LANL Experience while Creating & Validating ACE and Multi-Group Files from ENDF/B-VII.1

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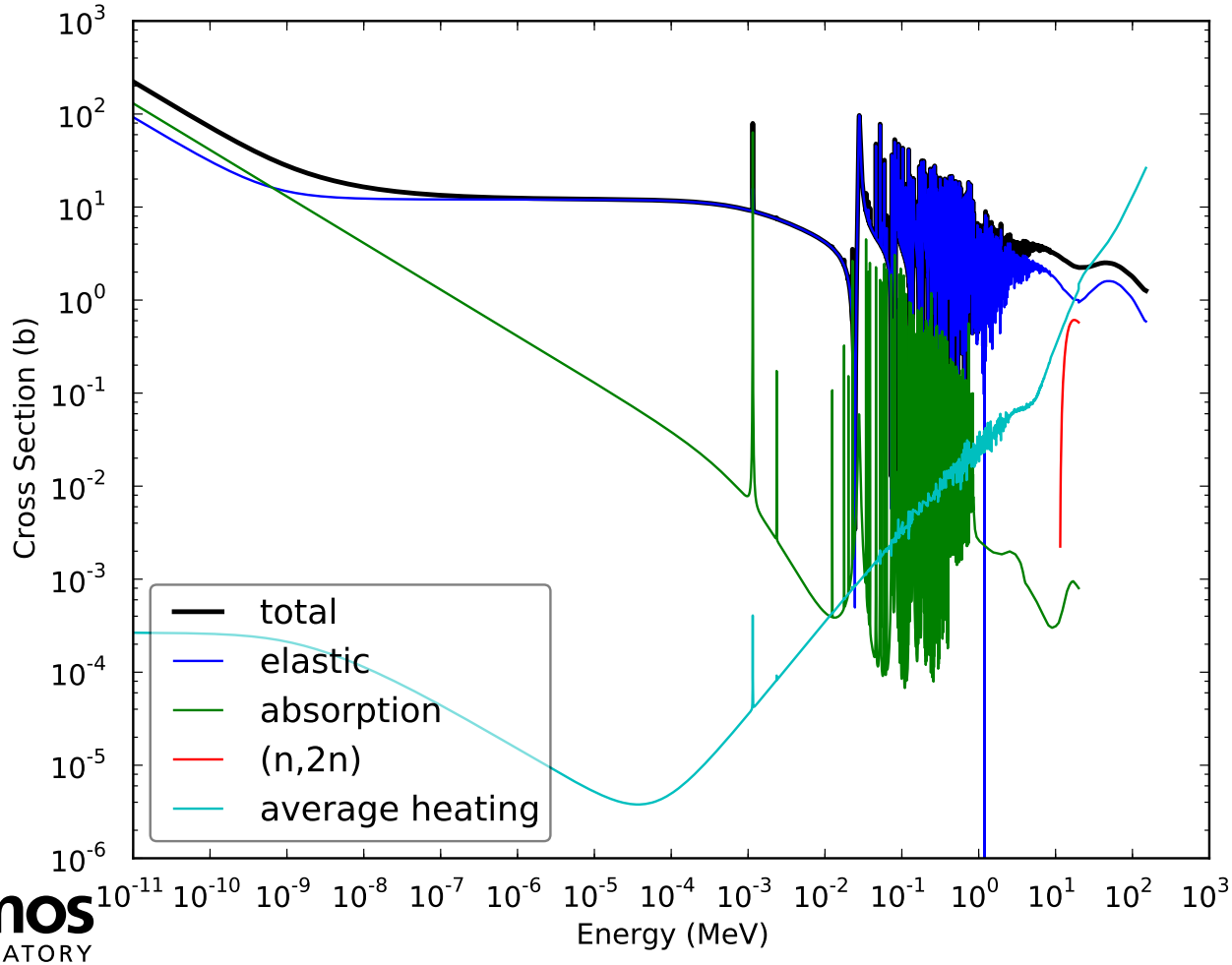
November 7, 2013

