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ENSDF analysis codes developments at the ANU (2023-2024)

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Codes developed at the ANU

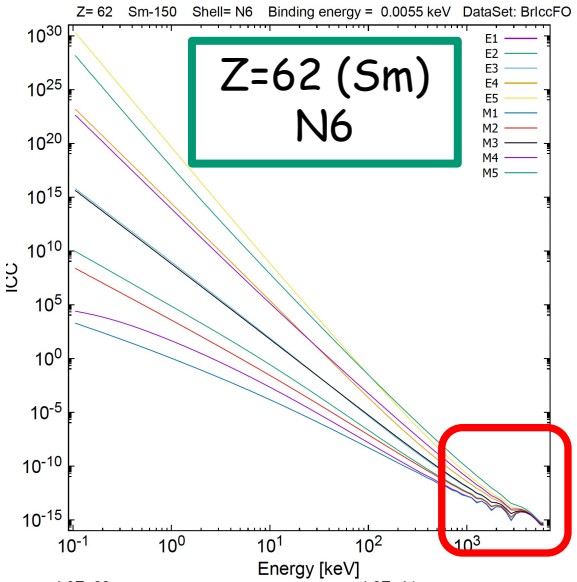
- BrIcc (2.3e 17-Jun-2020)
- BrIccMixing (2.3e 14-Aug-2020)
- GABS (20-Jun-2021)
- AveTools (10-Dec-2014)
- UncTools
- NS_RadList

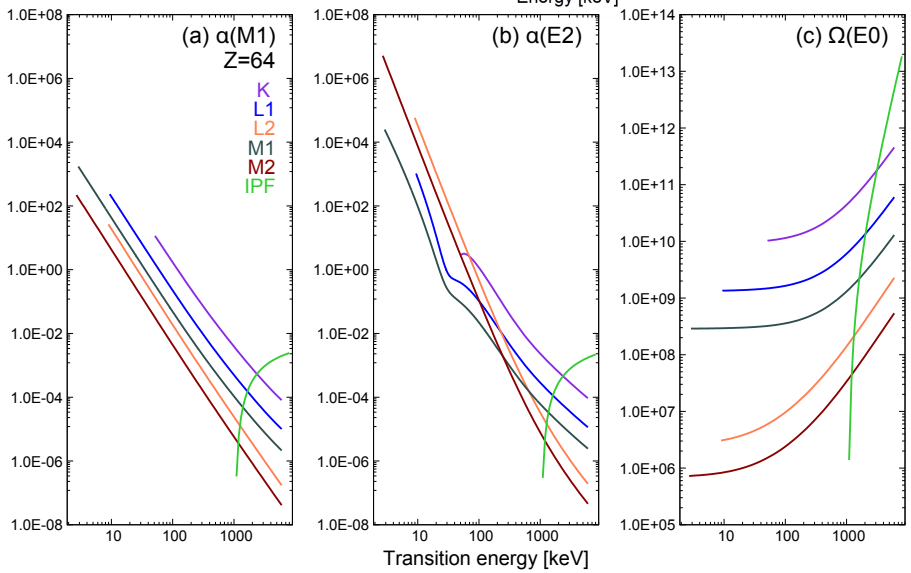
Stable version

BrIcc 2.3e (17-Jun-2020)

Developments

- BrIccFO transition energy range extended. Starting 0.3 keV above BE of all shells (Z=4- 126)
- Oscillations revisited; cutoff energies readjusted
- BrIcc V3.1 DB (19.7 MB) combines:
- BrIccFO (Z4-126) 2008Ki07, 2012Ki04
- IPC (Z=1-100) 1979Sc31, 1996Ho21
- Ω(E0, CE, Z=4-126) 2020Do01
- Ω(E0, PF, Z=4-100) 2020Do01
- Accessible through UncTools





UncTools

- A script driven tool to propagate uncertainties using Monte Carlo

  unctools <input script> -g *to plot PDF of the derived quantity*

  unctools <input script> -xs *to write results into XML file*

- Input parameters:
  - symmetric or asymmetric uncertainties, and limits

    [A_Sym] 12.45 14; [B_ASym] 12.45 +23-1 ; [C_Lim] +12.45 LT
  - ENSDF records

    [G_1] 87MO G 31.55 6 180 M1+E2 0.27 +18-1313.6 48
- Input parameters represented with Probability Density Functions (PDF) details in discussion on MC uncertainty propagation Thursday 11:30
- Equation parser
- Callable from other programs
- Output: ASCII report, PDF plot with GnuPlot, XML

