^{89}Zr – Comments on evaluation of decay data by A. L. Nichols

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Evaluation Procedures

Limitation of Relative Statistical Weight Method (LWM) and other analytical techniques were applied to obtain averaged data 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

^{89}Zr ($T_{½}$ = 78.42 h) undergoes 100 % electron capture/β^+ decay (Q(EC) = 2832.8 (28) keV) to various excited nuclear levels and the ground state of ^{89}Y. A reasonably well-defined decay scheme was derived from the gamma-ray measurements of 1968Hi12, 1969Ro02, 1971Ar18 and 1979Ba46, consisting of five EC transitions, one β^+ emission and five gamma rays. Weighted mean relative emission probabilities were calculated for the gamma rays. All of these relative emission probabilities have been defined in terms of the 871.094-keV gamma ray (100 %).

Nuclear Data

^{89}Zr decay is viewed as a potentially suitable β^+ emitter for application in positron emission tomography (PET).

Half-life of ^{89}Zr

The measurements of 1940Du05, 1953Sh48, 1960Ha26, 1961Ra06, 1964Va03, 1969Ro02 and 1984Sk01 were adopted to give a weighted mean half-life of 78.42 (13) hours based on the limitation of relative statistical weight method (LWM).

Reference	Half-life (h)
1938Sa01	70*
1940Du05	78 (1)
1940Sa08	68 (2)‡
1951Hy24	77*
1951Sh24	79.3*
1953Ka11	78*
1953Sh48	79 (2)
1960Ha26	79.0 (5)
1961Ra06	79.4 (16)
1962Ho10	79*
1964Va03	78.43 (8)†
1969Ro02	78.0 (2)
1984Sk01	78.62 (17)
Recommended value	**78.42 (13)#**

* Uncertainty unspecified – not included in weighted mean analysis of the data set.
‡ Defined as an outlier, and therefore not adopted in the analytical procedures.
† Uncertainty increased from ± 0.08 to 0.13 to reduce weighting below 0.50.
# Recommended uncertainty has been adjusted from ± 0.09 to 0.13, in alignment with the smallest uncertainty of the values used to calculate the average value.

A small change has been observed in the half-life of ^{89}Zr when bound at the lattice site of the Ti ion in $BaTiO_3$ as the crystal undergoes a phase transition at a temperature (T_c) of 120 °C (1970Ga03). This experimental study has been further assessed in terms of modelling the impact of changes in the chemical bonding and ligand field strength of the $BaTi(Zr)O_3$ lattice (1973Le13). Theoretical estimates of the relative change of the decay constant quantified in terms of the expression $\Delta\lambda_{EC}/\lambda_{EC}$ (where $\lambda = \ln2/t_{½}$) were of the order of 0.0015 and 0.0065 compared with the experimental observations of 0.00080 (3). Measured data represent observed changes in the EC-decay half-life of ^{89}Zr of the order of ~ 0.08 % (no more than 0.06 h).

Half-lives of ^{89m}Y and ^{89m}Zr metastable states

The measurements of 1955Sw92, 1962Br42, 1966Du07, 1967Yu01, 1968Bo52 and 1995ItZY were adopted to give a weighted mean half-life for ^{89m}Y of 15.84 (18) seconds, based on the limitation of relative statistical weight method (LWM).

Reference	^{89m}Y half-life (s)
1951Go42	14 (2)[‡]
1955Sw92	16.1 (3)
1962Br42	16.3 (13)
1966Du07	15.91 (17)
1967Yu01	16.06 (4)
1968Bo52	15.78 (11)
1995ItZY	15.663 (5)[†]
Recommended value	**15.84 (18)[#]**

[‡] Defined as an outlier, and therefore not adopted in the analytical procedures.
[†] Uncertainty increased from ± 0.005 to 0.04 to reduce weighting to 0.50.
[#] Weighted average adopted, with the recommended uncertainty increased to include the precise value of 15.66 (4) s.

The measurements of 1951Sh89, 1953Sh48, 1964Va03, 1969Ro02 and 1992KaZM were adopted to give a weighted mean half-life for ^{89m}Zr of 4.170 (19) minutes based on the limitation of relative statistical weight method (LWM).