LA-UR-13-28551

0.0 b σ_s in ^{56}Fe

0.0 b σ_s (MT=2) $E = 1.1971$ MeV



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```
1.196200+6 1.555300-1 1.196600+6 2.170100-1 1.197000+6 3.926200-22631 3  2  294
1.197100+6 0.000000+0 1.197300+6 8.537900-2 1.197500+6 3.621100-32631 3  2  295
1.197600+6 2.256600-1 1.198000+6 4.730800-1 1.198200+6 6.027800-12631 3  2  296
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```
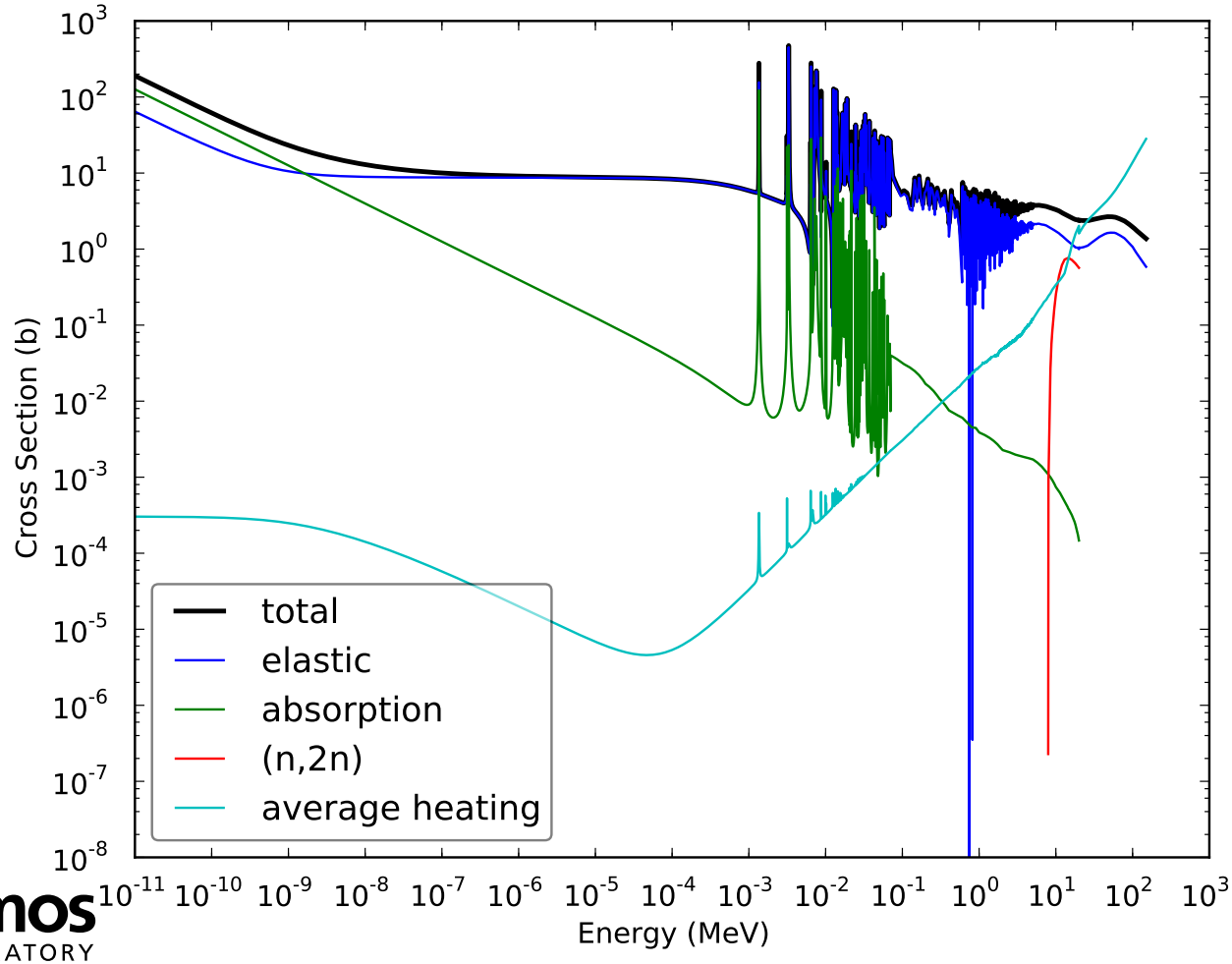

