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Improved Value for the Energy Splitting of the Ground-State Doublet in the Nucleus ^{229m}Th

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Abstract
We have made an improved estimate of the ^{229m}Th isomer energy. The new value, 7.8(5) eV, includes an estimate of possible spectral contamination effects due to the out-of-band E2 transition from the 42.43-keV 7/2+ member of the [633] ground state band to the 3/2+ [631] ^{229m}Th bandhead and so a weak and unresolved transition a few eV different in energy. We estimate a 2% branching ratio for this unobserved transition in the 42.43-keV 7/2+ [633] deexcitation. The excitation of the ^{229m}Th level is increased from the previously reported value of 7.6(5) eV to the new best value of 7.8(5) eV when this branch is included in the analysis.

1 Introduction

Beck, et al., report the energy difference between the ground state of ^{229}Th and the first excited state (^{229m}Th) as $\Delta E(^{229}Th) = 7.6(5)$ eV [Bec07]. Beck, et al., measured γ-rays following the α-decay of ^{233}U to ^{229}Th, and particularly the γ-ray cascade from the ^{229}Th 71.82-keV level. This level decays predominantly by 2 step γ-ray cascades, populating both members of the ground state doublet with (1) an inband [631] two-step γ-ray sequence to the isomeric level (71.82 → 29.19 → ^{229m}Th keV), and (2) an out-of-band transition to the 42.43-keV member of the ground state band (71.82 → 42.43 keV) followed by an inband [633] transition (42.43 → 0 keV) (Fig. 1). The relevant portion of the measured γ-ray spectrum consists of 2 doublets, each with an energy splitting of ~ 200 eV, one doublet composed of the 42.43 and 42.63-keV γ rays (ΔE_{42}), and the other doublet composed of the 29.18 and 29.39-keV γ rays (ΔE_{29}). The difference in the energy sum $\Delta E_{29} - \Delta E_{42}$ yields a first approximation to the energy splitting of the ^{229}Th ground-state doublet. Beck, et al., obtained 7.0(5) eV for the raw centroid difference. They noted that the peak in the γ-ray spectrum corresponding to the inband decay of the 29.19-keV state to the upper (isomeric) doublet member may be complex including a small contribution from an M1 ground state branch, 29.19 → 0 keV, and therefore a correction to the first-order centroid analysis is required to estimate $E(^{229m}Th)$. The correction is given by $E(^{229m}Th) = (\Delta E_{29} - \Delta E_{42})/(1 - b)$, where b is the branch 29.19 → 0 keV. Beck, et al., assumed the rotational model, used measured nuclear data, and estimated the 29.19 → 0 keV branching at 1/13; the correction for this unobserved branch amounts to + 0.6 eV, resulting in a value of the doublet splitting $\Delta E(^{229}Th, eV) = 7.0(5) + 0.6 = 7.6(5)$.

Singh [2] asked about the possible effect of a spectral contaminant due to the small out-of-band E2 branch 42.43 → ^{229m}Th, a branch also unresolved in the γ-ray spectroscopy but one that could have a small effect on the centroid analysis of ΔE_{42}. The effect of a 42.43 → ^{229m}Th keV branch on the value of ΔE was not included in the analysis presented in [1]. The issue may be important in this unique circumstance, the ~ eV energy splitting of the doublet and the extraordinary resolving power of the NASA microcalorimeter/spectrometer XRS [3, 4].

2 The 42.43 → ^{229m}Th keV Branching Ratio

The branching of the 42.43 → ^{229m}Th keV transition can be estimated with the rotational model parameters (Q_0, Q_2, $|g_K - g_R|$, [5] **)** which describe the electromagnetic transition strengths of inband and out-of-band γ-ray decays. These parameters can be obtained from comparison with the measured properties of the 97.13-keV level [6]. The lifetime of the 97.13-keV $J^\pi = 9/2^+$ member of the ground state band is measured to be 0.147 (12) nsec [7], and the inband and cross-over γ-ray branching ratios are also known, as are level spins and parities [6]. The rotational model equations for the electromagnetic transition rate strengths (inband, Eqs.1 and 2) and out-of- band (Eq. 3) are given in [5], and in standard notation they are:

$$B(E2; I_i \rightarrow I_f) = (5/16\pi)\, e^2 Q_0^2 \langle I_i\, K\, 2\, 0 \,|\, I_f\, K\rangle^2, \qquad (1)$$

$$B(M1; I_i \rightarrow I_f) = (3/4\pi)\, (g_K - g_R)^2 K^2 \langle I_i\, K\, 2\, 0 \,|\, I_f\, K\rangle^2, \text{ and} \qquad (2)$$

$$B(E2; I_i \rightarrow I_f) = (5/16\pi)\, e^2 Q_0^2 \langle I_i\, I_f\, 2\, \Delta K \,|\, K_i\, K_f\rangle^2. \qquad (3)$$

