Using EADL Atomic Relaxation Library Following Nuclear Decay

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a passion for discovery

Office of Science
U.S. DEPARTMENT OF ENERGY

Motivation

Need to have a more detailed description of X-ray and Auger production following nuclear decay.

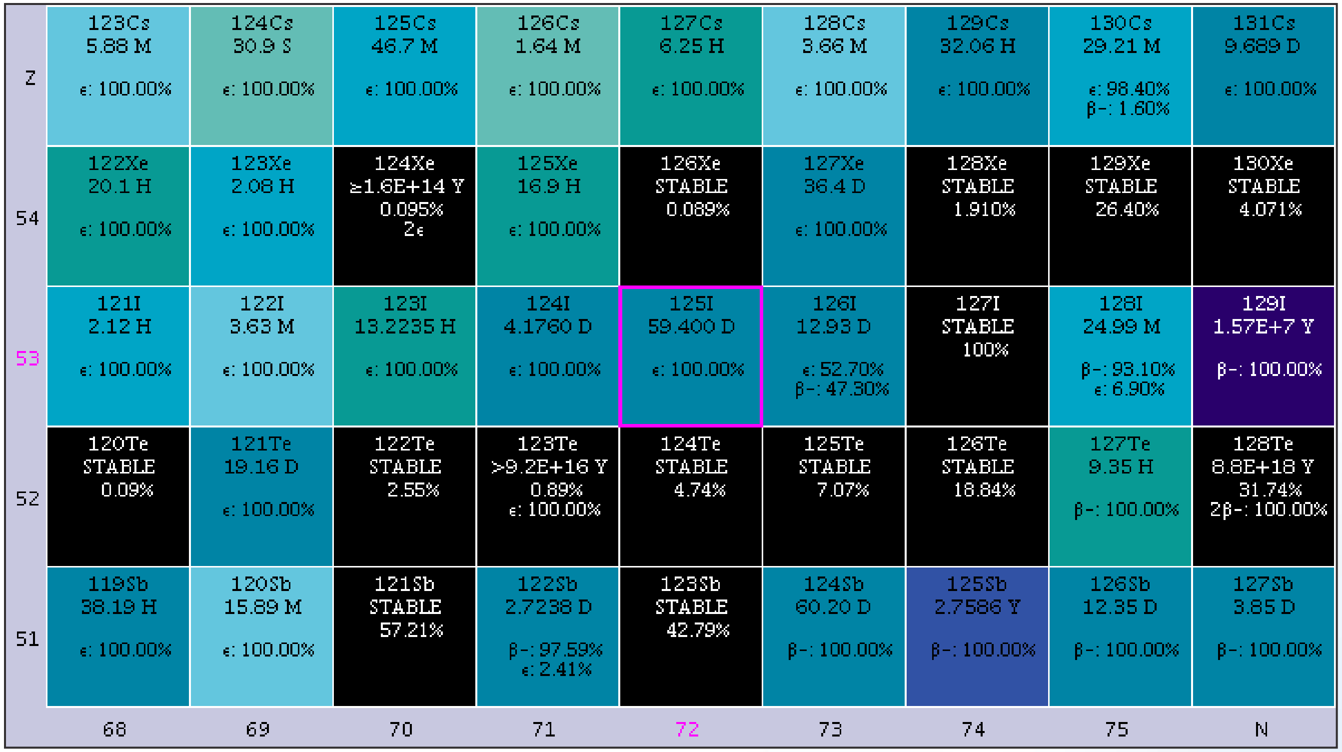
For many long-lived nuclides, atomic radiation is often the dominant type of ionizing radiation.

This topic has been extensively studied before, see:

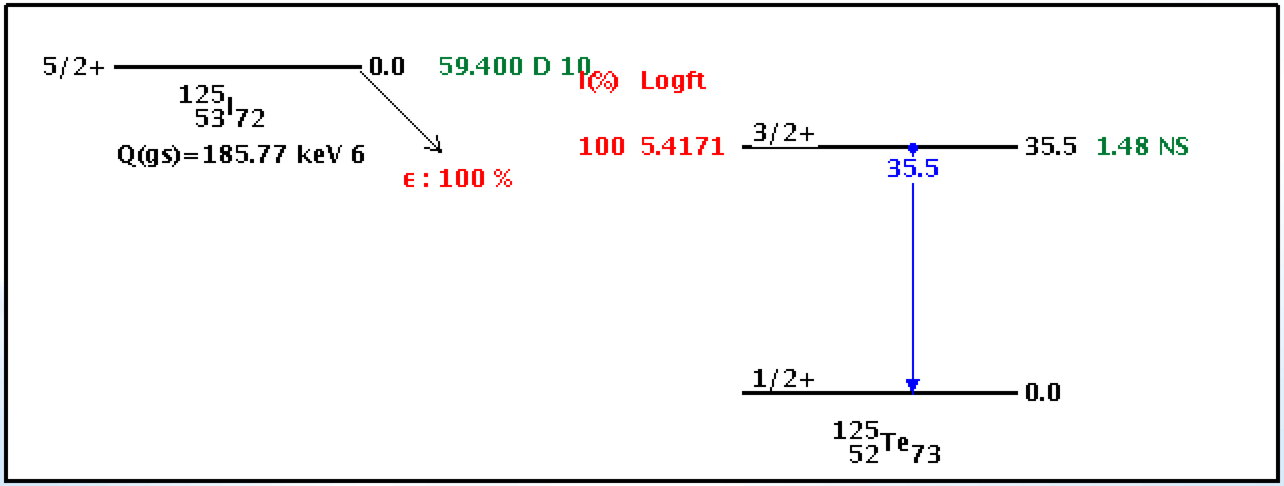
M.-M. Be, V. Chiste, C. Dulieu, Appl. Radiat. Isot. 64, 1435 (2006)
Detailed calculation of K- and L-Auger electron emission intensities following radioactive disintegration

J. Stepanek, Med. Phys. 27 (7), 1544 (2000)
Methods to determine the fluorescence and Auger
spectra due to decay of radionuclides or due to a single atomic subshell ionization and comparisons with experiments.

