THE AUSTRALIAN NATIONAL UNIVERSITY

Atomic Radiations in ENSDF (NS_RadList & UncTools)

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Aims

NS_RadList to evaluate Auger and X-ray spectrum following atomic vacancies created

a) Nuclear decay events: EC & CE

b) User specified initial vacancy distribution

c) Electron and/or Positron bombardment

BrIccEmisDB (225 MB):

- Calculations: BrIccEmis, 1M initial vacancy on all shells
- Atomic transition probabilities from EADL, Energies from RAINE with sem-empirical corrections
- Precompiled Auger and X-ray spectra for 72 atomic radiation groups (AU-tot, AU-Ktot, AU-KLL, …. X-tot, X-Ktot, X-KL, ….)
- Z=6-100
- 1 eV binned, individual transition types (AU-KL1L1) not preserved

ENSDF calculations

Syntax: ns_radlist -n ND147_beta.ens -u -g

NS_Radlist:

- Reads and validates all ENSDF records
- Calculates initial vacancies from EC (1995ScZY) and from IC (BrIccV3.1)
- Prepares UncTools scripts to propagate uncertainties using Monte Carlo
- Runs UncTools, Syntax: unctools NS_Radlist.unc -x

UncTools: Runs scripts, return results in XML: NS_Radlist.xml

NS_Radlist:

- Parse XML
- Generates calculation report file: ND147_beta_NS_Radlist.rpt
- Generates new ENSDF file: ND147_beta_NS_Radlist.new
- Prepare GnuPlot script and data files
- Runs GnuPlot. Syntax: gnuplot ND147_beta_Atomic.plt

UncTools script - CE

```
#   UncTools version: UncTools (18-Jul-2022)
# Input Parameters for UncTools ==================
#   Program version: NS_RadList v1.0 (18-Jul-2022)
#   BrIccEmis:       BrIccEmis (02-Mar-2021)
#   NSR Key:         2012Le09
#   ENSDF file:      ND147_beta.ens

[MAXTALLY]      10000   MC trials
[NR]         0.1311                    13   NORMALISATION
[BR]         1.0

[G_1]  147PM  G 91.1050   16 220.8  27 M1+E2    +0.089  5      2.03 G-record
[G_1_E]  Samples EG
[G_1_RI] Samples RI
[EQN]    G_1_AI=NR*BR*G_1_RI Evaluates AI
[G_1_MR1] Samples MR
[EQN]    G_1_CK_E=G_1_E -  45.1880 Calculates CKE
[G_1_CK_M1] Samples CK(M1) using Z and EG
[G_1_CK_E2] Samples CK(E2) using Z and EG
[EQN] G_1_CK_Icc=(G_1_CK_M1+G_1_MR1*G_1_MR1*G_1_CK_E2)/(1.0+G_1_MR1*G_1_MR1
                Calculates mixed CK
```

^{147}Nd β$^-$ decay
26 gamma rays
19 atomic shells/gamma
3090 CE lines
10000 MC events

NS_RadList Calculation report

```
#    Program version: NS_RadList v1.0 (18-Jul-2022)
#    BrIccEmis: BrIccEmis (02-Mar-2021)
#    NSR Key: 2012Le09
#    Command line: -n Nd147_beta_BrIcc.ens -u -g
#    Input ENSDF file:  Nd147_beta_BrIcc.ens
#    Output ENSDF file: Nd147_beta_BrIcc_NS_RadList.new
#    Parent: 147ND
#    Daughter: 147PM
#    DecayMode: B-
#    Half Life: 11.03 D
```

Q1: Rounding using rule "35"?
Q2: Should we symmetrize UNC if UNC_L ~ UNC_H at <5%

```
# NUCLEAR TRANSITIONS ========================================
# EM transitions (Intensity cutoff:  1.00E-03
# Transition            Energy [keV]              Probability
#                                                [per 100 decays]
G_1                     91.1050(16)                29.0(5)
G_1_CK                  45.9170(16)                49.6(+11-10)
G_1_CL                  83.7404(+32-31)             7.22(+15-14)
G_1_CM                  89.4794(19)                 1.547(+31-32)
G_1_CN                  90.7801(+16-17)             0.348(7)
G_1_CO                  91.0637(16)                 0.0522(11)
G_1_CP                  91.0995(16)                 0.00319(7)
```

