^{41}Ca - Comments on evaluation of decay data by X. Mougeot

This first evaluation was done in 2012, taking into account the available literature up to November 2012.

^{41}Ca plays an important role in the long-term evaluation of the safety of final repositories for nuclear waste and is used to study the fine-scale chronology of the formation of the Solar System (2012JO04).

1 Decay Scheme

The decay scheme is complete since ^{41}Ca can only decay through electron-capture to the ground state of ^{41}K: Q_ε = 421,63 (14) keV (from 2011AUZZ), and the first excited state of ^{41}K is $1/2^+$ at 980,476 (6) keV (from 2001CA59).

The J^π of the ground states of both ^{41}Ca ($7/2^-$) and ^{41}K ($3/2^+$) are from the 2001CA59 evaluation. The electron-capture transition is therefore first forbidden unique.

2 Nuclear Data

The first measurement of the Q value was detailed in 1950RI59. The Q value adopted in this evaluation is from Audi *et al.* 2011 (2011AUZZ).

A full list of the half-life measurements available by November 2012, including the reasons why certain have been excluded by the evaluator, is given in Table 1.

Three types of measurements were carried out:

1) using accelerator mass spectrometry, $T_{1/2}$(^{41}Ca) depends on $T_{1/2}$(^{36}Cl);

2) using specific activity deduced from X-ray intensity measurements, $T_{1/2}$(^{41}Ca) depends on neutron capture cross sections (σ_{40} and σ_{44}) and possibly on $T_{1/2}$(^{45}Ca), ω_K(K), P_K and P_L;

3) using liquid scintillation counting (TDCR method) for the activity and thermal ionization mass spectrometry for the absolute isotopic composition, the uncertainty on $T_{1/2}$(^{41}Ca) depends mainly on the uncertainty on P_K.

Thus, the available measurements have been recalculated using up-to-date values when it was necessary.

2.1 Half-life

In order to evaluate the ^{41}Ca half-life, the measured half-life values were recalculated using up-to-date values of parameters. The corresponding uncertainties were also calculated. The following parameter values have been used:

- N_A = 6,02214129 (27) 10^{23} mol^{-1} from 2008MO18.
- σ_{40} = 0,41 (2) b and σ_{44} = 0,88 (5) b from 2006MUZX.
- I_{ab}(^{40}Ca) = 0,9694 (16) from 2011BE53.
- ω_K(K) = 0,143 (4) from 1996SC06.
- LOGFT can calculate a first forbidden unique electron-capture transition. Using the Q value from 2011AUZZ, the following quantities have been calculated: P_K = 0,894 (9); P_L = 0,0916 (9); P_{M+} = 0,01482 (15). Thus, P_L/P_K = 0,1025 (10). A relative uncertainty of 1 % has been taken.
- $T_{1/2}$(^{36}Cl) = 3,02 (4) 10^5 *a* from the latest DDEP evaluation (2012).
- $T_{1/2}$(^{45}Ca) = 162,64 (11) *d* from the latest DDEP evaluation (2012).

Analysis of the publications

1962DR03 (Drouin *et al.*)

The source of ^{41}Ca had been prepared ten years before by high neutron irradiation of a sample of calcium carbonate. The number of ^{41}Ca atoms was calculated as:

$$N_{41} = \frac{N_A}{40 \cdot 1000} \times I_{ab}(^{40}Ca) \times \sigma_{40} \times (8{,}07 \cdot 10^{20})$$

where the factor 1000 is used for converting grams to milligrams, and the last factor is the integrated neutron flux. With the parameter values given above, the new N_{41} value is: 4,83 (24) 10^{15} atoms·mg^{-1}. The decay rate is then:

$$DR = 594\ (6) \times \frac{1}{0{,}86} \times \frac{1}{0{,}67} \times \frac{1}{\omega_K(K)} \times \left(1 + \frac{P_L}{P_K}\right) \times 2$$

where the first numerical term is the number of potassium K X-rays per min measured for 0,42 mg of Ca, the factor 2 corrects for the 50 % geometrical detection efficiency, 1/0,86 corrects for the self-absorption in the source (estimated to be 14 % in 1962DR03), and 1/0,67 corrects for the transmission of X-rays by the Auger electron absorber (estimated to be 67 % in 1962DR03).
Thus, the new value is: DR = 1,59 (5) 10^4 *min*$^{-1}$/(0,42 mg Ca). As:

$$T_{1/2} = \frac{N_{41} \cdot \ln 2}{DR/0{,}42}$$

the new half-life result is: $T_{1/2}$(^{41}Ca) = 8,8 (5) 10^{10} *min* = 1,68 (10) 10^5 *a*. The authors have estimated a relative uncertainty of about 15 %. Therefore, the final value is $T_{1/2}$(^{41}Ca) = 1,68 (25) 10^5 *a*.

