^{131}Cs – Comments on evaluation of decay data

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Evaluation Procedures

Limitation of Relative Statistical Weight Method (LWM) and other analytical techniques were applied to average numbers throughout the evaluation. The uncertainty assigned to the average value was always greater than or equal to the smallest uncertainty of the values used to calculate the average.

Decay Scheme

^{131}Cs ($T_{½}$ = 9.681 days) decays 100% by electron capture decay (Q_{EC} = 358.00 (18) keV) directly to the stable ground state of ^{131}Xe (2021Wa16). Thus, the very simple nuclear decay scheme consists only of one EC transition, along with arrays of atomic X-ray and Auger-electron emissions.

Nuclear Data

There is an interest in the EC decay of ^{131}Cs as a potentially suitable electron and X-ray emitter for microdosimetry and radiotherapy in nuclear medicine.

Half-life of ^{131}Cs

The measurements of 1960La06, 1972Em01, 1974Pl04 and 1975La16 were adopted to give a weighted mean half-life of 9.681 (16) days based on the LWM and NRM techniques (Avetools code, version 3.0, 11 December 2014, ENSDF utility program).

Reference	Half-life (d)	Comments
1947Ka01	10.2	uncertainty unspecified - therefore not included in weighted-mean analysis of the data set.
1947Yu01	10.0 ± 0.3	insufficient detail concerning activity analysis and assigned uncertainty; also defined as an outlier - therefore not included in weighted-mean analysis of the data set.
1949Ya02	9.6 ± 0.1	defined as an outlier - therefore not included in weighted-mean analysis of the data set.
1960Jo09	9.6	uncertainty unspecified - therefore not included in weighted-mean analysis of the data set.
1960La06	9.69 ± 0.05	
1963Ly02	9.83 ± 0.28	superseded by 1972Em01 (both measurements undertaken at ORNL) - therefore not included in weighted-mean analysis of the data set.
1972Em01	9.70 ± 0.03	
1974Pl04	9.688 ± 0.004	low questionable uncertainty increased from ± 0.004 to ± 0.016 d to reduce weighting to below 50%.
1975La16	9.66 ± 0.05	uncertainty expressed at the 3σ confidence level as ± 0.05 d; adjusted to the 1σ confidence level and rounded up to ± 0.02 d.
Recommended value	9.681 ± 0.016	uncertainty has been adjusted from ± 0.011 to ± 0.016 d to align with the smallest uncertainty of the values used to calculate the recommended average value.

Limitation of relative statistical weight method (LWM), normalised residual method (NRM), Rajeval technique, bootstrap method, and Mandel-Paule approach were considered in the analysis of the data set.

Analytical method	Half-life (d)	χ^2/(N-1)	$\chi^2/(N-1)_{critical}$
LWM	9.681 ± 0.011	0.58	3.78
NRM	9.681 ± 0.011	0.58	2.60
Rajeval	9.683 ± 0.012	0.48	–
Bootstrap	9.686 ± 0.010	0.65	–
Mandel-Paule	null result	–	–

A half-life of (9.681 ± 0.016) days is recommended, as quantified primarily by the LWM and NRM analytical procedures.

Q value

A high-precision measurement by means of the ISOLTRAP mass spectrometer at ISOLDE/CERN has furnished an accurately quoted value of 358.00 (17) keV (2019Ka48). This study impacted significantly on the atomic mass evaluation of Wang *et al* (2021Wa16) to furnish a recommended Q_{EC} value for ^{131}Cs EC decay to the stable ground state of ^{131}Xe of 358.00 (18) keV, which has been adopted.

Gamma-ray energies and emission probabilities

Although extensive studies have been undertaken of the complex collective structures of both ^{131}Cs (2005Ku10, 2008Si26) and ^{131}Xe (2006Vo04), their findings have little direct impact on defining the simple ground-state to ground-state EC-decay of ^{131}Cs. Nevertheless, these wide-ranging band structure studies do provide some supporting evidence for the spins and parities of the ^{131}Cs and ^{131}Xe ground states (2006Kh09).

Spins-parities of the ground-state nuclear levels of ^{131}Cs and ^{131}Xe (2006Kh09).

Nuclear level number	Nuclear level energy (keV)	Spin and parity‡		
0	0.0	5/2 +	9.681 (16) d	^{131}Cs
0	0.0	3/2 +	stable	^{131}Xe

‡ Spin and moments defined in regularly updated compilations and evaluations (1976Fu06, 2014StZZ, 2019StZV).

EC Transition

Energy

The energy of the ground-state to ground-state EC transition is defined by the adopted Q_{EC}-value of 358.00 (18) keV (2021Wa16).