NS_RadList Calculation report

Range containing 95% of the intensity

AUGER electrons ========

# Transition	Energy [keV] Mean	95% Confidence range	Probability [per 100 decays]
TOT	0.740	[0.001 : 4.949]	559(10)
K-TOT	33.443	[30.159 : 42.304]	3.75(8)
KLL	31.203	[30.159 : 32.080]	2.43(5)
KLX	37.003	[36.043 : 38.459]	1.186(+25-24)
KXY	42.751	[41.832 : 44.596]	0.1318(+28-27)
L-TOT	3.952	[0.188 : 5.937]	50.8(9)
CK-LLX	0.458	[0.053 : 0.944]	7.44(11)
LMM	4.254	[3.412 : 4.964]	31.8(6)
LMX	5.289	[4.722 : 6.105]	10.68(+20-19)
LXY	6.335	[5.864 : 7.115]	0.888(16)
M-TOT	0.555	[0.014 : 1.031]	124.3(22)
CK-MMX	0.140	[0.004 : 0.395]	34.1(6)
MXY	0.712	[0.481 : 1.056]	90.1(16)
N-TOT	0.060	[0.007 : 0.181]	295(5)
SCK-NNN	0.063	[0.005 : 0.117]	37.1(6)
CK-NNX	0.061	[0.009 : 0.138]	140.7(+25-24)
NXY			117.1(21)
O-TOT			85.5(15)
CK-OOX	0.007	[0.001 : 0.014]	83.6(15)

Evaluated from spectra

NS_RadList Calculation report

X-rays ==========

Transition	Energy [keV] Mean	95% Confidence range	Probability [per 100 decays]
TOT	34.358	[5.419 : 44.927]	55.1(11)
K-TOT	39.591	[38.171 : 44.949]	46.7(10)
KL2	38.171	[38.171 : 38.171]	13.38(+28-27)
KL3	38.724	[38.724 : 38.724]	24.3(5)
KM	43.791	[43.712 : 43.826]	7.16(15)
KM2	43.712	[43.712 : 43.712]	2.42(5)
KM3	43.826	[43.826 : 43.826]	4.66(10)
KN	44.943	[44.927 : 44.949]	1.547(+33-32)
KN2	44.927	[44.927 : 44.927]	0.525(11)
KN3	44.949	[44.949 : 44.949]	1.006(21)
L-TOT	5.772	[4.817 : 6.898]	7.68(14)
M-TOT	0.924	[0.781 : 1.370]	0.696(+13-12)
N-TOT	0.147	[0.097 : 0.332]	0.0458(8)
O-TOT	0.028	[0.025 : 0.029]	0.000

Output ENSDF file

D-record of program version
Do not delete it

```
147PM DM $Atomic relaxation from BrIccEmisDB(19-Apr-2021) (2022TeAA)
147PM cMA IM$Absolute intensity per 100 decays; as defined by 1991PeZY,
147PM2cMA uncertainties in theoretical Auger-electron emission probabilities
147PM3cMA are <15% for K and L shells (except for Coster-Kronig and super
147PM4cMA Coster-Kronig transitions) and 30% for outer shells.
147PM cMX IM$Absolute intensity per 100 decays; as defined by 1991PeZY,
147PM2cMX uncertainties in theoretical X-ray emission probabilities are 10% for
147PM3cMX K and L shells and 30% for outer shells.
```

Table footnote for java-NDS

All DM-, MA- and MX cards will
be replaced by NS_RadList
Only inserted if MA and/or MX

