 0
58-Ce-136 2 2 58-Ce-137 2	64-Gd-158 3 2 64-Gd-159 2	74-W -180 2 74-W -181 2 2	88-Ra-223 0 88-Ra-224 0	96-Cm-241 0 96-Cm-242 2 2
58-Ce-137 2 58-Ce-137m 2	64-Gd-159 2 64-Gd-160 3 2		88-Ra-224 0 88-Ra-225 0	96-Cm-242 2 2 96-Cm-243 2 2
58-Ce-13/m 2 58-Ce-138 2 2	65-Tb-158 2 2	74-W -182 7 2 74-W -183 7 2	88-Ra-226 2	96-Cm-243 2 2 96-Cm-244 2 2
58-Ce-139 2 2	65-Tb-156 2 2 65-Tb-159 2 2	74-W -183 7 2	89-Ac-225 0	96-Cm-245 2 2
58-Ce-140 2	65-Tb-160 2 2	74-W -185 2	89-Ac-226 0	96-Cm-246 2 2
58-Ce-141 2 2	65-Tb-161 2 2	74-W -186 7 2	89-Ac-227 0	96-Cm-247 2 2
58-Ce-142 2 2	66-Dy-154 2	75-Re-185 2 2	90-Th-227 0	96-Cm-248 2 2
58-Ce-143 2 2	66-Dy-155 2	75-Re-186m 2 2	90-Th-228 2 2	96-Cm-249 0
58-Ce-144 2	66-Dy-156 2 2	75-Re-187 2 2	90-Th-229 2 2	96-Cm-250 2 2
59-Pr-141 2 2	66-Dy-157 2	76-0s-184 2	90-Th-230 2 2	97-Bk-245 0
59-Pr-142 2 2	66-Dy-158 2 2	76-Os-185 2 2	90-Th-231 0	97-Bk-246 0
59-Pr-143 2 2	66-Dy-159 2	76-Os-186 2 2	90-Th-232 3 2	97-Bk-247 0
60-Nd-142 2 2	66-Dy-160 2 2	76-Os-187 2 2	90-Th-233 0	97-Bk-248 0
60-Nd-143 2 2	66-Dy-161 2 2	76-Os-188 2 2	90-Th-234 0	97-Bk-249 2 2
60-Nd-144 2 2	66-Dy-162 2 2	76-Os-189 2 2	91-Pa-229 0	97-Bk-250 0
60-Nd-145 2 2	66-Dy-163 2 2	76-Os-190 2 2	91-Pa-230 0	98-Cf-246 0
60-Nd-146 2 2	66-Dy-164 2 2	76-Os-191 2 2	91-Pa-231 3 2	98-Cf-247 2
60-Nd-147 2 2	67-но-165 2	76-Os-192 2 2	91-Pa-232 2 2	98-Cf-248 0
60-Nd-148 2 2	67-Ho-166m 2 2	77-Ir-191 2	91-Pa-233 3 2	98-Cf-249 2 2
60-Nd-149 2	68-Er-162 2	77-Ir-192 2 2	92-U -230 0	98-Cf-250 2 2
60-Nd-150 2 2 61-Pm-143 2 2	68-Er-163 2 68-Er-164 2	77-Ir-193 2 2 77-Ir-194m 2 2	92-U -231 0	98-Cf-251 2 2 98-Cf-252 2 2
61-Pm-143 2 2 61-Pm-144 2 2	68-Er-164 2 68-Er-165 2	77-Ir-194m 2 2 78-Pt-190 2 2	92-U -232 2 2 92-U -233 3 2	98-Cf-252 2 2 98-Cf-253 0
61-Pm-145 2 2	68-Er-166 2	78-Pt-191 2 2	92-U -234 2 2	98-Cf-254 0
61-Pm-146 2 2	68-Er-167 2 1	78-Pt-191 2 2 78-Pt-192 2 2	92-U -235 3 2	99-Es-251 0
61-Pm-147 2 2	68-Er-168 2	78-Pt-193 2 2	92-U -236 2 2	99-Es-252 0
61-Pm-148 2	68-Er-169 2 2	78-Pt-194 2 2	92-U -237 2 2	99-Es-253 2
61-Pm-148m 2	68-Er-170 2 2	78-Pt-195 2 2	92-U -238 3 2	99-Es-254 0
61-Pm-149 2	69-Tm-168 2	78-Pt-196 2 2	92-U -239 2 2	99-Es-254m 0
61-Pm-150 2	69-Tm-169 2 2	78-Pt-197 2 2	92-U -240 2 2	99-Es-255 0
61-Pm-151 2 2	69-Tm-170 2 2	78-Pt-198 2 2	92-U -241 2 2	100-Fm-255 0
62-Sm-144 2 2	69-Tm-171 2 2	79-Au-197 3 2	93-Np-234 0	
62-Sm-145 2 2	70-Yb-168 2 2	80-Hg-196 2	93-Np-235 0	
62-Sm-146 2	70-Yb-169 2	80-нд-197 2	93-Np-236 2 2	
62-Sm-147 2 2	70-Yb-170 2 2	80-Hg-197m 2	93-Np-236m 2	
62-Sm-148 2 2	70-Yb-171 2 2	80-Hg-198 2	93-Np-237 2 2	
62-Sm-149 2 2	70-Yb-172 2 2	80-Hg-199 2	93-Np-238 2 2	
62-Sm-150 2 2	70-Yb-173 2 2	80-Hg-200 2	93-Np-239 0	

# A Guide to Interpretation of the plots

Most of this report is a series of plots of the ENDF/B-VIII data [7]. All the plots were created using COMPLOT code [4] or PLOTTAB code [8]. Each plot displays the temperature dependent data for a single reaction from a given isotope; COLD (0 Kelvin) and room temperature data, HOT (293.6 Kelvin) are included on each plot. All of the data used here is from POINT2018 [9]; both COMPLOT and **PLOTTAB** codes and the POINT2018 data freely available are on-line. http://RedCullen1.net/HOMPAGE.NEW/; this allows anyone to create these or similar plots to meet individual needs.

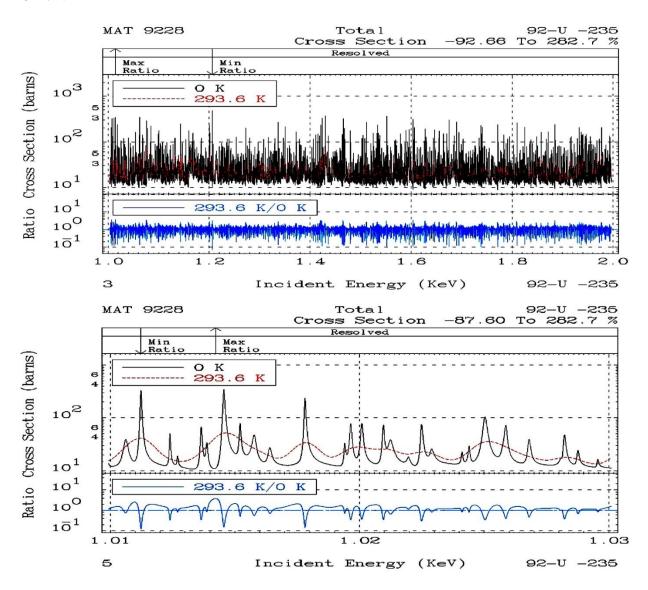
Each of the plots is divided into two sections: the upper two-thirds shows a comparison of the same reaction at two different temperatures: COLD (0 Kelvin) and room temperature, HOT (293.6 Kelvin). The lower one-third shows the ratio of the second set of data divide by the first set, i.e., HOT/COLD. Near the upper right-hand corner of each plot is shown the maximum % differences between the two sets of data; e.g., in the below figure the two sets differ by -92.66% to +426.3%. The position in energy of the minimum and maximum ratios is shown by upward (maximum) and downward (minimum) arrows near the top of each plot. If present, the resolved and unresolved resonance energy ranges are indicated at the top of each plot. If the ratio is extreme, I may restrain the plotted ratio to the range 10 to 1/10; this help clarify ratio.



# Doppler Broadening

The plots are designed to illustrate both the energy dependence of the reaction, as well as its temperature dependence. Even though in all cases the temperature difference here is quite small, i.e., 0 vs. 293.6 K, the effect on the energy dependent cross section can be quite large, and it can extend to surprisingly high energies. Even though 293.6 K corresponds to only 0.0253 eV, milli-eV wide capture cross sections into the KeV energy range can show large temperature effects.

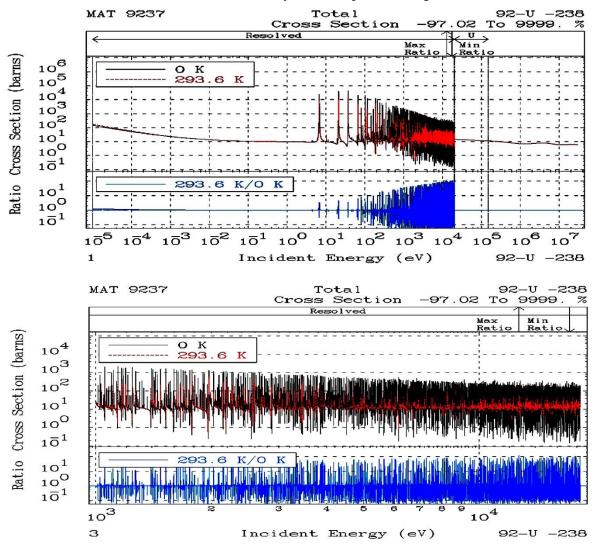
Because of their importance I have included here a few detailed plots of the U-235 and U-238 total cross sections, primarily to illustrate the important effect of temperature: Doppler broadening even from 0 Kelvin to 293.6 Kelvin has dramatic effects on the value of the cross section and this extends to rather high neutron incident energies: Here we even see the effect of 0 K to 293.6 K extending well into the KeV range. U-235 has a resolved resonance region extending up to 2.25 KeV and an unresolved region up to 25 KeV.



