Changes to Decay Data Sub-library

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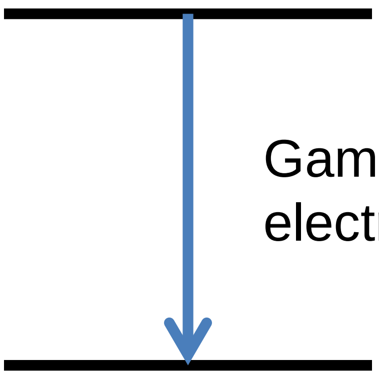
What has been done:

- Changed K X-ray energies for 60 materials with Z=88-94.
- Changed Beta intensities for some 40 fission products.
- Fixed a few minor issues.

Atomic Radiation

Atomic vacancies can be created following gamma emission or EC decay



Gamma emission or electron conversion

$E_k=E_\gamma-B_k$, $I_k/I_\gamma=\alpha_k$, K conv. coeff.
$E_{L1}=E_\gamma-B_{L1}$, $I_{L1}/I_\gamma=\alpha_{L1}$, L1 conv. coeff.
$E_{L2}=E_\gamma-B_{L2}$, $I_{L2}/I_\gamma=\alpha_{L2}$, L2 conv. coeff.
$E_{L3}=E_\gamma-B_{L3}$, $I_{L3}/I_\gamma=\alpha_{L3}$, L3 conv. coeff.
$E_{M1}=E_\gamma-B_{M1}$, $I_{M1}/I_\gamma=\alpha_{M1}$, LM conv. coeff.
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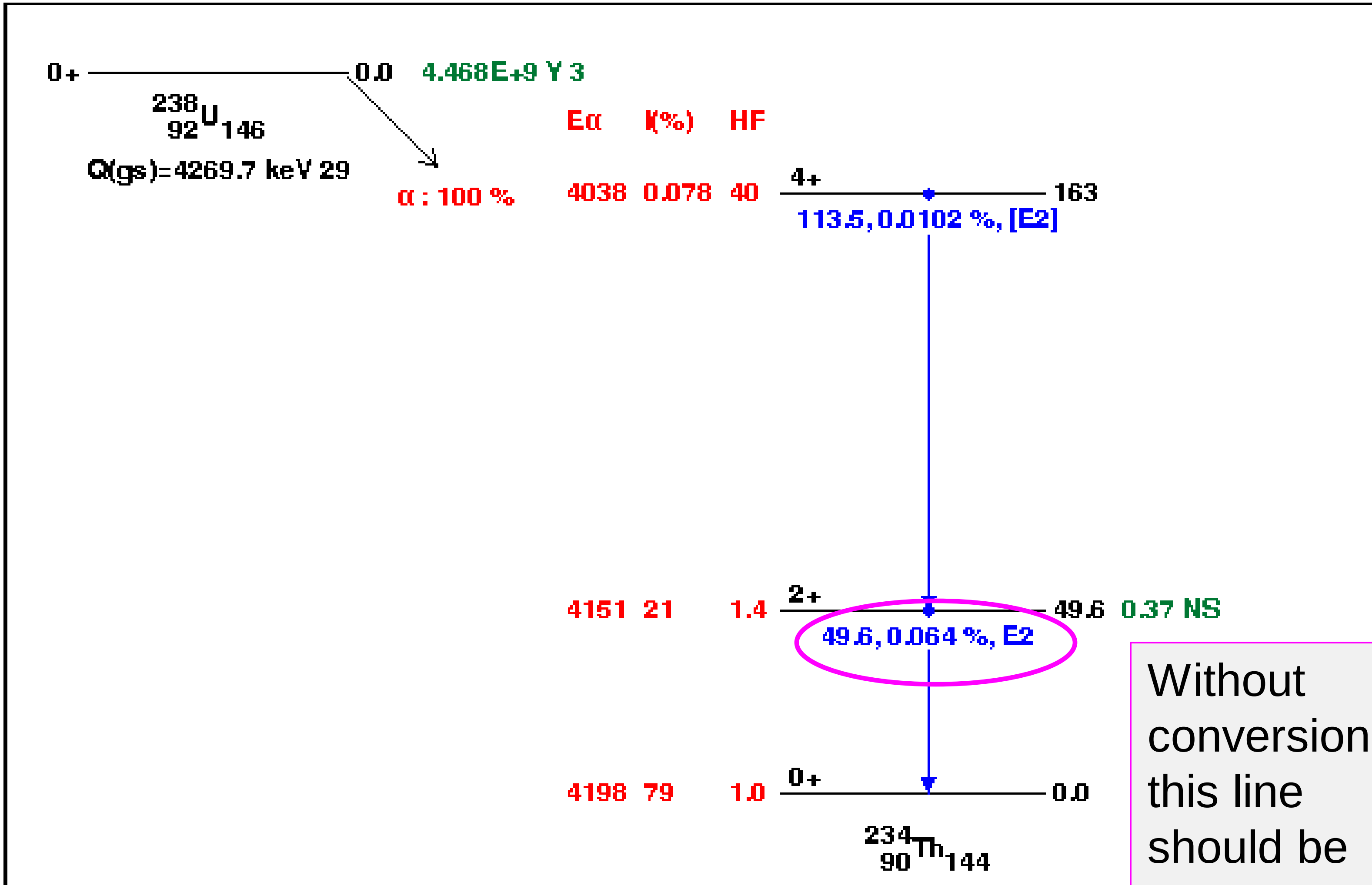
Conversion coefficients increase with Z, angular momentum and decreasing gamma energy. Decrease with increasing orbital. Also, $\alpha_K > \alpha_L > \alpha_M$

