Energies, Landé Factors, and Lifetimes for Some Excited Levels of Neutral Ytterbium ($Z = 70$)

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We have calculated relativistic energies, Landé factors, and lifetimes for some excited levels outside the core [Xe] in neutral ytterbium (Yb I, $Z = 70$) using two configuration interaction methods (multiconfiguration Hartree–Fock method within the framework of Breit–Pauli relativistic corrections developed by Fischer, and Cowan's relativistic Hartree–Fock method). Results obtained have been compared with other calculations and experiments.

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1. Introduction

The neutral and lowly ionized lanthanides ($Z = 57$–71) are characterized by the progressive filling of the $4f$ subshell of their electronic configurations. They possess the common feature of a xenon structure with addition of two or three outer electrons [1]. The basic spectroscopic characteristics of an atomic system are levels' location (the energies) and the lifetimes (decay probabilities). There is an increasing need of atomic data (wavelengths, transition probabilities, lifetimes, hyperfine structure constants, isotope shift data, the Landé factors) for the rare-earth elements and ions. Unfortunately, present knowledge of these characteristics, in particular for heavy-atomic systems, is rather insufficient. Such is the case for the rare earths in general [2].

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%). It has a fully filled $4f$ subshell. The main part of its spectrum looks like a two-electron spectrum; having $4f^{14}6s^2\ {}^1S_0$ as the ground state.

Theoretical knowledge of lanthanides was presented by Cowan [3]. The first spectrum of ytterbium was studied by King [4]. Meggers and co-workers studied atomic spectra of rare-earth elements, and reported wavelengths and relative intensities of 1668 lines and estimated intensities of 1791 lines of Yb I [5–7]. Camus and co-workers measured 73 absorption lines in the ultraviolet region and obtained the even-parity states with $J = 0$ and $J = 2$ belonging to the series $4f^{14}6sns$ ($n = 13$–62) $^1S_0$, $4f^{14}6snd$ ($n = 11$–64) $^1D_2$ and $4f^{14}6snd$ ($n = 11$–21) $^3D_2$ [8, 9]. Also, Wyart and Camus extended the analysis and identified some new levels of Yb I [10]. Spector identified the energy levels of $4f^{13}5d6s^2$ and $4f^{13}6s^26p$ configurations [11]. Mansfield and Baig photographed the $5p$-subshell spectrum of Yb I [12]. Maeda et al. studied optical-microwave double-resonance spectroscopy of highly excited Rydberg states of ytterbium [13]. Yi and co-workers investigated autoionizing states of ytterbium atom [14, 15]. Baig et al. reported innershell and double excitation spectrum of ytterbium involving the $4f$ and $6s$ subshells [16]. Ali and co-workers presented data on the even-parity autoionizing resonances, and two-colour three-photon excitation of the $6snf\ {}^{1,3}F_3$ and $6snp\ {}^1P_1$, $^3P_{1,2}$ Rydberg's states of Yb I [17, 18]. The Rydberg and autoionizing states of neutral ytterbium were also studied by Xu et al. [19]. Griesmann et al. presented photoionization cross-sections of doubly excited resonances in ytterbium [20]. Wu and co-workers measured some new energy levels belonging to the $4f^{14}6snp\ {}^3P_{0,2}$ series, and investigated sixteen autoionizing levels of Yb [21, 22]. Aymar and co-workers presented theoretical analysis of highly excited levels of Yb, and investigated high-lying odd-parity levels Yb I by the method of selective three-step laser spectroscopy [23, 24]. The interchannel interaction between single excitation from $4f^{14}$ and double excitation from $6s^2$ in Yb I was reported by Baig and Connerade [25]. Eliav et al. calculated transition energies of ytterbium using the relativistic coupled-cluster method [26].

