BrIccEmis & NS_RadList
Inclusion of absolute atomic radiation energies and emission probabilities in ENSDF decay data sets

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Atomic Data in ENSDF – ^{125}I EC

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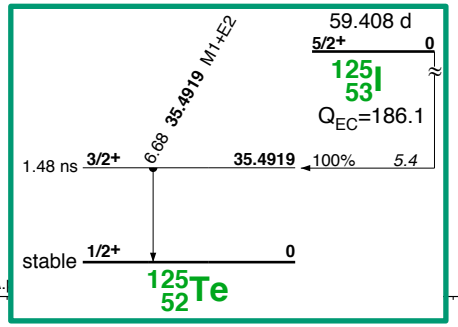
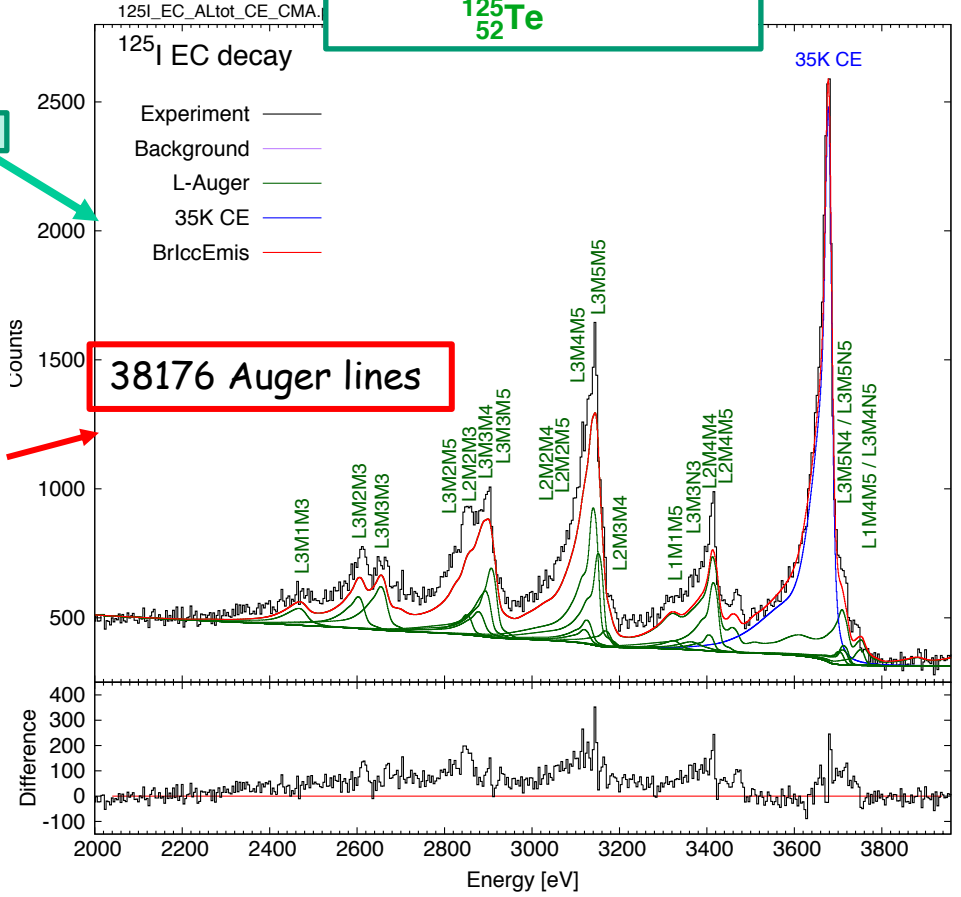
BrIccEmis

```
# AUGER electrons ==========================================
          AUGER transition types:      703
#                          Energy
# Trans        Mean[eV]    95% Conf. range       Prob.[per decay]
Auger_Tot        575.67        [0.67 : 3549.10]        1.984E+01
Auger_Ktot     24012.13    [21862.97 : 30041.68]        1.919E-01
Auger_KLL      22601.02    [21862.97 : 23073.01]        1.291E-01
Auger_KLX      26542.05    [25891.68 : 27430.52]        5.678E-02
Auger_KXY      30408.86    [29843.69 : 31587.48]        6.024E-03
Auger_Ltot      2779.82      [122.27 : 3992.71]        1.842E+00
CK_LLX           289.40       [65.01 : 549.65]        2.688E-01
Auger_LMM       3050.80     [2480.27 : 3744.61]        1.210E+00
Auger_LMX       3678.37     [3314.78 : 4270.55]        3.395E-01
Auger_LXY       4311.28     [4026.15 : 4851.10]        2.389E-02
Auger_Mtot       328.61       [21.81 : 632.80]        4.507E+00
CK_MMX           100.06        [8.36 : 246.72]        1.310E+00
Auger_MXY        422.29      [263.30 : 648.98]        3.197E+00
Auger_Ntot        16.01        [0.41 : 73.45]        1.330E+01
SCK_NNN           16.25        [0.52 : 55.53]        2.244E+00
CK_NNX            35.73        [0.97 : 108.81]       9.260E-01
Auger_NXY         14.15        [0.40 : 66.52]        1.013E+01
```