Transition Probability

The transition probability of the single EC decay is 100%. BetaShape code, version 2.2, 7 June 2021, was used to determine log*ft* and fractional electron-capture probabilities P_K, P_L, P_M, P_N and P_O (LNHB analysis program (2015Mo10, 2019Mo35)). Measurements of the P_K capture and P_L/P_K capture ratios provide significant support for these well-defined calculations (1960Jo09, 1967Sc15). However, the log*ft* value of 5.5804 (27) as calculated over-precisely to five significant figures has been modified to 5.580 (3) on the basis of more realistic datum.

EC-decay data of ^{131}Cs as calculated by the BetaShape code, version 2.2 (2015Mo10, 2019Mo35).

	E_{EC} (keV)*	P_{EC} (%)	^{131}Cs	^{131}Xe	transition type	log *ft*	P_K	P_L	P_{L1}	P_{L2}	P_{L3}
$EC_{0,0}$	358.00 (18)	100	5/2 +	3/2 +	allowed	5.580 (3)	0.83566 (30)	0.12757 (7)	0.12403 (10)	0.0003540 (29)	–

P_M	P_N	P_O
0.02824 (12)	0.00732 (9)	0.001214 (18)

Measurements of P_K and P_L/P_K ratio in the EC decay of ^{131}Cs.

P_K	P_L/P_K	
1974Pl04	1960Jo09	1967Sc15
0.832 (8)	0.0153 (8)	0.0155 (2)

Atomic Data

Experimental and theoretical datasets of X-ray and Auger-electron energies and emission probabilities for the atomic de-excitation of ^{131}Xe have been measured and calculated by various means (for example, 1995ScZY, 1996Sc06, 1998Sc28, 1998ScZM, 1999ScZX, 2000Sc47, 1998Ko78 and 2003De44). Accurate measurements of the emission probabilities are highly desirable to assist in defining with confidence these particularly important parameters identified with the EC decay of ^{131}Cs. Furthermore, relatively low-energy X-ray emissions need to be quantified with confidence and good accuracy in order to calculate excitation functions, and so ensure the optimum production and purity of ^{131}Cs with confidence.

Electron energies were determined from electron binding energies tabulated by Larkins (1977La19), and Xe: ω_K = 0.888 (5); ϖ_L = 0.097 (5); n_{KL} = 0.902 (4) were initially taken from 1996Sc06. Both the X-ray and Auger-electron spectra for the EC decay of ^{131}Cs have been calculated by means of the BrIccEmis code, as described in 2012Le09, 2016Le19 and 2020TeZY in order to achieve the necessary detail and resolution of spectral lines for confident application in microdosimetry. A vacancy reaching the valence shell is immediately filled by an electron from the surrounding condensed-phase material to generate more atomic radiation, and this process will terminate when all such vacancies are filled below the valence shell. Transition energies within each propagation step were derived from the atomic binding energies determined by means of the relativistic Dirac-Fock approach employed in the RAINE code (2002Ba85), along with the application of a semi-empirical correction procedure that aligns these energies more fully with known spectral data (2020TeZY). Fixed transition rates were obtained from the EADL database (1991PeZY, 1993Cu08). Resulting mean X-ray energies, 95% confidence energy ranges, and emission probabilities are listed below for ^{131}Cs, followed by the recommended Auger-electron energies, 95% confidence energy ranges, and emission probabilities. Intensity cut-off for these listings is 0.01 per 100 decays. As defined by

1991PeZY, uncertainties in these theoretical X-ray emission probabilities are 10% for the K and L shells and 30% for the outer shells, whereas uncertainties in the theoretical Auger-electron emission probabilities are <15% for the K and L shells (except for Coster-Kronig and super Coster-Kronig transitions) and 30% for the outer shells.

More detailed Auger-electron spectral measurements and individual component analyses can be found in the experimental studies of Kovalík *et al*. (1998Ko78). Absolute and relative energies of the LMM + LMX, KLL and KLM + KLX Auger transitions in Xe were determined along with their relative intensities. These and individual Auger transition data were shown to be in good agreement with *ab initio* calculations undertaken during a series of planned development phases of the BrIccEmis code (2013LeZX, 2020TeZY) that includes energy corrections to account for the Breit and quantum electrodynamic (QED) effects. The X-ray and Auger-electron data tabulated above were calculated from a more recent version of BrIccEmis (ENSDF analysis program, 26 May 2021), which continues to exhibit good agreement overall with the original measurements in terms of the shape of the spectrum, and the energies and intensities of the individual Auger peaks (1998Ko78). Future intentions are to focus on the introduction of the relativistic multiconfiguration Dirac-Fock method (MCDF) and Monte-Carlo techniques.