Example
125I



Z	123Cs 5.88 M ε: 100.00%	124Cs 30.9 S ε: 100.00%	125Cs 46.7 M ε: 100.00%	126Cs 1.64 M ε: 100.00%	127Cs 6.25 H ε: 100.00%	128Cs 3.66 M ε: 100.00%	129Cs 32.06 H ε: 100.00%	130Cs 29.21 M ε: 98.40% β-: 1.60%	131Cs 9.689 D ε: 100.00%
54	122Xe 20.1 H ε: 100.00%	123Xe 2.08 H ε: 100.00%	124Xe ≥1.6E+14 Y 0.095% 2ε	125Xe 16.9 H ε: 100.00%	126Xe STABLE 0.089%	127Xe 36.4 D ε: 100.00%	128Xe STABLE 1.910%	129Xe STABLE 26.40%	130Xe STABLE 4.071%
53	121I 2.12 H ε: 100.00%	122I 3.63 M ε: 100.00%	123I 13.2235 H ε: 100.00%	124I 4.1760 D ε: 100.00%	125I 59.400 D ε: 100.00%	126I 12.93 D ε: 52.70% β-: 47.30%	127I STABLE 100%	128I 24.99 M β-: 93.10% ε: 6.90%	129I 1.57E+7 Y β-: 100.00%
52	120Te STABLE 0.09%	121Te 19.16 D ε: 100.00%	122Te STABLE 2.55%	123Te >9.2E+16 Y 0.89% ε: 100.00%	124Te STABLE 4.74%	125Te STABLE 7.07%	126Te STABLE 18.84%	127Te 9.35 H β-: 100.00%	128Te 8.8E+18 Y 31.74% 2β-: 100.00%
51	119Sb 38.19 H ε: 100.00%	120Sb 15.89 M ε: 100.00%	121Sb STABLE 57.21%	122Sb 2.7238 D β-: 97.59% ε: 2.41%	123Sb STABLE 42.79%	124Sb 60.20 D β-: 100.00%	125Sb 2.7586 Y β-: 100.00%	126Sb 12.35 D β-: 100.00%	127Sb 3.85 D β-: 100.00%
	68	69	70	71	72	73	74	75	N



Energy Balance (keV)

Gammas	2.37 *5*
X-Rays	40.2 *24*
ß minus	0
ß plus	0
Conversion Electrons	6.98 *9*
Auger electrons	11.0 *3*
Neutrinos	123.98 *5*
Sum	184.6 *24*
Q-effective	185.77 *6*

EADL

Evaluated Atomic Data Library, developed in LLNL by Chen *et al*. Assembled in ENDF-6 format by Red Cullen.

Available from www.nndc.bnl.gov/sigma selecting Atomic Relaxation sub-library in ENDF/B-VII.0 library.

For each Z value, it lists:

Atomic sub-shells with corresponding binding energy.

For each sub-shell, it gives transition energy and probability for X-rays and Auger electrons.

For a given transition, it assumes that higher sub-shells are filled. So, corrections are needed if it is not the case.

Minor corrections may be needed for energies.

Using EADL coupled to ENSDF files

Must know vacancies generated by Electron Capture and Conversion.

LOGFT code only gives L capture, follow Stepanek to obtain L2 and L3 components (*also in RADLST*).

Must know conversion coefficients for sub-shells, possible now with BRICC.

Assume that vacancies propagate outwards from the K-shell in an isolated atom with EADL corrected probabilities, and vacancies can only be filled by bound electrons (Deterministic & Isolated).

The goal is to compare the use of EADL with the EMISSION code, which provides a more detailed atomic radiation output than RADLST. Once the quality control process is over, NuDat will offer EADL based values.

Fluorescence yield ωK: probability of filling vacancy in K-shell by X-ray emission