The range of differences on the plots can be better understood by remembering that,

- 1) The **minimum difference** is usually due to a decrease in the peak cross section of a resonance. For example, in the above plot -87.6% just above 1 KeV, means the peak of the broadened resonance is only 12.4% of the cold resonance, i.e., the hot peak is only 1/8 that of the cold resonance (an 8-fold decrease in the cross section).
- 2) The **maximum difference** is usually due to an increase in the minima between resonances. For example, in the above plot 282.7% near 1.014 KeV, means the hot cross section here is almost 3 times (nearly 300%) larger than the cold cross section in the minima between resonances (a 3-fold increase in the cross section)

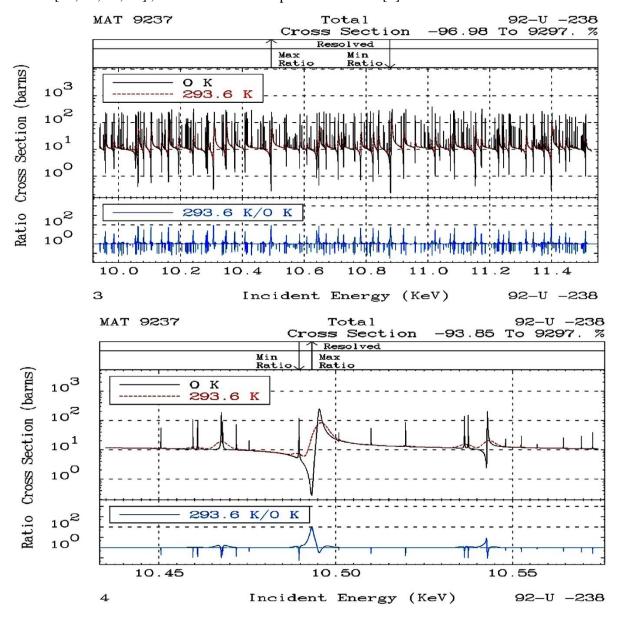
Above we can see the relatively wide overlapping resonance in U-235. In contrast below we can see the U-238 narrow, widely separated resonances. U-238 has a resolved resonance region extending up to 20 KeV and an unresolved region up to 149 KeV. Here the effect of temperature on U-238 is even more dramatic, due to the narrowness of the U-238 resonances. In the above U-235 plots we see differences due to Doppler broadening of factors of 3 to 8. Below for U-238 we see factors of up to 100!!! Remember, these are the differences we see over the relatively small temperature range 0 K and 293.6 K.



To summarize the effects of Doppler broadening that we see here,

- 1) For U-235 we saw decreases in peak cross sections of factors of 1/8 and increases in minima by about a factor of 3.
- 2) For U-238 the corresponding limits are much more dramatic: the **minimum** difference is -96.98%, which means the hot peak is only 3.02% of the cold, over 30 times smaller, and the **maximum** difference of 9297% mean the hot minima is 92.97 times the cold value.

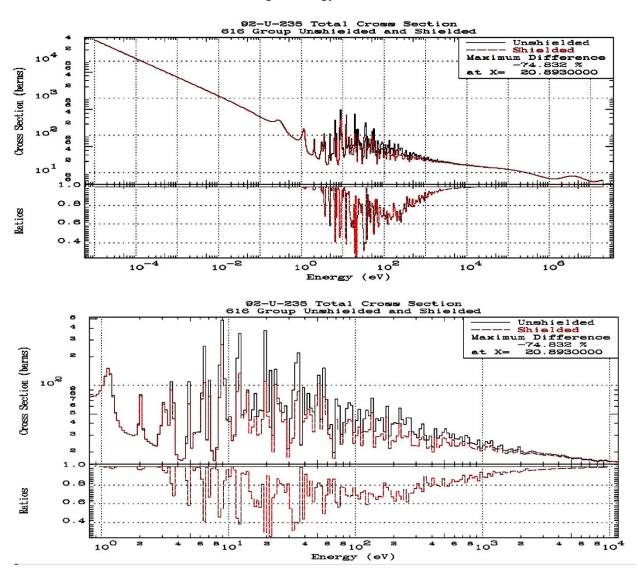
The plots shown here for U-235 and U-238 hopefully illustrate the importance of accurate Doppler broadening. All the Doppler broadening of the data shown in this report was performed using my SIGMA1 method [10, 11, 12, 13], which is included as part of PREPRO [4].



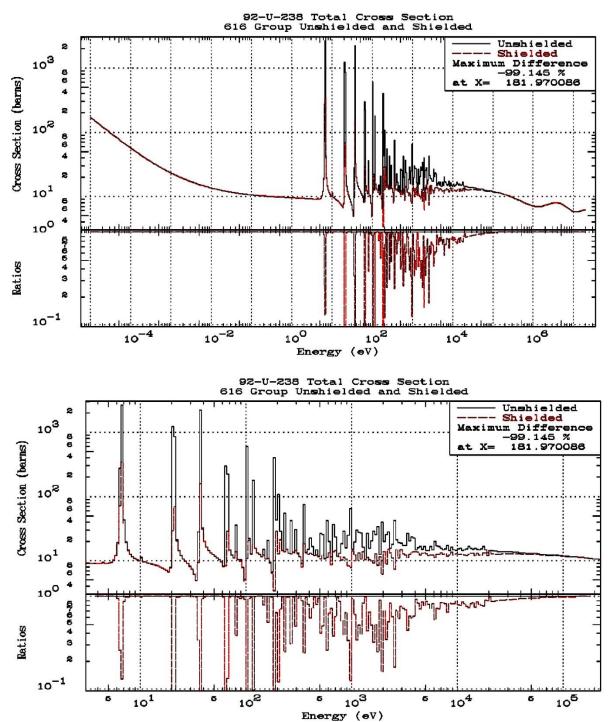
# Self-Shielding

Another important effect to consider in deciding the suitable of evaluations for use in our applications is self-shielding. I judge it to be beyond the scope of this report to cover this subject in detail; for more information see [11, 12]. However here I will briefly show the effect of self-shielding on U-235 and U-238 total cross sections; self-shielding can have a major impact on our results when we use evaluated data in our applications [2, 3].

Again, I will mention that U-235 has a resolved resonance region extending up to 2.25 KeV and an unresolved region up to 25 KeV. The below plot comparing unshielded and shielded (sigma0=0) cross sections [11, 12] show a difference of almost 75% near 182 eV, i.e., the shielded cross section is about 1/4 of the unshielded value. Note, that in the unresolved region 2.25 to 25 KeV the self-shielding is quite small and PREPRO [4] now defines self-shielding parameters to guarantee a smooth transition through the unresolved between the resolved and higher energy tabulated data.



Again, I will mention that U-238 has a resolved resonance region extending up to 20 KeV and an unresolved region up to 149 KeV. The below plot comparing unshielded and shielded (sigma0=0) cross sections [11, 12] show a difference of over 99% near 182 eV, i.e., the shielded cross section is less than 1% of the unshielded value (it is over 100 times smaller). Note, that in the unresolved region 20 to 149 KeV the self-shielding is quite small and PREPRO [4] now defines self-shielding parameters to guarantee a smooth transition through the unresolved between the resolved and higher energy tabulated data.



# The Overall Objective: Continuity of Cross Sections

This is all I will cover on self-shielding; I merely want the reader to be aware of the important role it plays to our applications. In many applications depending on energy, position, and direction the local neutron flux averaged cross sections can vary anywhere between the unshielded and shielded values [11, 12]. Be aware that to be physically acceptable the cross sections and flux MUST be continuous in energy; any non-physical discontinuity in the cross section will result in a corresponding non-physical discontinuity in the flux. This can be a problem in evaluations, particularly near what I will call transition points, such as: 1) At 20 MeV where many recent evaluation have extended the cross sections to higher energy, without regard to the importance of continuous cross sections, 2) At the resolved to unresolved and unresolved to tabulated higher energy data boundaries; today PREPRO [4] defines unresolved self-shielding parameters to guarantee a smooth, continuous cross section variation through the unresolved between resolved and higher energy tabulated data, 3) Thermal scattering law to low energy free atom data; no covered here.

Our aim is to eventually smoothly and continuously join all of these, which can be achieved ONLY if we have continuous, smoothly varying cross sections in our evaluations.

# Suggestion to Evaluators: Use the Available Tools

Since ENDF started over 50 years I estimate that over 1 billion dollar U.S. has been invested in ENDF infrastructure; much of this is in terms of computer codes designed to process [4, 5, 6] and apply [2, 3] the data. Over the years an enormous amount of time has been invested to VERIFY the accuracy of these codes, which for example, has allowed me to produce this report, including cross sections that have been reconstructed from resonance parameters to produce COLD (0 K) cross sections, and to Doppler broaden the cross sections to produce the HOT (293.6 K) data shown in this report; each step verified.

