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Experimental and theoretical energy levels, transition probabilities and radiative lifetimes in Yb III

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Abstract

The analysis of the spectrum of Yb III has been extended allowing us to establish 11 new energy level values. In addition, radiative lifetimes of two excited states of Yb III have been measured for the first time using time-resolved laser-induced fluorescence following two-photon excitation. The good agreement between experimental results and semi-empirical calculations performed with the relativistic Hartree–Fock method including core-polarization effects allows the determination of transition probabilities for 15 lines.

1. Introduction

Ytterbium is an even-Z rare-earth element ($Z = 70$) with seven natural isotopes, i.e. ^{168}Yb (0.13%), ^{170}Yb (3.04%), ^{171}Yb (14.28%), ^{172}Yb (21.83%), ^{173}Yb (16.13%), ^{174}Yb (31.83%) and ^{176}Yb (12.76%). Doubly ionized ytterbium has been considered much less in the literature than the neutral or singly ionized species. However, not only the first and second spectra of the lanthanides, but also their third spectra, and in particular those of the rare-earths with even atomic number, which have as a rule higher abundances than their odd-Z neighbours (see, e.g., Cowley 1976), have been observed in some chemically peculiar (CP) stars. As an example, some doubly ionized lanthanides such as Ce III ($Z = 58$), Pr III ($Z = 59$), Nd III ($Z = 60$), Sm III ($Z = 62$), Tb III ($Z = 65$), Dy III ($Z = 66$), Ho III ($Z = 67$) and Er III ($Z = 68$) have been identified recently in the spectrum of the Przybylski star between 3959 and 6632 Å (see, e.g., Cowley and Mathys 1998). The presence of the Yb III ion in a CP star has been revealed for the first time by Hensberge *et al* (1986) who used the wavelength coincidence statistics (WCS) method and traditional identification techniques to search for atoms and ions absorbing in the mid-ultraviolet spectrum of the star α^2CVn (HD112413).

Yb III is characterized by a simple atomic structure with a $4f^{14}$ ground configuration and with lowly excited configurations corresponding to one outer electron outside an ionic core of the type $[Xe]4f^{13}$. All but one of the Yb III levels compiled by the NIST (Martin *et al* 1978) were taken from Bryant's analysis (1961, 1965). The position of the $4f^{13}(^2F^o_{5/2})5d\left(\frac{5}{2},\frac{5}{2}\right)^o_0$ level was

