^{55}Fe - Comments on evaluation of decay data

P. Cassette

Faculty of Physics, Sofia University, "St. Kliment Ohridski"

The initial evaluation was completed in April 1998. A revised evaluation by M.M. Bé and V. Chisté was completed in 2005, covering the literature available by December 2005. The present revised evaluation was carried out in 2023, with a literature cut-off date of October 2023.

1 Decay Scheme

Fe-55 mostly disintegrates by electron capture to the ground state of ^{55}Mn. A very weak electron capture transition to the 7/2$^-$ excited level of ^{55}Mn was also identified.

An internal Bremsstrahlung electron capture spectrum was measured by ***Isaac et al. (1990)***, with an intensity of 3.24 (6) 10^{-5} in the 35 to 231 keV energy range, relative to the probability of the K-shell capture.

The J^{π} value and level energy are from ***NDS 109,787 (2008)***. The excited level energy has been determined to be 125.949 (10) keV.

2 Nuclear data

- The Q value (231.12 (18) keV), is from the AME 2020 atomic mass evaluation by ***Wang et al. (2021).***
- The half-life values considered are given in the following Table.

Reference	Value (days)	Method
Lagoutine (1982)	977.9 (23)	DSA PC
Houtermans (1980)	1000.4 (13)	PC
Hoppes (1982)	1009.0 (17)	PC, Si(Li)
Morel (1994)	996.8 (60)	Ge
Karmalitsyn (1998)	995.0 (30)	PC
Schötzig (2000)	1003.5 (21)	Si(Li)
Van Ammel (2006)	1005.2 (14)	DSA PC
Pommé (2019)	1006.70 (15)	PC
Kossert (2020)	1006.2 (10)	LSC

The measurement methods are: DSA = Defined Solid Angle, PC = Proportional Counter, Si(Li) = Lithium doped Silicon detector, Ge = germanium detector, LSC = Liquid Scintillation Counting.

The values 1 and 5 are rejected because they are discrepant from Chauvenet's criterion. We also decided to reject the value 4 because, in the publication, no detail is given on the uncertainty evaluation.

Value 2 exhibits a small relative uncertainty of 0.13 %, which surpasses the precision of most measurements reported in the literature at this time. This suggests that the uncertainty is greatly underestimated and this value was thus not considered.

Value 3 is cited in a report concerning the efficiency calibration of germanium spectrometer. In this report, this value is given as an unpublished result and thus was not considered.

An analysis of the publications cited showed that results 6 to 9 are associated with a comprehensive uncertainty evaluation, including study of possible systematic errors. The value 6 was obtained using Si(Li) photon detector, with an identified, albeit corrected, efficiency variation with time. Results 6 to 9 are consistent, and are based on different measurement techniques: Si(Li) detector for 6, DSA PC X-ray detector with a beryllium window for 7, pressurized proportional counter for 8 and Triple to Double Coincidence ratio LSC method for 9. The three first methods are only sensitive to X-rays and method 9 is sensitive to both X-rays and Auger electrons. Result 8 presents an uncertainty one order of magnitude lower than the other results, but the uncertainty budget is exhaustive and fully detailed. Value 8 has a relative weight of more than 96 %. The χ^2 value is 1.2, for a critical value 3.8 and the dataset is consistent.

The adopted value was calculated from results 6 to 9 using the Lweight program: **1006.66 (15) d or 2.75614 (41) a**. As the dataset is consistent, this value is the weighted average with internal uncertainty.

Other references were not used in this evaluation, due to their discrepancy or high uncertainty, compared with the set of more recent values considered. They are given in the following Table.

