Rates of transitions between the hyperfine-splitting components of the ground-state and the 3.5 eV isomer in $^{229}Th^{89+}$

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For the hydrogenlike $^{229}Th^{89+}$ ion, the rates of electromagnetic $M1$ transitions between hyperfine structure levels, originating from the nuclear $5/2^+$ ground state and the first excited 3.5 ± 1.0 eV $3/2^+$ isomeric state, are calculated. As a result of the mixing of the $F=2$ components, these transitions turn out to be faster than the nuclear isomeric γ transition in a bare nucleus by several orders of magnitude. The possibility of experimental observation of these transitions is discussed. [S0556-2813(98)06606-0]

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I. INTRODUCTION

In ^{229}Th, a nuclear level with spin and parity $3/2^+$ was indirectly established at an energy $E_{\rm isom}=3.5\pm1.0$ eV above the $5/2^+$ ground state [1]. Because of the extremely low energy of the $M1$ nuclear γ transition, the half-life of this excited state in a bare nucleus is expected to be within the range of hours [2,3].

This unique energy doublet is of great interest from various points of view.

For a neutral atom, the energy separation between the two nuclear levels is close to the electronic transitions $7s\rightarrow8s$, $7s\rightarrow9s$ of the same $M1$ multipolarity as the γ transition. This fact, taken with the closeness of the $7p$ and $8p$ levels, makes ^{229}Th a very likely candidate for discovering the effect of the drastic acceleration of nuclear decay by the externally applied laser radiation of the resonance frequency [4]. Because of the closeness of the level spacings, the electron shell can be also used as a resonator for radiative pumping the nuclear isomeric state [3].

In the hydrogenlike $^{229}Th^{89+}$ ion, an enormous magnetic field of about 28 MT is produced at the nucleus by a single electron in the $1s$ state [2]. In general, hyperfine interactions within such a coupled nucleus-electron system may mix nuclear states of the same parity that differ by one unit of spin. Of course, such mixing does not violate rotational invariance, as angular momentum is conserved for the whole system. The near degeneracy of the $5/2^+$ and $3/2^+$ nuclear states in $^{229}Th^{89+}$ should lead to a considerable mixing effect. Until now, such nuclear-spin mixing due to the magnetic interaction (predicted a long time ago [5]) was observed only in muonic atoms [6].

In the present paper we show that the spin mixing of the nuclear levels in $^{229}Th^{89+}$ is expected to manifest itself via an impressive enhancement of the radiative transitions between the pairs of the hyperfine-structure (hfs) components, relative to the nuclear γ transition. Ways of experimental detection of this effect are considered.

II. HYPERFINE LEVEL STRUCTURE AND RADIATIVE TRANSITIONS

A. Energy levels

Referring to paper [2], Fig. 1 shows level schemes of the bare nucleus $^{229}Th^{90+}$ and the hydrogenlike $^{229}Th^{89+}$ ion. The hyperfine structure indicated in the right part of this figure is determined by the magnetic interaction between the nucleus and the electron. This interaction is given by the Hamiltonian $H_{\rm magn}=-\boldsymbol{\mu}\boldsymbol{\sigma}_e B_{\rm eff}$, where $\boldsymbol{\mu}$ is the magnetic moment operator of the nucleus, $\boldsymbol{j}=\boldsymbol{\sigma}/2$ is the spin of the electron, and $B_{\rm eff}$ is an effective magnetic field produced by the electron at the nucleus. The level ordering and energy differences are determined by the energy matrix $\langle FI|H_{\rm magn}|I'F\rangle$ calculated within the basis of states enumerated by the values of nuclear spin I and total angular momentum F of the system ($\mathbf{F}=\mathbf{I}+\mathbf{j}$).