Radiative lifetimes of ytterbium have been studied by many authors. Rambow and Schearer measured the radiative lifetimes of some levels of Yb I [27]. Baumann and co-workers determined g_J factors and lifetimes of the excited states $6s6p\ {}^1P_1^{\circ}$ and $6s6p\ {}^3P_1^{\circ}$ of ytterbium, and performed lifetimes and g_J values in the D-states of the $4f^{14}6s6d$ configuration [28–30]. Also, they determined radiative lifetimes and g_J factors of low-lying even-parity levels in the Yb I spectrum, and measured radiative lifetimes in the even parity $6snd\ {}^1D_2$ ($n = 6$–13) and $6sns\ {}^1S_0$ ($n = 8$–14) level series of neutral Yb [31, 32]. Guo et al. measured lifetimes of the Rydberg levels in the perturbed $6snp\ {}^3P_2$ series of Yb I [33]. In addition, the lifetimes of 21 excited states in atomic Yb were measured by Bowers et al. [34]. Radiative lifetimes of levels of Yb I were compiled and analyzed by Blagoev and Komarovskii [35]. Doidge presented discussions concerning the lifetimes for the resonance transi-

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tions in Yb I [36]. Bai and Mossberg performed lifetime studies involving the $6s6p\ ^3P_1^o$ and $6s7s\ ^1S_0$ transition of atomic Yb [37]. Fang et al. measured radiative lifetimes of the Rydberg states of ytterbium for $6sns\ ^1S_0$ and $6snd\ ^1D_2$ (n = 21–27) [38]. Liu and Wang evaluated the lifetimes for the perturbed $6snd\ ^1D_2$ (n = 8–40) and $6snd\ ^3D_2$ (n = 10–26) Rydberg levels of Yb I [39]. Natural radiative lifetimes of ytterbium in the $6snd\ ^1D_2$ (n = 10–29) and $6snd\ ^3D_2$ (n = 10–20) Rydberg sequences were measured by Jiang et al. [40]. They presented natural radiative lifetimes of ytterbium in the $6sns\ ^1S_0$ (n = 12–22) Rydberg sequence of Yb [41]. Budick and Snir presented lifetimes of the two excited electronic states for ytterbium [42]. Jiang and Larsson studied perturbations in the $np\ ^{1,3}P$ Rydberg sequences and lifetime measurements of Yb I [43]. Migdalek and Baylis presented energies and oscillator strength for the spin-allowed $6s^2\ ^1S_0$–$6s6p\ ^1P_1^o$ transition in neutral ytterbium [44]. Later, they reported multiconfiguration Dirac–Fock (MCDF) calculations of lifetimes for the low-lying levels of neutral ytterbium [45]. A list of energy levels for excited levels was compiled and presented by Sansonetti and Martin [46], and can be found on the NIST web site [47].

TABLE I

Configurations considered in MCHF+BP and HFR calculations.