Unused reference	**Value (days)**
G. L. Brownell (1950)	1037 (11)
R. P. Schuman (1956)	950 (7) d
J. S. Evens (1965)	880 (44) d

2.1 Electron capture transitions

- The ec. transition energies are from the Q value and from individual levels energies.
- The transition probabilities are deduced from the gamma-ray transition probability balance at each level. Due to the very low probability of the $\varepsilon_{0,1}$ transition, the decay of ^{55}Fe can be considered as a pure electron capture to the ground level of ^{55}Mn.
- The electron capture probabilities, for each shell, were calculated using the ***BetaShape*** program for a Q energy of 231.12 (18) keV:

  P_K = 0.88044 (34), P_{L1} = 0.10188 (23), P_{L2} = 5.012E-4 (26), P_{M1} = 0.01599 (10)

  P_{M2} = 7.43E-5 (7), P_{N1} = 0.001120 (8), thus

  P_K = 0.88044 (34), P_L = 0.10238 (23), P_M = 0.01606 (10), P_N = 0.001120 (8)

  The log ft value is lg *ft* = 5.9869 (35)

  The values obtained using the ***EC-capture*** program are:

  P_K = 0.8853 (16), P_L = 0.0983 (13), P_M = 0.0157 (6), P_N = 0.0006 (1)

  The ***LOGFT*** program gives:

  P_K = 0.885 (9), P_L = 0.0974 (10), P_M = 0.0161 (2), P_N = 0.00106 (1)

The experimental values of ***Pengra et al.*** (1972) are:

P_K = 0.881 (4), P_L = 0.103 (4), P_{M+} = 0.0161 (8)

The ratio P_L/P_K were determined by ***Loidl et al.*** (2018) using a low-temperature calorimeter experiment. The values obtained, compared with the calculated values and the values from ***Pengra*** are given in the following Table.

Reference	P_L/P_K
Pengra et al.	0.117 (5)
Loidl et al.	0.1134 (25)
BetaShape	0.1162 (3)
EC-capture	0.1110 (14)
LOGFT	0.1101 (12)

Experimental and calculated results are consistent but the measured values of ***Pengra et al.*** are dependent on ω_K and on the intensity of K_α X-ray and the values of ***Loidl et al.*** only give ratio and not the absolute values of electron capture probabilities.

The recommended values are those of the ***BetaShape*** code.

The double K-shell ionization process was studied by several authors. The measured total probabilities for double K vacancies P_{KK} are given in the following Table.

Reference	P_{KK}
Kitahara et al. (1975)	1.01 (27) 10^{-4}
Campbell et al. (1991)	1.3 (2) 10^{-4}
Michel et al. (2014)	1.531 (79) 10^{-4}
EC- Bergman et al. (2016)	1.388 (37) 10^{-4}

These values are consistent with a weighted average of 1.405 (43) 10^{-4}.

2.2 Gamma transitions

A weak gamma transition of 126.0 keV was observed by ***Zlimen et al.*** (1992) following a second non-unique electron capture transition to an excited state of ^{55}Mn with a probability of 1.3 (1) 10^{-7} %.

The gamma emission intensity given by ***Zlimen et al.*** (1992) is 1.28 (2) 10^{-7} %, but only statistical fluctuations are considered in this publication and the uncertainty is underestimated. Thus the recommended value is 1.3 (1) 10^{-7} %. Multipolarity is M1(+E2) from ENSDF, which is based on measured conversion coefficient of K-shell.

3 Atomic data

Several data for ω_K are deduced from the measurements given in the following Table.

Reference	ω_K
Smith (1982)	0.320 (3)
Konstantinov et al. (1989)	0.312 (3)
Dobrilovic et al. (1973)	0.322 (5)
Kuhn et al. (1981)	0.310 (23)
Hubbell et al. (1994)	0.321 (7)

A theoretical value of 0.323 was also calculated by ***Chen*** (1980).

These values are in agreement with the recommended value of 0.321 (5) from the semi-empirical fit of ***Bambynek*** (1984).

ω_L and η_{KL} are from ***Schönfeld et al.*** (1995).

3.1 X radiations

The X-ray energies are from ***Bearden***, 1967.

The emission intensities are calculated by the EMISSION program from PTB (***Schönfeld et al.*** 1995).

