Theoretical Study of the $4f^{14}6s\ ^2S_{1/2}$–$4f^{13}6s^2\ ^2F^0_{7/2}$ $E3$ Transition in Yb II

E. Biémont[1,2] and P. Quinet[2]
[1]Institut d'Astrophysique, Université de Liège, B-4000 Liège, Belgium
[2]Astrophysique et Spectroscopie, Université de Mons-Hainaut, B-7000 Mons, Belgium
(Received 11 March 1998)

In view of the current interest of ion trap workers in the lifetime of the $4f^{13}6s^2\,^2F^0_{7/2}$ level in Yb II which may decay by electric octupole (E3) radiation to the ground $4f^{14}6s\,^2S_{1/2}$ level, we have used a pseudorelativistic Hartree-Fock method including configuration interaction and core polarization effects to estimate the value of the E3 matrix element $\langle 4f|r^3|6s\rangle$. The calculated lifetime, $\tau = 8.4$ yr, is in excellent agreement with the recent measurement due to Roberts *et al.* [Phys. Rev. Lett. **78**, 1876 (1997)] ($\tau = 10.1^{+7}_{-4}$ yr). [S0031-9007(98)07314-1]

PACS numbers: 32.10.–f, 32.30.–r, 32.70.Cs, 32.80.Pj

The development of ion traps, lasers, and photon counting techniques has allowed the determination (to within a reasonably high degree of accuracy) of experimental decay rates and branching ratios linking different energy levels from the observed fluctuations in laser-induced fluorescence of a transition in a single trapped ion. Forbidden transitions, emitted by a single atom at rest in free space, appear as interesting optical frequency reference. Electric quadrupole (E2) transitions, with linewidths of about 1 Hz, are usually considered for that purpose. Among the search for suitable frequency standards, Yb^+ ion has recently been the focus of particular attention. The work of Lehmitz *et al.* [1] has demonstrated excellent population trapping into the highly metastable low-lying $4f^{13}6s^2\,^2F^0_{7/2}$ state of Yb II. Laser cooling of trapped Yb^+ ions has also been successfully demonstrated [2].

Very recently, the $4f^{14}6s\,^2S_{1/2}$-$4f^{13}6s^2\,^2F^0_{7/2}$ electric octupole (E3) transition in singly ionized ytterbium has been detected by observing quantum jumps in a single laser cooled ion stored in an electrodynamic trap [3]. It is the first time that an atomic E3 transition has been driven. The $^2S_{1/2}$-$^2F^0_{7/2}$ transition has been observed at 642 116 785.3(0.7) MHz (1σ). From the rate at which the transition was driven, together with the laser parameters used, these authors gave, for the $4f^{13}6s^2\,^2F^0_{7/2}$ state, an estimated lifetime of 3700 days, which corresponds to 10.1 years. The standard deviation on this estimate due to uncertainties in the exact laser parameters used was $+7/-4$ yr. Previous to this observation, the experiment of Lehmitz *et al.* [1] put a lower limit of 8 days on the $^2F^0_{7/2}$ lifetime while theoretical estimates led to results considerably shorter than the measurement of Ref. [3], i.e., 650 [4] and 1533 days [5], respectively.

The aim of the present work is to provide a refined theoretical value for the lifetime of the $4f^{13}6s^2\,^2F^0_{7/2}$ metastable level of Yb II. The present study is part of a general investigation of the spectrum of singly ionized ytterbium. The details of the theoretical method used together with the detailed results (E1 transitions) will appear elsewhere [6].

The probability of an electric multipole transition of order K from the level γJ to the level $\gamma' J'$ is given by [7]

$$A_{\mathrm{EK}}(\gamma J, \gamma' J') = \frac{1}{2J+1}\,\frac{2(2K+1)(K+1)}{[(2K+1)!!]^2 K}\,\frac{k^{2K+1}}{\hbar} \times |\langle \gamma J \parallel r^K \parallel \gamma' J'\rangle|^2, \quad (1)$$

where $k = 2\pi/\lambda$, λ being the wavelength of the transition and $|\langle \gamma J \parallel r^K \parallel \gamma' J'\rangle|$ the reduced electric multipole matrix element. Consequently, in the case of an E3 transition, we have

$$A_{\mathrm{E3}}(\gamma J, \gamma' J') = \frac{1.69 \times 10^{-3}}{2J+1}\,\frac{(2\pi)^7}{\lambda^7 \hbar}\,|\langle \gamma J \parallel r^3 \parallel \gamma' J'\rangle|^2. \quad (2)$$