Levels	Configurations *A*	Configurations *B*	Configurations *C*	Configurations *D*
For MCHF+BP calculations:				
even-parity	$4f^{14}6s^2$, $4f^{14}5d6s$, $4f^{14}5d^2$, $4f^{14}6p^2$, $4f^{14}6sns$ (n = 7, 8), $4f^{14}6snd$ (n = 6, 7)	$4f^{14}6s^2$, $4f^{14}5dns$, $4f^{14}6snd$ (n = 6–9), $4f^{14}6sns$ (n = 7–9), $4f^{14}6p^2$, $4f^{14}5d^2$, $4f^{14}$5dnd (n = 6–8), $4f^{14}5d5g$, $4f^{14}5g^2$, $4f^{14}6sng$ (n = 5–7), $4f^{14}6p5f$, $4f^{14}5f7p$, $4f^{14}5f^2$	$4f^{14}ns^2$, $4f^{14}5dns$, $4f^{14}np^2$ (n = 6–9), $4f^{14}5d^2$, $4f^{14}6snd$ (n = 6, 7), $4f^{14}6sng$ (n = 5–7), $4f^{14}ns5g$ (n = 7, 8), $4f^{14}6p5f$, $4f^{14}5f7p$, $4f^{14}6sns$, $4f^{14}6pnp$ (n = 7–9), $4f^{14}7sns$, $4f^{14}7pnp$ (n = 8, 9), $4f^{14}8s9s$, $4f^{14}8p9p$	as in *B* calculation
odd-parity	$4f^{14}6snp$ (n = 6, 7), $4f^{14}6snf$ (n = 5, 6), $4f^{14}5f5g$	as in *A* calculation	$4f^{14}6snp$ (n = 6–9), $4f^{14}6snf$ (n = 5–9), $4f^{14}5dnp$ (n = 6, 7)	$4f^{14}6snp$ (n = 6–9), $4f^{14}6snf$ (n = 5, 6), $4f^{14}$7s5f, $4f^{14}6p5g$, $4f^{14}5f5g$, $4f^{14}$6pns, $4f^{14}$7snp (n = 7–9), $4f^{14}7pns$, $4f^{14}8snp$ (n = 8, 9), $4f^{14}8p9s$, $4f^{14}9s9p$
For HFR calculations:				
even-parity	$4f^{14}6s^2$, $4f^{14}5d6s$, $4f^{14}6p^2$, $4f^{14}6snd$ (n = 6, 7), $4f^{14}6s7s$	$4f^{14}6s^2$, $4f^{14}5d6s$, $4f^{14}6p^2$, $4f^{14}5d^2$, $4f^{14}6snd$ (n = 6–14), $4f^{14}6sns$ (n = 7–11)	$4f^{14}6s^2$, $4f^{13}6s^26p$	$4f^{14}6s^2$, $4f^{14}5d6s$, $4f^{13}6s^26p$, $4f^{13}5d6s6p$
odd-parity	$4f^{14}6snp$ (n = 6, 7), $4f^{14}6snf$ (n = 5, 6), $4f^{14}5d6p$	$4f^{14}6snp$ (n = 6–14), $4f^{14}6snf$ (n = 5–12), $4f^{14}5d6p$	$4f^{14}6s6p$, $4f^{13}5d6s^2$	$4f^{14}6s6p$, $4f^{13}5d6s^2$, $4f^{13}5d^26s$

The aim of this work is to carry out the relativistic energies, Landé factors, and lifetimes for $4f^{14}6s^2$, $4f^{14}5d6s$, $4f^{13}6s^26p$, $4f^{14}6sns$ (n = 7, 8), $4f^{14}6snd$ (n = 6, 7), $4f^{14}6p^2$, $4f^{14}5d^2$, $4f^{14}6snp$ (n = 6–8), $4f^{13}5d6s^2$, $4f^{14}6snf$ (n = 5, 6) and $4f^{14}5d6p$ excited levels outside the core [Xe] in Yb I (Z = 70). The ground of neutral ytterbium is $6s^2\ ^1S_0$ of closed shell formed by the $4f^{14}$ electrons. We have selected various configuration sets according to valence correlation for correlation effects. In addition, we have considered core–valence correlation in Hartree–Fock relativistic (HFR) calculation. Four various configuration sets outside the core [Xe] in neutral ytterbium are represented by *A*, *B*, *C*, and *D* for MCHF+BP and HFR calculations and presented in Table I.

The calculations have been carried out using the multiconfiguration Hartree–Fock (MCHF) code [48] in the framework of the Breit–Pauli corrections developed by Fischer and HFR code [49] developed by Cowan. We reported various atomic structure calculations such as transition energies, hyperfine structure, lifetimes, and electric dipole transitions for some rare-earth elements (La I, La II, Lu I and Ac I) [50–56].

2. Calculation methods: MCHF and HFR methods

In this work, the calculations have been performed using the MCHF method [57] and the HFR method [3]. The information about these methods can be found from Ref. [57] and Ref. [3]. We will here introduce these methods, briefly.