Obtained from theoretical calculations using the BRICC code

Example, ^{238}U alpha decay



Without conversion this line should be 21.078%

Electron Capture

For proton rich nuclides, the following weak interaction decay is possible:

$p + e^- \rightarrow n + \nu$

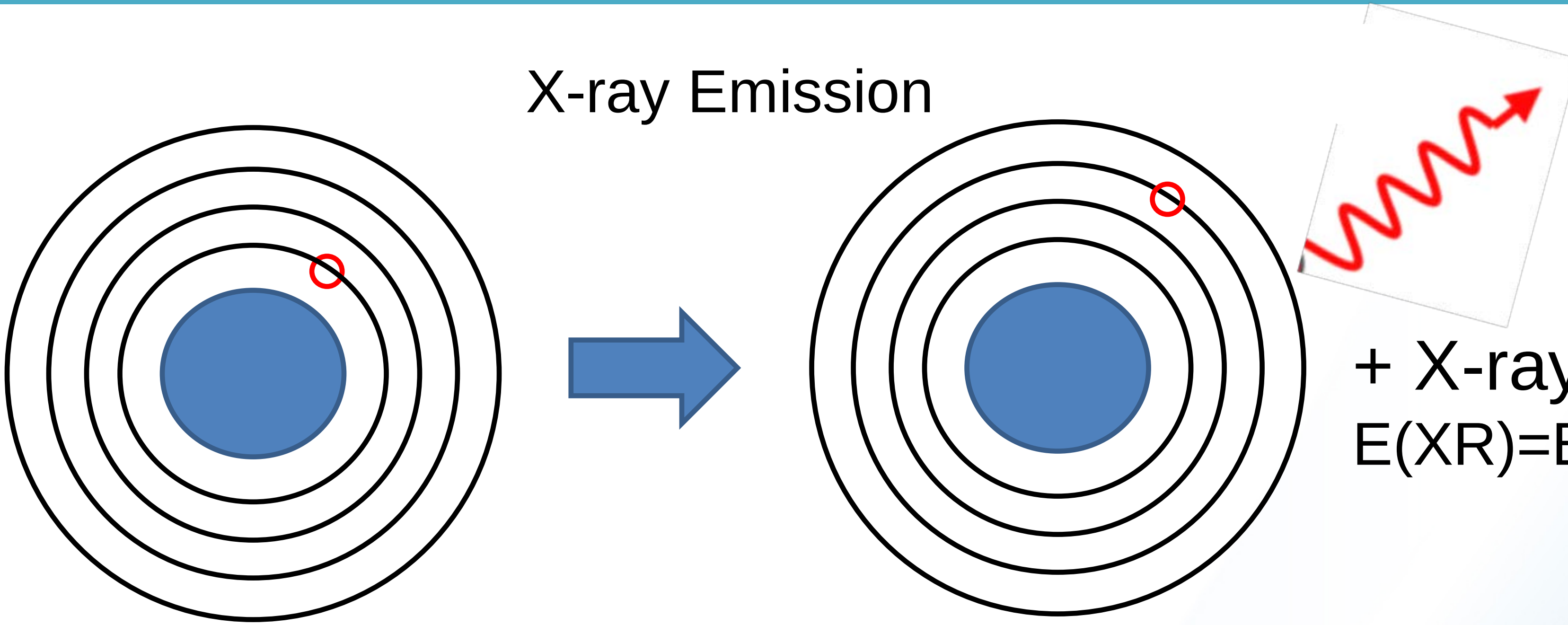
Electron capture creates atomic vacancies, Capture coefficients are given for each orbital, C_k, C_{L1}, etc.