In the present calculation, the reduced matrix element was estimated within the framework of the relativistic Hartree-Fock (HFR) approach of Cowan [8], including core-polarization effects. These effects were considered using the expressions of the core-polarization potential, V_P, and the corrected octupole moment of transition, $\vec{d}^3$, deduced from the work of Migdalek and Baylis [9]:

$$V_P(r) = \frac{-\alpha_d r^2}{2(r^2 + r_c^2)^3} \quad (3)$$

and

$$\vec{d}^3 = \left[-\vec{r} + \frac{\alpha_d \vec{r}}{(r^2 + r_c^2)^{3/2}}\right]^3. \quad (4)$$

The estimate of the core-polarization contributions (3) and (4) requires the knowledge of the dipole polarizability of the ionic core, α_d, and the cutoff radius, r_c. For the first parameter, we have used the value of the static dipole polarizability of Yb III computed by Fraga *et al.* [10], i.e., $\alpha_d = 7.35a_0^3$, a_0 being the value of the first Bohr orbit of hydrogen atom. The cutoff radius, r_c, usually taken as the expectation value of r for the outermost core orbitals has been chosen equal to $1.462a_0$; this corresponds to the HFR average value $\langle r\rangle$ for the outermost core orbitals ($5p^6$) of the investigated valence configurations. The adopted parameters agree well with those chosen by

0031-9007/98/81(16)/3345(2)$15.00

Migdalek [11,12] in his RMP (relativistic model potential) calculations with core polarization effects included.

Configuration interaction has been retained among the following configurations (limited to the $n \leq 7$ Layzer complexes): $4f^{14}6s + 4f^{14}7s + 4f^{14}5d + 4f^{14}6d + 4f^{14}7d + 4f^{13}5d6p + 4f^{13}6s6p + 4f^{13}6p6d + 5p^5 4f^{14}5d6p + 5p^5 4f^{14}6s6p$ for the even parity and $4f^{14}6p + 4f^{14}7p + 4f^{13}6s^2 + 4f^{13}6p^2 + 4f^{13}5d^2 + 4f^{13}6d^2 + 4f^{13}6s6d + 4f^{13}5d6s + 4f^{13}5d6d + 5p^5 4f^{14}5d^2 + 5p^5 4f^{14}6s^2 + 5p^5 4f^{14}5d6s$ for the odd parity, respectively. The consideration of additional configurations has been prevented by the computer capabilities. Nevertheless, these configuration lists extend considerably those previously considered [5].

The adequacy of the present physical model can be tested by considering different types of constraints imposed by the available experimental data as described in the following sections. The $4f^{14}5d\,^2D_{3/2}$ metastable level can decay to the $4f^{14}6s\,^2S_{1/2}$ ground state through M1 and E2 transitions, the M1 contribution appearing negligibly small when compared with the E2 one [5]. The lifetime of the $4f^{14}5d\,^2D_{3/2}$ level has been measured by Gerz *et al.* [13] as 52 ± 1 ms. Our theoretical estimate is 51.8 ms, which is substantially higher than the result quoted in Ref. [5] but in perfect agreement with experiment.

A useful test is also provided by the accurate experimental lifetimes recently measured by beam-laser [14,15] and laser-induced fluorescence [16,17] for some $4f^{14}6p$, $4f^{13}5d6s$, $4f^{13}5d^2$ odd levels and $4f^{13}5d6p$, $4f^{13}6s6p$ even levels, respectively. Table I shows such a comparison. The details concerning the method used for obtaining the electric dipole transition probabilities in Yb II will be given elsewhere [6]. For most of the levels, the agreement of theory and experiment is within a few percent, which is particularly gratifying in view of the complexity of the configurations considered. The only discrepancy observed is for the strongly perturbed level at 44941 cm^{-1} for which only one laser measurement is available.

For the reduced matrix element $\langle 4f \parallel r^3 \parallel 6s \rangle$, we have obtained a value of -2.15 a.u. which, when combined with the appropriate angular factors, yields an E3 probability for the $4f^{14}6s\,^2S_{1/2}$-$4f^{13}6s^{2}\,^2F^0_{7/2}$ of $3.80 \times 10^{-9}\ \text{s}^{-1}$. This leads to an estimate of the lifetime for the $4f^{13}6s^{2}\,^2F^0_{7/2}$ level of 3050 days (8.4 yr), which is in very good agreement with the experimental value of 3700 days (10.1^{+7}_{-4} yr) measured directly by Roberts *et al.* [3]. Fawcett and Wilson [5] have also used Cowan's code (including configuration interaction but without consideration of the core polarization effects) for calculating the lifetime of the $4f^{13}6s^{2}\,^2F^0_{7/2}$ level. When removing the core polarization corrections in our calculations, we found a lifetime value of 1700 days which is very close to the one obtained by these authors, i.e., 1533 days, the remaining difference being probably due to the different sets of configurations used in both calculations.