The hfs levels are composed according to the angular momentum addition rule

$$|Ij;FM\rangle=\sum_{m\mu}\langle Imj\mu|FM\rangle|X_{Im}\rangle|\Phi_{j\mu}\rangle, \qquad (1)$$

which consists of nuclear $|X_{Im}\rangle$ and atomic $|\Phi_{j\mu}\rangle$ factors. Three values of $F=1,2,3$ are allowed, but there are two $F=2$ components. The latter are exceptional as the $H_{\rm magn}$ interaction mixes them and thus generates two mixtures of

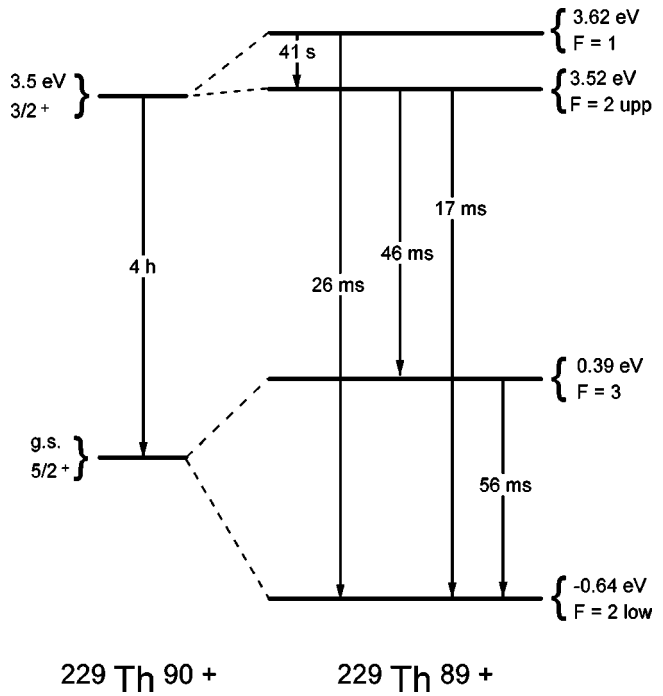

FIG. 1. Left: the ground and the first excited states in the bare ^{229}Th [1] nucleus, and the $M1$ γ transition between these states with the half-life estimated in Ref. [2]. For an account of the level-energy uncertainty, see Sec. III. Right: the relevant hfs components and electromagnetic $M1$ transitions in the hydrogenlike ion $^{229}Th^{89+}$. The mean lifetimes of these transitions are obtained in the present work taking into account the mixing of the two $F=2$ states. Positions of the levels are not to scale. Calculations have been performed for the magnetic-interaction matrix elements used in Ref. [2].

the primary nuclear $|5/2^+\rangle$ and $|3/2^+\rangle$ states. The new, mixed states are denoted by $|F=2i,M;\text{mixed}\rangle$, where the index i (= up, low) distinguishes one from the other:

$$|2\ \ \text{up},M;\text{mixed}\rangle=\{|3/2\ \ 1/2;2M\rangle+\beta|5/2\ \ 1/2;2M\rangle\}N_\beta,$$

$$|2\ \ \text{low},M;\text{mixed}\rangle=\{-\beta|3/2\ \ 1/2;2M\rangle+|5/2\ \ 1/2;2M\rangle\}N_\beta, \tag{2a}$$

where β is the mixing amplitude and $N_\beta=1/\sqrt{1+\beta^2}$.

For the other, nonmixed states,

$$|3,M\rangle=|5/2\ \ 1/2;3M\rangle,$$

$$|1,M\rangle=|3/2\ \ 1/2;1M\rangle. \tag{2b}$$

With the wave functions known, the rates of radiative transitions can be calculated.

B. Transition rates

The radiative $M1$ transition between the mixed states, 2 up$\rightarrow$2 low, is due to the electromagnetic interaction given by a tensor operator $H_\gamma(M1,q)$ of rank 1, where q is the projection of the photon angular momentum on the quantization axis. In the absence of nuclear-spin mixing, this operator connects different nuclear states. But as a consequence of nuclear-spin mixing, terms diagonal in the nuclear spin arise in the transition matrix element, $M_\gamma(2\ \text{up}\rightarrow 2\ \text{low})$, in the first order of perturbation theory:

$$\begin{aligned}M_\gamma(2\ \text{up}\rightarrow 2\ \text{low})&\equiv\langle 2\ \ \text{up},M;\text{mixed}|H_\gamma(M1,q)|2\ \ \text{low},M';\text{mixed}\rangle\\&=\beta N_\beta^2[\langle 5/2\ 1/2;2M|H_\gamma(M1,q)|5/2\ 1/2;2M'\rangle\\&\quad-\langle 3/2\ 1/2;2M|H_\gamma(M1,q)|3/2\ 1/2;2M'\rangle].\end{aligned} \tag{3}$$