Reference	^{89m}Zr half-life (min)
1940Du05	4.5[*]
1951Sh89	4.4 (1)
1953Ka11	4.25[*]
1953Sh48	) 4.5 (5)
	) 4.40 (4)
	) 4.4 (3)
1964Va03	4.18 (1)
1969Ro02	4.16 (6)
1992KaZM	4.145 (9)[†]
Recommended value	**4.170 (19)**

[*] Uncertainty unspecified – not included in weighted mean analysis of the data set.
[†] Uncertainty increased from ± 0.009 to 0.010 to reduce weighting to no more than 0.50.

Q-value

Q_{EC}-value for ^{89}Zr EC/β^+ decay of 2832.8 (28) keV was adopted from Wang *et al*. (2012Wa38).

Gamma-ray energies and emission probabilities

Energies

The well-defined nuclear level energies of 2013Si03 were used to calculate the gamma transition energies and their uncertainties, and these data were adjusted to account for gamma recoil in the formulation of recommended gamma-ray emission energies and uncertainties. Greater confidence was placed on this overall method of assignment because of the more wide-ranging origins of the gamma transition data in 2013Si03.

Adopted energies, spins, parities and half-lives of the nuclear levels of ^{89}Y (2013Si03).

Nuclear level number	Nuclear level energy (keV)	Spin and parity	Half-life	
0	0.0	1/2 −	stable	^{89}Y
1	908.97 (3)	9/2 +	15.84(18) s	^{89m}Y
2	1744.74 (18)	5/2 −	0.62(14) ps[*]	
3	2529.80 (20)	7/2 +	0.08(3) ps[†]	
4	2566.55 (15)	11/2 +		
5	2622.1 (3)	9/2 +	0.21(10) ps[*]	

[*] Determined from Döppler shift attenuation measurements of the ^{87}Rb(α,2nγ)^{89}Y reaction by 1992Fu04.
[†] Determined from Döppler shift attenuation measurements of the ^{89}Y(p,p'γ)^{89}Y reaction by 1973BeYD.

Gamma transition energies, and measured and recommended gamma-ray energies.

E_{TP} (keV)[#]	E_γ (keV)										
	1953Sh48	1961Mo12	1964Va03	1968Dr02	1968Hi12	1969GuZV	1969Ro02	1971Ar18	1974HeYW	1992Fu04	Recommended[§]
–	–	511	511	511	511.0	511	–	–	511.006	–	annihilation radiation
908.97 (3)	920 (10)	915	908	908 (2)	909.1 (1)	909.1 (1)	909.2 (1)	908 (1)	909.14 (7)	909.1 (1)	908.97 (3)
1620.83 (20)	–	–	1621 (9)	1617 (2)	1620.6 (7)	–	1620.8 (2)	1620 (1)	1620.76 (19)	1620.9 (5)	1620.81 (20)
1657.58 (15)	–	–	–	1655 (2)	1656.9 (7)	–	1657.3 (2)	1657 (1)	1657.26 (19)	1657.5 (2)	1657.56 (15)
1713.1 (3)	–	) 1750 (20)	1705 (4)	1712 (2)	1713.0 (6)	1713.4 (2)	1712.9 (8)	1712 (1)	1712.8 (4)	1713.3 (4)	1713.1 (3)
1744.74 (18)	–	)	–	1744 (2)	1744.4 (7)	–	1744.5 (2)	1744 (1)	1744.47 (19)	1744.9 (3)	1744.72 (18)

[#] Determined from the nuclear level energies of 2013Si03.
[§] Calculated by subtracting gamma recoil from gamma transition energy (E_{TP} (keV)).

Measured and recommended gamma-ray emission probabilities relative to P_γ(908.97 keV) of 100 %.