UncTools

Script to calculate total ICC

```
[MAXTALLY] 100000
[G_1] 177HF  G 71.6418  6    1.58 5E1+M2    -0.018  9    0.89  6          p
[G_1_CC_E1]   <αT(E1) from BrIcc>
[G_1_CC_M2]   <αT(M2) from BrIcc>
[G_1_MR1]     <M2/E1 mixing ratio>
[EQN] G_1_CC = (G_1_CC_E1 + G_1_MR1*G_1_MR1*G_1_CC_M2)/(1.0+G_1_MR1*G_1_MR1)
```

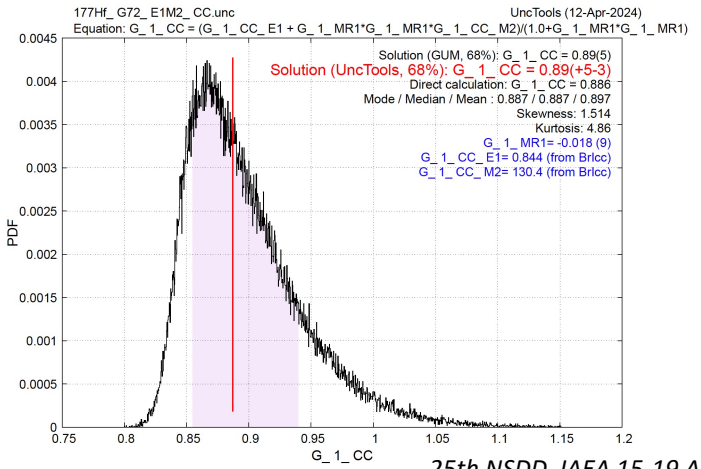
$$\alpha_T = \frac{\alpha_T(M1) + \delta^2 \alpha_T(E2)}{1 + \delta^2}$$

unctools <input script> -g **to plot PDF of output quantity**

α_T(E1+M2, 71.6418)

UncTools: 0.89(+5-3)

BrIcc v2.3e: 0.89(6)



Script to calculate total ICC

[MAXTALLY] 100000

[G_1] 177HF G 71.6418 6 1.58 5E1+M2 -0.018 9 0.89 6 p

[G_1_CC_E1] <α_T(E1) from BrIcc>

[G_1_CC_M2] <α_T(M2) from BrIcc>

[G_1_MR1] <M2/E1 mixing ratio>

$$\alpha_T = \frac{\alpha_T(M1) + \delta^2 \alpha_T(E2)}{1 + \delta^2}$$

[EQN] G_1_CC = (G_1_CC_E1 + G_1_MR1*G_1_MR1*G_1_CC_M2)/(1.0+G_1_MR1*G_1_MR1)

unctools <input script> -xs **to report in XML**

```
<?xml version="1.0"?>
<UncTools ProgVersion="UncTools (12-Apr-2024)" InputFile="177Hf_G72_E1M2_CC.unc">
<G_1_CC_UEqn cUEqnPar="G_1_CC" cUEqn="(G_1_CC_E1 +
        G_1_MR1*G_1_MR1*G_1_CC_M2)/(1.0+G_1_MR1*G_1_MR1)">
 <G_1_CC_Solution cUnc="+5-3"> 0.89 </G_1_CC_Solution>
</G_1_CC_UEqn>
</UncTools>
```