50 years ago, with the first versions of ENDF we were flying in the blind, in the sense that we did not have these tools. It was not until the release of ENDF/B-III [14] that we could even "see" the energy dependent COLD cross sections, by reconstructing the energy dependent cross sections. It was only later that we could accurately Doppler broadened cross sections [10, 11, 12, 13]. For decades as each version of ENDF/B was released I have produced temperature dependent libraries that have always been FREELY available, as in POINT2018 [9] today, through my website: <a href="http://RedCullen1.net/HOMEPAGE.NEW">http://RedCullen1.net/HOMEPAGE.NEW</a>

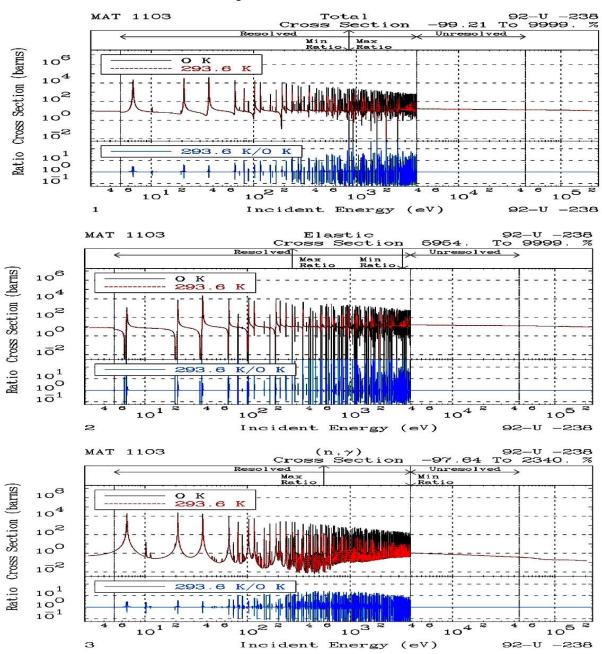
Today we have an abundance of computer resources that are FREELY available to anyone. My suggestion to evaluators is **USE THEM**. From talking to evaluators, I have been amazed at how many of them have never "seen" their own evaluated data. So many of the problems I (we) see in this report could have been so easily avoided if the evaluators, rather than I, created the plots in the report. This would be a win-win situation, where evaluators have everything to gain and nothing to lose; certainly, we data users would gain, in terms of improved evaluated data.

# Suggestion to Evaluator Users: Close the Circle

ENDF/B is designed to be continuously used and more or less continuously improved based upon this use. So please be aware that feedback from evaluation and code users can be so important in improving our future evaluations. If you publish any reports, or even have informal suggestions, or questions, PLEASE send them to the evaluators or code designers, and the National Nuclear Data Center (NNDC), Brookhaven National Laboratory (BNL). This is definitely a win-win situation, where we ALL gain by pooling our experience toward improving future evaluations. Personally I keep repeating in the documentation for my own codes [3, 4] THE MOST IMPORTANT improvements to these codes is due to feedback from users; their experience is invaluable and most appreciated.

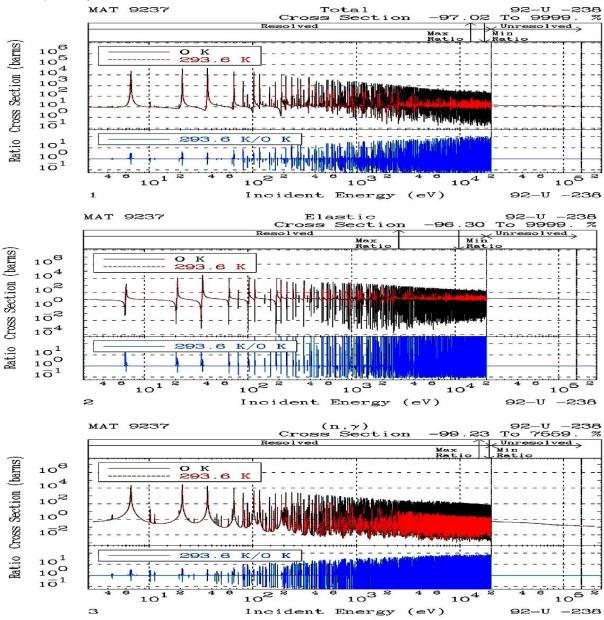
# The Way We Were

50 years ago, ENDF/B-II was the current ENDF/B data library. At the time we did not have the computer tools we have today to reconstruct the energy dependent cross sections. Even if we had the energy dependent cross sections, we could not accurately Doppler broaden them. And we could not even "see" them. Today I find it interesting to use today's tools to see where we were 50 years ago. Below is a plot of the ENDF/B-II U-238 major cross sections. With the single level (LRF=1) parameters used at the time it would have come as a shock to us to see the negative elastic cross sections, at many energies for the COLD (0 K) data and even at a few energies for the HOT (293.6 K) data.



#### Back to the Future

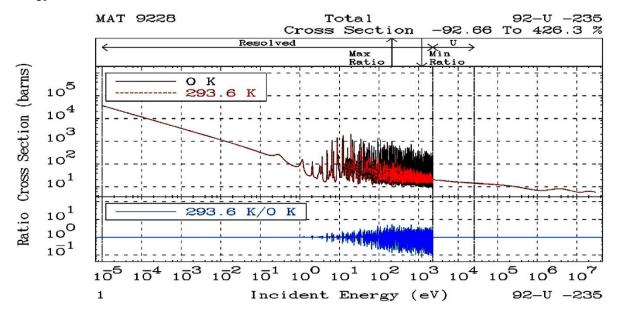
We have come a long way since then; here is today's corresponding ENDF/B-VIII U-238 data. Comparing the above and below plots, the most obvious difference is that using Reich-Moore (LRF=3) there are no negative elastic cross sections, in the COLD or HOT data. 50 years ago, the resolved resonance region extended up to 3.91 KeV, and the unresolved up to 45 KeV; see the above plots. Today the resolved resonance region extends up to 20 KeV, and the unresolved up to 149 KeV; see the below plots. Based on merely looking at these plots, 3.91 KeV to 20 KeV may seem like a minor area of the plot, but it means today's evaluations extend over five times higher in energy and include many more resolved resonances: 250 vs. 3345. In addition, the unresolved region today starting at 20 KeV plays a much smaller role than it did 50 years ago when it started at 3.91 KeV.

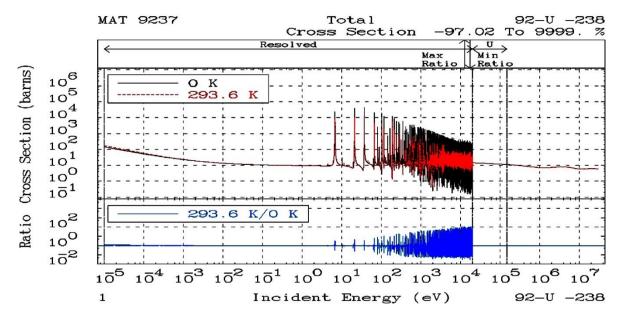


#### In Praise of Evaluators

We have come so far in improving our evaluations and our evaluators should be praised for what they have accomplished. Here I will point out a few areas of excellence, but also a few areas in which our evaluations can be still further improved.

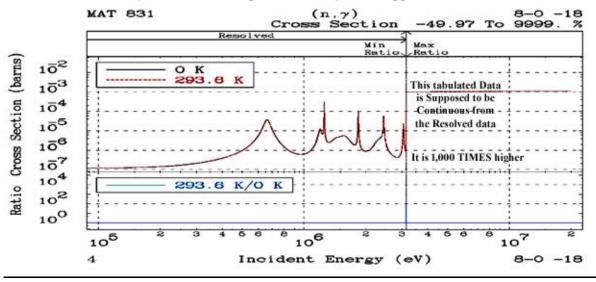
For starters I will mention the U-235 and U-238 cross sections, which because of their importance illustrate examples of well-defined cross sections, across the entire energy range from thermal up to high energy.

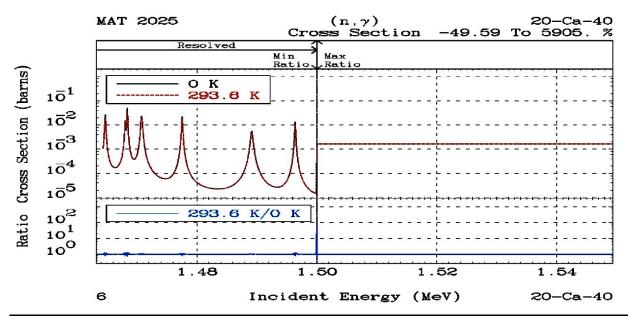




# No Unresolved Region

Now I address problems I see with today's data. I should mention that these problems appear in many current evaluated data files, not just ENDF/B-VIII [7]. Including a resolved region, but no unresolved region makes it difficult to define cross sections that are continuous in energy. There are a number of excellent evaluations where this has been accomplished by joining resolved resonances to high energy measurements, including resonance-like fluctuations in the high energy data. In contrast, here are two examples, where in the first the discontinuity at the upper energy limit of the resolved energy range is roughly a factor of 1,000, and in the second at factor of 100. There are far too many of these examples in our data libraries; again, not just ENDF/B-VIII. With the computer tools that we have today these are easy to find and correct early in the evaluation process, so they do not appear in our finished evaluations.





# Experimentalist vs. Evaluator and Resolved vs. Unresolved

I like to think that the difference between an experimentalist and an evaluator can best be summarized by asking the answer: What is the total neutron cross section at 10 MeV in Ardvarknium-187? An experimentalist might answer I do not know, because it has never been measured. In contrast an evaluator does not have the luxury of ever saying I do not know. Evaluation is not pure science; it is an art, and a very important part of evaluation is to supply the "best" estimate, based on measurement, theory, personal experience, probability, or when all else fails, just their blind best guess. An evaluator cannot answer I do not know; if you don't know, guess; that's part of the job.