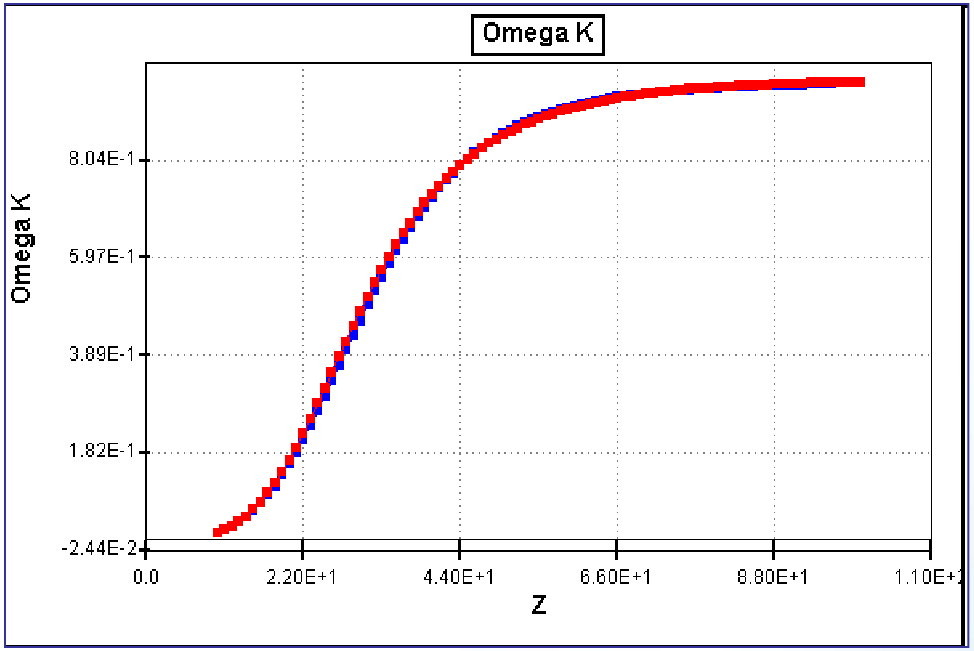
ωK=sum of K-(other shell) X-ray intensities

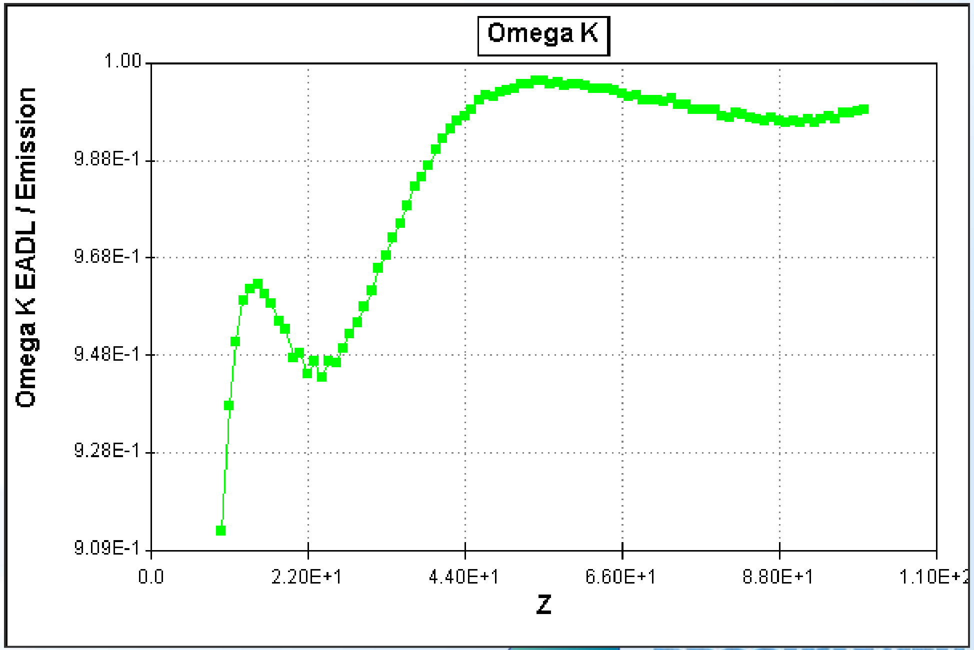
Blue: from EADL

Red: from EMISSION

Green: ratio of EADL to EMISSION.

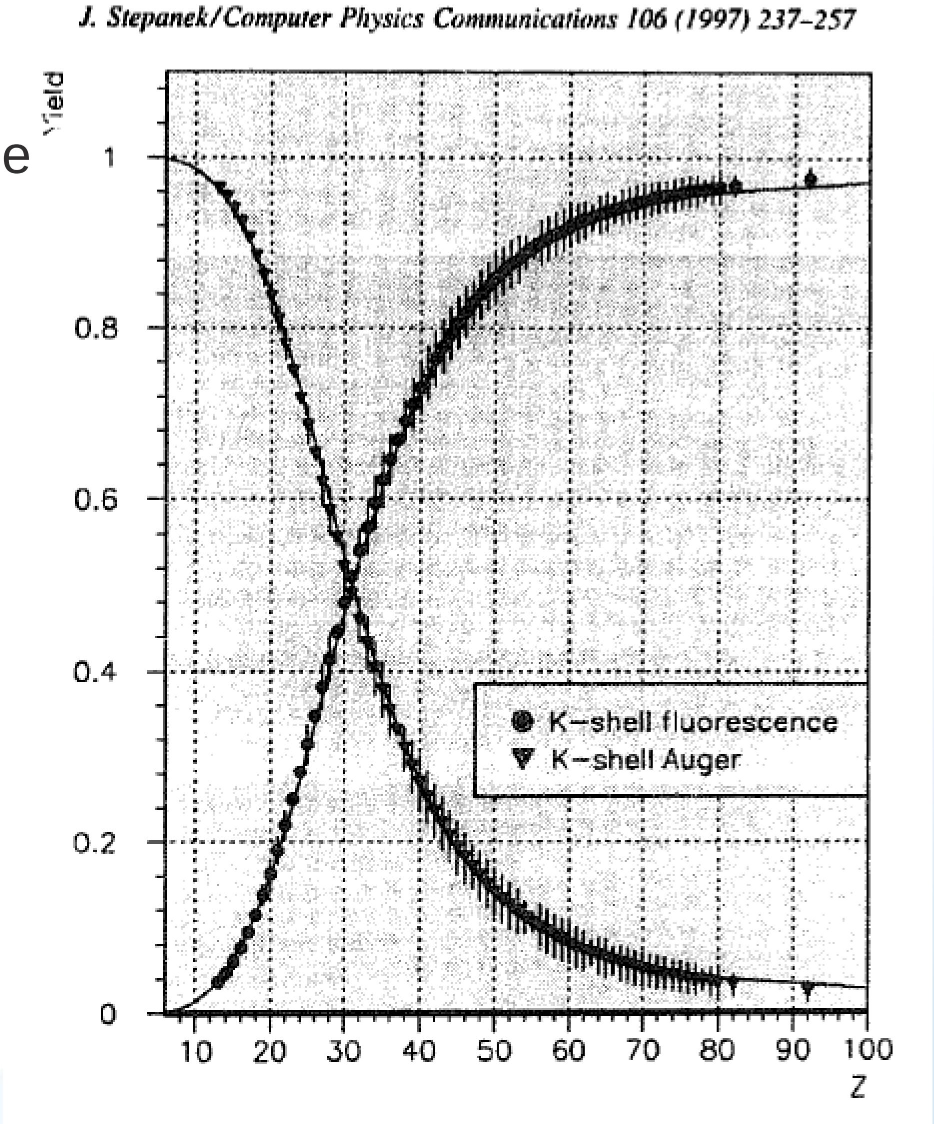
For **ωK**, the ratio is close to 1.0, and the expected uncertainties are about 10%.