If the energy available is larger than 1.022 MeV, it competes with positron emission:

$p \rightarrow n + \nu + e^+$

How vacancies are filled

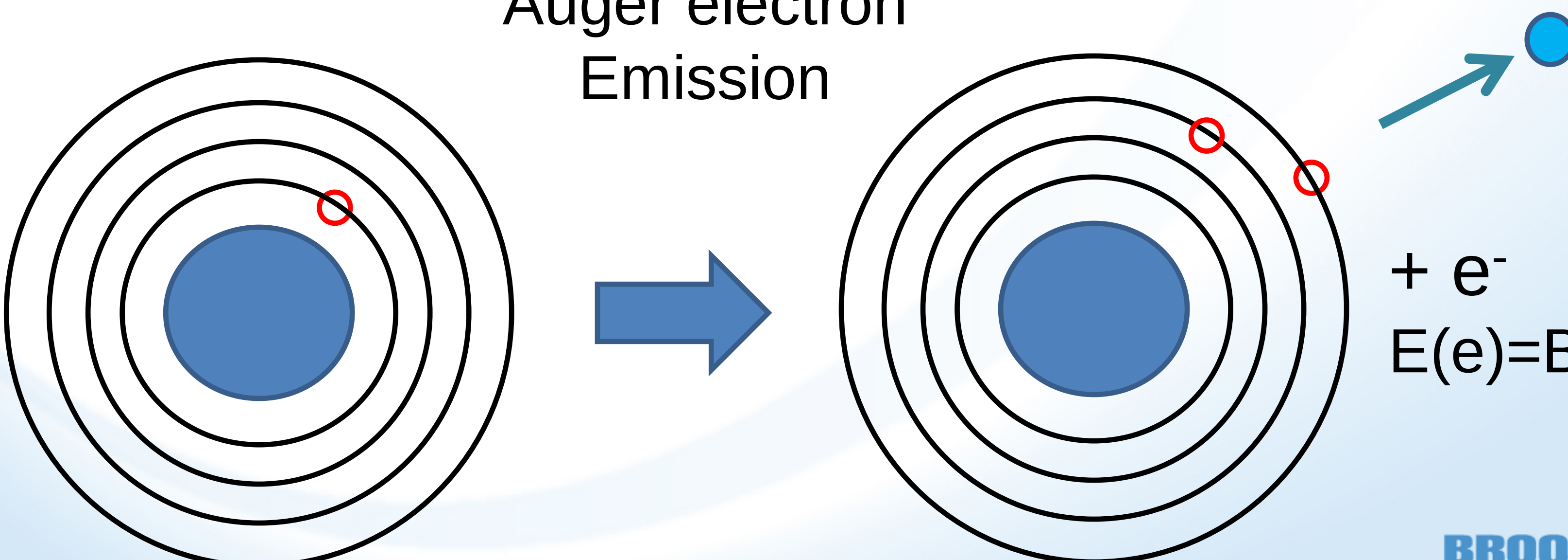
X-ray Emission



+ X-ray

$E(XR)=B_i-B_f$

Auger electron Emission



$+ e^-$

$E(e)=B_i-B_{f1}-B_{f2}$

Atomic Radiation in ENDF/B-VII.1

We used the EADL library to obtain energies and intensities of the X-rays. For instance for ^{235}U:

	Energy	ΔEnergy	Intensity	ΔIntensity
M XR	3065.349	396.5345	0.04553829	0.005930909
L α XR	12960.11	1325.288	0.1184198	0.01204844
other L XR	13197.49	820.5491	0.01522813	9.74183E-4
L β	16125.43	1434.188	0.1308145	0.01150638
L γ	19185.05	1697.594	0.02883229	0.002554897
K-L2 ($K_{\alpha 2}$)	90330.0	903.3	0.03289313	0.003518737
K-L3 ($K_{\alpha 1}$)	93795.0	937.95	0.05631759	0.006024565
K-M2 ($K_{\beta 3}$)	105278.0	1052.78	0.006747349	7.217965E-4
K-M3 ($K_{\beta 1}$)	106074.0	1060.74	0.01324711	0.001417108
K-M4 ($K^{II}_{\beta 5}$)	106608.0	1066.08	2.274561E-4	2.433208E-5
K-M5 ($K^{I}_{\beta 5}$)	106771.0	1067.71	2.62765E-4	2.810925E-5
K-N2 ($K^{II}_{\beta 2}$)	108948.0	1089.48	0.001690858	1.808793E-4
K-N3 ($K^{I}_{\beta 2}$)	109154.0	1091.54	0.003397445	3.634411E-4
K-N4 ($K^{II}_{\beta 4}$)	109395.0	1093.95	6.575589E-5	7.034225E-6
K-N5 ($K^{I}_{\beta 4}$)	109433.0	1094.33	7.612251E-5	8.143193E-6

We were aware that the K binding energies in EADL was affecting the K X-rays energies, shifting up by 0.2-0.4 keV.

Atomic Radiation in ENDF/B-VII.1

Auger electrons are given for groups.

	Energy	ΔEnergy	Intensity	ΔIntensity
CK MMX	493.7612	21.27332	0.3203093	0.01292212
CK LLX	1524.159	73.38183	0.08857388	0.005513789
Auger MXY	2387.489	75.4484	0.822061	0.02509419
Auger LMM	5799.095	50.0081	8.009999E-5	2.673895E-5
Auger LMX	12963.23	352.2304	0.09721805	0.002724669
Auger LXY	16119.98	450.9654	0.01158554	3.35071E-4
Auger KLL	71370.5	200.0004	0.003003	3.089302E-4
Auger KLX	87216.23	3775.481	0.001399327	6.131373E-5
Auger KXY	102582.3	4312.696	2.045445E-4	8.71038E-6

Atomic Radiation in ENDF/B-VIII.0

We are using NIST K X-rays for Z=88-94, about 60 materials.

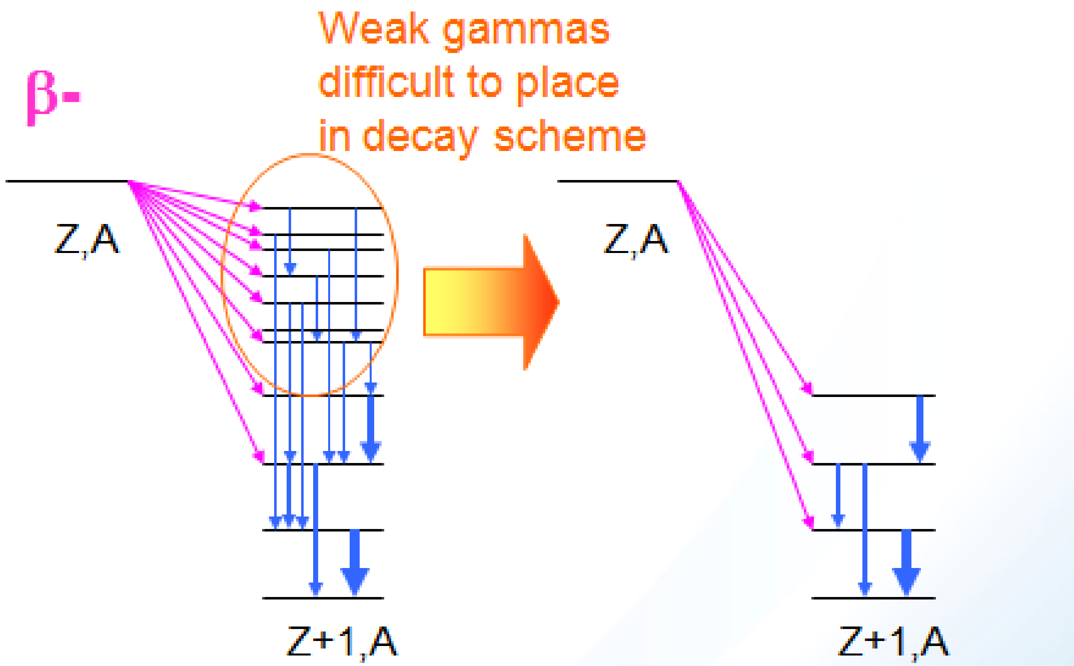
The rest of the atomic radiation is not modified.