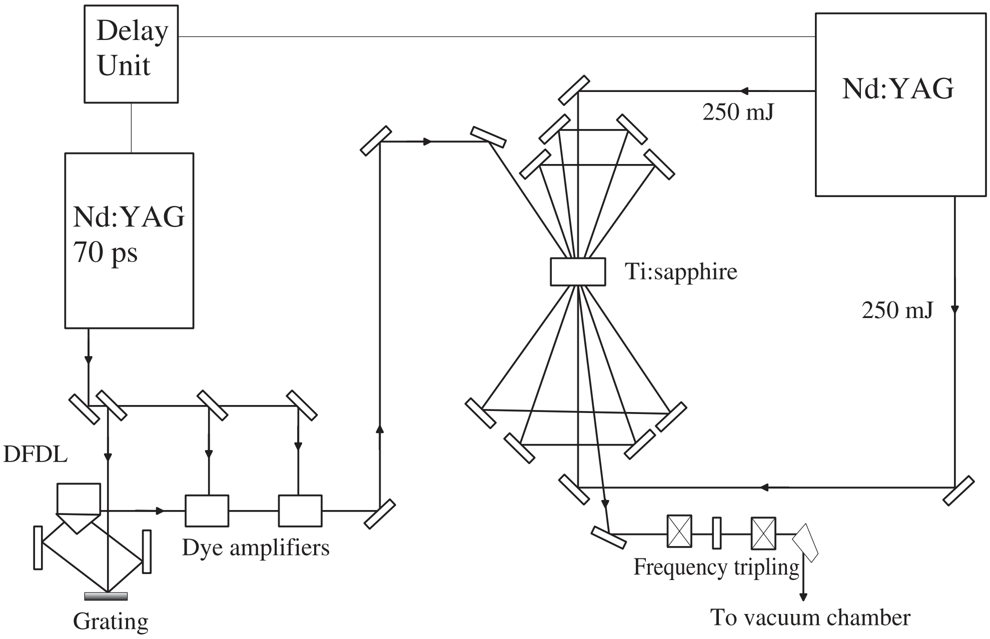

Figure 1. Picosecond laser system.

suggested by Sugar (1970). In the NIST compilation, the $4f^{14}$, $4f^{13}6p$ even configurations and the $4f^{13}5d$, $4f^{13}6s$, $4f^{13}7s$ odd configurations are complete, while 10 of the 20 levels expected for $4f^{13}6d$ are located with tentative spectroscopic designations. In this paper, a new analysis of the Yb III spectrum has been realized, providing new identifications of some levels belonging to the $4f^{13}7p$, $4f^{13}5f$ and $4f^{13}6d$ configurations and allowing one to refine or reject some $4f^{13}6d$ levels reported in the NIST compilation.

Up to now, neither transition probabilities nor radiative lifetimes have been available for Yb III. A classical way to determine transition probabilities in an atom or ion relies upon the measurement of lifetimes and on an independent (theoretical or experimental) determination of branching fractions. This paper combines experimental lifetimes with theoretical branching ratios in order to deduce a first set of transition probabilities. The feasibility of precise lifetime measurements of doubly ionized rare-earths at the Lund Laser Centre (LLC) in Sweden using time-resolved laser spectroscopy provides a unique opportunity for testing the adequacy of the physical model retained in the calculations. In the present paper, we report lifetime measurements of two $4f^{13}6p$ energy levels in Yb III together with a comprehensive calculation performed using the relativistic Hartree–Fock (HFR) method taking both intra-valence correlation and core-polarization effects into account.

This paper extends lifetime measurements and calculations in Yb ions previously reported by Biémont *et al* (1998), Li *et al* (1999) and Wyart *et al* (2001).

2. Lifetime measurements

A two-photon excitation from the $4f^{14}$ ground state has allowed the measurements of radiative lifetimes for two $4f^{13}6p$ excited states of Yb III by time-resolved laser-induced fluorescence. As the details of the experimental set-up can be found elsewhere (see, e.g., Li *et al* 1999,