TABLE I. Radiative lifetimes for selected levels of Yb II.

Config.	J	E (cm^{-1})[a]	τ_{exp} (ns)	τ_{calc} (ns)[b]
$4f^{14}6p$	1/2	27062	8.07 ± 0.09[c]	8.60
			8.10 ± 0.13[d]	
			8.0 ± 0.2[e]	
$4f^{14}6p$	3/2	30392	6.15 ± 0.09[c]	7.23
			6.3 ± 0.3[e]	
$4f^{13}5d^2$	3/2	44941	20.3 ± 0.3[d]	14.46
$4f^{13}5d6s$	3/2	45737	30.9 ± 0.6[f]	27.70
$4f^{13}5d6s$	3/2	47005	19.7 ± 0.5[f]	19.02
$4f^{13}5d6p$	5/2	56376	3.78 ± 0.07[f]	3.76
$4f^{13}6s6p$	9/2	57765	2.87 ± 0.11[f]	2.80
$4f^{13}5d6p$	5/2	58824	3.59 ± 0.07[f]	3.73
$4f^{13}6s6p$	7/2	59090	2.31 ± 0.10[f]	2.40
$4f^{13}5d6p$	7/2	61823	3.01 ± 0.13[f]	2.64
$4f^{13}5d6p$	13/2	65876	3.30 ± 0.09[f]	2.81

[a]From Ref. [18]. [b]Present work (theory). [c]Pinnington *et al.* [15]. [d]Berends *et al.* [14]. [e]Lowe *et al.* [17]. [f]Pinnington *et al.* [16].

The authors thank the Belgian National Fund for Scientific Research (FNRS) for financial support.

[1] H. Lehmitz, J. Hattendorf-Ledwoch, R. Blatt, and H. Harde, Phys. Rev. Lett. **62**, 2108 (1989).
[2] H. A. Klein, A. S. Bell, G. P. Barwood, and P. Gill, Appl. Phys. B **50**, 13 (1990).
[3] M. Roberts, P. Taylor, G. P. Barwood, P. Gill, H. A. Klein, and W. R. C. Rowley, Phys. Rev. Lett. **78**, 1876 (1997).
[4] V. Shevelko (private communication to Lehmitz *et al.* [1]).
[5] B. C. Fawcett and M. Wilson, At. Data Nucl. Data Tables **47**, 241 (1991).
[6] E. Biémont, J.-F. Dutrieux, I. Martin, and P. Quinet, J. Phys. B **31**, 3321 (1998).
[7] I. I. Sobel'man, *An Introduction to the Theory of Atomic Spectra* (Pergamon Press, New York, 1972).
[8] R. D. Cowan, *The Theory of Atomic Structure and Spectra* (University of California Press, Berkeley, CA, 1981).
[9] J. Migdalek and W. E. Baylis, J. Phys. B **11**, L497 (1978).
[10] S. Fraga, J. Karwowski, and K. M. S. Saxena, *Handbook of Atomic Data* (Elsevier, Amsterdam, 1976).
[11] J. Migdalek, J. Phys. B **13**, L169 (1980).
[12] J. Migdalek, J. Quant. Spectrosc. Radiat. Transf. **28**, 61 (1982).
[13] C. Gerz, J. Roths, F. Vedel, and G. Werth, Z. Phys. D **8**, 235 (1988).
[14] R. W. Berends, E. H. Pinnington, B. Guo, and Q. Ji, J. Phys. B **26**, L701 (1993).
[15] E. H. Pinnington, G. Rieger, and J. A. Kernahan, Phys. Rev. A **56**, 2421 (1997).
[16] E. H. Pinnington, R. W. Berends, and Q. Ji, Phys. Rev. A **50**, 2758 (1994).
[17] R. M. Lowe, P. Hannaford, and A.-M. Mårtensson Pendrill, Z. Phys. D **28**, 283 (1993).
[18] W. C. Martin, R. Zalubas, and L. Hagan, *Atomic Energy Levels*, NSRDS-NBS **60** (Washington, D.C., 1978).