^{44}Sc – Comments on evaluation of decay data

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The *Limitation of Relative Statistical Weights* [1] (LWM) method, used for averaging numbers throughout this evaluation, provided a uniform approach for the analysis of discrepant data. The uncertainty assigned to the recommended value was always greater than or equal to the smallest uncertainty of the values used to calculate the average.

Decay Scheme

^{44}Sc ($T_{1/2}$ = 3.97 h) decays 94.27(5)% by β^+, and 5.73(5)% by electron capture (Q(EC)=3653.3(19) keV (95Au04)[2]) allowed transitions to levels at 1157.0-, 2656.5-, and 3301.5-keV in ^{44}Ca (stable). A β^+ transition from ^{44}Sc ($J^\pi = 2^+$) to the ground state of ^{44}Ca ($J^\pi = 0^+$) has not been observed. Such transition would be second-forbidden non unique, for which the systematic trend of log *ft* predicts a value > 10.6 (98Si17)[4]. For ^{44}Sc this value corresponds to a β^+ transition probability limit of < 0.005%. Therefore, I used no β^+ feeding to the ground state, and normalized the decay scheme using the sum of the relative transition probabilities of the 1157.0-, 2656.4-, and 3301.3-keV gamma rays. This procedure produced a normalization factor $N = (9.9875(3) \times 10^{-4})$, as it will be shown in below.

Nuclear Data

The recommended half-life of ^{44}Sc, 3.97(4) h, is a weighted average (LWM, σ_{int}=0.01, χ^2/ν= 8.0) of 3.927(8) h (69Ra16)[5], 4.00(2) h (66Ta01)[6], and 4.05(3) h [7]. Other values are: 4.04 h [8], 4.01 h [9], and 3.9 h [10], were not used because they have no uncertainties.

Gamma Rays

Tables Ia and Ib give gamma-ray energies and relative emission probabilities, respectively, reported by 90Me15[11], 83Gu11[12], 76Co06 [13], 74HeYW [14], 73Si05 [15], and 90Sc08 [16]. Recommended values (weighted averages (LWM)) are given on columns 5 and 7, respectively.

Table Ia - Gamma-Ray Energies

90Me15[11] & 76Co06[13] keV	83Gu11[12] keV	74HeYW[14] keV	73Si05[15] keV	Rec. Value keV	χ^2/ν
	646.55 (62)		646.5 (20)		
726.49	726.3 (15)		726.0 (15)		
	772.7 (12)		774		
1157.031 (15)	1157.015 (15)	1156.92 (15)	1156.9 (5)	1157.020 (15)	0.37
1499.489 (25)	1499.436 (15)	1499.20 (20)	1499.4 (3)	1499.460 (20)	1.3
2144.3 (1)	2144.43 (20)		2144.8 (8)	2144.33 (10)	0.34
2656.478 (30)	2656.435 (50)	2657.14 (20)	2656.4 (5)	2656.48 (7)	3.9
3301.3 (1)	3301.361 (55)	3301.6 (15)	3301.35 (6)	0.16	

Table Ib - Relative Gamma-Ray Emission Probabilities

Energy keV	90Me15[11] & 76Co06[13]	90Sc08[16]	83Gu11[12]	74HeYW[14]	73Si05[15]	Rec. Value	χ^2/ν
646.5			0.040		0.043 (18)		
726.3	=0.014		0.053 (10)		0.051 (21)		
772.7	=0.0067*		0.062 (16)		0.041 (23)		
1157.020	1000(3)	1000 (1)	1000 (3)#	1000 (50)	1000 (3)#	1000 (3)	
1499.46	9.0 (2)	9.12 (15)	9.22 (37)	9.0 (10)	9.1 (4)	9.09 (15)	0.10
2144.33	0.02 (2)		0.035 (10)#		0.039 (7)	0.036 (7)	0.41
2656.48	1.11 (4)	1.15 (6)	1.11 (3)	1.4 (5)	1.3 (1)	1.12 (3)	0.98
3301.35	0.0064 (8)		0.016 (2)		0.018 (3)	0.017 (2)&	0.31

* From ^{44}K decay, relative to 9.0 for the emission probability of 1499-keV gamma ray._

\# Estimated by evaluator.