solution

E0 review

2022Ki03 Prog. Part. Nucl. Phys. 123 (2022) 103930

```
##  74SE  L     853.83 9 0+              0.75 NS 5
##  74SEX L XREF=BCFGHIJLP$
##  74SE cL J$(219|g)(635|g)(|q) in {+74}Br |e (46 min). L(p,p')=L(p,t)=0
##  74SE cL T        from B(E2) in Coul. ex. others:
##  74SE2cL 0.83 ns {I14} (|g|g(t) in {+74}Br |e (25.4 min)), 0.52 ns {I6}
##  74SE3cL (centroid-shift in (p,p'))
##  74SE  G  219.06   10100     4  E2                0.047
##  74SEB G BE2W=77 7
##  74SE  G  853.8              E0                        0.82    9
##  74SE cG $ q{+2}{-K}(E0/E2)=0.203 {I14}, X(E0/E2)=0.011 {I5},
##  74SE2cG |r{+2}(E0)=0.0231 {I22} (2005Ki02, evaluation)
#
## REFERENCES
#    EKC       1983Pa10,1984Ma35
##    ENSDF      2006Si19
#
[MAXTALLY]      100000
# ------------------------------------------------------------------------
[L_1] 74SE  L     853.83 9 0+              0.75 NS 5
[L_1_T]                                    #
[EQN]       tau = L_1_T/log(2.)
```

User Comments

UncTools commands

Parameter values

E0 review 2022Ki03

```
[G_1]  74SE  G  219.06   10100    4  E2              0.047
[G_1_E]
[G_1_RI]
[G_1_CK_E2]
[G_1_CC_E2]
[EQN]    G1_TI = G_1_RI * (1.+G_1_CC_E2)
[G_2]    74SE  G  853.8            E0                    0.82   9
[G_2_E]
[G_2_CK_E0]
[G_2_CC_E0]
[q2_KE0_GE2]       7.8E-3    6                          # 1983Pa10
[EQN]    q2_K_Pas =  q2_KE0_GE2 / G_1_CK_E2            # 1983Pa10  q2_K_Pas = 0.194(15)
[q2_K_Mak]  0.26      4                                 # 1984Ma35
[q2_K]    0.202    14                                   # ADOPTED LWM & NRM of 1983Pa10, 1984Ma35
[EQN]    G2_CK_RI = G_1_RI * G_1_CK_E2 * q2_K
[EQN]    G2_TI = G2_CK_RI * G_2_CC_E0 / G_2_CK_E0
[EQN]    tau_E0 = tau * (G1_TI + G2_TI) / G2_TI
[A]       74.
[EQN]    X = 2.54E+9 * (A**(4./3.)) * ((G_1_E/1000.)**5.) * q2_K * G_1_CK_E2 / G_2_CK_E0  # ADOPTED X = 0.0104(9)
[EQN]    rho2_mU = 1000.0/(tau_E0 * G_2_CC_E0)         # ADOPTED   rho2_mU = 22.9(25)
```

User Comments

UncTools commands

Parameter values

NS_RadList – nuclear decay mode with B. Tee

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Aim: Calculate α, β, γ–ray, CE, X-ray and Auger electron energies and absolute intensities and total energy released per decay

- Reads and parses ENSDF file
- Evaluates EC rates using probabilities from BetaShape 2019MO35
- Evaluates IC rates using BrIcc v3.1 (UncTools) 2008Ki07, 2012Ki04, 1979Sc31, 1996Ho21, 2020Do01
- Propagates uncertainties in nuclear structure parameters (energy, intensity, mixing ratio, etc) using UncTools (10,000 MC trials)
- Evaluates atomic radiation spectre (BrIccEmis 2012Le09, 2020TeZY) using atomic radiation probabilities from EADL 1991PeZY
- Generates: calculation report, new ENSDF file with atomic records and plots full X-ray and Auger electron spectra

NS_RadList calculation

Calculations for Decay Data Library for Monitoring Applications (IAEA Dec 2023)

Command:

NS_RadList -n ce139_decay_fgk_BS.ens -u -g -csv_fr ce139_decay_fgk_ecbp.csv

-n ce139_decay_fgk_BS.ens - nuclear decay mode & input ENSDF file

-u - propagates uncertainties using UncTools

-g - plots atomic radiation spectra

-csv_fr ce139_decay_fgk_ecbp.csv – EC/B+ data from BetaShape

Output files:

ce139_decay_fgk_BS_NS_RadList.new – ENSDF

ce139_decay_fgk_BS_Atomic.plt, ce139_decay_fgk_BS_Atomic.spe, ce139_decay_fgk_BS_Atomic.pdf