Fluorescence yield ωK:

There was a question during the ICTP workshop on this topic.



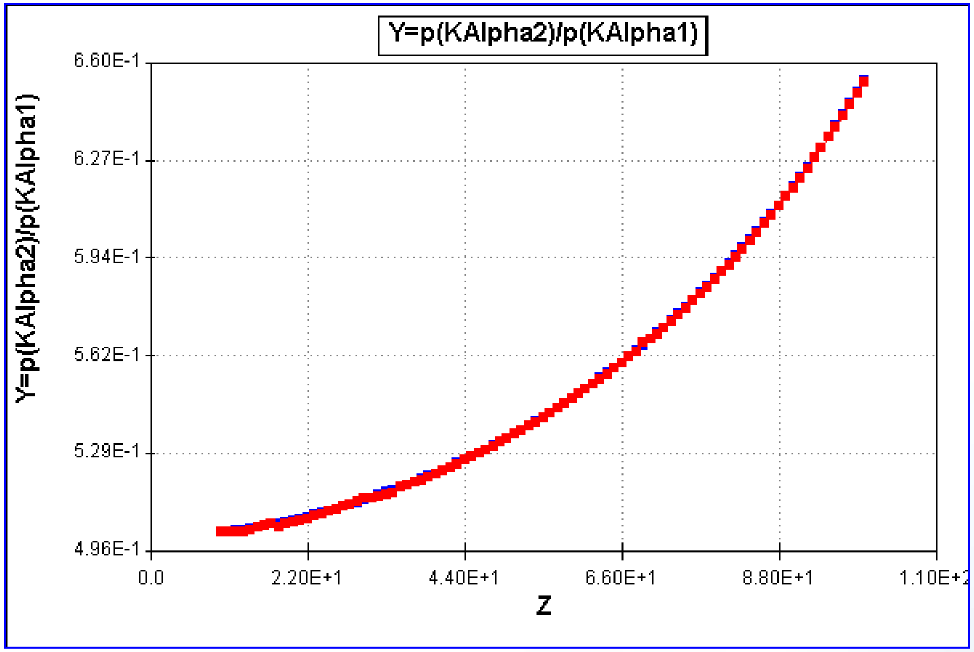
J. Stepanek/Computer Physics Communications 106 (1997) 237–257

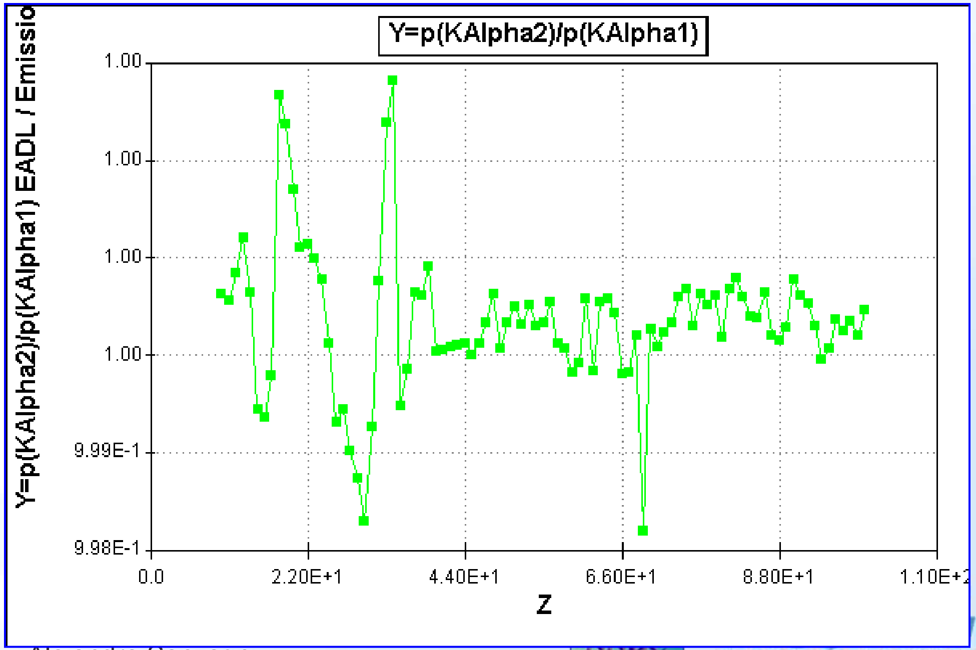
Y=I(Kα2)/I(Kα1)

Y=I(K-L2)/I(K-L3)

Ratio of intensities for the most intense, lowest energies K X-rays.