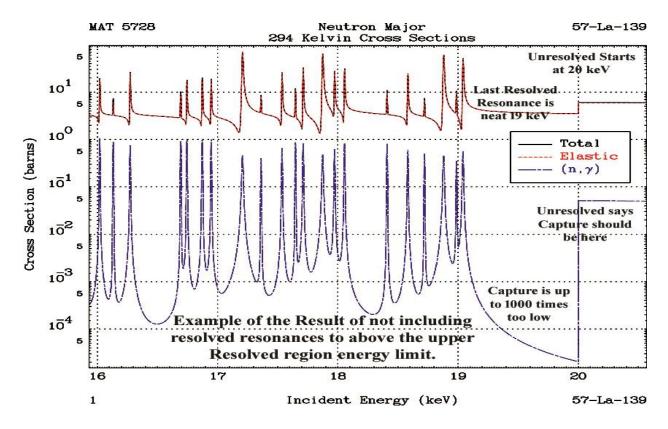
To be of any use evaluations, for better or worse, must be complete. As far as users are concerned, if something is not included it is ZERO. So, evaluators can, or should, only omit something if their best guess and/or highest probability truly is that it is ZERO.

There is a BIG difference between the meaning of resolved and unresolved for experimentalists versus evaluators; or rather there should be, but too often there is not. To an experimentalist the dividing line between resolved and unresolved is where the resolution of their measuring equipment can no longer "see" (resolve) ALL the individual resonances. This energy may be different for the wider L=0, (s wave) resonances, than for the narrower L>0 (p, d.,,,wave) resonances. For experimentalists this might be considered to be a somewhat soft line; is not necessarily unique and is somewhat of a judgement call between different experimentalists. As such it may be viewed as merely a definition, not of any great consequence.

# No Resolved Resonances Above Resolved Energy Range

In contrast to the evaluators who produces data for use in ENDF the resolved and unresolved energy ranges are each a fixed energy range, where the physics and mathematics used in each energy range is quite different. For use in ENDF data evaluators are forced to draw an energy line in each evaluator and understand that on one side of this line they can uniquely define cross sections versus neutron energy (the resolved range) and on the other side they can only define cross sections statistically (the unresolved range). This is not as easy as it sounds, and too often where evaluators define the dividing line between resolved and unresolved may not be the most probable or useful place to draw this line in the sand.

The most frequent mistake that today's evaluations make is to define the dividing line between resolved and unresolved not where they start to lose sight of resonances (as an experimentalist would define it), but rather where they completely run out of all resonances; they draw the "line" between resolved and unresolved above the last resolved resonance that they tabulate in their evaluation. The result can be a "hole" in the cross section near the resolved/unresolved boundary. It important to include resonances whose peaks are above the upper energy limit of the resolved range, so that following ENDF rules, the tails of these resonances extend down into the resolved energy range and produce a smooth join between resolved and unresolved. The below plot shows an example where there are no resolved resonances between about 19 KeV and the upper limit of the resolved region at 20 KeV. The result is a "hole" where relative to the elastic, there is almost no capture; in applications this produces a non-physical "bump" in the neutron flux.

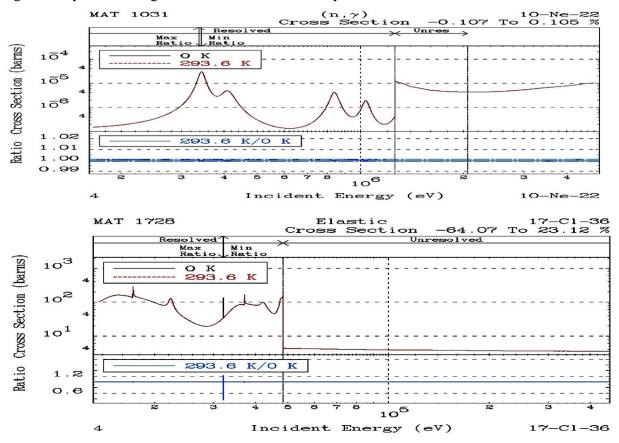


Here the evaluators know that there is almost zero probability that there are no more resonance above the highest energy one they tabulate, so not including additional resonance is the worst possible guess. Indeed, including an unresolved region says they know there are definitely resonances above the resolved range. A much better guess is to either lower the resolved/unresolved boundary or use theory to sample a few additional resonances above the resolved energy range. Either one of these guesses would produce more probable results; again, I suggest evaluators consider probability.

#### Resolved to Unresolved Mismatch

Let me repeat: physically both the neutron flux and neutron cross sections MUST be continuous as a function of energy; the two are coupled together. Any discontinuity in cross section will produce a discontinuity of the flux. Therefore, it is VERY important that evaluations include cross sections that are continuous in energy. The boundary between the resolved and unresolved region is one point where I feel not enough effort is made to guarantee, let alone allow the possibility of continuity.

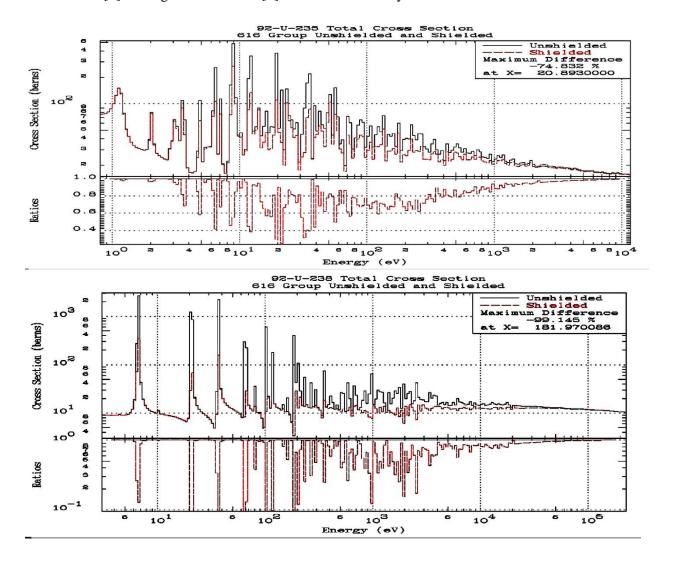
Keep in mind that the unresolved region is supposed to be a continuation of the resolved region; the only difference between the two being that in the resolved region we can uniquely define the energy dependence, whereas in the unresolved we can only define a statistical spread of values. But to be acceptable the average of the unresolved data, MUST be consistent with the average of the energy dependent resolved data. The *mean value theorem* tells us that the average of anything must be somewhere between the minimum and maximum of the distribution. Unfortunately, ENDF/B-VIII includes a number of examples where the unresolved average is way outside the limits of the tabulated resolved data. In the below first example the unresolved average is obviously at least an order of magnitude higher than the resonance peaks in the resolved; my eye suggests maybe closer to 50 times too high to allow any kind of physical match or continuity. In the second example it is an order of magnitude to low. Again, today after "seeing" these results it should be easy to correct and make the data consistent.



# Unresolved to Tabulated High Energy Continuity

The Unresolved resonance region is supposed to serve as a transition between the uniquely defined variations of the cross section in the resolved region, below it in energy, and the uniquely defined tabulated high energy cross sections, above it in energy. By definition, only within the unresolved region do we not uniquely define an energy dependent cross section.

Within ENDF-102 rules it is difficult to both smoothly join the fluctuations due to resonances at lower energy end of the unresolved and the smooth, uniquely defined tabulated cross sections at higher energies above the tabulated range. Unfortunately, most of our current ENDF unresolved data still produces a discontinuity at the unresolved to tabulated high energy interface. Strictly, for illustrative purposes, below I illustrate what the unshielded and shielded U-235 and U-238 total cross sections should look like; smoothly varying across the unresolved from resolved to high energy. I mention this in the hope of recognizing this problem and encouraging discussions: continuity of flux and cross sections are our ultimate goal, and we cannot achieve this goal without continuity at this interface. For my personal use in Monte Carlo [3] and together PREPRO [4] forces the continuity shown below.



# **Brief Survey**

Below I present a brief graphic, survey of ENDF/B-VIII resonance parameters, grouped together based on whether or not they include resolved and/or unresolved resonance regions (four groups). I have chosen to treat the R-Matrix Limited (LRF=7) separately as a fifth group, because it is relatively new to ENDF, quite different from the other resonance formalisms, and yet not widely used.

# Scope of this Survey: The Good, the Bad and the Ugly

In each case I first show a GROUP including selected: total, elastic & capture cross sections, followed by a section including selected fission cross sections (if any). There are far too many evaluations in ENDF/B-VIII (553 evaluations) to allow me to present graphic results for all of them. For a comparison, I suggest you see results from almost 50 years ago, when I was able to present all the data for the much smaller ENDF/B-III [14].

Here I have tried to present only a selection to illustrate mostly the extremes of very good evaluations, ready for prime-time, and in the other extreme those that could use some improvements (what I refer to as "The Good, the Bad, and the Ugly"; an Italian spaghetti western). Fortunately, today most of our evaluation fall into the good, or even better, and need not be included here. It is never my intent to embarrass anyone; none of us are perfect, and my intent here is only to use my over 50 years of experience with ENDF formatted data (everything from the original, first released version of ENDF/B, to the current ENDF/B-VIII) to suggest improvements that will make any ENDF formatted evaluation more physically acceptable for use in our applications [2, 3]. Please maintain focus: ENDF/B is not an end in and of itself, rather it is intended for use in our applications [2, 3].

For this report initially I began adding comments directly onto some of the plots, mostly highlighting the good or bad points, and their relationship to the above described problem areas. I did this in the hope of guiding readers. However, as I proceeded there was so much redundancy in my comments, that I decided: by now readers gets the idea, so I stopped my comments. I think/hope you the reader can take it from there.