NS_RadList calculation

```
#   Program version: NS_RadList v1.0 (7-Dec-2023)
#   BrIccEmis: BrIccEmis (02-Mar-2021)
#   NSR Key: 2012Le09
#   EC rates from BetaShape
#      X. Mougeot, Applied Radiation and Isotopes 154 (2019) 108884
#      CSV file: ce139_decay_fgk_ecbp.csv
#   Command: -n ce139_decay_fgk_BS.new -u -g -csv_fr ce139_decay_fgk_ecbp.
#       Monte Carlo Uncertainty propagation
#   Input ENSDF file:  ce139_decay_fgk_BS.new
#   Output ENSDF file: ce139_decay_fgk_BS_NS_RadList.new
#   Parent: 139CE
#   Daughter: 139LA
#   Decay Mode: EC
#   Half Life: 137.64 D
```

NS_RadList calculation

```
# NUCLEAR TRANSITIONS ============================================================
# ELECTRON CAPTURE
================================================================
# Trans              E-decay       E_fin          EC Prob.      Shell EC Prob.
#                     [keV]         [keV]        [/100 dec]     (2019Mo15)
EC -  1            264.6(20)        0.0         5E-7(5)
EC -  2             98.8(20)      165.8576(11)  100
# EM TRANSITIONS (Intensity cutoff:  1.00E-03%) ====================================
# GAMMA                            Energy          Intensity          Dose
#                                 [keV/decay]          [%]          [MeV/Bq s]
G_1                           165.8575(11)       79.90(5)           0.13252(8)
# CONVERSION ELECTRONS  Energy          Intensity          Dose
#                                 [keV/decay]          [%]          [MeV/Bq s]
CE-K       EG=165.8575     126.9295(11)       17.83(25)          0.02263(32)
CE-L       EG=165.8575     159.6230(12)        2.394(31)         0.00382(5)
CE-M       EG=165.8575     164.5071(11)        0.497(6)          0.000818(11)
CE-N       EG=165.8575     165.5898(11)        0.1094(14)        0.0001811(24)
CE-O       EG=165.8575     165.8225(11)        0.01779(24)       2.95E-05(4)
CE-P       EG=165.8575     165.8519(11)        0.001386(20)      2.299E-06(32)
```

NS_RadList calculation

AUGER electrons

Transition	Energy [keV] Mean	95% Confidence range	Intensity [%]	Dose [MeV/Bq s]
TOT	0.696	[0.003 : 4.328]	889(6)	0.00618(4)
K-TOT	28.978	[26.235 : 36.549]	8.03(6)	0.002327(17)
KLL	27.122	[26.235 : 27.785]	5.28(4)	0.001432(11)
KLX	32.056	[31.233 : 33.219]	2.476(18)	0.000794(6)
KXY	36.912	[36.146 : 38.440]	0.2749(20)	0.0001015(7)
L-TOT	3.499	[0.150 : 4.935]	79.4(6)	0.002778(21)
CK-LLX	0.296	[0.067 : 0.656]	8.13(5)	2.406E-05(15)
LMM	3.627	[2.939 : 4.154]	52.7(4)	0.001909(14)
LMX	4.475	[4.041 : 5.011]	17.28(12)	0.000773(5)
LXY	5.328	[4.976 : 5.871]	1.342(10)	7.15E-05(5)
M-TOT	0.437	[0.011 : 0.795]	197.8(14)	0.000864(6)
CK-MMX	0.102	[0.004 : 0.310]	52.6(4)	5.37E-05(4)
MXY	0.558	[0.369 : 0.842]	145.2(10)	0.000810(6)
N-TOT	0.042	[0.006 : 0.089]	491.9(35)	0.0002075(15)
SCK-NNN	0.022	[0.003 : 0.053]	1.852(13)	4.128E-07(29)
CK-NNX	0.046	[0.005 : 0.106]	133.8(9)	6.19E-05(4)
NXY	0.041	[0.006 : 0.077]	356.2(25)	0.0001452(10)
O-TOT	0.007	[0.002 : 0.011]	111.7(8)	8.36E-06(6)
CK-OOX	0.007	[0.002 : 0.011]	109.1(8)	7.55E-06(6)

