THE AUSTRALIAN NATIONAL UNIVERSITY

Proposal
Inclusion of absolute atomic radiation energies and emission probabilities in decay data sets

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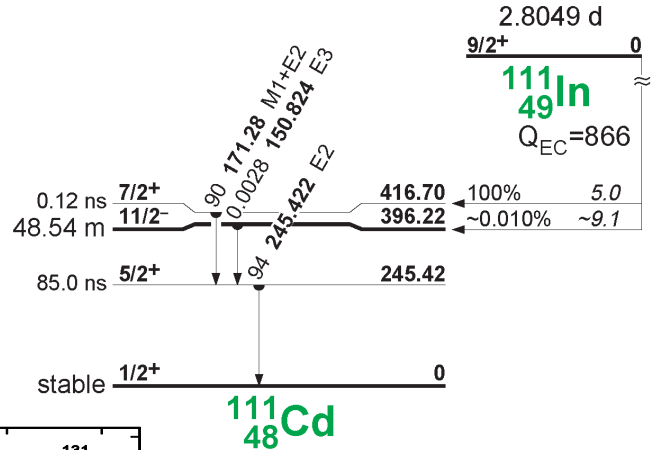
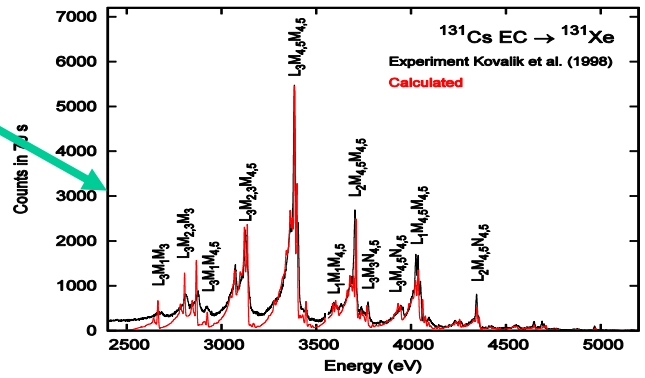
Atomic Data in ENSDF

BrIccEmis (Dec-2014)

```
# AUGER electrons ==============================
                  AUGER electrons:  5911659
           AUGER transition types:      482
# Trans        Energy[eV]    Prob.[/decay]
Auger tot         1125.49    5.912E+00
Auger Ktot       20318.39    1.548E-01
Auger KLL        19222.36    1.067E-01
Auger KLX        22461.82    4.384E-02
Auger KXY        25631.33    4.321E-03
Auger Ltot        2306.76    1.189E+00
Auger LLM           32.20    4.729E-02
Auger LLX          229.91    1.288E-01
Auger LMM         2580.25    8.166E-01
Auger LMX         3054.43    1.852E-01
Auger LXY         3531.82    1.086E-02
Auger Mtot         244.28    2.975E+00
Auger MMX           94.58    8.572E-01
Auger MXY          304.87    2.118E+00
Auger Ntot          24.10    1.593E+00
Auger NNN           17.89    7.272E-01
Auger NNX           17.30    5.928E-01
Auger NXY           55.37    2.732E-01
```





Transitions:

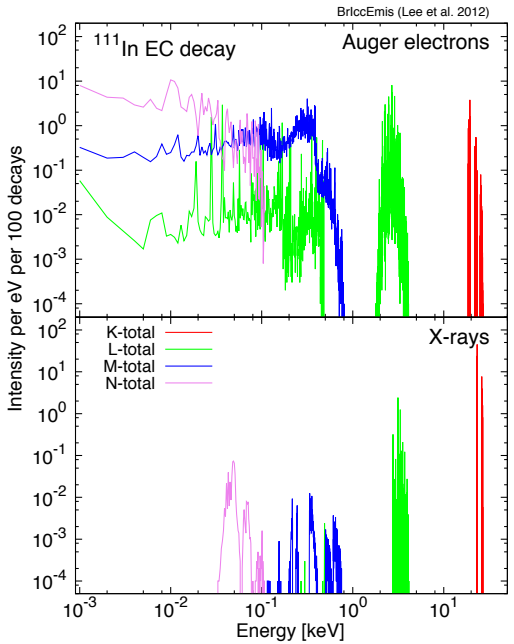
Auger 300 k of 453 types

X-ray: 17.4 k of 55 types

Need to

- ❑ Contain energy and intensity for the users
- ❑ Readable by computer codes
- ❑ Use standard notation

Uncertainties of atomic radiations from nuclear decay



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:15% (Auger) 10% (X-ray)
- M, N ..: unknown (Auger), 100% (KC-Auger), 30% (X-ray below 100 eV)

NOTE2: EADL calculated for single initial vacancies!