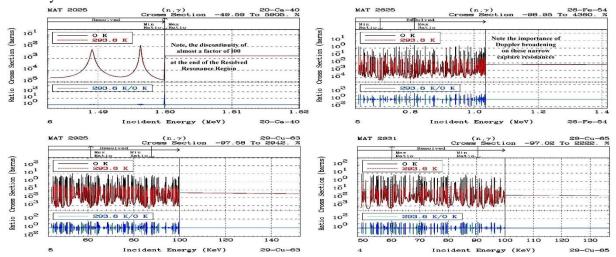
Before I begin I will again remind readers that you can use on-line resources to produce any and all of the plots presented here, or other plots that meet your own individual needs or interests, through my website, <a href="http://redCullen1.net/HOMEPAGE.NEW">http://redCullen1.net/HOMEPAGE.NEW</a>

# R-Matrix Limited (RML) (LRF=7): 10 Evaluations

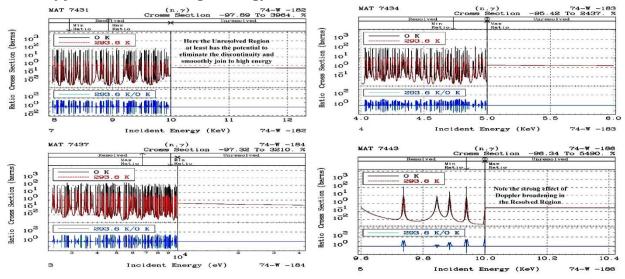
This most recent addition to the ENDF Resonance Formalisms (LRF=7) has the potential to greatly improve the accuracy of resolved resonance region cross sections. As yet this potential has not been met, in the sense that only ten (10) of the 553 evaluations in ENDF/B-VIII use this formalism, and these have some important limitations that we should note.

There are six evaluations in the Z=17 to 29 range, and all of these suffer from the fact that each only included a resolved, but no unresolved resonance region. In addition, there are four evaluations of Z=74 isotopes; these include both resolved and unresolved resonance regions. Fission is not included in any of these evaluations.

The first four plots below shows evaluations that include a resolved, but no unresolved resonance region. The result is a discontinuity in the cross section at the resolved to tabulated higher energy cross section boundary.



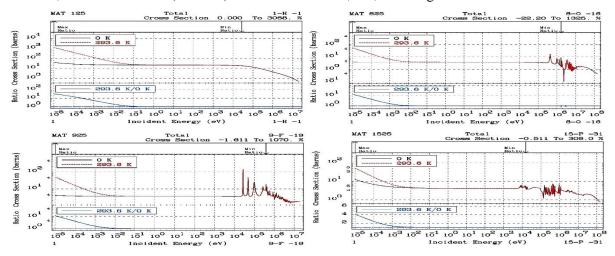
The next four plots show isotopes of Z=74, all of which include both resolved and unresolved resonance regions. The inclusion of an unresolved region at least has the potential to eliminate the discontinuity and smoothly join to the tabulated higher energy cross sections.



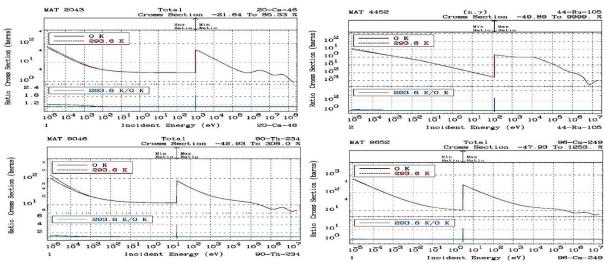
# No Parameters (LRU=0): 64 evaluations

These evaluations are used for all the low Z (light) evaluations (Z=1 through 9, and Z=15), where tabulated data can be accurately defined without using any resonance models within the evaluations. This is followed by many low naturally abundant isotopes, with very crude cross sections, including order of magnitude discontinuities in the cross sections. These crude evaluations extend from about Z=30 up to Z=100, the highest Z included in ENDF/B-VIII. Half of the highest Z evaluations include fission; usually a very crude approximation for lower abundance isotopes.

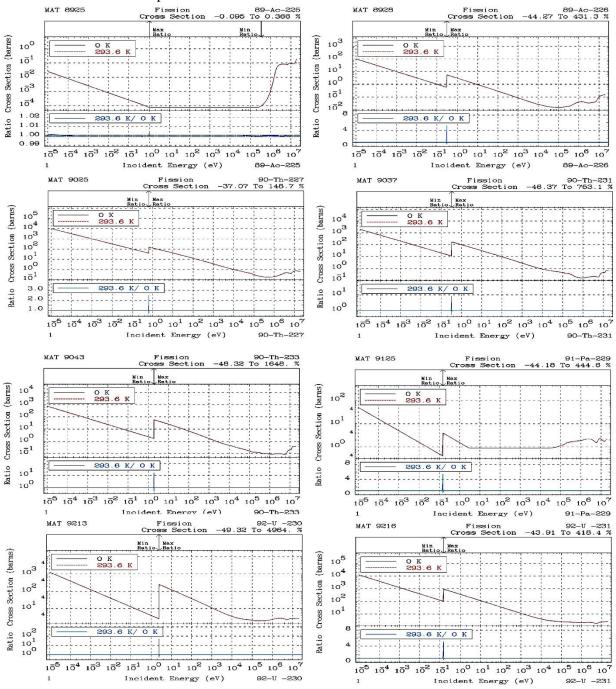
The first four plots below show low Z evaluations, which include anywhere from no resonances, Z=1, up to Z=15, which include high energy, well resolved resonances. The one DANGER to look for with these low Z evaluations is to ensure that the tabulated data (MF=3) [1] is for 0 K for use in ENDF, not room temperature experimental data. Note the large effect that temperature has on the low energy low Z cross sections; any uncertainty in the actual temperature of this evaluated data can result in large uncertainties in the cross section we use in our applications. As but one example: The 1-H-1 COLD (0 K) data is about 20 barns, whereas the HOT (293.6 K) data about 30 barns, i.e., 50 % higher.

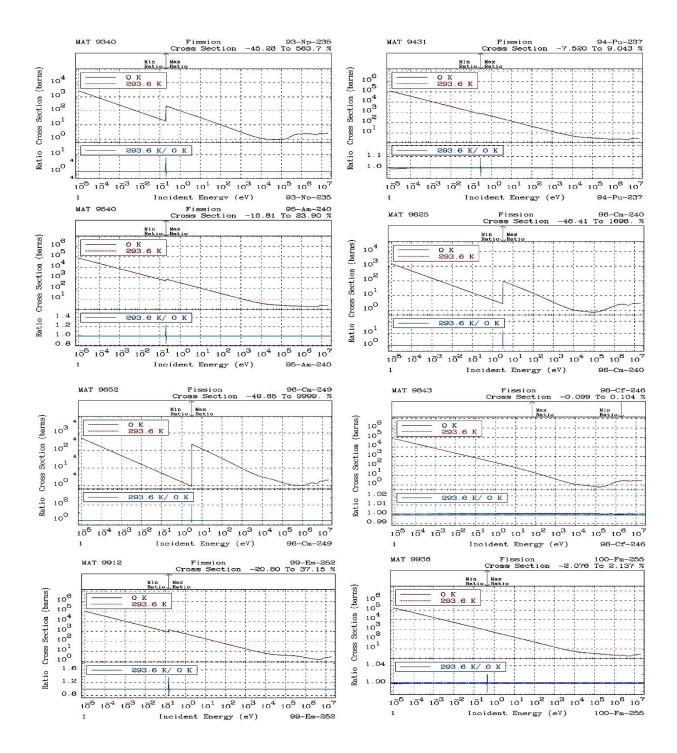


The next four plots show higher Z evaluations, Z=20 to 98, which are very crude, showing no resolved resonances, but large discontinuities in the cross sections, inferring resonances above the energy of the discontinuity. These are obviously not intended for high precision transport calculations.



Fission is included for many low abundance isotopes for elements Z = 89 through 100; all of these are very crude, with no clear resonance structure and a large discontinuity where it is assumed resonances start. Here are a few examples.