L X-rays and Auger electrons are not affected by EADL binding energies. K Augers are.

For the next major release of the decay data sub-library, we will use more precise binding energies for all materials.

Beta intensities in ENDF/B-VIII.0

Ge gamma spectroscopy data can lead to an oversimplification of decay schemes.



As a result the beta spectrum will be overestimated.

A possible solution is to use TAGS data.

Beta intensities in ENDF/B-VIII.0

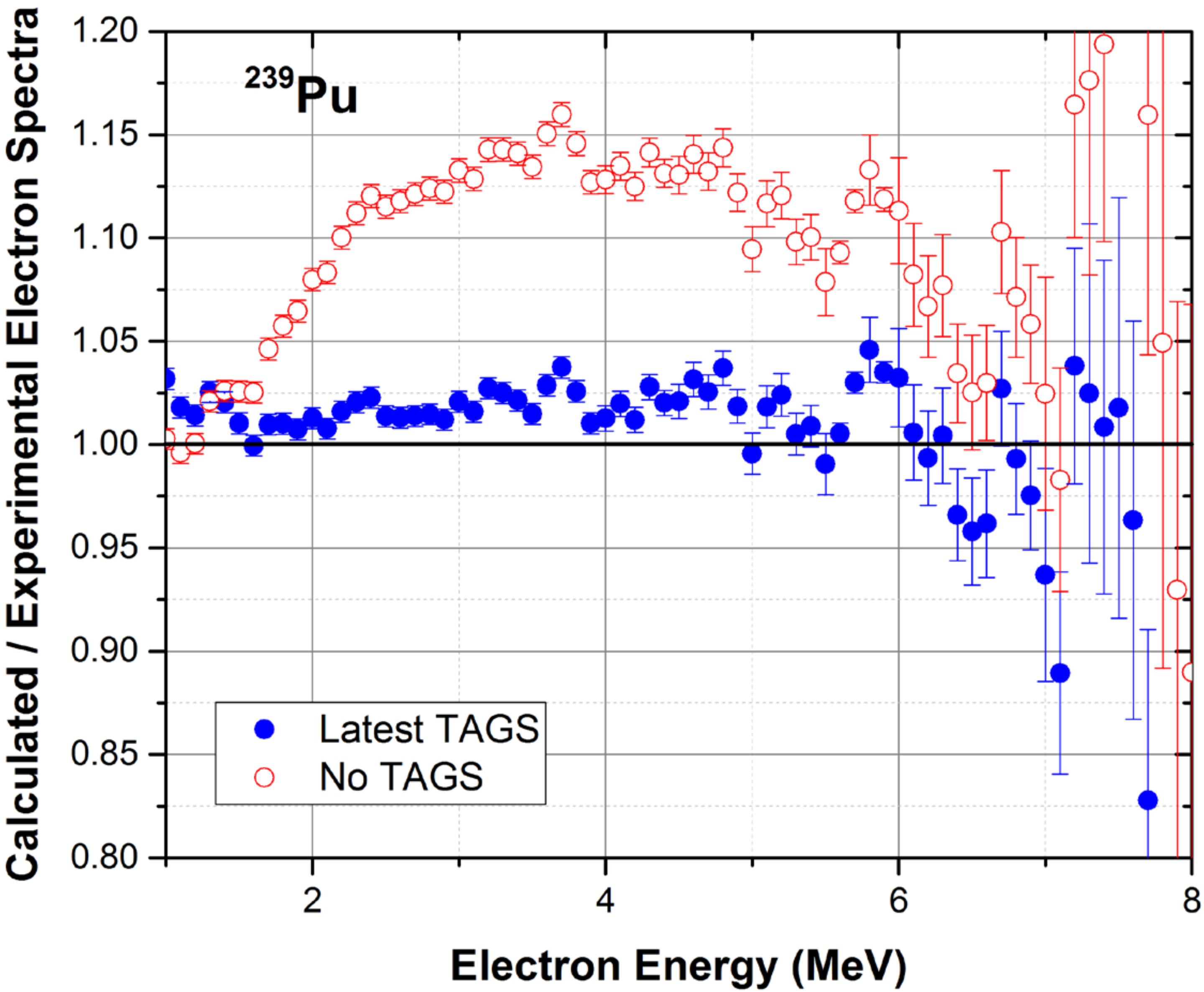
ENDF/B-VII.1 included TAGS data in the mean gamma and beta energies to calculate decay heat.