Thus, transitions between components with the same nuclear spins occur via a spin flip of the orbital electron, like transitions between normal components of hyperfine structure. They are much faster than the radiative transition between the isomeric and ground states of the bare nucleus.

A straightforward calculation gives the following expression for the matrix element in the nonmixed basis:

$$\begin{aligned}&\langle F_2M_2;jI|H_\gamma(M1,q)|Ij;F_1M_1\rangle\\&\quad=(-1)^{j+I+F_1+1}\sqrt{2F_1+1}\begin{Bmatrix}j & I & F_1\\ F_2 & 1 & j\end{Bmatrix}\\&\quad\times\langle F_1M_1 1q|F_2M_2\rangle\langle j\|H_\gamma(M1)\|j\rangle,\end{aligned} \tag{4}$$

where $\langle j\|H_\gamma(M1)\|j\rangle$ is the reduced matrix element of the $1s$ electron interaction with the electromagnetic field. We have used the fact that $H_\gamma(M1,q)$ is a tensor operator.

The presence of the one-electron reduced matrix element in the right side of Eq. (4) allows one, by means of a simple algebra, to obtain the expression for the transition rate between the hfs components in the following transparent form:

$$W(2\ \text{up}\rightarrow 2\ \text{low})=2\beta^2N_\beta^4\ \ (2F_2+1)\times\left|\sum_{I=3/2,5/2}\begin{Bmatrix}F_2 & j & I\\ j & F_1 & 1\end{Bmatrix}\right|^2W_0. \tag{5}$$

In Eq. (5), W_0 is the radiative width of the spin-flip transition of the electron. The electron is in the $1s$ shell in both the initial and final states, as explained above. The value of W_0 can be expressed as follows:

$$W_0=\pi|\langle j\|H_\gamma(M1)\|j\rangle|^2=4\alpha\omega\left[\int_0^\infty GFj_1(\omega r)dr\right]^2, \tag{6}$$

where α is the fine structure constant, ω is the transition energy, $j_1(\omega r)$ is the spherical Bessel function, and G and F are the large and small components of the radial wave function, correspondingly. In the case of a transition between the hfs components corresponding to the same nuclear state, without spin mixing, formulas (5) and (6) reduce to the corresponding equations of Ref. [7]. Finally, with the numerical values of the coefficients, the transition rate (5) is obtained as

$$W(2\ \text{up}\rightarrow 2\ \text{low})=2(5/6)^2W_0\beta^2N_\beta^4. \tag{7}$$

If the Dirac wave function of an electron in the Coulomb field of the point charge is used in Eq. (6), the result for W_0 is

$$W_0^{\mathrm{Coul}}=\frac{\alpha}{m^2}\left(\frac{1+2\gamma}{3}\right)^2\omega^3. \quad (8)$$

An account of the nuclear size produces a small effect, which was, however, studied in the present paper, as it is of interest itself. Higher-order effects, such as vacuum polarization and magnetization density, are neglected, since they lead to corrections much less than the expected uncertainties; see Sec. III.

The other transition rates are found in the same fashion to be

$$W(1\rightarrow 2\ \mathrm{up})=5/6\ W_0\ N_\beta^2,$$

$$W(1\rightarrow 2\ \mathrm{low})=5/6\ W_0\ \beta^2\ N_\beta^2,$$

$$W(2\ \mathrm{up}\rightarrow 3)=7/6\ W_0\ \beta^2\ N_\beta^2,$$

$$W(3\rightarrow 2\ \mathrm{low})=5/9\ W_0\ N_\beta^2. \quad (9)$$

For each transition, the factor W_0 gives the time scale as explained above. The latter is also characterized by the transition energy ω. Notice that rates of three transitions are proportional to the amount of mixing, β^2, which is rather small. However, small values of β^2 are compensated by the larger energies involved in these three transitions.