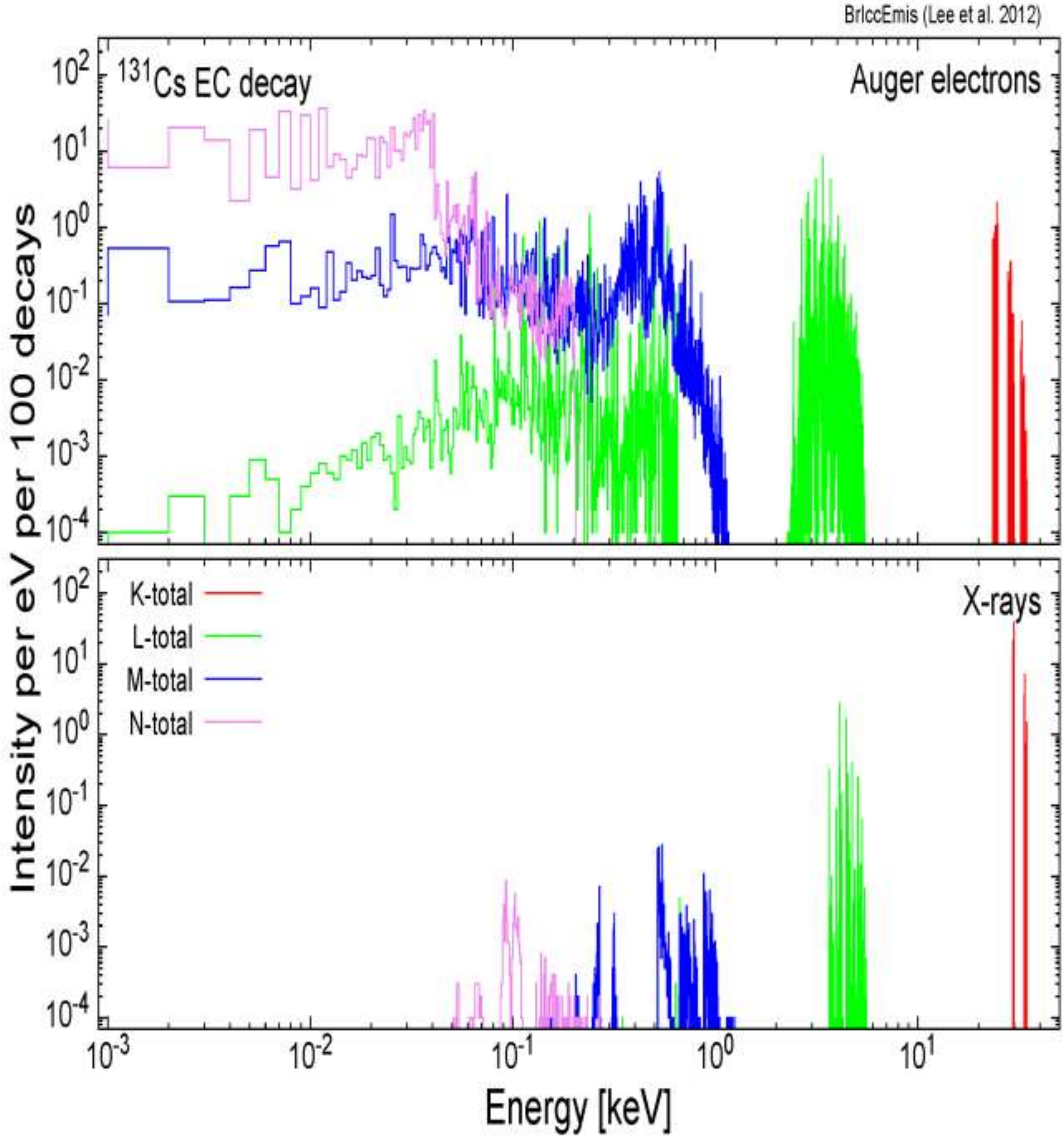
X-ray energies and emission probabilities of ^{131}Cs (BrIccEmis code).