Transitions:

Auger: 320279 energies of 703 transition types

X-ray: 9158 energies of 73 transition types

M Alotiby et al., Phys. Med. Biol. ***63*** *(2018) 06NT04*

M Alotiby et al., J. Phys. Elect. Spect. and Rel. Phenom. ***232*** *(2019) 73*

Uncertainties

Uncertainties should be evaluated from

ΔE: nuclear transition energies (CE only) and atomic binding energies calculated for ionic systems

NOTE: RAINE tend to overestimate binding energies (magnitude depends on Z and shell)

ΔRI: nuclear transition (γ, EC) intensities, conversion coefficients and transition rates from EADL

NOTE1: Accuracy of EADL

- K, L: Auger: 15%; X-ray: 10%
- M, N ..: Auger: unknown, KC-Auger: 100%, X-ray below 100 eV: 30%;

NOTE2: EADL calculated for single initial vacancies!

NOTE3: To propagate uncertainties BrIccEmis need to be modified significantly

At present we will not be able report uncertainties

Notation

Comment	X-rays	Auger electrons
Notation: from IUPAC ❑ International Union of Pure and Applied Chemistry ❑ Based on initial and final atomic levels involved	K-L_3	K-L_1-L_2
Group sub-shells to reduce number of transitions ❑ Summed decay rates ❑ Use the mean transition energy for the group. Mean energy evaluated from the full energy spectrum	L (for L_1-M_2, … L_3-O_4) But not for K $K_{\alpha 1}$ for K-L_3 $K_{\alpha 2}$ for K-L_2 K_{β} for K-M_3&K-M_2	KLL (for K-L_1-L_1, … K-L_3-L_3) KLX (X=M_1….,N_1….) KXY (X&Y=M_1….,N_1….)

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NS_RadList

- Reads and validates ENSDF input
- Calculates primary vacancy distribution following EC (1995SCZX, 1998Sc28) and IC (2008Ki07)
- Calculates full Auger and X-ray spectra using BrIccEmis data base; generates new ENSDF cards, calculation report files and optional plots using GnuPlot
- Second pass to merge new ENSDF cards (same as BrIcc)
- NS_Radlist based on NS_Lib, shared routines with BrIcc, TRuler, UncTools. Comprehensive error checking of the ENSDF file. Runs on all operating systems
- BrIccEmis data base: calculated for Z=6-100, ~70 Mb binary data
- To be completed in 2019 (ANU)

NS_RadList - calculation report: ^{103}Pd EC

```
#  Programs ================================================
#    Program version: NS_RadList v1.0 (01-Dec-2018)
#    NS_Library version: NS_Lib v1.0 (24-Nov-2018)
#    Atomic relaxation program: BrIccEmis (18-Apr-2017)
#    BrIccEmis data base: (21-Jun-2017)
#    NSR Key: 2012Le09

#  Nuclear decay data ======================================
#    ENSDF file: 103Pd_EC.ens
```