The ratio is very close to 1.





X=I(Kβ)/I(Kα)

X=[I(K-M3)+

I(K-N2)+I(K-N3)+

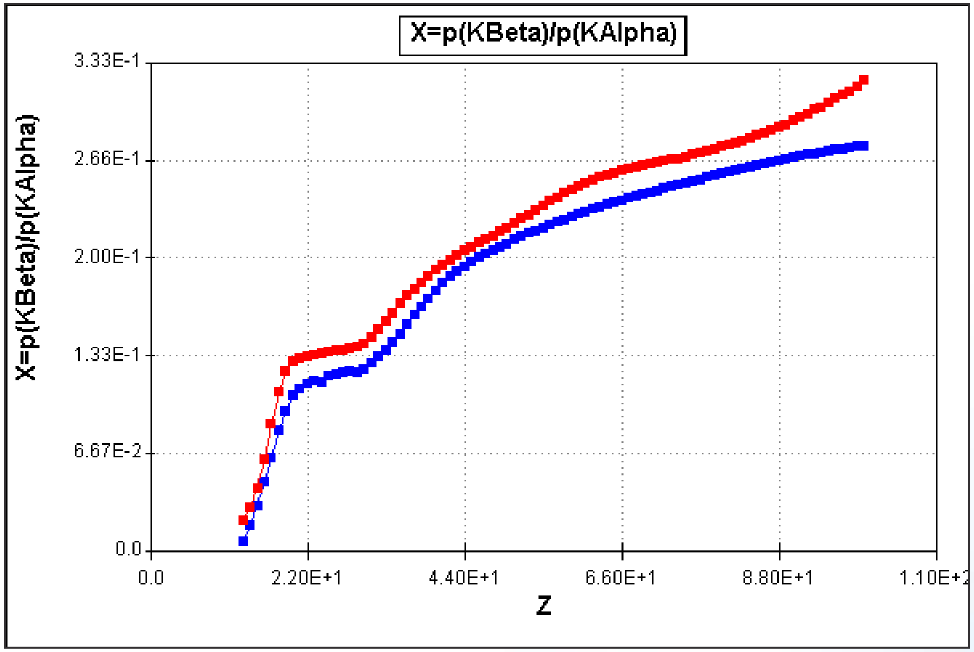
I(K-M2)+

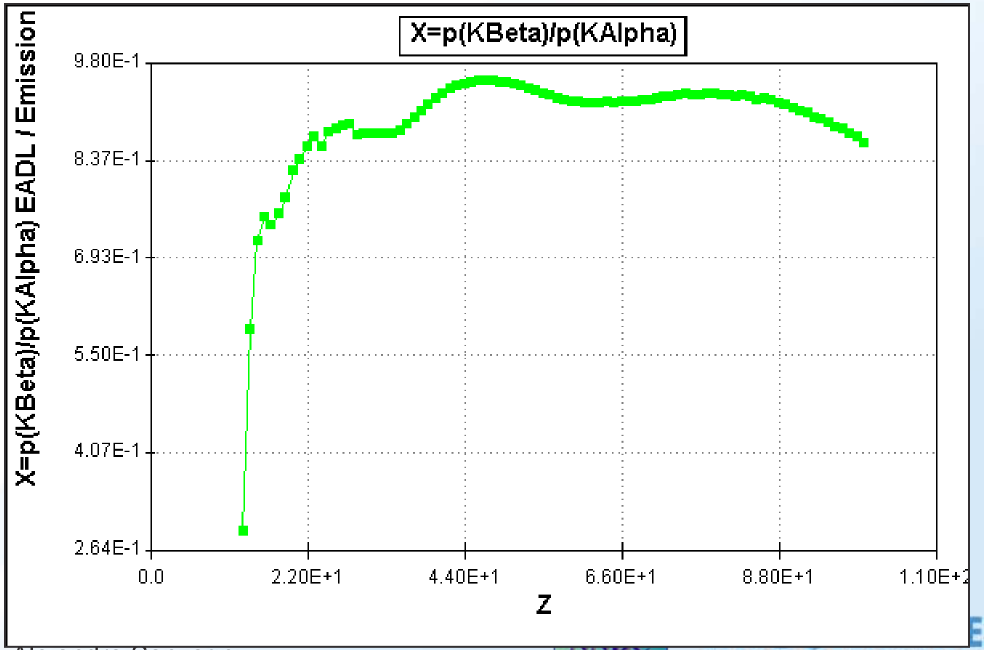
I(K-N4)+I(K-N5)+

I(K-M4)+I(K-M5)] /

[I(K-L2) + I(K-L3)]

The ratio is close to 1 for Z > 44.