		Mean Energy (keV)	Energy (keV), 95% confidence range	Photons per 100 disint.
X_{tot}	(Xe)	28.559	4.2876 – 35.819	83.91
XK_{tot}	(Xe)	31.632	30.631 – 35.819	74.52
XKL_2	(Xe)	30.631	30.631	21.37
XKL_3	(Xe)	30.978	30.978	39.64
XKM	(Xe)	34.972	34.925 – 34.993	10.98
XKM_2	(Xe)	34.925	34.925	3.697
XKM_3	(Xe)	34.993	34.993	7.193
XKM_4	(Xe)	35.252	35.252	0.0354
XKM_5	(Xe)	35.266	35.266	0.0520
XKN	(Xe)	35.828	35.819 – 35.832	2.307
XKO	(Xe)	35.980	35.979 – 35.981	0.2287
XL_{tot}	(Xe)	4.4876	3.7956 – 5.2886	8.648
XM_{tot}	(Xe)	0.6797	0.2769 – 1.0378	0.5394
XN_{tot}	(Xe)	0.1173	0.0929 – 0.2088	0.2050

Auger-electron energies and emission probabilities of ^{131}Cs (BrIccEmis code).

		Mean Energy (keV)	Energy (keV), 95% confidence range	Electrons per 100 disint.
Auger total	(Xe)	0.7072	0.00197 – 4.0972	900.7
Auger K_{tot}	(Xe)	26.859	24.398 – 33.721	9.056
Auger KLL	(Xe)	25.218	24.398 – 25.789	6.046
Auger KLX	(Xe)	29.727	28.987 – 30.780	2.719
Auger KXY	(Xe)	34.161	33.493 – 35.569	0.291
Auger L_{tot}	(Xe)	3.0998	0.1350 – 4.5518	93.75
Auger Coster-Kronig LLX	(Xe)	0.3073	0.0661 – 0.5900	13.84
Auger LMM	(Xe)	3.3875	2.7428 – 4.1477	60.65
Auger LMX	(Xe)	4.1474	3.7300 – 4.7935	17.92
Auger LXY	(Xe)	4.9133	4.5912 – 5.5289	1.338
Auger M_{tot}	(Xe)	0.3791	0.0146 – 0.7217	227.2
Auger Coster-Kronig MMX	(Xe)	0.0965	0.0067 – 0.2834	61.96
Auger MXY	(Xe)	0.4921	0.3183 – 0.7582	162.7
Auger N_{tot}	(Xe)	0.0298	0.0018 – 0.0974	570.7
Auger super Coster-Kronig NNN	(Xe)	0.0115	0.0020 – 0.0554	10.82
Auger Coster-Kronig NNX	(Xe)	0.0475	0.0043 – 0.0938	141.0
Auger NXY	(Xe)	0.0244	0.0014 – 0.1056	418.9

Auger-electron (upper panel) and X-ray (lower panel) spectra of ^{131}Cs EC decay:



Total energy release per decay as determined from the BrIccEmis studies:

Gamma rays:	0.0000 keV
Conversion electrons:	0.0000 keV
X-rays:	23.9637 keV
Auger electrons:	6.3699 keV

The final X-ray and Auger-electron spectra were effectively evaluated from one million simulated nuclear decay events – these spectra consist of 76 X-ray transition types, and 685 Auger-electron transition types. Both component spectra of the Auger-electron and X-ray emissions as calculated by the BrIccEmis code (26 May 2021) for the EC decay of ^{131}Cs are shown in the figure above.

Main Production Modes for ^{131}Cs

^{130}Ba(n,γ)^{131}Ba(EC)^{131}Cs, ^{nat}Ba(n,xn)^{131}Ba(EC)^{131}Cs, ^{131}Xe(p,n)^{131}Cs,

^{133}Cs(p,3n)^{131}Ba(EC)^{131}Cs

Data Consistency

A Q_{EC}-value of 358.00 (18) keV has been adopted from the atomic mass evaluation of Wang *et al.* (2021Wa16), and compared with the Q-value calculated by summing the contributions of the individual emission(s) of the ^{131}Cs EC-decay process (i.e., only a single EC transition):

calculated Q-value = 358.00 (18) keV

Percentage deviation from the Q-value of Wang *et al.* is (0.00 ± 0.05)%, which supports the derivation of a fully consistent decay scheme with a small variant based only on ± 0.18 keV uncertainty of Q_{EC}. This particularly high consistency is based on the simplicity of the decay scheme, with only one allowed EC transition probability of 100% directly from the ^{131}Cs ground state to the daughter ^{131}Xe ground state.

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ENSDF Analysis Programs: BrIccEmis, 26 May 2021

ENSDF Utility Program: Avetools, version 3.0, 11 December 2014

LNHB Analysis Program: BetaShape, version 2.2, 7 June 2021

The above codes have undergone and will continue to undergo various forms of modification and improvement, which will be reflected in changes to the version number and date of issue into the public domain. Assistance from Xavier Mougeot (LNHB, CEA Saclay, France – BetaShape) and Tibor Kibédi (ANU, Australia – particularly BrIccEmis) concerning improved operational features of some of the above codes is gratefully acknowledged by ALN.