	E_γ (keV)[#]	P_γ^{rel}									
		1961Mo12	1964Va03	1968Dr02[*]	1968Hi12	1969GuZV[*]	1969Ro02	1971Ar18	1974HeYW[†]	1979Ba46	Recommended[‡]
$\gamma^\pm$	511	44.5 (15)	44.2 (9)	–	44.3 (20)	0.47 → 47.5	–	–	45.1 (6)	–	46.0 (6)[§] annihilation radiation
$\gamma_{1,0}$	908.97 (3)	100	100	100	**100**	0.99 → 100	**100**	**99.86 → 100**	99.871 (3) → 100	**100**	100
$\gamma_{3,1}$	1620.81 (20)	–	0.12 (1)	0.077	**0.068 (9)**	–	**0.071 (7)**	**0.08 (1)**	0.072 (5)	**0.075 (5)**	0.075 (5)[#]
$\gamma_{4,1}$	1657.56 (15)	–	–	0.098	**0.105 (5)**	–	**0.10 (1)**	**0.12 (1)**	0.107 (4)	**0.108 (5)**	0.107 (5)[+]
$\gamma_{5,1}$	1713.1 (3)	) 0.4 (1)	0.98 (3)	0.77	**0.760 (10)**	0.0067 → 0.68	**0.77 (7)**	**0.86 (5)**	0.763 (13) → 0.764 (13)	**0.731 (13)**	0.752 (10)[Δ]
$\gamma_{2,0}$	1744.72 (18)	)	–	0.096	**0.127 (4)**	–	–	**0.14 (1)**	0.129 (3)	**0.118 (4)**	0.124 (4)[θ]

[*] Unquantified uncertainties – not included in weighted mean analysis of the data set.
[†] Described as obtained from the 1998 version of ENSDF when prepared as an electronic spectral database in 1998 - not included in weighted mean analysis of the data set.
[‡] Emission probabilities expressed relative to P_γ(908.97 keV) of 100 %.
[§] Relative emission probability of 46.0 (6) % for the 511-keV annihilation radiation was calculated from the total absolute positron emission probability of 22.8 (3) % and normalisation factor of 0.9903 (2).
[#] Recommended uncertainty has been adjusted from ± 0.004 to 0.005, in alignment with the smallest uncertainty of the values used to calculate the average value.
[+] Recommended uncertainty has been adjusted from ± 0.003 to 0.005, in alignment with the smallest uncertainty of the values used to calculate the average value.
[Δ] Recommended uncertainty has been adjusted from ± 0.008 to 0.010, in alignment with the smallest uncertainty of the values used to calculate the average value.
[θ] Recommended uncertainty has been adjusted from ± 0.003 to 0.004, in alignment with the smallest uncertainty of the values used to calculate the average value.

Gamma-ray emissions: multipolarities, and theoretical internal-conversion (frozen orbital approximation) and internal-pair formation coefficients.

E_γ (keV)	Multipolarity	α_K	α_L	α_{M+}	$\alpha_{ICCtotal}$	α_{IPF}	α_{total}
908.97 (3)	100%M4	0.007 43 (11)	0.000 906 (13)	0.000 174	0.008 51 (12)	–	0.008 51 (12)
1620.81 (20)	M1 + E2	–	–	–	–	–	–
1657.56 (15)	M1 + E2	–	–	–	–	–	–
1713.1 (3)	M1 + E2 1984HaZC, 1985HaZI	–	–	–	–	–	–
1744.72 (18)	E2	0.000 172 2 (25)	0.000 018 6 (3)	0.000 003 6	0.000 194 4 (25)	0.000 188 (3)	0.000 382 (6)

Emission Probabilities

All of the relative emission probabilities were quantified in terms of the emission probability of the 908.97-keV gamma ray (100.0 %), and the gamma-ray measurements of 1968Hi12, 1969Ro02, 1971Ar18 and 1979Ba46 were used to derive weighted-mean relative emission probabilities.