NOTE3: To propagate uncertainties BrIccEmis need to be modified significantly

Action: report experimental X-ray and Auger energies and intensities in ENSDF

At present we will not able report uncertainties

Notation

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

Inclusion of atomic relaxation data into ENSDF

```
111CDSAD AKtot=20.298 [0.1526]$AKLL=19.223 [0.1058]$AKLX=22.464 [0.0428]$
...
111CDSXD Xtot=10.843 [1.855]$XKtot=23.706 [0.836]$XKL2=23.058 [0.2415]$
...
111CD  L   0.0       1/2+            STABLE
```

- New ENSDF record type "D" (col. 8) and "S" (col. 6) with "A" (Auger) and "X" (X-ray) in column 7; 16 records for ^{111}In
- Only appears in DECAY data sets just before the ground state level record
- Each entry: (a) Radiation group ("Aktot="); (b) Mean energy in keV; (c) Intensity (on the same scale as gammas; "[RI]")
- Intensities cut off: 0.0001/decay
- Detailed spectra (list and figure) stored on the ENSDF file server
- Uncertainties: need further study how to deduce

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 (in preparation); 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=70, ~40 Mb binary data
- To be completed in late 2017 (ANU)

NS_RadList - calculation report

Header

```
#   Program version: NS_RadList v1.0 (10-May-2017)#   BrIccEmis:
BrIccEmis (18-Apr-2017)
#   NSR Key: 2012Le09
#   ENSDF file: 103Pd_EC.ens
#   Parent: 103PD#   Daughter: 103RH
#   DecayMode: EC#   Half Life: 16.991 D
```

List of Gamma-rays and CEs – in development

NS_RadList - calculation report

Auger electrons

# Transition	Energy [keV] Mean	95% Confidence range	Probability [per 100 decays]
Auger_Tot	0.6537	[0.0020 : 2.6570]	1.257E+03
Auger_Ktot	17.7580	[16.3210 : 21.9800]	1.824E+01
Auger_KLL	16.8571	[16.3210 : 17.1390]	1.276E+01
Auger_KLX	19.6269	[19.1830 : 20.2040]	5.019E+00
Auger_KXY	22.3323	[21.9800 : 22.9530]	4.618E-01
Auger_Ltot	2.0301	[0.0480 : 2.7680]	1.908E+02
CK_LLM	0.0462	[0.0090 : 0.0560]	9.229E+00
CK_LLX	0.1428	[0.0310 : 0.3930]	1.418E+01
Auger_LMM	2.2358	[1.8420 : 2.4960]	1.400E+02
Auger_LMX	2.6045	[2.3730 : 2.8250]	2.613E+01
Auger_LXY	2.9813	[2.8510 : 3.2660]	1.329E+00
Auger_Mtot	0.1997	[0.0360 : 0.3730]	5.014E+02
CK_MMX	0.0937	[0.0110 : 0.1760]	1.456E+02
Auger_MXY	0.2431	[0.1460 : 0.4040]	3.558E+02
Auger_Ntot	0.0184	[0.0010 : 0.0410]	5.461E+02
SCK_NNN	0.0183	[0.0010 : 0.0400]	5.038E+02
CK_NNX	0.0185	[0.0020 : 0.0600]	4.232E+01

NS_RadList - calculation report

X-rays

Transition	Energy [keV] Mean	95% Confidence range	Probability [per 100 decays]
X-ray tot	18.6729	[2.7030 : 22.7880]	8.634E+01
X-ray Ktot	20.6614	[20.1340 : 23.2330]	7.682E+01
X-ray KL2	20.1340	[20.1340 : 20.1340]	2.220E+01
X-ray KL3	20.2790	[20.2790 : 20.2790]	4.197E+01
X-ray KM	22.7806	[22.7630 : 22.7880]	1.056E+01
X-ray KM2	22.7630	[22.7630 : 22.7630]	3.551E+00
X-ray KM3	22.7880	[22.7880 : 22.7880]	6.955E+00
X-ray KN	23.2371	[23.2330 : 23.2390]	2.086E+00
X-ray KN2	23.2330	[23.2330 : 23.2330]	7.095E-01
X-ray KN3	23.2390	[23.2390 : 23.2390]	1.372E+00
X-ray Ltot	2.7511	[2.3780 : 3.1180]	9.074E+00
X-ray Mtot	0.3321	[0.1860 : 0.5700]	2.504E-01
X-ray Ntot	0.0599	[0.0350 : 0.0780]	1.980E-01

S_G records from BrIcc

Current record created by BrIcc

```
71GE  G 23.438    15 0.0226 13 M2                  208
71GES G  KC=169.5 25$LC=32.7 5$MC=5.03 8
71GES G  NC=0.265 4
```

No CE energy given

Modified records, ICC ratios not changed

```
71GES G KC=12.33 [169.5 25]$LC=22.07 [32.7 5]$MC=23.27 [5.03 8]$
```

ICC DICC

Energy

- Given to the precision of the g-ray
- For L, M, etc shells weighted using Icc