III. NUMERICAL RESULTS

In this section the calculations for the hfs energy levels and radiative transition rates are presented. These are based on experimental input which is presented and discussed.

The most recent value of the isomer energy is 3.5 ± 1.0 eV [1]. For E_{isom} assumed to be 4.5, 3.5, or 2.5 eV, the half-life values for the nuclear γ transition are estimated to be 1.7, 4, and 10 h, respectively [2]. These estimates apply to a bare nucleus. In the presence of complete electron shells, the radiative transition rates might be enhanced by the specific effect of an ''electron bridge'' considered in Refs. [10,3,11].

The hfs energy levels and relevant transition energies, the mixing amplitude β, and the decay rates are determined by the energy E_{isom}, the magnetic moments of the ground and isomeric states, and the mixing matrix element.

In Ref. [2], the magnetic moments of the ground and isomeric states were adopted to be $(0.45\pm 0.06)\mu_n$ and $(-0.08\pm 0.08)\mu_n$, respectively. The mixing matrix element was found to be $\langle 2\ 3/2|H_{\mathrm{magn}}|5/2\ 2\rangle=0.59\pm 0.06$ eV.

The values of W_0 for different transition energies of interest have been calculated by means of the package of the computer codes RAINE [8]. Finite nuclear size is taken into account. Calculated values of W_0 for all the transitions were equal to $1.9558\times 10^{-14}\omega^3$ eV. These values may be compared with the pure Coulomb widths (8), which turn out to be $1.9535\times 10^{-14}\omega^3$ eV. The comparison shows the influence of the nuclear size on the radiative widths.

Now, to calculate the mean lifetimes τ of the radiative transitions between the hfs components of $^{229}Th^{89+}$ the values given above were taken, in the first step, with no account for experimental uncertainties. The results for the three input E_{isom} values are presented in Table I and only for $E_{\mathrm{isom}}=3.5$ eV in Fig. 1.

TABLE I. Calculated energies ω and mean lifetimes τ for radiative transitions between the four states of hfs in the $^{229}Th^{89+}$ ion. Calculations have been performed for the magnetic-interaction matrix elements used in Ref. [2]. For a discussion of the role of uncertainties in these matrix elements, especially dramatic for the $F_i=1\rightarrow F_f=2$ up transition, see Sec. III.

E_{isom} [eV]	4.5		3.5		2.5	
Mixing β^2 [%]	1.35		2.06		3.51	
Transition $F_i\rightarrow F_f$	ω [eV]	τ [s]	ω [eV]	τ [s]	ω [eV]	τ [s]
$1\rightarrow 2$ up	0.12	24.0	0.10	41	0.08	82
$1\rightarrow 2$ low	5.24	0.022	4.26	0.026	3.28	0.033
2 up $\rightarrow 3$	4.11	0.031	3.13	0.046	2.15	0.085
2 up $\rightarrow 2$ low	5.12	0.013	4.16	0.017	3.20	0.023
$3\rightarrow 2$ low	1.01	0.060	1.03	0.056	1.05	0.054

Next, the role of uncertainties of the magnetic moments is investigated for $E_{\mathrm{isom}}=3.5$ eV and $\langle 2\ 3/2|H_{\mathrm{magn}}|5/2\ 2\rangle=0.59$ eV.

First, the magnetic moment of the isomer is fixed to $-0.08\mu_n$ and the two extreme values $0.51\mu_n$ and $0.39\mu_n$, defined by the error limits, are taken for the ground state. The relevant energies of the $F=2$ low level are -0.71 and -0.56 eV. The energy differences between the $F=3$ and $F=2$ low states are then 1.15 and 0.90 eV, respectively. The corresponding values of β^2 are 1.99% and 2.14%. For the $F=3\rightarrow F=2$ low transition, the relevant mean lifetimes are 41 and 85 s. Changes of the $F=2$ up state energy, with respect to that given in Fig. 1, are below 0.01 eV.