ENDF/B-VIII.0 will have TAGS beta intensities to improve the calculation of antineutrino spectra.

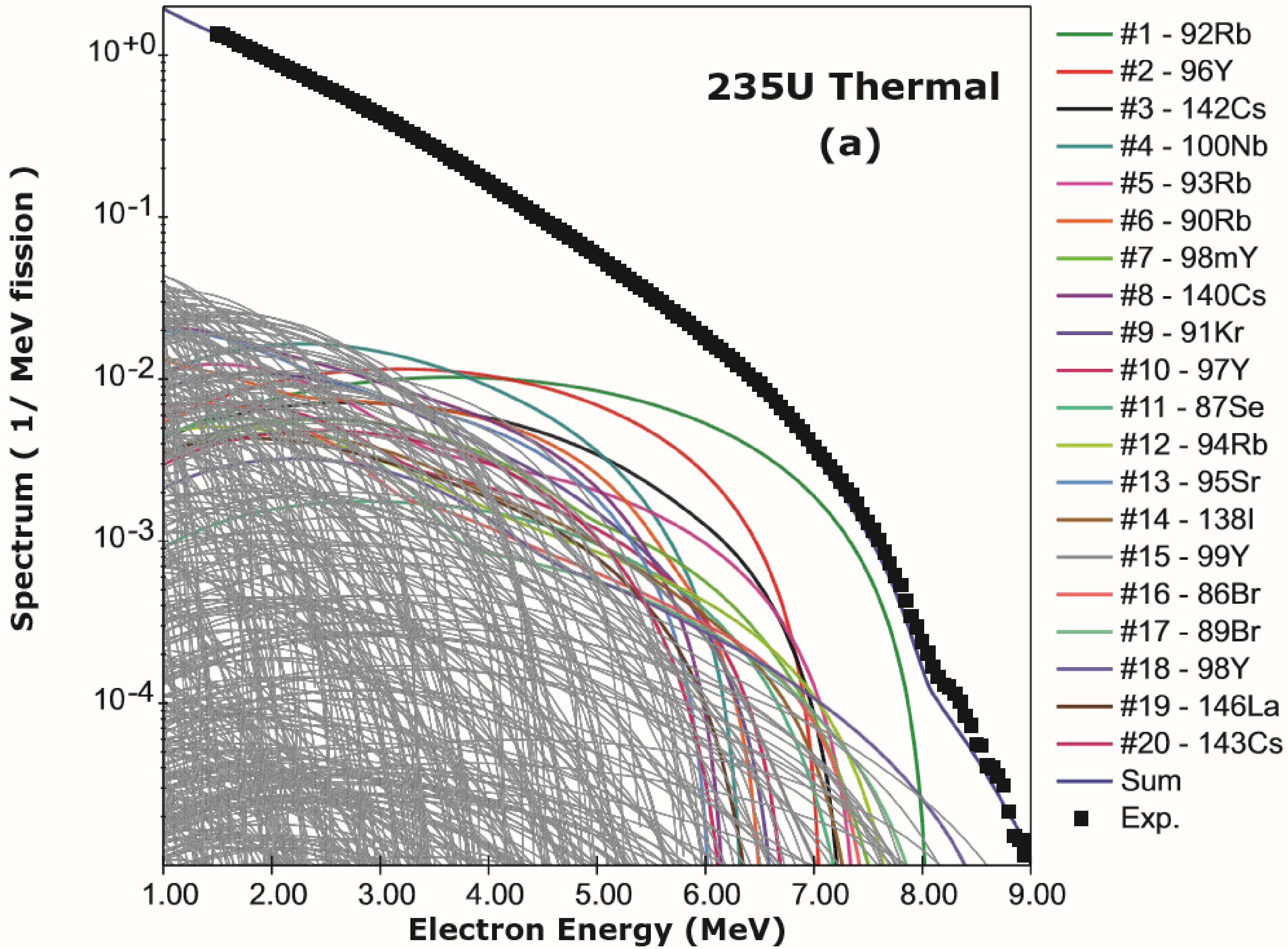
As a benchmark, we will use the electron spectra for ^{235,238}U(n,fission) and ^{239,241}Pu(n,fission) were measured in ILL and Munich.