Header

```
# EC decay ================================================
# Transition    Decay Energy [keV]              Probability
#                                             [per 100 decays]
   1              5.43E+02                       1.000E-01 LE
   2            503.4(8)                        99.90(10)
   3            248.1(8)                         0.00044(11)
   4            185.7(8)                         0.0248(8)
   5              6.3(8)                         0.00400(20)
```

EC decay

```
# Electromagnetic decay ===================================
# Transition    Energy                          Probability
#                [keV]                        [per 100 decays]
  G_1           39.748(8)                        6.83E-02
  K_1           16.528(8)                        9.24E+00
  L_1           36.683(14)                       7.03E+01
  M_1           39.245(18)                       1.430E+01
  N_1           39.700(18)                       2.091E+00
  O_1           39.741(8)                        9.04E-04
  G_2           53.29(1)                         3.E-05(3)
  G_3           62.41(3)                         0.00104(4)
  K_3           39.19(3)                         0.001186(12)
  L_3           59.02(6)                         1.460E-04
  M_3           61.79(7)                         2.72E-05
  G_5          294.98(15)                        0.00280(8)
  G_6          317.72(5)                         1.50E-05(7)
  G_7          357.45(8)                         0.0221(8)
  K_7          334.23(8)                         0.000302(3)
  L_7          354.11(14)                        3.98E-05
  G_8          443.79(5)                         1.50E-05(7)
  G_9          497.080(13)                       0.00396(15)
```

EM transitions

NS_RadList – calculation report: ^{103}Pd EC

Auger electrons

# Transition	Energy [keV] Mean	95% Confidence range	Probability [per 100 decays]
Auger_Tot	0.416	[0.002 : 2.490]	9.78E+02
Auger_Ktot	17.758	[16.321 : 21.980]	1.77E+00
Auger_KLL	16.857	[16.321 : 17.139]	1.24E+00
Auger_KLX	19.627	[19.183 : 20.204]	4.88E-01
Auger_KXY	22.332	[21.980 : 22.953]	4.49E-02
Auger_Ltot	1.695	[0.048 : 2.767]	1.71E+02
CK_LLM	0.053	[0.048 : 0.056]	3.24E+01
CK_LLX	0.209	[0.031 : 0.394]	1.48E+01
Auger_LMM	2.238	[1.842 : 2.571]	1.03E+02
Auger_LMX	2.607	[2.378 : 3.004]	1.95E+01
Auger_LXY	2.987	[2.851 : 3.316]	1.01E+00
Auger_Mtot	0.203	[0.039 : 0.369]	3.83E+02
CK_MMX	0.093	[0.012 : 0.178]	1.03E+02
Auger_MXY	0.243	[0.147 : 0.394]	2.80E+02
Auger_Ntot	0.018	[0.001 : 0.041]	4.22E+02
SCK_NNN	0.018	[0.001 : 0.040]	3.92E+02
CK_NNX	0.019	[0.003 : 0.061]	3.05E+01

NS_RadList – calculation report: ^{103}Pd EC

X-rays

# Transition	Energy [keV] Mean	95% Confidence range	Probability [per 100 decays]
X-ray tot	11.995	[2.378 : 22.788]	1.44E+01
X-ray Ktot	20.661	[20.134 : 23.233]	7.47E+00
X-ray KL2	20.134	[20.134 : 20.134]	2.16E+00
X-ray KL3	20.279	[20.279 : 20.279]	4.08E+00
X-ray KM	22.781	[22.763 : 22.788]	1.03E+00
X-ray KM2	22.763	[22.763 : 22.763]	3.45E-01
X-ray KM3	22.788	[22.788 : 22.788]	6.76E-01
X-ray KN	23.237	[23.233 : 23.239]	2.03E-01
X-ray KN2	23.233	[23.233 : 23.233]	6.90E-02
X-ray KN3	23.239	[23.239 : 23.239]	1.33E-01
X-ray Ltot	2.748	[2.378 : 3.154]	6.69E+00
X-ray Mtot	0.328	[0.186 : 0.559]	1.89E-01
X-ray Ntot	0.056	[0.033 : 0.067]	5.32E-02