Output ENSDF file

```
147PM  MA E(TOT)= 0.740$ I(TOT)= 559 9$
147PM2 MA E(K-TOT)= 33.443$ I(K-TOT)= 3.75 7$
147PM3 MA E(KLL)= 31.203$ I(KLL)= 2.43 5$
147PM4 MA E(KLX)= 37.003$ I(KLX)= 1.185 +24-23$
147PM5 MA E(KXY)= 42.751$ I(KXY)= 0.1316 26$
147PM6 MA E(L-TOT)= 3.953$ I(L-TOT)= 50.8 8$
147PM7 MA E(CK-LLX)= 0.458$ I(CK-LLX)= 7.43 11$
. . . .
. . . .
147PMk MX E(TOT)= 34.359$ I(TOT)= 55.1 11$
147PMl MX E(K-TOT)= 39.591$ I(K-TOT)= 46.6 9$
147PMm MX E(KL2)= 38.171$ I(KL2)= 13.37 +27-26$
147PMn MX E(KL3)= 38.724$ I(KL3)= 24.3 5$
147PMo MX E(KM)= 43.791$ I(KM)= 7.16 14$
147PMp MX E(KM2)= 43.712$ I(KM2)= 2.42 5$
147PMq MX E(KM3)= 43.826$ I(KM3)= 4.66 9$
147PMr MX E(KN)= 44.943$ I(KN)= 1.545 +31-30$
147PMs MX E(KN2)= 44.927$ I(KN2)= 0.525 10$
147PMt MX E(KN3)= 44.949$ I(KN3)= 1.004 20$
147PMu MX E(L-TOT)= 5.772$ I(L-TOT)= 7.67 13$
147PMv MX E(M-TOT)= 0.924$ I(M-TOT)= 0.695 12$
147PMz MX E(N-TOT)= 0.147$ I(N-TOT)= 0.0458 8$
147PMx MX E(O-TOT)= 0.028$ I(O-TOT)= 0.000$
```

All MA- and MX cards will be replaced by NS_RadList
Only inserted if MA and/or MX

Java-NDS Output

Auger electrons (^{147}Pm)

Transitions	E(keV)	I(%)†	Transitions	E(keV)	I(%)†
TOT	0.740	558 *+9–10*	M-TOT	0.555	124.1 *+21–23*
K-TOT	33.443	3.74 *+7–8*	CK-MMX	0.140	34.1 *+5–6*
KLL	31.203	2.43 *5*	MXY	0.712	90.0 *+16–17*
KLX	37.003	1.184 *+24–25*	N-TOT	0.060	294 *5*
KXY	42.751	0.1315 *+26–28*	SCK-NNN	0.063	37.1 *+6–7*
L-TOT	3.952	50.8 *+8–9*	CK-NNX	0.061	140.4 *+24–25*
CK-LLX	0.458	7.43 *11*	NXY	0.059	116.9 *+20–21*
LMM	4.254	31.8 *6*	O-TOT	0.007	85.4 *+14–16*
LMX	5.289	10.66 *+18–20*	CK-OOX	0.007	83.5 *+14–15*
LXY	6.335	0.887 *+15–17*			

Auger electrons (^{147}Pm) (continued)

† Absolute intensity per 100 decays; as defined by 1991PeZY, uncertainties in theoretical Auger-electron emission probabilities are <15% for K and L shells (except for Coster-Kronig and super Coster-Kronig transitions) and 30% for outer shells.

X rays (^{147}Pm)

Transitions	E(keV)	I(%)†	Transitions	E(keV)	I(%)†	Transitions	E(keV)	I(%)†
TOT	34.358	55.0 *11*	KM2	43.712	2.42 *5*	L-TOT	5.772	7.67 *+13–14*
K-TOT	39.591	46.6 *+9–10*	KM3	43.826	4.65 *+9–10*	M-TOT	0.924	0.695 *+12–13*
KL2	38.171	13.36 *+27–29*	KN	44.943	1.544 *+31–33*	N-TOT	0.147	0.0457 *8*
KL3	38.724	24.3 *5*	KN2	44.927	0.524 *+10–11*	O-TOT	0.028	0.000
KM	43.791	7.15 *+14–15*	KN3	44.949	1.004 *+20–21*			

† Absolute intensity per 100 decays; as defined by 1991PeZY, uncertainties in theoretical X-ray emission probabilities are 10% for K and L shells and 30% for outer shells.

Symmetrize uncertainties if
0.90 < |UncL/UncR| < 1.10
(less than 10% different)

Question / Future plans

Know issues

- Testing, testing, … bug fixes
- There are hundreds of SYS values given in the ENSDF files. Many of them already defined in NS_Radlist.
- NS_RadList performs a format check, based on FMTCHK (under development; ~50% complete)
- The GnuPlot PDF may need to be adjusted, as fonts may not show up correctly. It depends on the actual OS, GnuPlot and Adobe font installations.
- Summary of mean gamma, CE, Auger and X-rays energies to be listed at the end of the report

Questions to decide / thinks in the pipeline

- Symmetrize uncertainties if |UncL| and |UncR| differ only less than 10%, adopt the larges one as symmetric
- Use EC rates from BetaShape
- CPU time: ~10 s to 30 m (MC uncertainty propagation, to be improed)