The normalisation factor for the relative gamma-ray emission and EC/β^+ transition probabilities can be calculated via two related routes:

(a). A total value of 100 % can be assigned to the gamma transition probabilities directly populating the 0.0-keV nuclear level of ^{89}Y, assuming zero EC/β^+ decay directly to the ground state on the basis of spin-parity considerations (9/2+ ⟶ 1/2− constitutes a third forbidden unique transition (4, yes)):

$$\sum_{0.0\ keV}^{\gamma\ population} TP_\gamma = 100$$

Thus: 100.975 (13) F = 100

where F is the normalisation factor for the relative gamma-ray emission probabilities.

$$F = 100 / 100.975\ (13) = 0.99034 \pm 0.00013$$

(b). Gamma population-depopulation of the various nuclear levels of ^{89}Y provide a means of determining the relative EC/β^+ transition probabilities from the relative γ-ray transition probabilities. Imbalances for each proposed nuclear level of Y-89 (at energies of 2622.1, 2566.5, 2529.8, 1744.7 and 908.97 keV) can be calculated on the basis of the evaluated relative gamma-ray emission probabilities, and their adopted total internal conversion coefficients. These population-depopulation imbalances in the relative gamma-transition probabilities constitute relative EC (EC + positron) transition probabilities of 0.752 (10) F, 0.107 (5) F, 0.075 (5) F, 0.124 (4) F and 99.917 (17) F to give a total of 100.975 (18) F in which the uncertainties of the $EC_{0,2}$, $EC_{0,3}$, $EC_{0,4}$ and $EC_{0,5}$ transitions are correctly included once in the summation. The total relative EC transition probability can be set to 100 % EC decay, assuming zero EC/β^+ decay directly to the ground state based on spin-parity considerations (third forbidden unique):

$$\sum_{0}^{EC/\beta^+\ populations} TP_{EC} = 100$$

Thus: 100.975 (18) F = 100

where F is the normalisation factor for the calculated relative EC/β^+ transition probabilities (and relative gamma-ray emission probabilities).

$$F = 100 / 100.975\ (18) = 0.99034 \pm 0.00018$$

On the basis of the above, a normalization factor of (0.9903 ± 0.0002) was adopted for the relative gamma-ray emission and EC/β^+ transition probabilities.

Multipolarities and Internal Conversion Coefficients

The nuclear level scheme specified by Singh has been used to define the multipolarities of the gamma transitions on the basis of known spins and parities (2013Si03). Only the significant emission probability of the 908.97-keV gamma ray merits the determination of the internal conversion coefficients for this 100 % M4 transition, although such data have also been derived for the 1744.72-keV E2 gamma-ray emission. Recommended internal conversion coefficients have been determined from the frozen orbital approximation of Kibédi *et al*. (2008Ki07), based on the theoretical model of Band *et al*. (2002Ba85, 2002Ra45), while the internal-pair formation coefficient for the 1744.72-keV E2 gamma transition was quantified from the tabulations of 2008Ki07.

Energies and emission probabilities of noteworthy internal conversion electrons.

		Energy (keV)	Electrons per 100 disint.
$ec_{1,0\ T}$	(Y)	891.93 – 908.97	0.84 (3)
$ec_{1,0\ K}$	(Y)	891.93 (3)	0.73 (3)
$ec_{1,0\ L}$	(Y)	906.60 – 906.89	0.089 (3)
$ec_{1,0\ M+}$	(Y)	908.58 – 908.97	0.017 (1)

Recommended gamma-ray energies, relative and absolute emission probabilities, and transition probabilities

	Eγ (keV)	P_{γ}^{rel} (%)	P_{γ}^{abs} (%)	Transition probability (%)
$\gamma^{\pm}$	511 annihilation radiation	46.0 (6)[§]	45.6 (6)	–
$\gamma_{1,0}$	908.97 (3)	100	99.03 (2)	99.87 (2)
$\gamma_{3,1}$	1620.81 (20)	0.075 (5)	0.074 (5)	0.074 (5)
$\gamma_{4,1}$	1657.56 (15)	0.107 (5)	0.106 (5)	0.106 (5)
$\gamma_{5,1}$	1713.1 (3)	0.752 (10)	0.745 (10)	0.745 (10)
$\gamma_{2,0}$	1744.72 (18)	0.124 (4)	0.123 (4)	0.123 (4)

[§] Relative emission probability of 46.0 (6) % for the 511-keV annihilation radiation was calculated from the total absolute positron emission probability of 22.8 (3) % and normalisation factor of 0.9903 (2).