1966WA (Wahlin)

$T_{1/2}$(^{41}Ca) = 1,00 (25) 10^5 *a* was determined proportionally to $T_{1/2}$(^{36}Cl) = 2,60 (8) 10^5 *a*. The up-to-date value of $T_{1/2}$(^{36}Cl) provides directly the up-to-date value of $T_{1/2}$(^{41}Ca) = 1,16 (29) 10^5 *a*.

1974MA30 (Mabuchi *et al.*)

The authors gave a value of $T_{1/2}$(^{41}Ca) = 1,03 (4) 10^5 *a* using a neutron capture cross section on ^{40}Ca with a relative uncertainty of 10 %. The uncertainty on $T_{1/2}$(^{41}Ca) in 1974MA30 was clearly underestimated and has been recalculated by the evaluator to be 0,14 10^5 *a*. The half-life is calculated as follows:

$$T_{1/2}(^{41}Ca) = 108\ (4) \times 5{,}29 \cdot 10^3 \times \frac{\sigma_{40}}{\sigma_{44}} \times T_{1/2}(^{45}Ca) \times \frac{1}{0{,}9750}$$

where the first numerical term is the ratio of measured activity of ^{45}Ca on measured activity of ^{41}Ca, the second numerical term is the ratio (resulting from mass spectroscopy analysis) of the number of ^{40}Ca atoms on the number of ^{44}Ca atoms irradiated using a thermal neutron flux, and the last numerical term takes into account the time duration of irradiation and depends on experimental conditions. Thus, the up-to-date value is: $T_{1/2}$(^{41}Ca) = 1,22 (10) 10^5 *a*.

1991PA10 (Paul *et al.*)

The authors gave a value of $T_{1/2}$(^{41}Ca) = 1,01 (10) 10^5 *a* derived from the specific activity determined from ^{41}K X-ray measurements. They obtained: S(^{41}K) = 23,98 (186) X-rays *min*$^{-1}$ng^{-1}.
As:

$$S(^{41}Ca) = \frac{S(^{41}K)}{\omega_K P_K}$$

one has the new value: S(^{41}Ca) = 188 (16) *min*$^{-1}$ng^{-1}, and the half-life is given by:

$$T_{1/2} = \frac{N_A \cdot \ln 2}{S(^{41}Ca) \cdot 41}$$

namely $T_{1/2}$(^{41}Ca) = 1,03 (9) 10^5 *a*.

1991KL06 (Klein *et al.*)

The authors obtained a value of $T_{1/2}$(^{41}Ca) = 1,03 (7) 10^5 *a* which depends on the half-life of ^{36}Cl, taken as $T_{1/2}$(^{36}Cl) = 3,01 (2) 10^5 *a*. As they measured a ratio $T_{1/2}$(^{36}Cl)/ $T_{1/2}$(^{41}Ca) = 2,91 (9), the updated value is $T_{1/2}$(^{41}Ca) = 1,04 (7) 10^5 *a*. It is noteworthy that the authors estimated a final uncertainty two times larger, from 0,035 10^5 *a* to 0,07 10^5 *a*, to take into account the dispersion of their measurements.

Evaluation

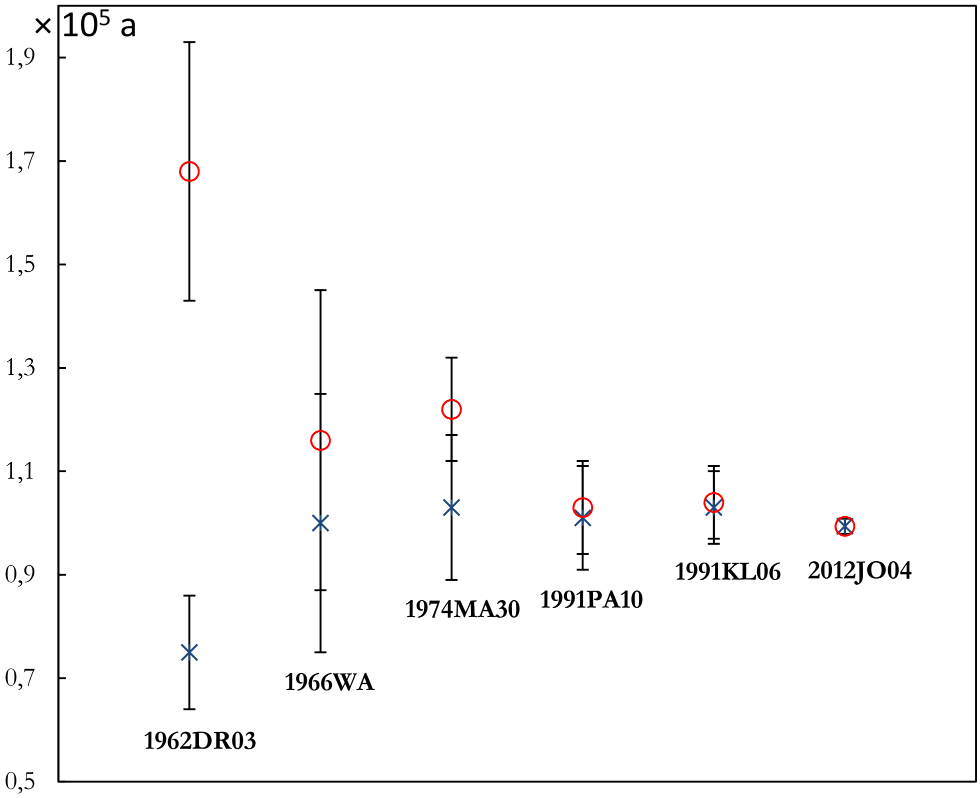
The half-life value and the reasons why some of them have been excluded by the evaluator are given in Table 1.