0.0 b σ_s in ^{61}Ni

0.0 b σ_s (MT=2) $E = 0.7429251 - 0.7439620$ MeV $E = 0.8184120$ MeV



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```
7.414711+5 1.146780+0 7.416770+5 1.063260+0 7.421590+5 2.461800-12834 3  2  483
7.425731+5 6.247990-2 7.429251+5 3.900000-8 7.435471+5 0.000000+02834 3  2  484
7.439620+5 2.581600-7 7.447940+5 1.643870+0 7.452091+5 2.426830+02834 3  2  485
7.456951+5 1.193080+0 7.458341+5 9.596160-1 7.459731+5 1.092830+02834 3  2  486

...

8.157041+5 1.424090+0 8.162591+5 1.423930+0 8.164981+5 1.257190+02834 3  2  545
8.174531+5 7.069040-1 8.181721+5 1.900300-1 8.184120+5 3.506000-72834 3  2  546
8.188110+5 2.066800-5 8.191311+5 2.307450-2 8.192910+5 2.396970-12834 3  2  547
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```

Negative PDF Values in ^{153}Eu; MF=6, MT=91

- 16 MeV incident energy MT=91
- Legendre Coefficients Representation (LANG=1)

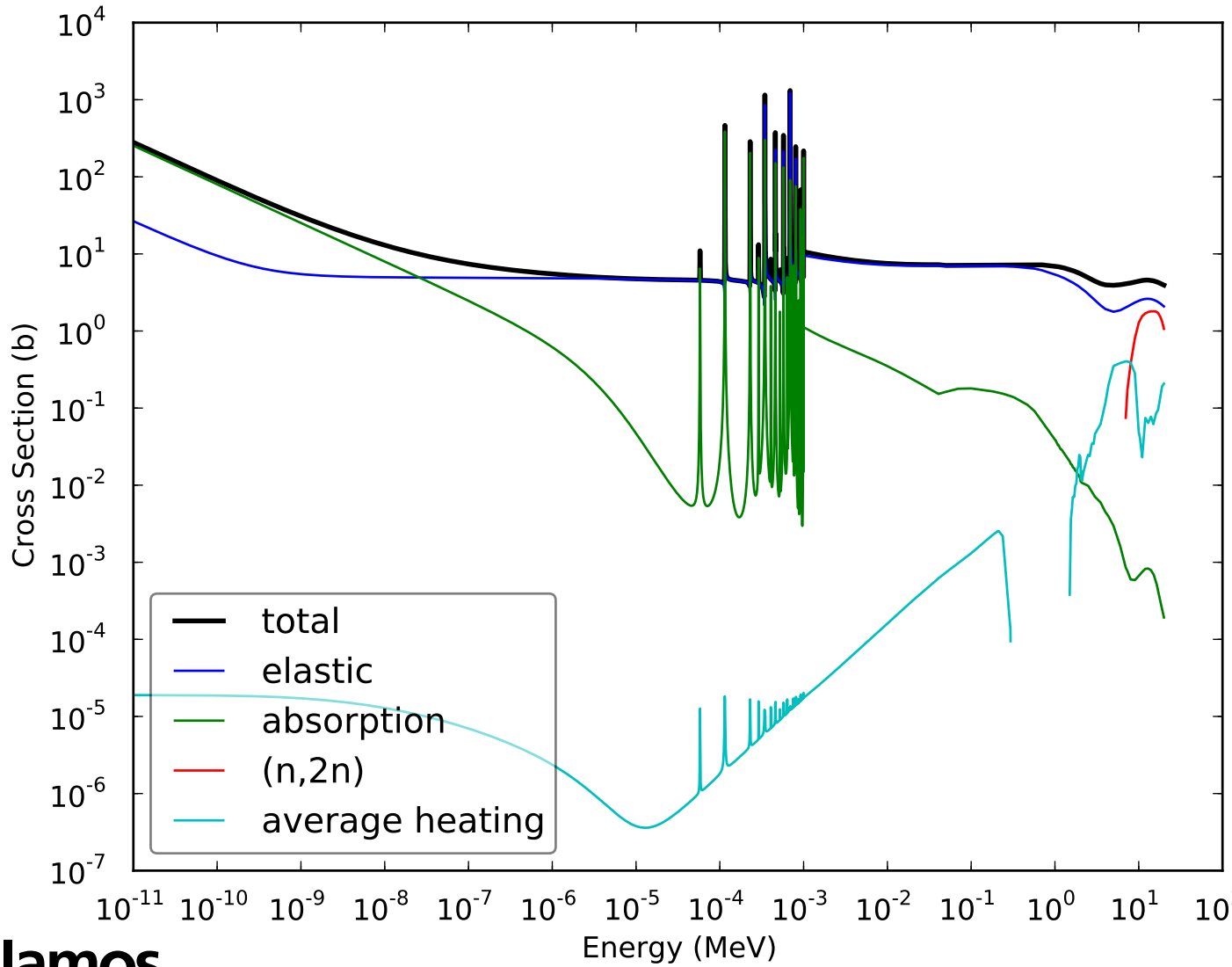
$$f_l(\mu, E, E') = \sum_{l=0}^{NA} \frac{2l+1}{2} f_l(E, E') P_l(\mu)$$

```