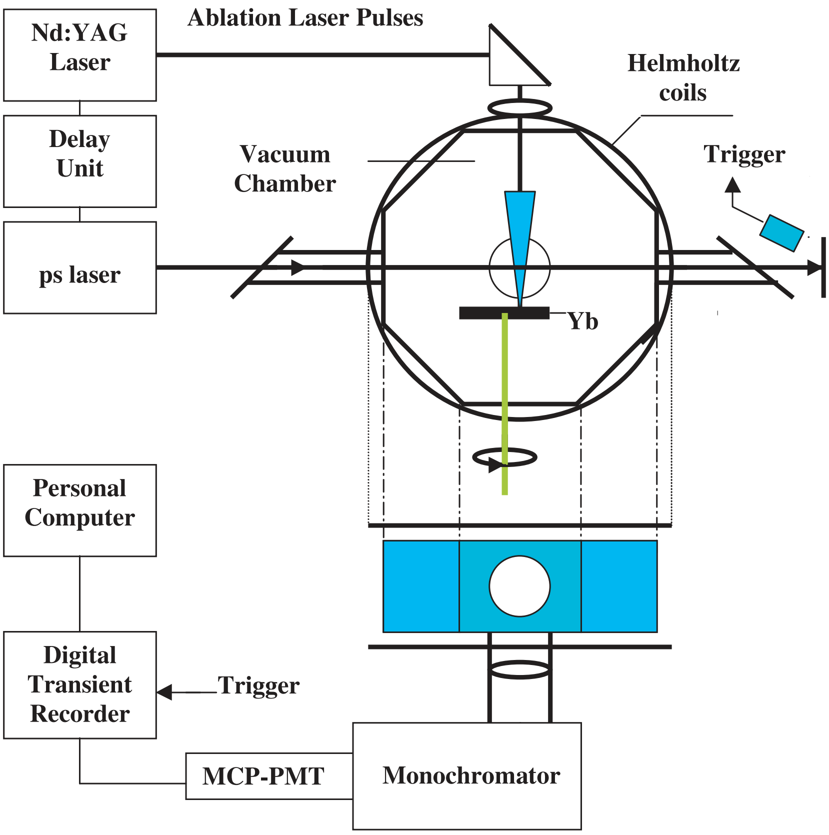

Figure 2. Experimental set-up.
(This figure is in colour only in the electronic version, see `www.iop.org`)

2001), only a short summary is presented here. The picosecond laser system employed is shown schematically in figure 1, while the set-up of the whole system is shown in figure 2.

A distributed feedback dye laser (DFDL) pumped from the 5320 Å output of a mode-locked and Q-switched Nd:YAG laser, was used to produce ultrashort picosecond pulses in the 7200–7900 Å region (using different dyes, i.e. LDS751 and LDS768). The energy of the pulse was subsequently increased by going, firstly, through a two-cell dye amplifier pumped by the same Q-switched Nd:YAG and, secondly, by a butterfly amplifier based on a Ti:sapphire crystal pumped with another Q-switched Nd:YAG laser. To obtain the required ultraviolet wavelength in the 2400–2600 Å region, the amplified DFDL radiation was frequency tripled in a nonlinear crystal system. The resulting laser pulse, which has a duration of about 60 ps and an energy of a few mJ, was sent to a vacuum chamber where the beam from another Nd:YAG laser (Continuum Surelite), which provided 10 ns pulses of about 5 mJ energy at 5320 Å, was focused on a rotating ytterbium metallic target to produce Yb III ions by laser ablation. These three Nd:YAG lasers were triggered by two connected Stanford Research Systems Model 535 digital delay generators. By a careful tuning of the short pulse wavelength, a two-photon selective excitation of Yb III levels was possible and the decay photons were observed with a monochromator acting as a wavelength selector and detected by a fast MCP photomultiplier. The signal was recorded

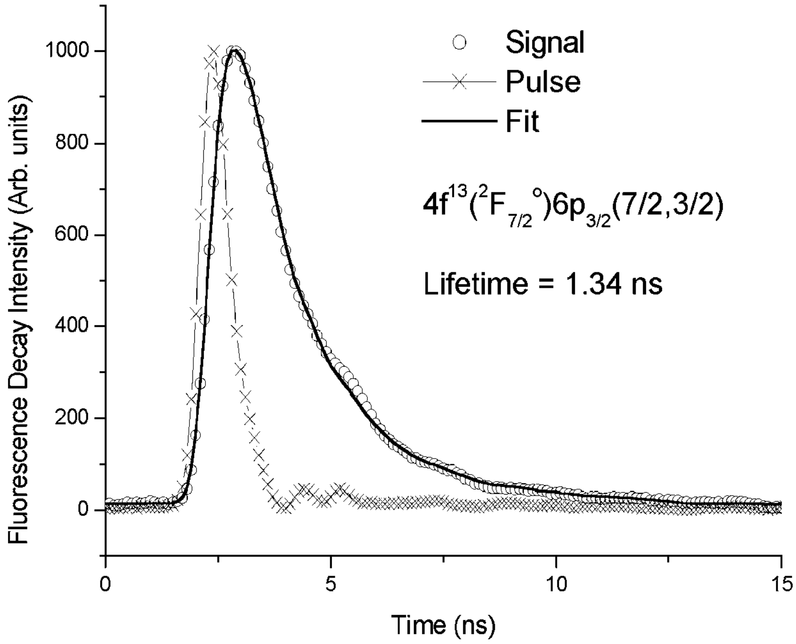

Figure 3. A typical detected fluorescence signal from a $4f^{13}6p$ level, with a convolutional fitting.

by a Tektronix TDS684A 5GS/s oscilloscope and analysed online by a PC. The oscilloscope was triggered from a Thorlabs SV2-FC photodiode (120 ps rise time) driven by the excitation beam.