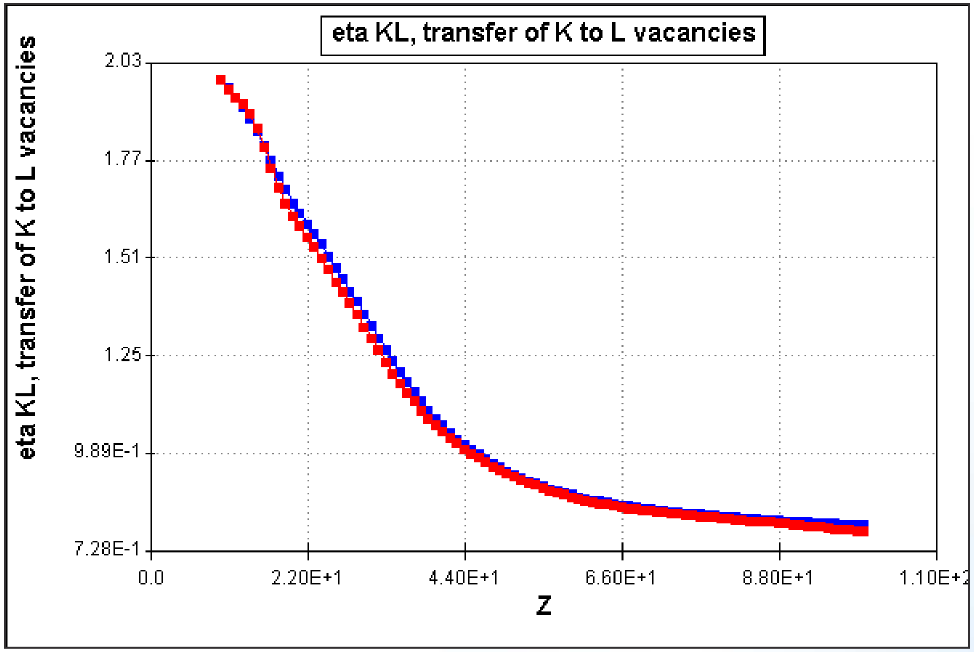
ηKL=Transfer of K to L vacancies.

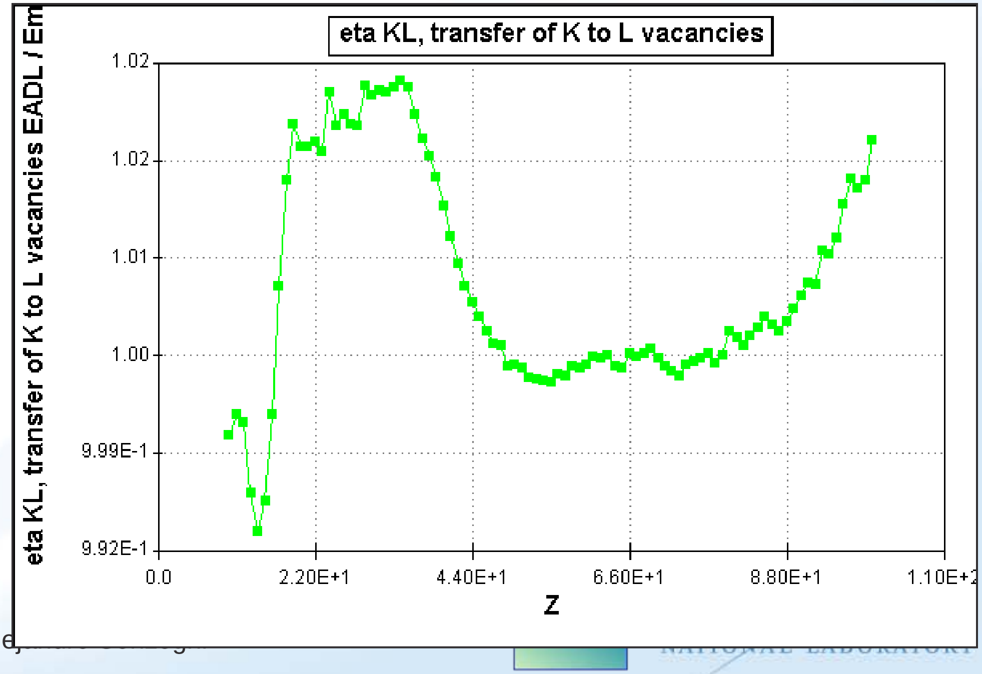
ηKL=sum of K-L X-rays plus K-L-L Auger intensities.

The ratio is very close to 1.

However, ratio for the individual **ηKL2**, **ηKL3** deviates from 1 if Z < 44.

We calculate less **ηKL2** and more **ηKL3** than Emission for Z < 44, about a 30% discrepancy.