The electrons are produced by the beta-minus decay of the neutron rich fission products.

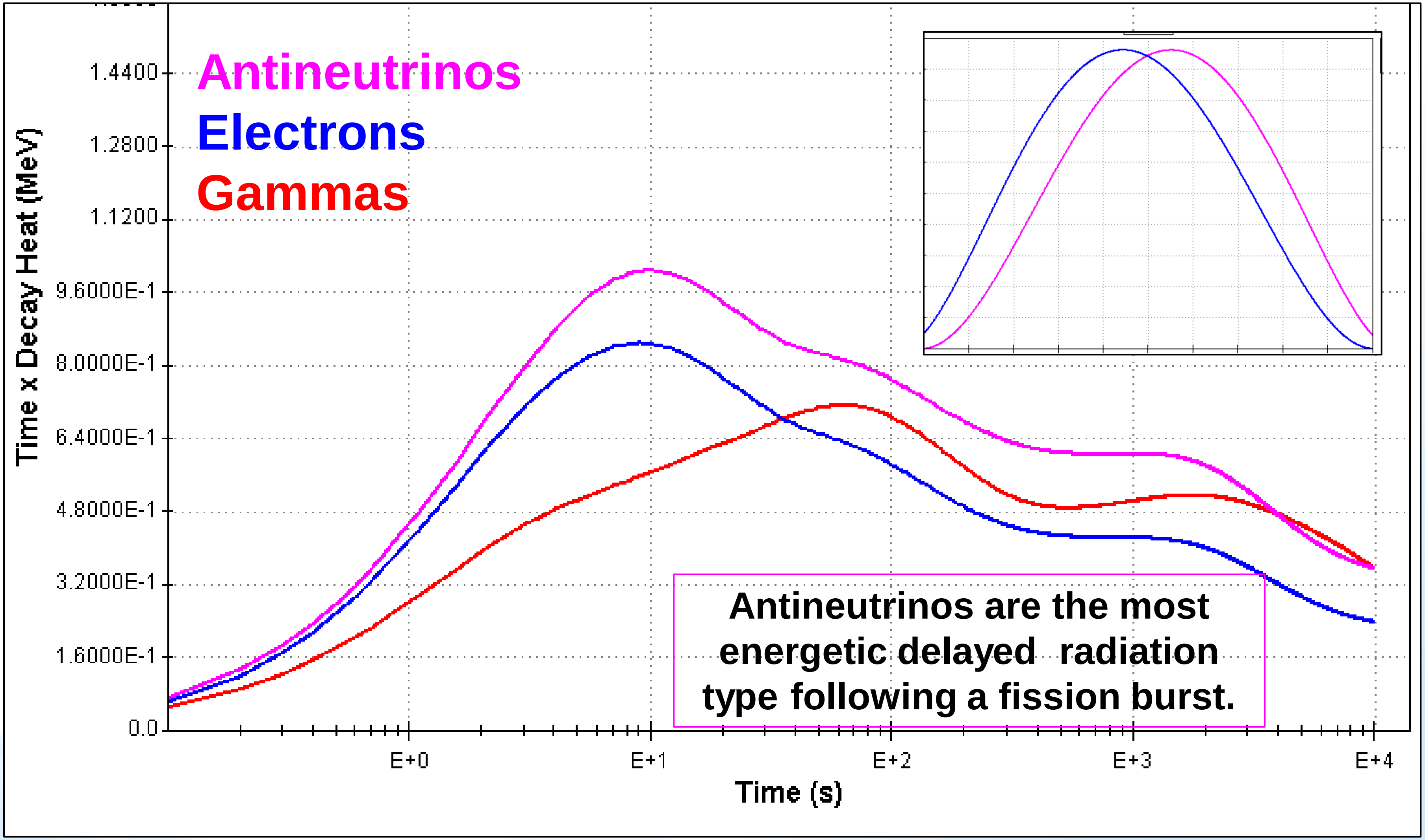
TAGS effects



Calculation of antineutrino spectra



‘Decay Heat’ for 3 radiation types



Decay Energy Systematics