NS_RadList – new ENSDF cards: ^{103}Pd EC

```
#  Nuclear decay data ============================
#    ENSDF file: 103Pd_EC.ens
103RH  AM E(Tot)= 0.416$ I(Tot)= 9.78E+02$
103RH2 AM E(Ktot)= 17.758$ I(Ktot)= 1.77E+00$
103RH2 AM E(KLL)= 16.857$ I(KLL)= 1.24E+00$
103RH2 AM E(KLX)= 19.627$ I(KLX)= 4.88E-01$
103RH2 AM E(KXY)= 22.332$ I(KXY)= 4.49E-02$
103RH2 AM E(Ltot)= 1.695$ I(Ltot)= 1.71E+02$
103RH2 AM E(CK_LLM)= 0.053$ I(CK_LLM)= 3.24E+01$
103RH2 AM E(CK_LLX)= 0.209$ I(CK_LLX)= 1.48E+01$
103RH2 AM E(LMM)= 2.238$ I(LMM)= 1.03E+02$
103RH2 AM E(LMX)= 2.607$ I(LMX)= 1.95E+01$
103RH2 AM E(LXY)= 2.987$ I(LXY)= 1.01E+00$
103RH2 AM E(Mtot)= 0.203$ I(Mtot)= 3.83E+02$
103RH2 AM E(CK_MMX)= 0.093$ I(CK_MMX)= 1.03E+02$
103RH2 AM E(MXY)= 0.243$ I(MXY)= 2.80E+02$
103RH2 AM E(Ntot)= 0.018$ I(Ntot)= 4.22E+02$
103RH2 AM E(SCK_NNN)= 0.018$ I(SCK_NNN)= 3.92E+02$
103RH2 AM E(CK_NNX)= 0.019$ I(CK_NNX)= 3.05E+01$
103RH  XM E(tot)= 11.995$ I(tot)= 1.44E+01$
103RH2 XM E(Ktot)= 20.661$ I(Ktot)= 7.47E+00$
103RH2 XM E(KL2)= 20.134$ I(KL2)= 2.16E+00$
103RH2 XM E(KL3)= 20.279$ I(KL3)= 4.08E+00$
103RH2 XM E(KM)= 22.781$ I(KM)= 1.03E+00$
103RH2 XM E(KM2)= 22.763$ I(KM2)= 3.45E-01$
103RH2 XM E(KM3)= 22.788$ I(KM3)= 6.76E-01$
103RH2 XM E(KN)= 23.237$ I(KN)= 2.03E-01$
103RH2 XM E(KN2)= 23.233$ I(KN2)= 6.90E-02$
103RH2 XM E(KN3)= 23.239$ I(KN3)= 1.33E-01$
103RH2 XM E(Ltot)= 2.748$ I(Ltot)= 6.69E+00$
103RH2 XM E(Mtot)= 0.328$ I(Mtot)= 1.89E-01$
103RH2 XM E(Ntot)= 0.056$ I(Ntot)= 5.32E-02$
```

- New ENSDF record type "M" (col. 8) and with "A" (Auger) and "X" (X-ray) in column 7
- Only appears in DECAY data sets just before the ground state level record
- Entry E(tot)=<mean energy>$ I(tot)=<total intensity>;
- Energy 3 digits (eV);
- Intensity 3 significant digits
- Intensities cut off: 1.0E-4/decay
- I(511)=sum(I_beta+)+sum(I_g*ICC_Tpf)
- No spaces in AM XM records
- Use 2_AM, 2_XM

What next

- Testing, testing and testing. Benchmarking against BrIccEmis
- Few issues already identified:
  - N-Auger rates seems high
  - EC decay probabilities
  - Need to handle pure E0 and mixed M1+E2+E0; BrIccV3.1 has Ω(E0) values for all atomic shells
  - Gnuplot could not be called from NS_RadList
- Publish BrIccEmis data base and NS_Radlist