With P_K = 0.88044 (34) for the allowed transition, and ω_K = 0.321 (5), the total K X-ray emission intensity is 0.2826 (30), in good agreement with the experimental values of 0.279 (8) (***Schötzig***, 2000) and 0.283 (2) (***Smith***, 1982). An experimental K X-ray emission of 0.273 was reported by (***Martin***, 1994), but without uncertainty.

The ratio $X_{K\beta}/X_{K\alpha}$ calculated from the results of the EMISSION program is 0.1359 (32) and this value is coherent with the experimental values of ***Lépy et al.***, 1994, 0.1388 (15), considering the radiative Auger effect in the X-ray spectrum analysis. The ratio $X_{K\beta}/X_{K\alpha}$ reported by ***Bonnelle et al.***, 2020, is 0.138 (4) for metal manganese, which is also coherent with these previous values. This is not the case for the $X_{K\beta}/X_{K\alpha}$ value of 0.1188 (11) reported by ***Yalcin***, 2007 but the reason of this discrepancy is not clear.

3.2 Auger electrons

Measurement of the K Auger spectrum of manganese was performed by ***Kovalik et al.*** (1990), giving the following relative intensities of the Auger groups:

KLM/KLL = 0.26 (2)

KMM/KLL = 0.018 (2)

These values are in good agreement with the recommended values calculated with the EMISSION program:

KLM/KLL = 0.272 (3)

KMM/KLL = 0.0185 (4)

The energies are from ***Larkins*** (1977) or calculated from the electron binding energies ***Bé et al.*** (2006). ***Kovalik et al.*** (1990) also measured the energies and found good agreement with the KLM spectrum but discrepancies were observed for the KLL and KMM groups.

4 Gamma emissions

A weak gamma emission, superimposed on the inner-bremsstrahlung photon emission was observed by ***Zlimen et al.*** (1992) and associated to the deexcitation of the first state of ^{55}Mn. The gamma ray energy is given as 126.0 (1) keV, with an emission intensity of 1.3 (1) 10^{-7} %.

From the energy level of 125.949 (10) keV and a recoil energy of 0.2 eV, the adopted gamma energy is 125.949 (10) keV. Because of the very low probability of this transition, the conversion coefficients and the associated conversion electron emission are not reported.

5 References

G.L. Brownell, C.J. Maletskos. Phys. Rev. 80, 1102 (1950) [Half-life]

R.P. Schuman, M.E. Jones, A.C. McWherter. J. Inorg. Nuclear Chem, 3, 160 (1956) [Half-life]

J.S. Evans, R.A. Naumann. PPAD-2137-566, 10 (1965) [Half-life]

J.A. Bearden, Reviews of Modern Physics, 39, 78 (1967) [X-ray energies]

J.G. Pengra, H. Genz, J.P. Renier, R.W. Fink. Phys. Rev. C5,6, 2007 (1972) [P_L/P_K, P_M/P_L]

L. Dobrilovic, D. Bek-Uzarov, M. Simovic, K. Buraei, A. Milojevic. Proc. of the International Conference on Inner-shell Ionization Phenomena, CONF-720404, 128 (1973) [K fluorescence yield]

T. Kitahara, S. Shimizu. Phys. Rev. C11,3 920 (1975) [Ionization probability]

F.P. Larkins, At. Data Nucl. Data Tables 20,4, 338 (1977) [Auger Electrons]

***J.E. Martin**, *M.D.K. Liaw**, Appl. Radiat. Isot. 45, 121 (1994) [X-ray emission intensities]

H. Houtermans, O. Milosevic, F. Reichel. Int. J. Appl. Radiat. Isotop., 31, 153 (1980) [Half-life]

M.H. Chen, Phys. Rev. A21-2, 436 (1980) [K fluorescence yield]

U. Kuhn, H. Genz, W. Löw, A. Richter, H.W. Müller. Z. Phys. A - Atoms and Nuclei, 300, 103 (1981) [K fluorescence yield]

D.D. Hoppes, J.M.R. Hutchinson, F.J. Schima, M.P. Unterweger. NBS-Special publication, 626, 85 (1982) [Half-life]