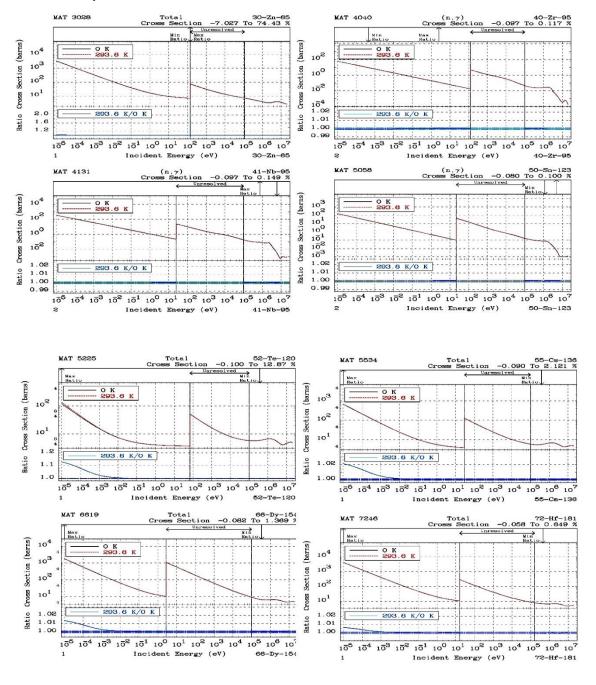




# Only Unresolved (LRU=2): 31 Evaluations

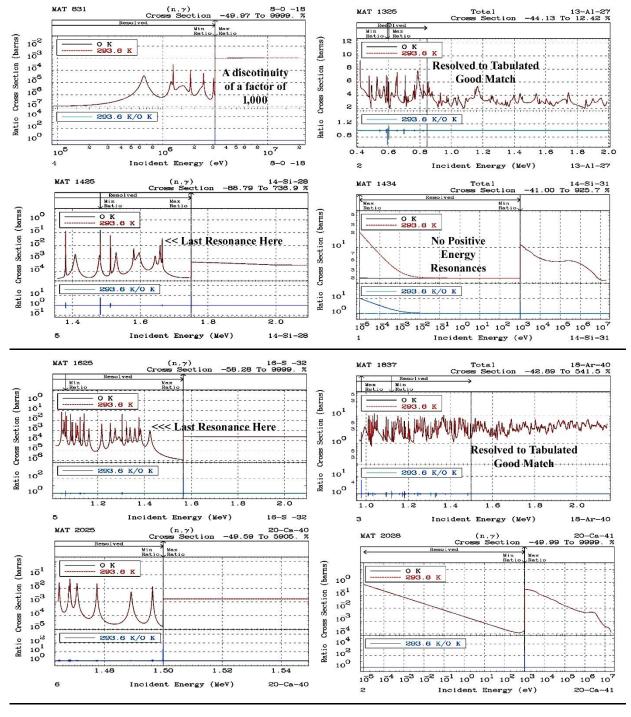
The above evaluations (with no resonance data) may be able to accurately represent the data for low Z isotopes, but is crude for higher Z. Here all these evaluations are extremely crude across the entire range Z = 30 to 72.

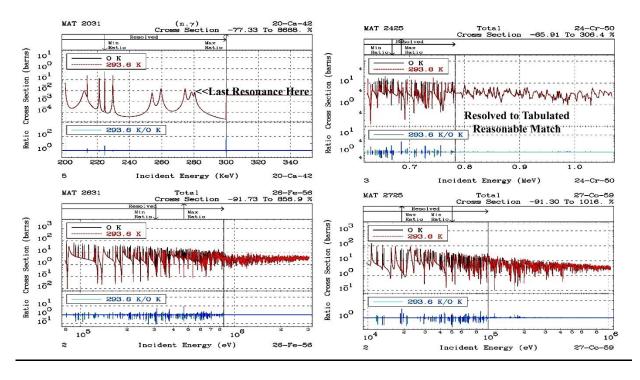
Below are a few examples. All show no resonances, and enormous discontinuities in the cross section. Unlike the above evaluations (with no resonance data), here in principle the unresolved resonance region may be able to correct for this discontinuity, but in fact these must all be judged to be crude. Fission is not included in any of these evaluations.

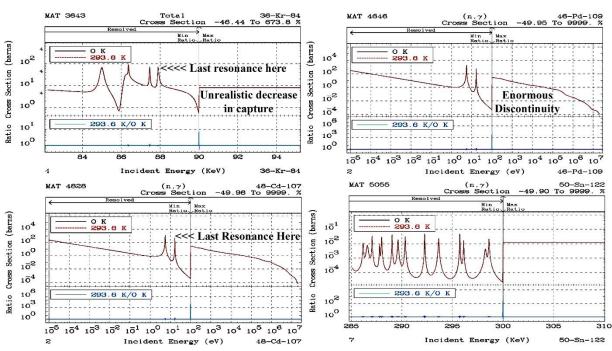


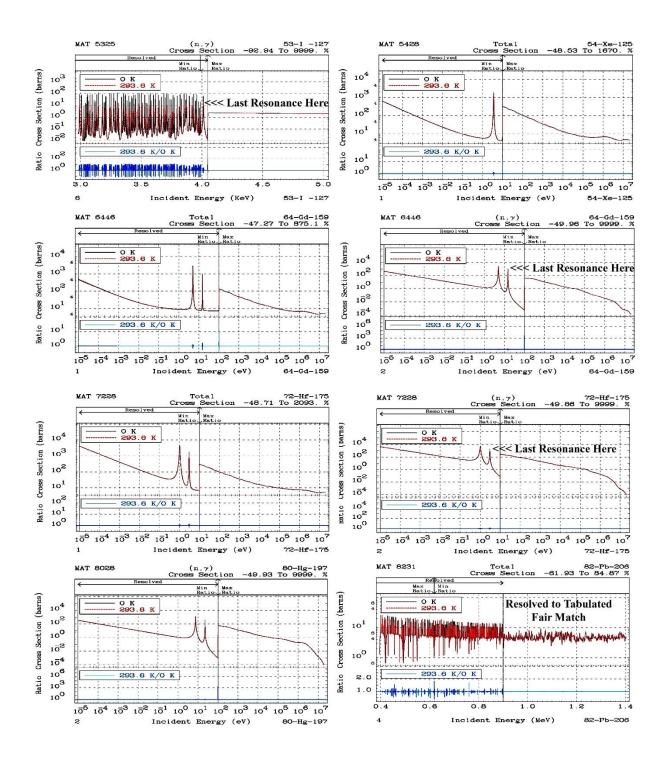
# Only Resolved (LRU=1): 143 Evaluations

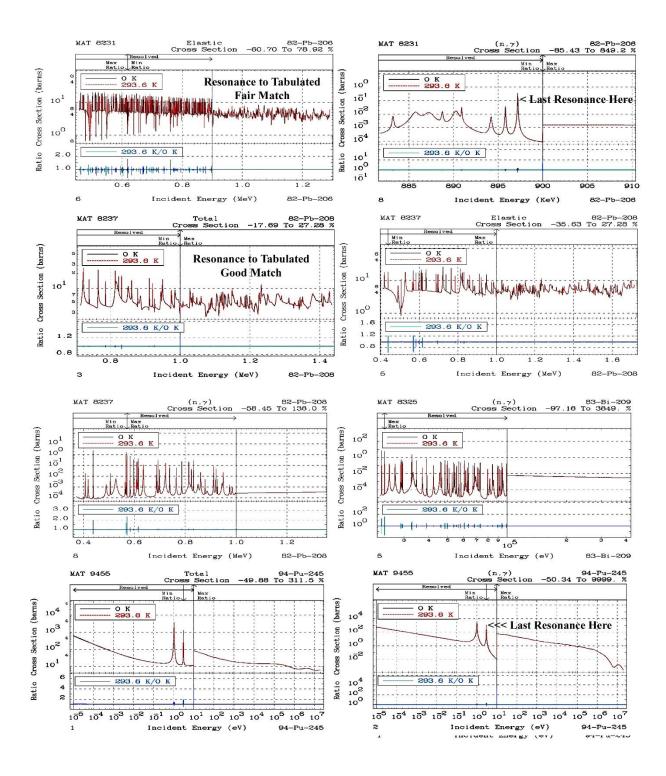
These vary in quality from exceptionally good to poor. Without an unresolved resonance region many include a large discontinuity in the cross section at the resolved directly to higher energy tabulated interface. Many include resonance sequences that do not extend beyond the end of the resolved energy range; this is most evident in the large discontinuities in the capture cross section. Some, particularly the metals, include a good match between the resolved and higher energy tabulated, by including detailed higher energy tabulated data, with fluctuations similar to the data within the resolved range. Fission is included in five of these evaluations; these five are crude approximations for low abundance isotopes.