EC/β+ transitions

Energies

All EC/β^+ energies were derived from the structural details of the proposed decay scheme. The nuclear level energies of 2013Si03 and evaluated Q_{EC}-value of 2832.8 (28) keV (2012Wa38) were used to determine the recommended energies and uncertainties of the EC transitions and β^+ emissions.

Transition and Emission Probabilities

^{89}Zr undergoes 100 % EC/β^+ decay. All resulting EC transition probabilities were derived from the population-depopulation imbalances of the relative emission probabilities of the gamma rays, their theoretical internal-conversion and internal-pair formation coefficients. However, an EC transition directly to the ground state of ^{89}Zr was assumed to be zero, based on spin-parity considerations alone (third forbidden unique (4, yes)). A value of 0.9903 (2) was adopted as the normalisation factor in order to determine the absolute transition and emission probabilities of the EC and β^+ particles from their resulting relative transition and emission probabilities. Component EC and β^+ transition and emission probabilities were determined from EC/β^+ ratios (1971Go40), and log*ft* values and average $E_{\beta+}$ energies were derived by means of the LOGFT code. Fractional EC probabilities P_K, P_L, P_M and P_N were calculated by means of the EC-CAPTURE code (1998Sc28) as developed from the data tabulations of 1995ScZY.

Measurements by 1953Sh48, 1961Mo12, 1964Va03, 1968Hi12 and 1979Ba46 have been made to determine or provide a means of calculating the EC/β^+ ratio for the 1924-keV EC transition. All relevant EC/β^+ data for ^{89}Zr are summarised in the table below.

EC/β^+ ratio for the 1924-keV EC transition of ^{89}Zr.

Reference	ϵ/β^+(1924-keV EC transition)
Gove and Martin (1971Go40), theory	3.36 (5)
derived from 1953Sh48, and quoted by Bambynek *et al.* (1977Ba48)	4 (1)
1961Mo12, as adjusted and quoted by Bambynek *et al.* (1977Ba48)	3.54 (14) → 3.48 (15)
1964Va03, and quoted by Bambynek *et al.* (1977Ba48)	3.43 (10)
derived from 1968Hi12, and quoted by Bambynek *et al.* (1977Ba48)	3.47 (21)
Baillie *et al.* (1979Ba46)	3.634 (55)

The absolute emission probability of the 511-keV annihilation radiation was derived from the total absolute positron emission probability of 22.8 (3) % as determined during the evaluation of the EC/β^+ transitions/emissions:

$$absolute\ P_{\gamma}^{\pm} = 2 \text{ x } 22.8\,(3) = 45.6\,(6)\ \%$$

$$[\,relative\ P_{\gamma}^{\pm} = \frac{absolute\ P_{\gamma}^{\pm}}{F} = \frac{45.6(6)}{0.9903(2)} = 46.0\,(6)\ \%\,]$$

where *F* is the normalisation factor for the gamma-ray emission probabilities.

A decay scheme was derived that consists of five EC transitions, one β^+ emission and five gamma rays. Furthermore, 511-keV annihilation radiation was also observed, with an absolute emission probability of 45.6 (6) %.

Recommended energies and transition probabilities of the EC/β^{+} decay of ^{89}Zr.

	E_{EC} (keV)*	$E_{\beta+}$ (keV)	Av. $E_{\beta+}$ (keV)	P_{EC}(total)	ϵ/β^{+} (theory) 1971Go40	P_{EC}	$P_{\beta+}$	^{89}Zr	^{89}Y	transition type	log *ft*	P_K	P_L	P_M	P_N
$EC_{0,5}$	211 (3)	–	–	0.745 (10)	–	0.745 (10)	–	9/2 +	9/2 +	allowed	6.18	0.8575 (17)	0.1165 (13)	0.0223 (5)	0.0036 (2)
$EC_{0,4}$	266 (3)	–	–	0.106 (5)	–	0.106 (5)	–	9/2 +	11/2 +	allowed	7.25	0.8615 (16)	0.1134 (13)	0.0216 (5)	0.0035 (2)
$EC_{0,3}$	303 (3)	–	–	0.074 (5)	–	0.074 (5)	–	9/2 +	7/2 +	allowed	7.52	0.8632 (16)	0.1120 (13)	0.0213 (4)	0.0035 (2)
$EC_{0,2}$	1088 (3)	–	–	0.123 (4)	–	0.123 (4)	–	9/2 +	5/2 –	first forbidden unique	9.09^{1u}	0.8677 (15)	0.1082 (12)	0.0208 (4)	0.0033 (2)
$EC_{0,1}$	1924 (3)	902 (3)	395.7 (14)	98.95 (2)	3.36	76.2 (3)	22.8 (3)	9/2 +	9/2 +	allowed	6.152	0.8731 (15)	0.1041 (12)	0.0196 (4)	0.0032 (2)
				∑ 99.998		∑ 77.248	∑ 22.8								
						∑ 100.048									