The temporal shape of the excitation laser pulse, recorded by the fluorescence detection system, appears as a pulse of about 1 ns wide. As the laser pulse width is much shorter, we assumed that the observed signal describes the response function of the apparatus. Thus, the lifetimes were evaluated by fitting the observed fluorescence signals with a convolution between the recorded laser pulse with a single exponential decay. Measurements under different conditions were performed to avoid systematic errors.

The $4f^{13}(^2F^o_{7/2})6p_{3/2}\left(\frac{7}{2},\frac{3}{2}\right)_2$ (78 183.44 cm^{-1}) and $4f^{13}(^2F^o_{5/2})6p_{1/2}\left(\frac{5}{2},\frac{1}{2}\right)_2$ (82 907.42 cm^{-1}) levels were excited by two-photon absorptions from the ground state (2560.56 and 2412.33 Å). The signals were observed in lines at 2591.4 and 2651.7 Å, respectively. About 20 fluorescence curves were recorded for each level, and the mean values were taken as the final results. The quoted error bars include the random scattering and a conservative estimate of the possible systematic errors. A typical fluorescence curve with a convolutional fit is shown in figure 3. The experimental measurements are reported in table 1, where they are compared with the theoretical data obtained using the procedure described in the following section.

3. Theoretical approach

3.1. General method

The theoretical approach considered in the present paper is the relativistic Hartree–Fock method of Cowan (1981) in which we have incorporated the core-polarization effects. The

Table 1. Experimental and calculated lifetimes obtained in this paper for the $4f^{13}6p$ levels of Yb III.

Term	J	Energy (cm^{-1})	τ_{exp} (ns)	τ_{HFR} (ns)
$4f^{13}(^2F^o_{7/2})6p_{1/2}\ (\frac{7}{2}, \frac{1}{2})$	3	72 140.35		2.18
	4	72 486.97		2.19
$4f^{13}(^2F^o_{7/2})6p_{3/2}\ (\frac{7}{2}, \frac{3}{2})$	5	78 020.45		1.49
	2	78 183.44	1.34 ± 0.10	1.53
	3	78 779.29		1.50
	4	79 282.92		1.44
$4f^{13}(^2F^o_{5/2})6p_{1/2}\ (\frac{5}{2}, \frac{1}{2})$	3	82 546.33		2.21
	2	82 907.42	2.53 ± 0.20	2.22
$4f^{13}(^2F^o_{5/2})6p_{3/2}\ (\frac{5}{2}, \frac{3}{2})$	1	87 612.61		1.52
	4	88 497.90		1.50
	2	88 977.09		1.47
	3	89 397.41		1.47