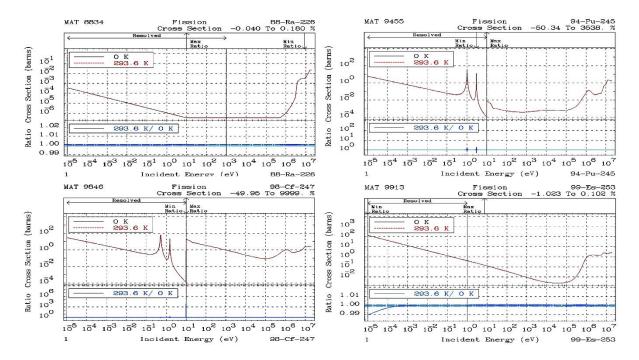






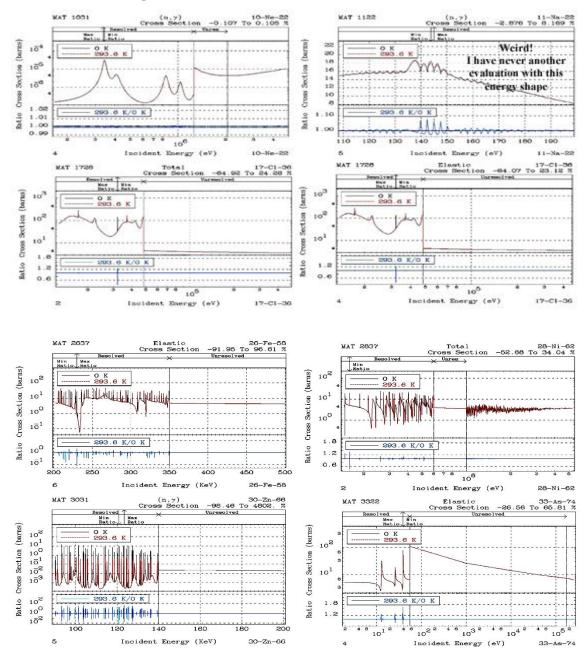


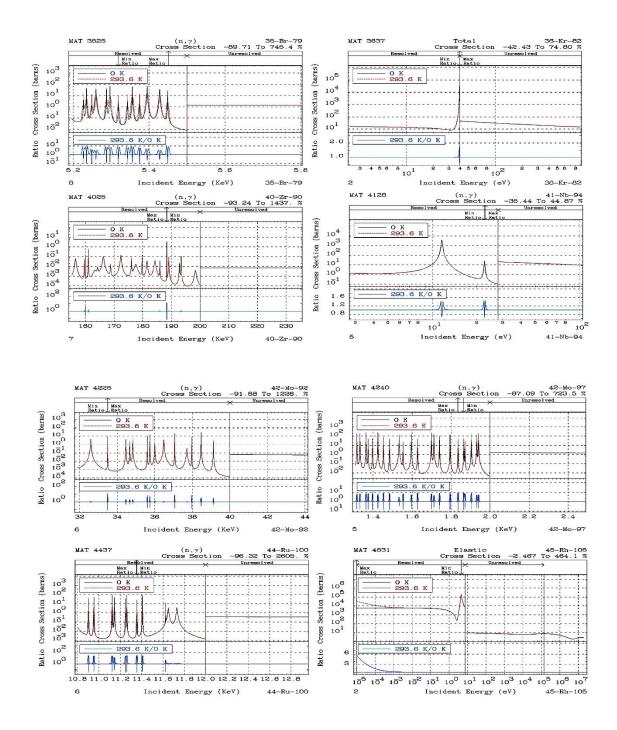
Fission is included for five low abundance isotopes for elements Z = 88 through 99; all of these are very crude, with no or minima resonance structure and a discontinuity where it is assumes resonances start. Here are four examples (only 93-Np-236m is omitted),

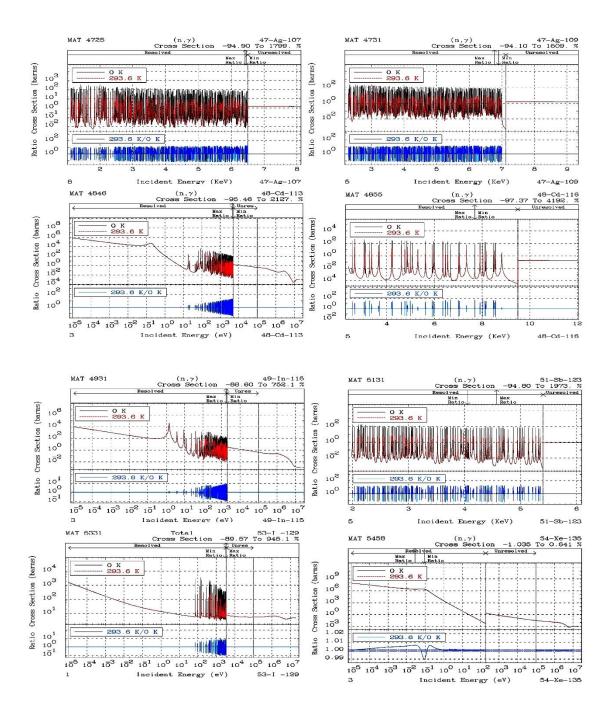


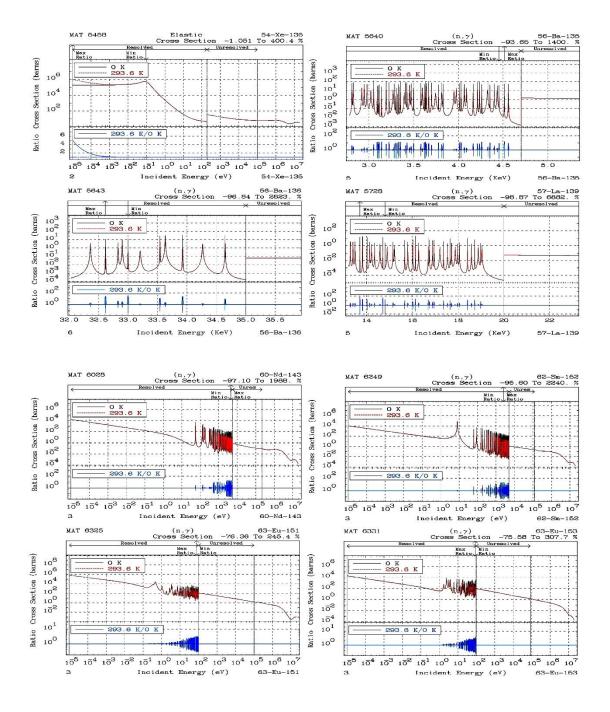
## Resolved & Unsolved (LRU=1 & 2)): 315 Evaluations

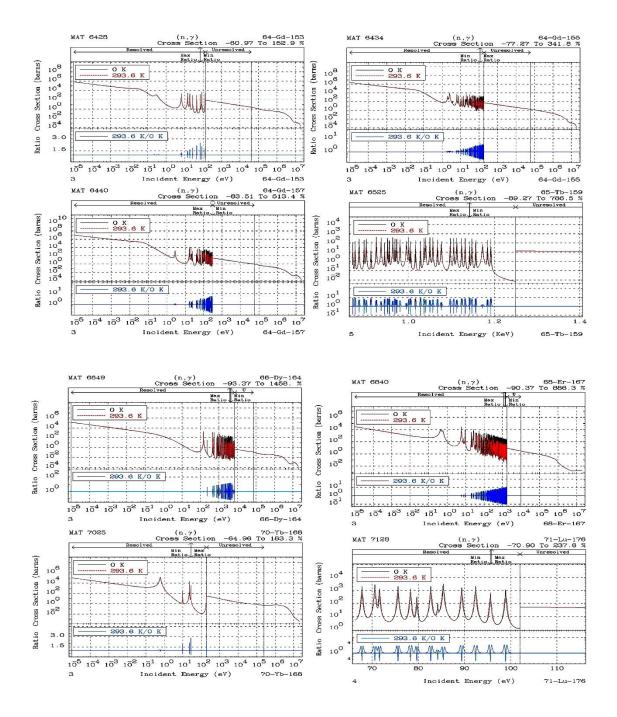
Generally, these are the best quality evaluations for heavier (higher Z=10 through 98) elements. With an unresolved resonance region at least in principle the fluctuations in the resolved range can smoothly approach the higher energy tabulated interface. Many have the limitation that they include resonance sequences that do not extend beyond the end of the resolved energy range; this is most evident in the large discontinuities in the capture cross section. Fission is included in 45 of these evaluations.