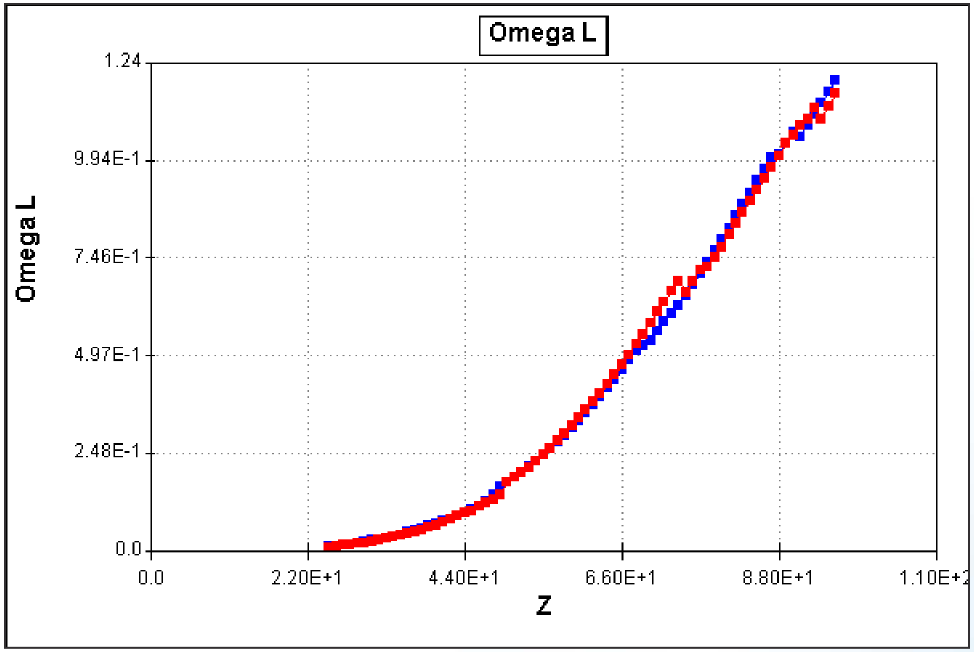


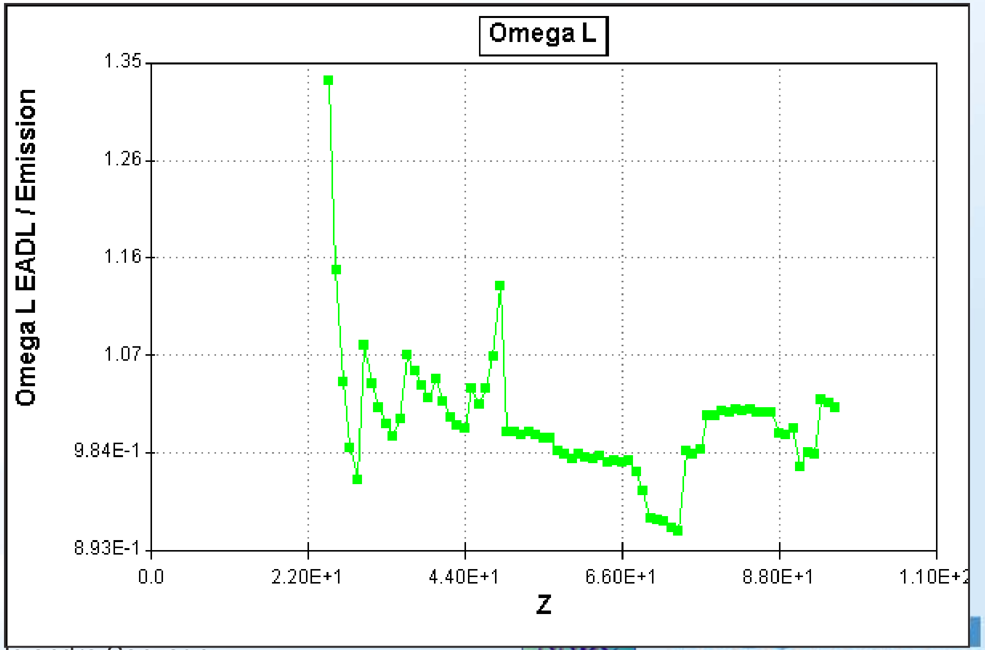


Fluorescence yield ωL: probability of filling vacancy in L-shells by X-ray emission

ωL=sum of L1-(other shell) + L2-(other shell) + L3-(other shell) X-ray intensities

Ratio is close to 1.0, shell effects are mainly due to **ωL1**





Comparison with Stepanek 2000 and Be 2006 for 125I

Radiation Label	Energy[a]	Intensity[a]	Energy[b]	Intensity[b]	Intensity[c]
Auger KLL	2.36E+04	1.22E-01	2.27E+04	1.21E-01	1.32E-01
Auger KLX	2.76E+04	5.41E-02	2.65E+04	5.50E-02	6.00E-02
Auger KXY	3.16E+04	5.40E-03	3.03E+04	5.99E-03	6.80E-03
CK LLX	3.13E+02	2.48E-01	2.91E+02	2.25E-01	2.72E-01
Auger LMM	3.21E+03	1.20E+00	3.09E+03	1.18E+00	1.23E+00
Auger LMX	3.84E+03	3.56E-01	3.68E+03	3.48E-01	3.29E-01
Auger LXY	4.53E+03	2.55E-02	4.29E+03	2.56E-02	2.18E-02
CK MMX	1.18E+02	1.40E+00	1.21E+02	1.31E+00	
Auger MXY	4.82E+02	3.20E+00	4.57E+02	3.14E+00	3.07E+00
K-L3 (Ka1)	2.86E+04	7.57E-01	2.75E+04	7.50E-01	7.40E-01
K-L2 (Ka2)	2.83E+04	4.10E-01	2.72E+04	4.01E-01	3.97E-01
K-M3 (Kb1)	3.23E+04	1.33E-01	3.10E+04	1.34E-01	2.12E-01
K-N2+K-N3 (Kb2)	3.30E+04	4.25E-02	3.17E+04	4.24E-02	4.60E-02
K-M2 (Kb3)	3.22E+04	7.09E-02	3.09E+04	6.91E-02	
K-N4+K-N5 (Kb4)	3.31E+04	3.00E-04	3.18E+04	2.46E-04	
K-M4+K-M5 (Kb5)	3.25E+04	1.60E-03	3.12E+04	1.46E-03	