NS_RadList calculation

X-rays

Transition	Energy [keV]	Intensity	Dose
	Mean	95% Confidence range	[%]	[MeV/Bq s]
TOT	30.802	[4.661 : 38.719]	90.9(7)	0.02798(22)
K-TOT	34.172	[33.035 : 38.733]	80.5(6)	0.02751(21)
KL2	33.035	[33.035 : 33.035]	23.06(17)	0.00762(6)
KL3	33.442	[33.442 : 33.442]	42.40(31)	0.01418(10)
KM	37.779	[37.722 : 37.804]	12.10(9)	0.004572(34)
KM2	37.722	[37.722 : 37.722]	4.060(30)	0.001531(11)
KM3	37.804	[37.804 : 37.804]	7.94(6)	0.003000(23)
KN	38.729	[38.719 : 38.733]	2.560(19)	0.000991(7)
KN2	38.719	[38.719 : 38.719]	0.860(6)	0.0003328(23)
KN3	38.733	[38.733 : 38.733]	1.676(12)	0.000649(5)
L-TOT	4.886	[4.123 : 5.806]	9.61(7)	0.0004697(34)
M-TOT	0.756	[0.358 : 1.138]	0.706(5)	5.34E-06(4)
N-TOT	0.130	[0.072 : 0.286]	0.03147(22)	4.091E-08(29)
O-TOT	0.025	[0.025 : 0.025]	0.0	0(0)