technique appears to be adequate for predicting (with an accuracy of 10–15% in most cases) radiative lifetimes for complex configurations observed in lanthanide spectra such as La III, Lu III (Biémont *et al* 1999), Ce II (Palmeri *et al* 2000b, Zhang *et al* 2001), Pr III (Palmeri *et al* 2000a, Biémont *et al* 2001b), Er III (Biémont *et al* 2001a), Tm II (Quinet *et al* 1999a), Tm III (Li *et al* 2001), Yb II (Biémont *et al* 1998), Yb IV (Wyart *et al* 2001) and Lu II (Quinet *et al* 1999b). The estimate of core-polarization contributions requires knowledge of the dipole polarizability of the ionic core, α_d, and of the cut-off radius, r_c. For the first parameter, we have used the value of the static dipole polarizability computed by Fraga *et al* (1976) for Yb IV, i.e. $\alpha_d = 5.40\ a_0^3$. The cut-off radius has been chosen as equal to 1.40 a_0 which corresponds to the HFR average value $\langle r \rangle$ of the outermost core orbital ($5p^6$). Polarization corrections were not introduced in the atomic orbital calculations of the ground configuration, $4f^{14}$. For the 4f–5d transitions, polarization corrections to the dipole operator as described, for example, by Quinet *et al* (1999b) (equation (6)) are no longer valid because 4f orbitals are deeply embedded in the 5s and 5p core-orbitals. Instead, we have introduced a scaling factor, equal to 0.82, to the $\langle 4f|r|5d \rangle$ matrix element which is equal to 1.0415 a_0 for the $4f^{14}$–$4f^{13}5d$ transitions. This factor can be deduced from a curve showing the ratio between core-polarization-corrected, d_{pol}, and uncorrected, d_{nopol}, transition matrix elements for transitions not involving a 4f electron as a function of the uncorrected matrix element. This procedure has already been used successfully in the cases of Ce II (Zhang *et al* 2001), Pr III (Biémont *et al* 2001b), Er III (Biémont *et al* 2001a), Tm III (Li *et al* 2001) and Yb IV (Wyart *et al* 2001). This correction, although empirical, does provide a better agreement between calculated and measured lifetimes and, consequently for the derived oscillator strengths, particularly for the 4f–5d transitions.

3.2. Optimization process

The configuration sets retained for the calculations were $4f^{14}$, $4f^{13}6p$, $4f^{13}7p$, $4f^{13}5f$, $4f^{13}6f$, $4f^{13}7f$ for even parity and $4f^{13}5d$, $4f^{13}6d$, $4f^{13}7d$, $4f^{13}6s$, $4f^{13}7s$ for odd parity. The weak interactions of the lowest excited configurations of present interest with the configurations of the type $4f^{12}nln'l'$ are implicitly included in the polarization potential and, consequently, these configurations were not retained in the adopted configuration sets. In addition, the

Table 2. New energy levels in Yb III.

Configuration	Term	J	Energy (cm^{-1})
$4f^{13}6d$	$(\frac{7}{2}, \frac{3}{2})^o$	3	125 560.5
		5	125 167.1
	$(\frac{7}{2}, \frac{5}{2})^o$	5	126 671.4
		6	125 730.9
$4f^{13}7p$	$(\frac{7}{2}, \frac{1}{2})$	3	133 653.8
		4	133 933.4
	$(\frac{7}{2}, \frac{3}{2})$	3	137 102.0
		4	136 755.5
$4f^{13}5f$	$(\frac{7}{2}, \frac{7}{2})$	5	139 081.9
		6	138 987.1
		7	138 272.2

radial parameters (E_{av}, F^k, G^k and ζ_{nl}) were adjusted with a least-squares optimization program, minimizing the discrepancies between calculated and experimental energy levels. The levels were taken from the NIST compilation of Martin *et al* (1978) for $4f^{14}$, $4f^{13}6p$, $4f^{13}5d$, $4f^{13}6s$ and $4f^{13}7s$. For the levels of $4f^{13}6d$ (Bryant 1965) which displayed large differences $E_{exp} - E_{th}$, we used two linelists (Bryant 1961, Meggers and Corliss 1966) to check the classifications. Large wavelength inaccuracies in the former reference and bad correlations of intensities with transition probabilities, gA_{HFR}, led us to conclude that the levels at 132 864, 133 997 and 135 355 cm^{-1} are results of fortuitous coincidences. Conversely, four new levels of $4f^{13}(^2F_{7/2})6d$, each with more than seven transitions, are given in table 2. In the even-parity case, the lowest doubly excited levels of $4f^{12}(5d + 6s)^2$ had been predicted above 103 000 cm^{-1} (Brewer 1971), which leaves $4f^{13}6p$ free of close configuration-interaction effects, but makes $4f^{13}5f$ and $4f^{13}7p$ totally overlapped. During a recent investigation of Yb IV (Wyart *et al* 2001), more lines with Yb III character than expected for the transition arrays $4f^{13}(5f + 7p)$–$4f^{13}(5d + 6s)$ were found in the 950–1150 Å region, due to many $4f^{12}5d^2$–$4f^{13}5d$ transitions. The search for upper even levels leads to dozens of energies in addition to the final seven entries of table 2. A final description of the high even levels has not yet been obtained and the 5f and 7p level designations reported in table 2 result from a fair correlation between observed intensities and gA_{HFR} values.