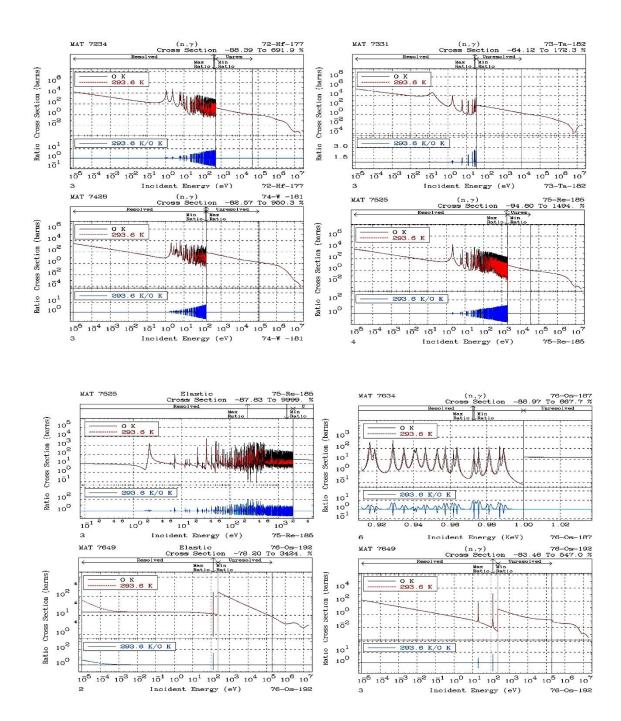


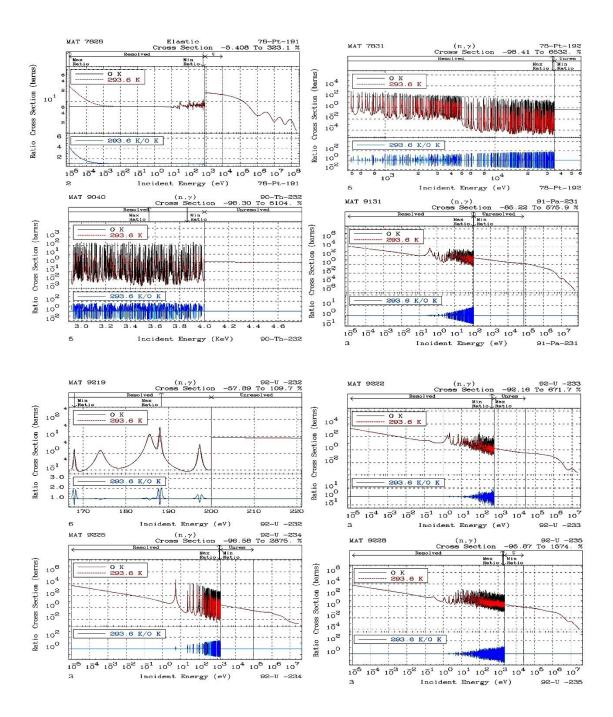


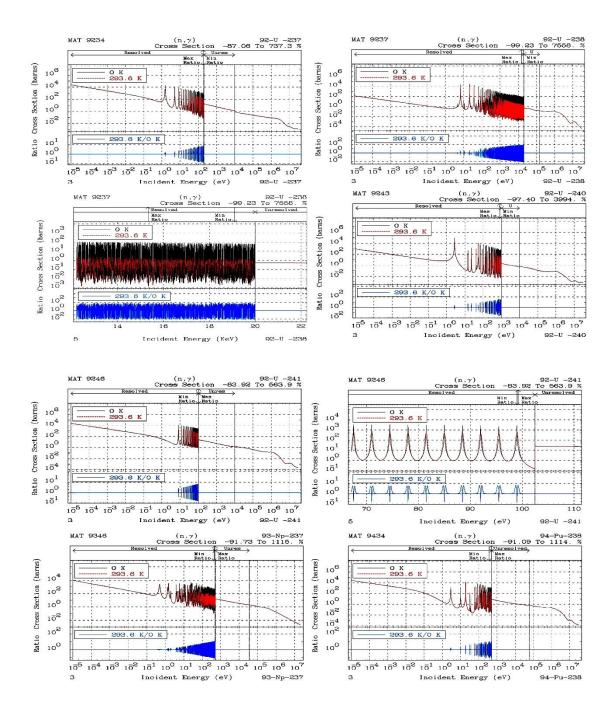


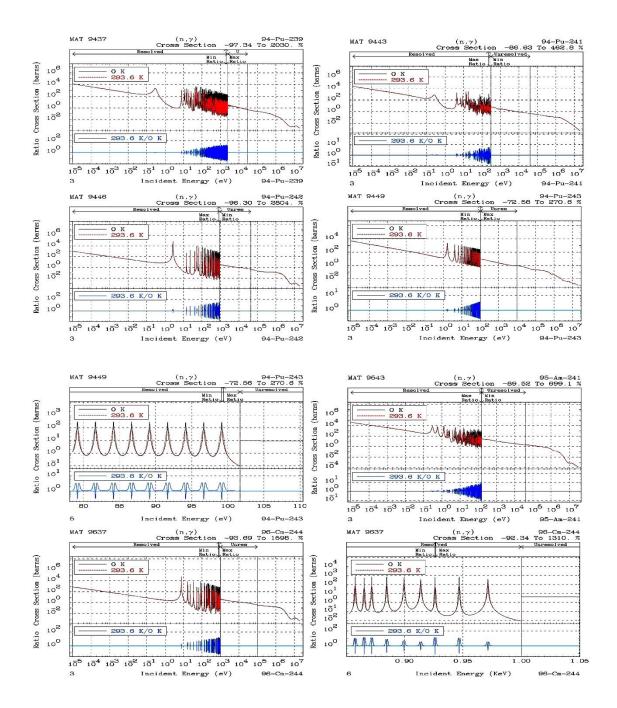


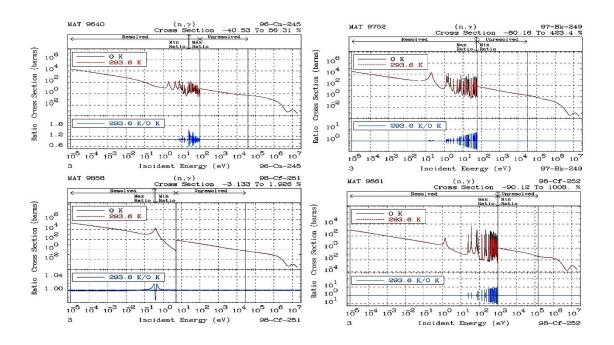




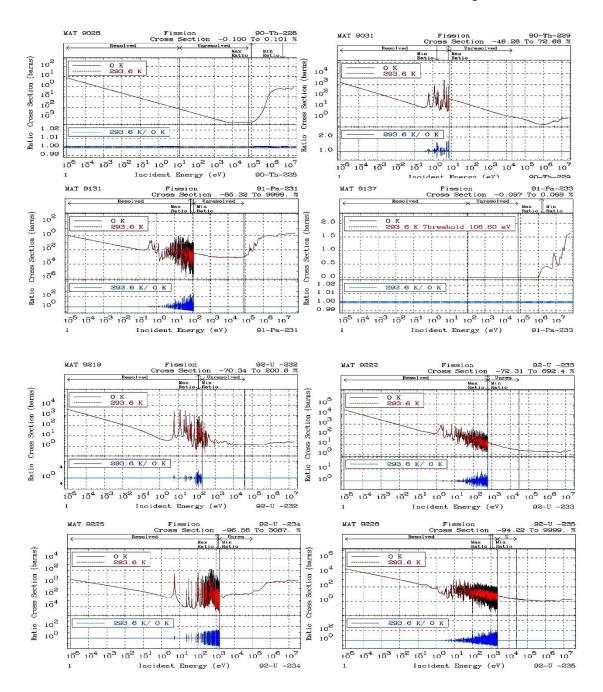


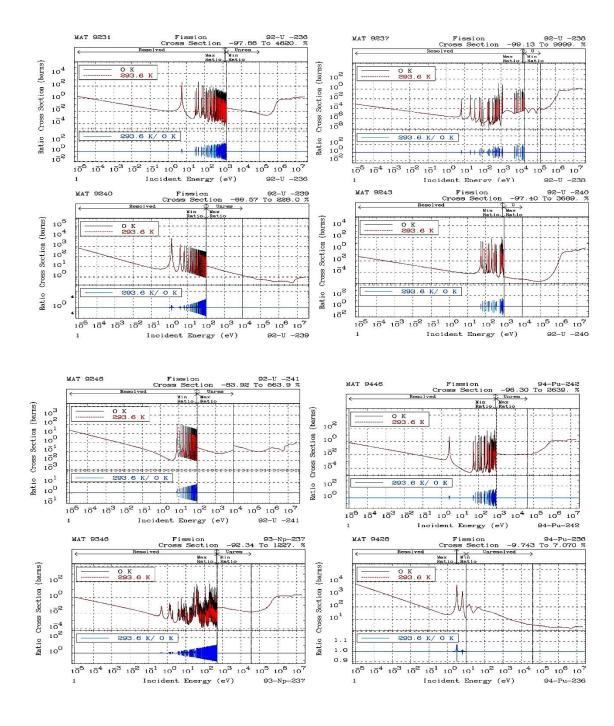


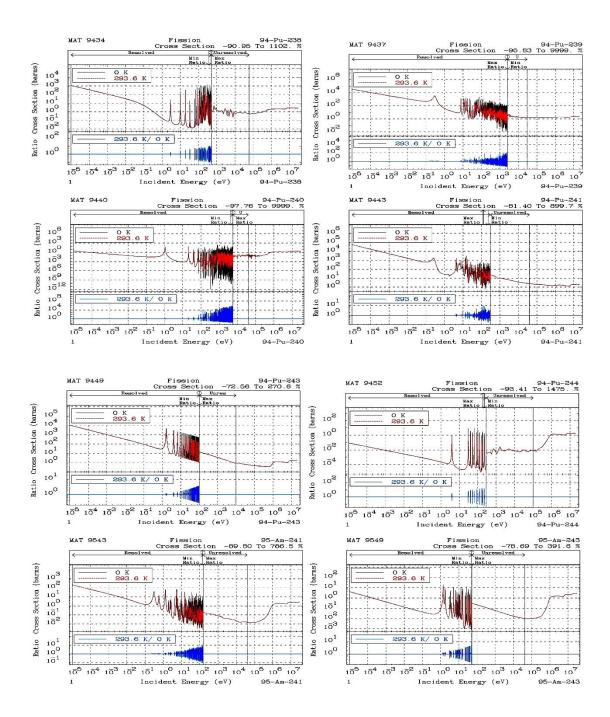


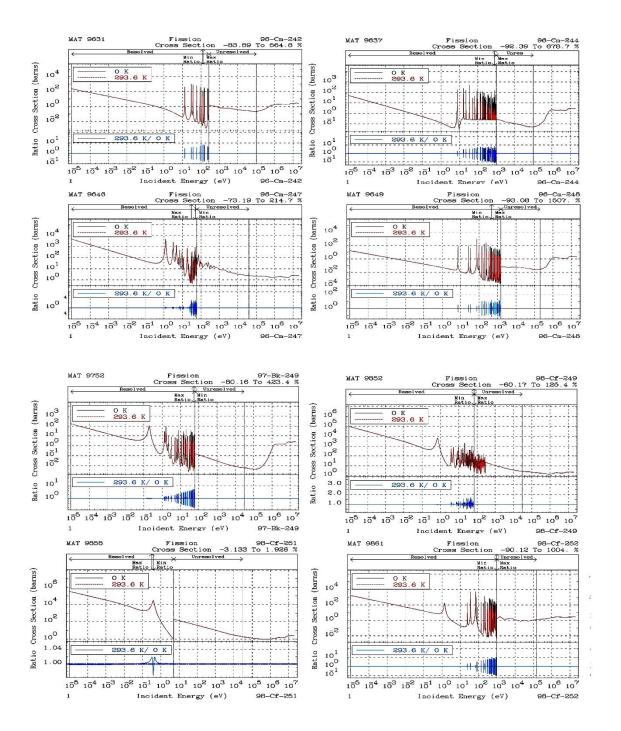


Fission is included for 45 isotopes for elements Z = 90 through 98. Because of the importance of these fission reactions many are shown here: included are all isotopes of U and Pu, and at least one isotope of the each of other fissionable elements that include resolved and unresolved regions.









## Conclusion

This report is a graphic survey of ENDF/B-VIII Resonance Parameters. The intent is to present the status of this data today (2020), compared to the development of ENDF/B over the last more than fifty years, and based on our experience to recommend how we can continue to improve in the future. Let me assure you that we have made enormous progress in our evaluated data compared to where we were 50 years ago, and this report is only intended to present what I hope will be constructive criticism, of our already excellent data.

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