& Weighted average of 0.016(2) and 0.018(3).

The 726- and 772-keV gamma rays reported by 83Gu11 [12] and 73Si05 [15] were not observed by 90Me15 [11] and 76Co06 [13], who reported upper limits four and nine times lower, respectively, for their relative emission probabilities. Therefore, they probably do not belong to the decay of ^{44}Sc.

The 646-keV gamma ray was observed with about the same relative emission probability by both 83Gu11 [12] and 73Si05 [15]. These authors placed this gamma ray de-exciting a 3301-keV level, which is also de-excited by the 2144- and 3301-keV transitions. 90Me15 [11] and 76Co06 [13] did not report the 646-keV gamma ray. However, 76Co06 [13] have seen it in the β^- decay of ^{44}K. Table II shows the relative emission probabilities of the 646-, 2144-, and 3301-keV gamma rays, which de-excite the 3301-keV level, from both ^{44}Sc electron-capture and ^{44}K β^- decay.

Table II - Relative Emission Probabilities for the 646-, 2144-, and 3301-keV Gamma Rays from the 3301-keV Level

Energy keV	83Gu11[12] P_γ	73Si05[15] P_γ	76Co06[13] P_γ
	From ^{44}Sc EC Decay		From ^{44}K β^- Decay
646.5	0.040	0.043 (18)	1.5 (5)
2144.33	0.035	0.039 (7)	12.9 (8)
3301.35	0.016 (2)	0.018 (3)	5.5 (9)
R(646/2144)	1.1	1.1	0.12
R(2144/3301)	2.2	2.2	2.3

Table II shows that the ratio R(646/2144) is ten times lower from ^{44}K β^- decay than from ^{44}Sc electron-capture decay. Consequently, the 646-keV gamma-ray, observed from ^{44}K decay, does not de-excite the 3301-keV level, as 83Gu11 had suggested, and therefore, its existence is uncertain.

Multipolarities and Conversion Coefficients

A total measured conversion coefficient [17] α_t=6.3 (3)x10^{-5} for the 1157.020-keV gamma-ray suggests an E2 multipolarity for this gamma-ray. The 1499.46-keV gamma-ray has an M1+1.8 (4)% E2 multipolarity (δ = +0.137(7)), determined in a $\gamma\gamma(\theta)$ measurement (68Wa21)[3].The theoretical conversion coefficients in Table 2.3 (Tables Section) for these transitions are from 76Ba63 [18]. Conversion coefficients for pair creation are theoretical values from 79Sc31[30].

Absolute Emission Probabilities.

As mentioned before, the gamma-ray normalization factor *N* can be obtained as follows:

$$N = 1/[P_{\gamma(1157)}(1+\alpha_{1157}) + P_{\gamma(2256)} + P_{\gamma(3301)}] = 1/[1000\ (3)\ (1 + 6.68 \times 10^{-5}) + 1.12\ (3) + 0.064\ (8)]$$
$$= 9.9875(3) \times 10^{-4}$$

The internal pair conversion coefficients (from 79Sc31[19]) for these gamma-rays are: α_{IP}(1157, E2) = 4.0 $\times 10^{-6}$, α_{IP}(2256, E2) = 5.9 $\times 10^{-4}$, and α_{IP}(3301, E2) = 9.0 $\times 10^{-4}$. These coefficients were not included in the calculation shown above because their effect is negligible.

The fractional uncertainty in *N* should be added in quadrature to those in the relative emission probabilities. For the 1157.020-keV gamma-ray, which dominates this normalization, the correct propagation of this uncertainty is as follows:

$$P_\gamma(\text{abs},1157) = P_\gamma(\text{rel},\ 1157) \times N = 1000\ (3)/[1000\ (3)\ (1 + 6.68 \times 10^{-5}) + 1.12\ (3) + 0.064\ (8)] =$$
$$= 1/\ [1.0000668 + 1.18\ (3)/1000\ (3)] = 1/[1.0000668 + 0.00118\ (3)] = 0.99875(3)$$

Notice that the fractional uncertainty of the relative emission probability is 0.3% , however, because of the effect of covariances, that in the absolute emission probability is just 0.003% . Table III shows the gamma-ray absolute emission probabilities.