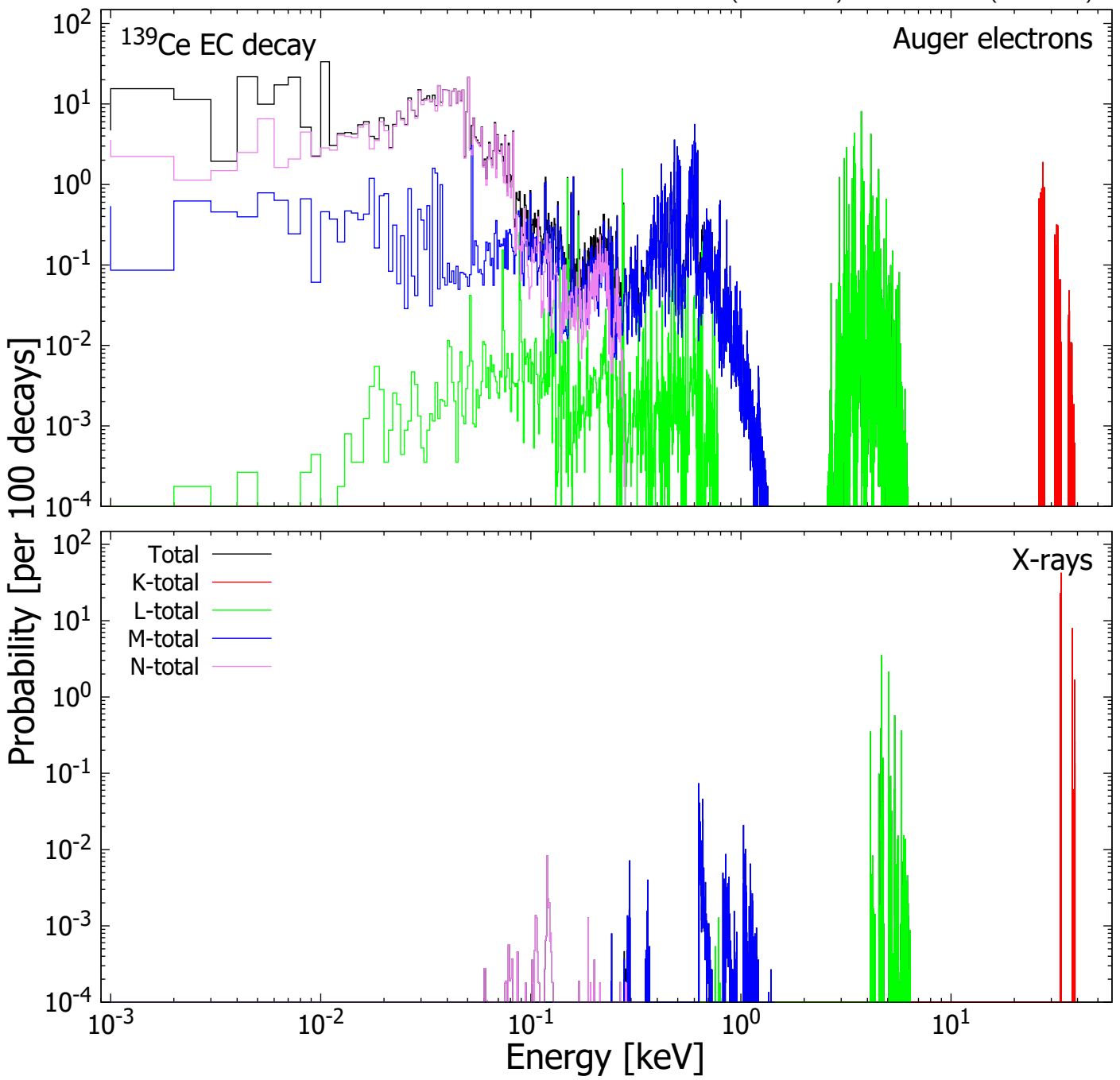
NS_RadList calculation

TOTAL ENERGY RELEASED PER DECAY ==========

# Radiation	Total Energy [keV/decay]	Total Intensity [%]	Dose [MeV/Bq s]
Neutrino	70.1(16)		
G-rays	132.52(8)	79.90(5)	0.13252(8)
CE	27.48(32)	20.85(25)	0.02748(32)
Auger	6.18(5)	889(6)	0.00618(5)
X-rays	27.98(22)	90.9(7)	0.02798(22)
Summed total	**264.3(17)**		0.2643(17)

EXPECTED:

(Q+Eini)*BR	**264.6(20)**


BrIccEmis (02-Mar-2021) & NS RadList v1.0 (7-Dec-2023)
^{139}Ce EC decay
Auger electrons
X-rays
Total
K-total
L-total
M-total
N-total
Probability [per 100 decays]
Energy [keV]

NS_RadList calculation

X rays (^{139}La)

Transitions	E(keV)	I(%)†
TOT	30.802	90.9 *7*
K-TOT	34.172	80.5 *6*
KL2	33.035	23.06 *17*
KL3	33.442	42.40 *31*
KM	37.779	12.10 *9*

Transitions	E(keV)	I(%)†	Transitions	E(keV)	I(%)†	Transitions	E(keV)	I(%)†
KM2	37.722	4.060 *30*	KN2	38.719	0.860 *6*	M-TOT	0.756	0.706 *5*
KM3	37.804	7.94 *6*	KN3	38.733	1.676 *12*	N-TOT	0.130	0.03147 *22*
KN	38.729	2.560 *19*	L-TOT	4.886	9.61 *7*	O-TOT	0.025	0.0

† Absolute intensity per 100 decays; quoted uncertainties include direct contributions from only electron capture and internal-conversion electrons (2020TeZY) – these data do not include the significant uncertainties from the more complex but less well-defined atomic radiation probabilities as considered semi-quantitatively in EADL (1991PeZY).

Auger electrons (^{139}La)

Transitions	E(keV)	I(%)†	Transitions	E(keV)	I(%)†
TOT	0.696	889 *6*	M-TOT	0.437	197.8 *14*
K-TOT	28.978	8.03 *6*	CK-MMX	0.102	52.6 *4*
KLL	27.122	5.28 *4*	MXY	0.558	145.2 *10*
KLX	32.056	2.476 *18*	N-TOT	0.042	491.9 *35*
KXY	36.912	0.2749 *20*	SCK-NNN	0.022	1.852 *13*
L-TOT	3.499	79.4 *6*	CK-NNX	0.046	133.8 *9*
CK-LLX	0.296	8.13 *5*	NXY	0.041	356.2 *25*
LMM	3.627	52.7 *4*	O-TOT	0.007	111.7 *8*
LMX	4.475	17.28 *12*	CK-OOX	0.007	109.1 *8*
LXY	5.328	1.342 *10*			

† Absolute intensity per 100 decays; quoted uncertainties include direct contributions from only electron capture and internal-conversion electrons (2020TeZY) – these data do not include the significant uncertainties from the more complex but less well-defined atomic radiation probabilities as considered semi-quantitatively in EADL (1991PeZY).