We use the equations above and deduce (1) the intrinsic quadruple moment Q_0 from the average of the measured inband 97.13 → 42.43 keV and 97.13 → 0 keV E2 transition rates, (2) the g-factor $|g_K – g_R|$ from the inband 97.13–42.43 keV M1 transition, and (3) Q_2 from the cross- over transition 97.13 → 29.19 keV , and then use these parameters to predict the inband and cross-over transition rates for the 42.43-keV level. Numeric values are given in Table 1. The calculated 42.34 → 0 keV transition rates are $\lambda[E2, s^{-1}] = (1.86 \times 10^{-6}) \times 10^{12}$ and $\lambda[M1, s^{-1}]\ (8.12 \times 10^{-6}) \times 10^{12}$, and for the 42.43 → ^{229m}Th keV E2 transition rate $\lambda[E2, s^{-1}] = 0.222 \times 10^{-6}\ (\times 10^{12})$. Thus the magnitude of the 42.43 → ^{229m}Th keV branch is 0. 22/(0. 22 + 8.12 + 1.86) = 0.02, and the energy correction $(\Delta E_{29} - \Delta E_{42})/(1 - b)$ amounts to + 0.2 eV when the correction is considered on an individual basis. The sense of the correction (+) is the same as for contamination in spectral analysis due to the possible 29.19 → 0 branch. The formula for the correction when both branches are considered is $(\Delta E_{29} - \Delta E_{42})/(1 – b_{29} – b_{42})$, and so including both corrections for possible spectral contaminations a better description of the energy splitting of the ground-state doublet of ^{229}Th is ΔE = 7.8(5) eV.

3 Summary

The best value for the energy splitting of the ^{229}Th ground state doublet is 7.8(5) eV when corrections for spectral contaminations due to unobserved 42.43 → ^{229m}Th keV and 29.19 → 0 keV out-of-band transitions are included in the analysis. The corrections are + 0.2 eV and + 0.6 eV, respectively. The best estimate of ΔE is important for a precision energy determination. This extremely unusual and rare doublet may remain a scientific curiosity or else it may represent an important pathway in the field of atomic-nuclear coupling. Work on the nuclear and atomic properties of the excited doublet state continues to be reported; Inamura and Haba [8] report excitation of ^{229m}Th in a hollow cathode electrode discharge; they report the isomer halflife and excitation as $1 \leq T_{1/2}(\mathrm{min}) \leq 3$, $3 \leq E_x(\mathrm{eV}) \leq 7$. Burke and his colleagues [9] are mounting an experiment at LLNL to measure the nuclear properties of the isome. Chapman *et al.*, have trapped and cooled ^{232}Th 3+ ions [10]; currently they are mounting an experiment with the goal of measuring the hyperfine structure of $^{229\mathrm{Th}}$ 3+ ions.

Table 1: Rotational band parameters Q_0, Q_2, and $|g_K-g_R|$ for ^{229}Th ground state band [633] deduced from data summarized in [6] , and from equations for B(ML) given in [5]. Entries for the 42.43-keV level transition rate are calculated with B(ML) values obtained from analysis of the 97.13–keV level.

$E_i \rightarrow E_f$ (keV)	E_γ (keV)	B(E2) (e^2fm^4)	B(M1) (μ_n^2)	Q_0 (eb)	Q_2 (eb)	$\lvert g_K-g_R \rvert$ (μ_n^2)	λ[E2] (s^{-1})	λ[M1] (s^{-1})
97.13 → 0	97.13	3.4(8) x10^3		5.86				
97.13 → 42.43	54.70	4.3(27) x10^3		5.57				
97.13 → 42.43	54.70		9.2(19)x10^{-3}			0.014		
97.13 → 29.19	67.94	1.6(4)x10^3			2.20			
42.43 → 0	42.43			5.71[a]		0.014	1.8 x10^6	8.21x10^6
42.43 → ^{232m}Th	42.43				2.20		0.22x10^6	

[a] Unweighted average of Q_0^2 determined from B(E2; 97.13 → 0 keV) and B(E2; 97.13→ 42.43 keV).

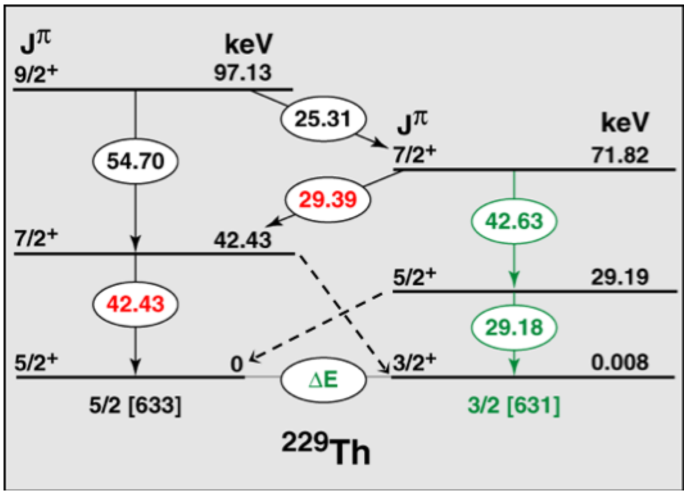

Fig. 1: Partial level scheme for ^{229}Th. The 71.82-keV level decays both to the ground state [red] and to the excited member [green] of the ground state doublet at 0.8 eV. Transitions suggested by the dashed lines are degenerate with the cascade decays of the 71.82-keV level.

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