Table III - Absolute Gamma-ray Emission Probabilities

Energy (keV)	P_γ(%)
1157.020 (15)	99.875 (3)
1499.460 (20)	0.908 (15)
2144.33 (10)	3.6 (7) $\times 10^{-3}$
2656.48 (7)	0.112 (3)
3301.35 (6)	1.7 (2) $\times 10^{-3}$

Electron-Capture and b$^+$ **Transitions**

The electron-capture plus β^+ probabilities shown in the decay scheme have been deduced from gamma-ray transition intensity balances at each level. For the transition to the 1157-keV level, the values of the individual β^+ and electron-capture probabilities (given in Tables 2.2 and 2.1, respectively) are based on the recommended ε/β^+ = 0.0499(5) ratio. This ratio is a weighted average of the experimental values 0.0499(5) (83Ba41) [20] and 0.0497(23) (76St21) [21]. Theory predicts 0.0489 [22].

Electron-capture probabilities to the various atomic sub-shells, i.e., P_K, P_L, P_{M+} in Table 2.1 are theoretical values (98Sc28)[23] calculated with the computer program EC-CAPTURE[24].

90Sc08 [16] measured the annihilation emission probability $P_{\gamma\pm}(511) = 1.88(3)$, which includes a 2.4% correction for positron annihilation-in-flight. I confirmed the value of this correction using the calculation procedure presented in Appendix D of the *Table of Radioactive Isotopes* [25], as described below in Table IV.

Table IV - Annihilation-in-flight Correction Factor

E(bin) keV	$<\beta^+>^*$ keV	β^+ (%)$^\#$ %	$E_{avg}{}^{\&}$ keV	$P(E_{avg})^\wedge$ %	$\beta^+{}_{fl}{}^{@}$ %
0-10	0.000434	0.0056	7.75		
10-20	0.0056	0.0355	15.77		
20-40	0.060	0.191	31.41		
40-100	1.12	1.50	74.67	0.5	0.0075
100-300	26.8	12.6	212.69	1.0	0.126
300-600	140.0	30.7	456.03	2.1	0.645
600-1300	418.0	48.6	860.0	3.4	1.652
1300-2497	10.8	0.80	1350.0	4.8	0.038
	Total β^+ branching	**94.0**		Correction factor	**2.47**

*Average β^+ energy per decay
$^\#$ β^+ bin probability
$^\&$ Average β^+ bin energy = 100 < β^+>/β^+(%)
$^\wedge$ Positron annihilation-in-flight probability (from Fig.3, Appendix D, *Table of Radioactive Isotopes*)
$^@$ Fraction (in %) of β^+ transitions that annihilate in flight = 0.01xβ^+(%)x $P(E_{avg})$

The final result, 2.47%, agrees with 2.4%, used by 90Sc08 [16].

Then, the β^+ probability is $P_{\beta+}$(1157) = 1.88(3)/2 = 0.940(15). The electron-capture probability, P_{EC}(1157) = 0.9897(5) - 0.940(15) = 0.0497(15), although less accurate, is in agreement with the recommended value given in Table 2.1.

Levels half-life

The following half-life values: 2.61(14) ps (1157-keV level), 30(3) fs (2656-keV level), and 35 (18) fs (3301-keV level), shown on the level scheme, are from 90En08 [26].

Atomic Data

The X-ray and Auger-electron probabilities in Section 4 have been calculated with the computer program EMISSION[27], using the gamma-ray and electron-capture data from Section 2, and atomic data from 96Sc06[28]

Total Average Radiation Energy

The calculated (RADLST[29]) total average radiation energy of 3653.3(25) keV (which includes all the radiations emitted by ^{44}Sc), agrees very well with Q(EC) =3653.3(19) keV (1995Au04[2]) and confirms the self consistency of the ^{44}Sc decay scheme.

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