The LWEIGHT program excluded the result from 1962DR03, which was found to be an outlier by Chauvenet's criterion. A weighted average was adopted from the resulting consistent data set, with a reduced-χ^2 value of 1,43. The data used for the evaluation of the ^{41}Ca half-life can be seen in Figure 1. The main contribution comes from 2012JO04, amounting to 91 %. The quality of this measurement leads the evaluator to keep this high contribution to the weighted average. The recommended value for the ^{41}Ca half-life is then: **$T_{1/2}(^{41}Ca)$ = 1,002 (17) × 10^5 *a*.**

Table 1: Measured half-lives used for the evaluation.

Reference	Measured $T_{1/2}(^{41}Ca)$ (10^5 a)	Updated $T_{1/2}(^{41}Ca)$ (10^5 a)	Comments
~~1951BR94~~	~~1,2 (4)~~	-	Excluded: same authors as in 1962DR03
~~1953BR71~~	~~1,1 (3)~~	-	Excluded: same authors as in 1962DR03
~~1962DR03~~	~~0,75 (11)~~	~~1,68 (25)~~	Excluded by LWEIGHT (Chauvenet's criterion)
1966WA	1,00 (25)	1,16 (29)	
1974MA30	1,03 (14)	1,22 (10)	
~~1990FI13~~	~~1,03 (7)~~	~~1,04 (7)~~	Excluded: same authors as in 1991KL06
1991PA10	1,01 (10)	1,03 (9)	
1991KL06	1,03 (7)	1,04 (7)	
~~1992KU~~	~~1,01 (10)~~	~~1,03 (9)~~	Excluded: same authors as in 1991PA10
2012JO04	0,994 (15)	0,994 (15)	No updating required
Adopted	-	**1,002 (17)**	Weighted average using LWEIGHT

Figure 1: $T_{1/2}$ measurements used for the present evaluation. Blue crosses: measured. Red circles: updated.



2.2 Electron Capture Transition

^{41}Ca can only decay through electron-capture to the ground state of ^{41}K.

The LOGFT program can calculate this first forbidden unique electron-capture transition. The log *ft* value is: log *ft* (1U) = 10,53 (3). LOGFT provides also the P_K, etc. values:

- P_K = 0,894 (9)
- P_L = 0,091 6 (9)
- P_{M+} = 0,014 82 (15)
- P_{L2}/P_{L1} = 0,002 61 (3)
- P_{L3}/P_{L1} = 0,014 1 (1)

Thus: P_L/P_K = 0,102 5 (10); P_{L1} = 0,090 1 (9); P_{L2} = 0,000 235 1 (24); P_{L3} = 0,001 270 (13). A relative uncertainty of 1 % has been taken by the evaluator.

3 Atomic Data (K, Z=19)

3.1 X Radiations and Auger electrons

The X-ray and Auger electron data were computed using the EMISSION program with the atomic data of Schönfeld and Janßen (1996SC06).

The authors of 1951SA31 measured $E_{XK}(^{41}K)$ = 3,40 (15) keV. The authors of 1970SI24 measured $E_{XK}(^{41}K)$ = 3,17 (10) keV. The adopted value from 1996SC06 is: $E_{XK}(^{41}K)$ = 3,31 keV.

4 Radiation Emissions

4.1 Electron Emission

Internal ionization has been studied in 1988JA11. In this process, an orbital electron is ejected due to the sudden change of Coulomb potential and rearrangements in the electronic structure caused by the capture of another orbital electron by the nucleus. The energy released is statistically shared between the electron and the neutrino, giving rise to a continuous energy spectrum of emitted electrons that spans from 0 keV to the Q value of the transition. The integrated probability of electron ejection with an energy greater than 38 keV was found to be 1.7 (2) 10^{-6} per K-capture.

4.2 Photon Emissions

In ordinary electron-capture decay, the energy is shared statistically between the neutrino and the nucleus. A second-order process, the internal bremsstrahlung, makes possible the emission of a photon together with the neutrino. The energy is thus shared between three bodies, giving rise to a continuous energy spectrum of photons that spans from 0 keV to the Q value of the transition. The probability of this process was measured in 1987HO16 to be: $P_{IB(1s)}$ = 2.5 (3) 10^{-4} per K-capture.

Measurements of the photon spectrum can be found in 1973MY03, 1987HO16 and 1991PA10. Internal bremsstrahlung calculations can be found in 1992KA05 and 1973ZO03.

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