In the MCHF approximation, Hamiltonian is used for obtaining the best radial functions for the set of non--relativistic energies of the interacting terms. The wave function is approximated by a linear combination of orthonormal configuration state functions. In this method, the relativistic effects are considered in the framework of the Breit–Pauli Hamiltonian. This Hamiltonian is a first-order perturbation correction to the non-relativistic Hamiltonian and includes non-relativistic Hamiltonian plus relativistic shift operator including mass correction, one- and two-body Darwin terms, spin–spin contact term and orbit–orbit term, and the fine structure operator including the spin–orbit, spin–other orbit, and spin–spin terms. Therefore, the Breit–Pauli wave functions are obtained as a linear combination of the form

$$\Psi(\gamma JM) = \sum_{i=1}^{M} c_i \Phi(\gamma_i L_i S_i JM), \tag{1}$$

where $\Phi(\gamma LSJM)$ are LSJ coupled configuration state functions (CSFs). Also, γ_i and c_i represent configurations and mixing coefficients of configurations, respectively. The mixing (or expansion) coefficients c_i are obtained by diagonalizing the Breit–Pauli Hamiltonian. The radial functions building the CSFs are taken from a previous non-relativistic MCHF calculation and only the expansion coefficients are optimized.

In HFR method [3], Hamiltonian includes spin–orbit interaction besides nuclear–electron and electron–electron interactions. This method calculates one--electron radial wave functions for each of any number of specified electron configurations, using the Hartree–Fock or any of several more approximate methods. There was obtained the center-of-gravity energy of each configuration, and those radial Coulomb and spin–orbit integrals required to calculate the energy levels for the configuration. After the wave functions have been obtained, they are used to calculate the configuration interaction Coulomb integrals between each pair of interacting configurations. Then, it is set up energy matrices for each possible value of J and diagonalized each matrix to get eigenvalues (energy levels) and eigenvectors. In this method, relativistic corrections have limited calculations to the mass-velocity and Darwin corrections, taking as relativistic correction to total binding energy.

The Landé g factor of an atomic level is related to the energy shift of the sublevels having magnetic number M by

$$\Delta E = gM\mu_0 B\,, \tag{2}$$

where B is the magnetic field intensity and μ_0 is the Bohr magneton. In pure LS coupling, the g-factor can be taken given by formula (8) in [58]. The Landé factors for energy levels are a valuable aid in the analysis of a spectrum. These factors which are a measure of the magnetic sensitivity of atomic levels can be calculated using the code developed by Jönsson and Gustafsson [58] according to MCHF wave functions. In HFR method, Landé factors have been calculated using wave functions obtained from HFR calculation.

Most experiments yield the lifetime of the upper level because of easy measuring. In this case the sum over multipole transitions to all lower lying levels must be taken. The lifetime, $\tau_{\gamma' J'}$, of upper level $(\gamma' J')$ is

$$\tau_{\gamma' J'} = \frac{1}{\sum_{\pi k,\gamma J} A^{\pi k}(\gamma' J', \gamma J)}\,. \tag{3}$$

In the formula (3), $A^{\pi k}$ is the transition rate (or probability) for emission from the upper level to the lower level in the form

$$A^{\pi k}(\gamma' J', \gamma J) = 2C_k \left[\alpha\left(E_{\gamma' J'} - E_{\gamma J}\right)\right]^{2k+1} \frac{S^{\pi k}(\gamma' J', \gamma J)}{g_{J'}}\,, \tag{4}$$

where $C_k = (2k+1)(k+1)/k[(2k+1)!!]^2$, and $S^{\pi k}(\gamma' J', \gamma J)$, k and $g_{J'}$ denote line strength, rank of a spherical tensor operator and statistical weight of the upper level, namely $g_{J'} = 2J'+1$, respectively. If each multipole is described by transition operator $O_q^{\pi(k)}$ (a spherical operator of rank k and parity π), the line strength can be written as the summation over M, M' of the expected values of operator $O_q^{\pi(k)}$.