 6.315300+4 1.516080+2          0          2          3          06331 6 91     1
 1.000000+0 1.000000+0          0          1          1          26331 6 91     2
 ...
 0.000000+0 1.600000+7          0         12        784         566331 6 91  1502
 0.000000+0 2.22750-10-7.70107-19 0.000000+0 0.000000+0 0.000000+06331 6 91  1503
 0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+06331 6 91  1504
 ...
 0.000000+0 0.000000+0 3.704600+6-3.88100-10-1.75209-12-1.11431-126331 6 91  1533
 3.84332-13-1.59787-13 7.62323-14 6.55549-15 1.32716-13 2.85685-146331 6 91  1534
 4.34154-15 2.88240-15 2.49306-14 2.17400-15 3.989600+6-5.014980-96331 6 91  1535
-3.18764-11-2.16201-11 6.60057-12-3.02087-12 1.46726-12-8.92714-146331 6 91  1536
 2.20506-12 5.75437-13 1.97253-13 9.65643-14 4.15861-13 1.71800-146331 6 91  1537
```

Unresolved Resonance Problems

1. ^{22}Na
2. ^{36}Ar
3. ^{58}Co
4. ^{65}Zn
5. ^{70}Ge
6. ^{106}Cd
7. ^{170}Tm
8. ^{182}W
9. ^{186}W
10. ^{203}Tl
11. ^{232}U
12. ^{236}Pu
13. ^{249}Bk
14. ^{249}Cf
15. ^{250}Cf.