Second, the magnetic moment of the isomer is set equal to 0, and $0.45\mu_n$ is kept for the ground state. This yields 3.50 and 3.58 eV for the energies of the $F=1$ and $F=2$ up levels (with $\beta^2=2.00\%$). Compared to Fig. 1, the order of these two levels becomes reversed. This is a result of the mixing and the related mutual repelling of the $F=2$ up and $F=2$ low states. The energy of the $F=2$ low state is changed only a little to -0.63 eV.

Next, E_{isom} and the magnetic moments are fixed to the experimental values, but the mixing-matrix element is changed to 0.65 or 0.53 eV. This leads to a minor change in the spacing of the $F=3$ and $F=2$ low levels, which becomes 1.05 or 1.01 eV. The relevant β^2 value is 2.47% or 1.68%, correspondingly.

IV. PERSPECTIVES OF EXPERIMENTAL STUDIES

At GSI, in Darmstadt, hydrogenlike ions of heavy atoms can be produced either via in-flight stripping of lower charge ions accelerated in SIS or as products of fragmentation reactions. After injection into the storage ring ESR, these ions can be exposed to interactions with collinear laser pulses.

Recently, the first method was applied to inject into ESR a beam of $^{209}Bi^{82+}$ ions [9]. In this pioneering experiment, the 5.4 eV $M1$ transition between the $F=4$ and $F=5$ hfs levels of the $9/2^-$ ground state was observed by the detection of laser-induced fluorescence. The distance between the two levels could be calculated in advance with reasonable accu-

racy because the magnetic moment of the ^{209}Bi ground state was known with high precision. This facilitated the search for the resonance condition. The lifetime of the $F=5$ level was determined as $\tau=0.351(16)$ ms.

In principle, one can carry out a similar experiment with $^{229}Th^{89+}$ ions in the ESR. Collinear laser beams of appropriate wavelengths could be used to excite the $F=3$, 2 up and 1 hfs levels. The time dependence of the induced fluorescence would contain information on the lifetimes. At present, poor initial knowledge of the transition energies (Sec. III) may make the experiment more difficult. A possible preceding high-precision measurement of the ground-state magnetic moment would be only a partial solution of the problem.

As this approach may be difficult, another one could be considered. In a fragmentation of ^{238}U nuclei on a Be target, the ground and isomeric states of ^{229}Th are presumably produced with a comparable yield. In view of the long half-life of the isomer, in the beam of bare $^{229}Th^{90+}$ nuclei injected into the ring, both states would be present. A transformation of $^{229}Th^{90+}$ into hydrogenlike $^{229}Th^{89+}$ by an electron capture inside the ring would be followed by transitions with the lifetimes between 10 and 100 ms; see Table I and Fig. 1. Efforts should be made to detect these transitions.

An additional encouragement for these experiments comes from a very recent observation [12] of ultraviolet and visible photons from samples of ^{233}U, suggesting the deexcitation of a 3.5 eV level in ^{229}Th.

V. SUMMARY AND CONCLUSIONS

The doublet of the $5/2^+$ ground state and the 3.5 ± 1.0 eV $3/2^+$ isomer in the ^{229}Th nucleus offers interesting research possibilities.

As shown in the present paper, nuclear-spin mixing in $^{229}Th^{89+}$ is expected to have a drastic influence on the electromagnetic transitions between pairs of hfs components related to the isomer ($F=1$ and 2) and to the ground state ($F=3$ and $F=2$). The calculated rates of these transitions are enhanced by several orders of magnitude with respect to the isomeric nuclear γ transition.

From an experimental observation of these transitions and a determination of their rates, one could obtain the exact value of the unperturbed isomer energy and the matrix elements responsible for both the hyperfine splitting of the nuclear levels and the nuclear-spin mixing of the $F=2$ components. Good knowledge of the isomer energy is important for testing the available theoretical predictions on the coupling of the nuclear and atomic degrees of freedom in a neutral ^{229}Th atom.

With the use of the GSI storage ring a relevant although difficult experiment could be conceived.

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