3. Results and discussion

In this work, we have calculated the relativistic energies, Landé factors, and radiative lifetimes for some excited levels in Yb I ($Z = 70$) using MCHF+BP [48] and HFR [49] codes. In MCHF+BP calculation, four various calculations have been performed to obtain configuration state functions (CSFs) according to valence–valence correlation.

The configuration sets selected for investigating correlation effects are given in Table I. Correlation effects in atoms can often be classified as valence–valence, core–valence and core–core contributions. Generally, these contributions can be evaluated by multiconfiguration techniques. As introduced by Migdalek and Baylis [44], especially for oscillator strength calculations, only the first two contributions are usually important, in particular valence–valence correlation although the core–valence correlation in many electron atoms is important. However, excitations from core to valence produce too many configurations.

In Table I, the configuration sets are selected according to increasing number of configurations. We tried to perform the various correlations (core–core and core–valence correlation) other than valence–valence correlation. But, these type configurations occur resulting in large configuration state function expansions due to open core and valence subshells and cause the optimization problems. Therefore we have often restricted our calculations with valence–valence correlation. Only in HFR calculation, we have considered core–valence correlation (in C and D) besides valence–valence correlation (in A and B). In C calculation we have only taken one configuration excited from core besides the ground and first excited levels. In D calculation $4f^{14}5d6s$ valence and one configuration excited from valence have added those in C calculation. That is, we have not selected more configurations excited from core and valence together because of the optimization constraints and computer limits.

Electron correlation effects and relativistic effects play an important role in the spectra of heavy elements. Thus we have to consider these effects for lanthanides. However, it is very difficult to calculate the electron correlation for these atoms because of their complex structure. In addition, it may be needed to take highly excited levels of these type atoms. Therefore this has provided useful information for understanding correlation effect. But, in this case the computer constraints occur. Therefore, we varied some parameter values increasingly in the MCHF atomic-structure package (maximum number of eigenpairs, maximum number of configuration state functions, maximum number of terms and maximum number of coefficients) so that the calculations for the configurations above can reasonably be made. In the atomic structure calculation and accurate prediction of radiative atomic properties for heavy atom such as Yb I, complex configuration interaction and relativistic effects must be considered simultaneously. But some constraints related to method and available computer limitations occur.

In this work, the relativistic energies (cm^{-1}) relative to the $4f^{14}6s^2\ ^1S_0$ ground state and the Landé factors have been calculated for configuration sets denoted by A, B, C and D. In Table II, $4f^{14}6s^2$, $4f^{14}5d6s$, $4f^{13}6s^26p$, $4f^{14}6sns$ (n = 7, 8), $4f^{14}6snd$ (n = 6, 7), $4f^{14}6p^2$, $4f^{14}5d^2$, $4f^{14}6snp$ (n = 6–8), $4f^{13}5d6s^2$, $4f^{14}6snf$ (n = 5, 6) and $4f^{14}5d6p$ excited levels of neutral ytterbium (Yb I) are presented to facilitate comparison with these levels in the literature. We have also calculated Landé factors for these levels using the Zeeman program developed by Jönsson and Gustafsson [58]. This code has used MCHF wave functions. References for other comparison values are typed below the table with a superscript lowercase letter. Only odd-parity states in tables are indicated by the superscript "o".

The MCHF+BP calculations obtained by the MCHF atomic-structure package [48] are performed with various configuration sets displayed in Table I. Table II displays relativistic energies and Landé factors. When energies obtained from MCHF calculations are compared with others, the agreement is usually good except some highly excited levels. D and B calculations for $4f^{14}5d6s$ level and D calculation for $4f^{14}6s7p$ level agree with other works. For $4f^{14}6p^2$ and $4f^{14}6s6d$ levels the results from A calculation are better than B, C and D. The results obtained from C are good, especially for $4f^{14}6s7s$ and $4f^{14}6s8s$. For the energies of odd-parity levels the results from C calculation (for $4f^{14}6s6p$, $4f^{14}6s6f$, and $4f^{14}5d6p$) agree with others. A and B calculations also agree for some levels. The Landé factors are also in agreement with others. It is noted that the MCHF+BP calculations are performed according to valence–valence correlation. It will be probably correct to consider the configurations including excitations from core. But, as mentioned above, it was not possible because of the optimizing constraints for all orbitals in these configurations. Our results obtained within the framework of the MCHF+BP approximation can be improved when the configurations including more unfilled d and f subshells and the excited from $4f^{14}$ are considered. But a huge number of levels arise from these configurations, making the analysis of the ytterbium spectra extremely complex and time consuming such as in other lanthanide atoms.