* Determined from the nuclear level energies of 2013Si03 and Q-value of 2832.8 (28) keV (2012Wa38).

Atomic Data

The X-ray and Auger-electron data have been calculated using the evaluated gamma-ray data, and atomic data from 1996Sc06, 1998ScZM and 1999ScZX. Both the X-ray and Auger-electron emission probabilities were determined by means of the EMISSION computer program (version 4.02, 28 February 2012), as described in 2000Sc47. This program incorporates atomic data from 1996Sc06, along with the adoption of a capture probability ratio P_{L1}/P_{L2} from 1997ScZY and P_{L3} of zero, and the evaluated gamma-ray data.

K and L X-ray energies and emission probabilities of ^{89}Zr.

			Energy (keV)	Photons per 100 disint.	Relative probability
XL		(Y)	1.686 – 2.347	2.36 (5)	8.74
	XL_l	(Y)	1.686	0.0568 (15)	
	XL_α	(Y)	1.920 – 1.923	1.48 (4)	
	XL_η	(Y)	1.762	0.0234 (7)	
	XL_β	(Y)	1.996 – 2.078	0.778 (19)	
	XL_γ	(Y)	2.153 – 2.347	0.01331 (24)	
XK_α	$XK_{\alpha2}$	(Y)	14.8829 (1)	14.08 (13)	52.1
	$XK_{\alpha1}$	(Y)	14.9585 (1)	27.01 (20)	100
$XK'_{\beta1}$	$XK_{\beta3}$	(Y)	16.7259 (7)	)	
	$XK_{\beta1}$	(Y)	16.7381 (5)	) 6.78 (8)	25.1
	$XK_{\beta5}$	(Y)	16.880 (2)	)	
$XK'_{\beta2}$	$XK_{\beta2}$	(Y)	17.0156 (9)	) 0.94 (4)	3.48
	$XK_{\beta4}$	(Y)	17.0362 (12)	)	

Auger-electron energies and emission probabilities of ^{89}Zr.

		Energy (keV)	Electrons per 100 disint.	Relative probability
e_{AK}	(Y)		19.4 (3)	
	KLL	12.205 – 12.784	13.72 (21)	100
	KLX	14.238 – 14.956	5.16 (9)	37.6
	KXY	16.251 – 17.034	0.484 (11)	3.53
e_{AL}	(Y)	1.27 – 1.89	79.5 (7)	579

Y: ω_K = 0.716 (4); ϖ_L = 0.0289 (7); n_{KL} = 1.081 (4) were taken from 1996Sc06.

Electron energies were determined from electron binding energies tabulated by Larkins (1977La19) and the evaluated gamma-ray energies. Absolute electron emission probabilities were calculated from the evaluated absolute gamma-ray emission probabilities and associated internal conversion coefficients.

Data Consistency

A Q_{EC}-value of 2832.8 (28) keV has been adopted from the atomic mass evaluation of Wang *et al.* (2012Wa38) for the EC decay of ^{89}Zr. This value has subsequently been compared with the Q-value calculated by summing the contributions of the individual emissions to the ^{89}Zr EC-decay process (i.e. EC/β^+, electron, γ, etc.):

$$\text{calculated Q-value} \quad = \quad \sum (E_i \ x \ P_i) \quad = \quad 2834\ (7)\ \text{keV}$$

Percentage deviation from the Q-value of Wang *et al*. is 0.04 (28) %, which supports the derivation of a reasonably consistent decay scheme albeit with a significant variant.

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