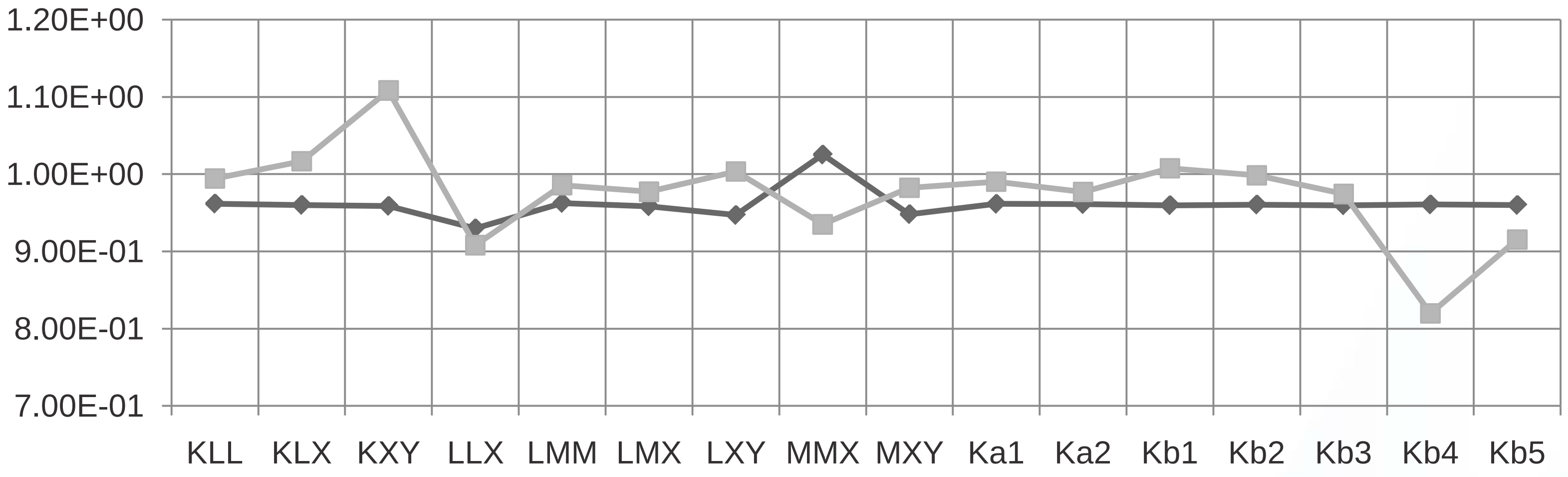
a: Stepanek 2000, Table IV, Deterministic

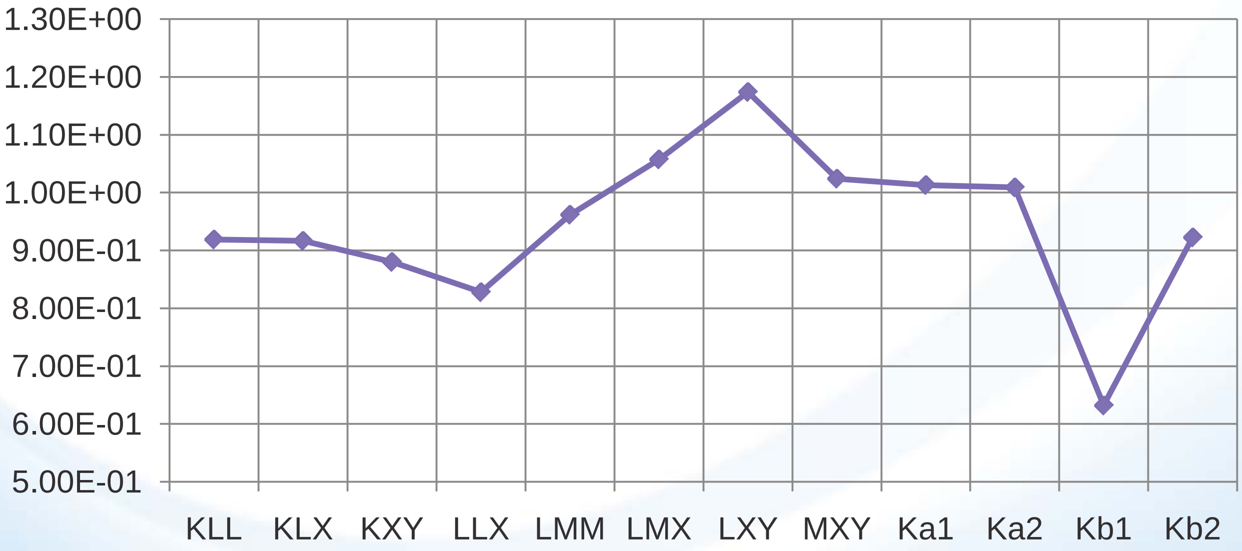
b:This work

c: Be 2006

K intensities have 10% uncertainties. Higher values for less bound sub-shells

E(EADL)/E(Stepanek) & I(EADL)/I(Stepanek)





I(EADL)/I(Be 2006)

Conclusions

We plan to upgrade the current Radlist available from NuDat using EADL. Highly detailed X-rays and Auger data for all decay datasets in ENSDF.

Deterministic & Isolated calculations agree well with earlier works. Discrepancies are observed for transitions with negligible impact in energy balance (possible exception of Kb1)

Still some work has to be done to understand some minor discrepancies.

Any experience using EADL?