KERMA Problems



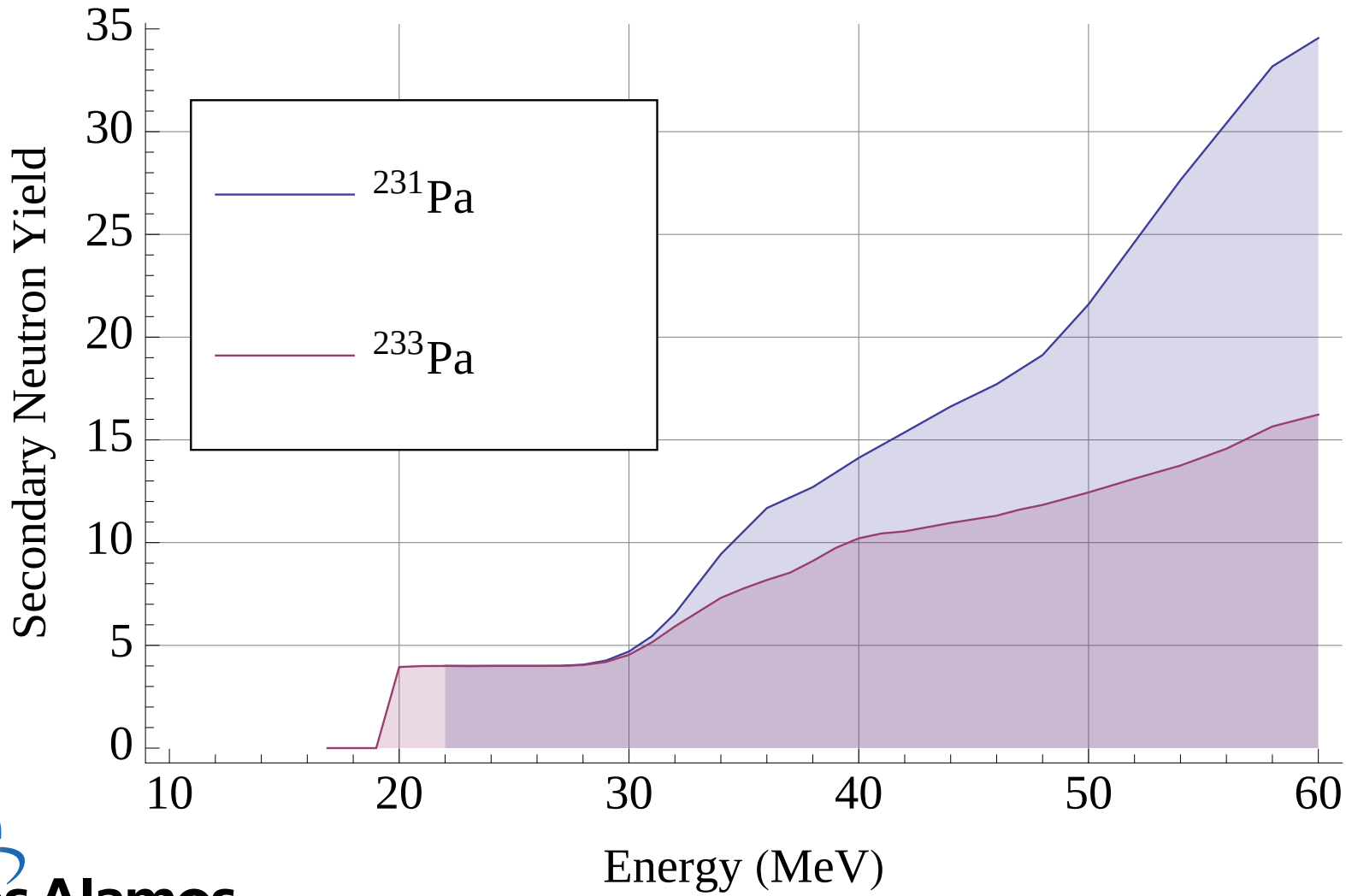
KERMA Problems

1.	^{3}H	13.	^{59}Ni	25.	^{82}Kr	37.	^{92}Mo	49.	^{110m1}Ag
2.	^{4}He	14.	^{74}Se	26.	^{84}Kr	38.	^{94}Mo	50.	^{106}Cd
3.	^{30}Si	15.	^{76}Se	27.	^{86}Kr	39.	^{96}Mo	51.	^{111}Cd
4.	^{40}Ca	16.	^{77}Se	28.	^{85}Rb	40.	^{97}Mo	52.	^{113}In
5.	^{42}Ca	17.	^{78}Se	29.	^{87}Rb	41.	^{98}Mo	53.	^{115}In
6.	^{43}Ca	18.	^{79}Se	30.	^{86}Sr	42.	^{99}Mo	54.	^{112}Sn
7.	^{44}Ca	19.	^{80}Se	31.	^{87}Sr	43.	^{96}Ru	55.	^{113}Sn
8.	^{46}Ca	20.	^{82}Se	32.	^{90}Sr	44.	^{98}Ru	56.	^{114}Sn
9.	^{48}Ca	21.	^{79}Br	33.	^{91}Y	45.	^{99}Ru	57.	^{115}Sn
10.	^{49}Ti	22.	^{81}Br	34.	^{96}Zr	46.	^{100}Ru	58.	^{116}Sn
11.	^{55}Mn	23.	^{78}Kr	35.	^{94}Nb	47.	^{106}Ru	59.	^{117}Sn
12.	^{58}Co	24.	^{80}Kr	36.	^{95}Nb	48.	^{107}Pd	60.	^{118}Sn

KERMA Problems

61.	^{119}Sn	73.	^{125}Te	85.	^{129}Xe	97.	^{136}Ba	109.	^{149}Pm
62.	^{120}Sn	74.	^{126}Te	86.	^{133}Xe	98.	^{137}Ba	110.	^{152}Eu
63.	^{122}Sn	75.	^{128}Te	87.	^{135}Xe	99.	^{138}Ba	111.	^{156}Eu
64.	^{123}Sn	76.	^{132}Te	88.	^{136}Xe	100.	^{138}La	112.	^{159}Tb
65.	^{124}Sn	77.	^{127m1}Te	89.	^{134}Cs	101.	^{140}La	113.	^{180}Ta
66.	^{126}Sn	78.	^{129m1}Te	90.	^{135}Cs	102.	^{140}Ce	114.	^{181}Ta
67.	^{124}Sb	79.	^{129}I	91.	^{136}Cs	103.	^{142}Ce	115.	^{185}Re
68.	^{125}Sb	80.	^{131}I	92.	^{137}Cs	104.	^{144}Ce	116.	^{187}Re