3.3. Calculated lifetimes and transition probabilities

The calculated radiative lifetimes for the $4f^{13}6p$ levels of Yb III are reported in table 1 where they are compared with the present measurements. As can be seen from this table, the agreement between theoretical and experimental results is good (within 13%) for the two levels at 78 183.44 and 82 907.42 cm^{-1}. Using the experimental lifetimes as measured in this work and the HFR branching ratios, it has been possible to deduce the transition probabilities reported in table 3. Data for additional transitions are available in our database accessible from the website http://www.umh.ac.be/∼astro/dream.shtml.

Table 3. Oscillator strengths, log gf, and probabilities of the transitions, gA, depopulating the two $4f^{13}6p$ levels of table 1 for which radiative lifetimes have been measured in this paper. Only lines with $gA > 10^7$ s^{-1} are reported in the table.

Wavelength[a] (Å)	Lower level[b] (cm^{-1})	J	Upper level[b] (cm^{-1})	J	log gf_{HFR}	gA_{HFR} (s^{-1})	log gf_{norm}[c]	gA_{norm}[c] (s^{-1})
2314.490	34 991 (o)	3	78 183 (e)	2	0.27	2.35E+09	0.33	2.68E+09
2314.820	39 721 (o)	1	82 907 (e)	2	−1.27	6.61E+07	−1.33	5.80E+07
2506.248	43 019 (o)	3	82 907 (e)	2	−1.81	1.64E+07	−1.87	1.44E+07
2560.559	39 141 (o)	3	78 183 (e)	2	−1.94	1.18E+07	−1.88	1.35E+07
2599.148	39 721 (o)	1	78 183 (e)	2	−0.52	2.99E+08	−0.46	3.41E+08
2627.073	44 854 (o)	2	82 907 (e)	2	−0.71	1.89E+08	−0.77	1.66E+08
2638.059	40 288 (o)	2	78 183 (e)	2	−0.37	4.05E+08	−0.31	4.62E+08
2651.746	45 208 (o)	3	82 907 (e)	2	0.15	1.35E+09	0.09	1.18E+09
2842.959	43 019 (o)	3	78 183 (e)	2	−0.72	1.56E+08	−0.66	1.78E+08
2898.310	48 415 (o)	2	82 907 (e)	2	−0.41	3.05E+08	−0.47	2.68E+08
3040.663	50 029 (o)	1	82 907 (e)	2	−1.78	1.20E+07	−1.84	1.05E+07
3191.350	51 582 (o)	3	82 907 (e)	2	−0.65	1.48E+08	−0.71	1.30E+08
3384.013	53 365 (o)	1	82 907 (e)	2	−0.58	1.54E+08	−0.64	1.35E+08
3550.876	50 029 (o)	1	78 183 (e)	2	−1.68	1.12E+07	−1.62	1.28E+07
4028.155	53 365 (o)	1	78 183 (e)	2	−1.11	3.20E+07	−1.05	3.65E+07

[a] Air wavelength.
[b] (o) and (e) denote odd and even parity, respectively.
[c] Normalized using experimental lifetimes reported in table 1.

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