D. Smith, Nucl. Instrum. Methods, 200, 383 (1982) [$P_K\omega_K$]

F. Lagoutine, J. Legrand, C. Bac. Int. J. Appl. Radiat. Isotop., 33, 711 (1982) [Half-life]

W. Bambynek, A. Meisel Ed. Leipzig Aug. 20-23, (1984) [K fluorescence yield]

A.A. Konstantinov, T.E.Sazonova, S.V. Sepman, E.A. Frolov. Metrologia 26, 205 (1989) [K fluorescence yield]

M.C.P. Isaac, V.R. Vanin, O.A.M. Helene. Z. Phys. A. 335, 243 (1990) [Beta emission energies]

A. Kovalik, V. Brabec, J. Novak, O. Dragoun, V.M. Gorozhankin, A.F. Novgorodov, Ts. Vylov. J. Elec. Spectro. Rel. Phenomena, 50, 89 (1990) [Auger electrons]

J.L. Campbell, J.A. Maxwell, W.J. Teesdale. Phys. Rev. C. 43,4, 1656 (1991) [Double K capture probability]

I. Zlimen, E. Browne, Y. Chan, M.T.F. Da Cruz, A. Garcia, R.-M. Larimer, K.T. Lesko, E.B. Norman, R.G. Stokstad, F.E. Wietfeldt. Phys. Rev. C. 46,3, 1136 (1992) [Gamma Emission]

J. Morel, M. Etcheverry, M. Vallée. Nucl. Instrum. Methods Phys. Res. A339, 232 (1994) [Half-life]

J.H. Hubbell, P.N. Trehan, Nirmal Singh, B. Chand, D. Mehta, M.L. Garg, R.R. Garg, Surinder Singh, S. Puri. J. Phys. Chem. Ref. Data, 23-2, 339 (1994) [K fluorescence yield]

M.C. Lépy, J. Plagnard, J. Morel. Nucl. Instrum. Methods Phys. Res. A339, 241-247 (1994) [K_β/K_α]

E. Schönfeld, H. Janssen. Report PTB Ra-37 (1995) [L fluorescence yield, K_β/K_α]

N.I. Karmalitsyn, T.E. Sazonova, A.V. Zanevsky, S.V. Sepman. Appl. Rad. Isotopes 49,9-11, 1363 (1998) [Half-life]

U. Schötzig, Appl. Rad. Isotopes 53, 469 (2000) [Half-life, X-ray emission intensities]

C. Bonnelle, P. Jonnard, M.M. Bé, M.C. Lépy. Bulletin du BNM 120, 7-16 (2001) [K_β /K_α]

R. Van Ammel, S. Pommé, G. Sibbens. Appl. Rad. Isotopes 64, 1412 (2006) [Half-life]

M.M. Bé, V. Chisté, C. Dulieu. Appl. Radiat. Isotopes 64, 1435-1439 (2006) [Auger electrons]

T. Michel, B. Bergmann, J. Durst, M. Filipenko, T. Gleixner, K. Zuber. Physical Review C 89, 014609 (2014) [Double K ionization]

B. Bergmann, T. Michel, A. Surzhykov, S. Fritzsche. Physical Review C 94, 014611 (2016) [Double K ionization]

M. Loidl, M. Rodrigues, R. Mariam. Appl. Radiat. Isotopes 134, 395-398 (2018) [EC probabilities]

S. Pommé, H. Stroh, R. Van Ammel. Appl. Rad. Isotopes 148, 27-34 (2019) [Half-life]

K. Kossert, Appl. Radiat. Isotopes 155, 108931 (2020) [Half-life]

P. Yalcin, Nucl. Instrum. Methods Phys. Res B254, 182 (2007) [K_β/K_α]

M. Wang, W.J. Huang, F.G. Kondev, G. Audi, S. Naimi. Chinese Physics C 45, 3, 030003 (2021) [Q-value]