69.	^{120}Te	81.	^{123}Xe	93.	^{130}Ba	105.	^{142}Pr	117.	^{204}Pb
70.	^{122}Te	82.	^{124}Xe	94.	^{132}Ba	106.	^{143}Pr	118.	^{206}Pb
71.	^{123}Te	83.	^{126}Xe	95.	^{134}Ba	107.	^{147}Pm	119.	^{207}Pb
72.	^{124}Te	84.	^{128}Xe	96.	^{135}Ba	108.	^{148}Pm	120.	^{208}Pb

Too Many Secondaries in ^{231,233}Pa, MT=5



Missing Fission Q-value

1. ^{223}Ra
2. ^{226}Ra
3. ^{251}Es
4. ^{252}Es
5. ^{253}Es
6. ^{254m1}Es
7. ^{255}Es

n-099_Es_253.endf

```
...
                                                  9913 1451   303
  1          451          361                   19913 1451   304
  1          452            5                   19913 1451   305
  1          455            7                   19913 1451   306
  1          456            4                   19913 1451   307
  2          151            6                   19913 1451   308
  3            1           39                   19913 1451   309
  3            2           39                   19913 1451   310
...
```

Conclusion

- ^{56}Fe and ^{61}Ni have unphysically small resonances
- ^{153}Eu has negative PDF values for `MT=91`
- 15 evaluations have problems with the unresolved resonance range
- 120 evaluations have problems with the heating or KERMA data
- ^{231,233}Pa has far too many secondary particles for `MT=5` above 20 MeV
- Isotopes of Ra and Es are missing `MT=458`—no fission Q-value