We have studied with four various configuration sets again for considering correlation effects in the HFR calculations performed using Cowan's computer code [49]. These configuration sets are also given in Table I. This approach, although based on the Schrödinger equation, includes the relativistic effects like the mass–velocity corrections and the Darwin contribution besides spin–orbit effect. In this calculation, the calculated eigenvalues of the Hamiltonian were optimized to the observed energy levels via a least-squares fitting procedure using the available experimental energy levels. In fact, all the levels taken from the NBS compilation (NIST) were included in the fitting procedure. The scaling factors of the Slater parameters (F^k and G^k) and of configuration interaction integrals (R^k), not optimized in the least-squares fitting, were chosen equal to 0.75, while the spin–orbit parameters were left at their *ab initio* values. This low value of the scaling factors has been suggested by Cowan for neutral heavy elements [3].

The agreement between our energies and the Landé factors (in column represented by HFR in Table II) obtained according to A, B, C and D configuration sets and other works is very good. Here, C and D configuration sets include the configuration excited from $4f^{14}$ ($4f^{13}6s^26p$, $4f^{13}5d6s6p$, $4f^{13}5d6s^2$, and $4f^{13}5d^26s$) for considering core–valence correlation contribution. These configurations have not been taken together with the configurations in A and B. In this case Cowan's code has been not executed. In the D calculation, therefore, we have considered only $4f^{14}5d6s$ valence and $4f^{13}5d6s6p$ core configurations, and $4f^{13}5d^26s$ core configuration besides those in C calculation for even- and odd-parity, respectively.

TABLE II

Energies, E, and Landé factors for some excited levels in Yb I.

Levels		E [cm^{-1}]			Landé factors		
		This work		Other works	This work		Other works
Configuration	Term	MCHF+BP	HFR		MCHF+BP	HFR	
For even-parity:							
$4f^{14}6s^2$	$^1S_0$	0.00[A,B,C,D]	0.00[A,D]	0.00[a]			
			0.03[B], 0.001[C]	−1[b]			
$4f^{14}5d6s$	$^3D_1$	24094.77[A]	24489.390[A]	24489.102[a]	0.499[A,B,C,D]	0.499[A,B,D]	0.50[a,b]
		23740.08[B,D]	24484.649[B]	24489[b]			
		28871.97[C]	24489.586[D]				
	$^3D_2$	24505.97[A]	24751.614[A]	24751.948[a]	1.147[A]	1.164[A,B,D]	1.16[a]
		24171.81[B,D]	24752.449[B]	24751[b]	1.150[B,D]		1.164[b]
		28973.71[C]	24751.119[D]		1.142[C]		
	$^3D_3$	25860.31[A]	25271.096[A]	25270.902[a]	1.334[A,B,C,D]	1.334[A,B,D]	1.34[a]
		25499.96[B,D]	25275.501[B]	25270[b]			1.333[b]
		29374.42[C]	25271.295[D]				
$4f^{14}5d6s$	$^1D_2$	26984.49[A]	27677.700[A]	27677.665[a]	1.020[A]	1.003[A,B,D]	1.01[a]
		26841.47[B,D]	27636.403[B]	27654[b]	1.017[B,D]		1.003[b]
		29633.76[C]	27677.700[D]		1.026[C]		
$4f^{13}(^2F^o_{7/2})6s^26p_{1/2}$	$(7/2,\ 1/2)_3$	–	32028.422[C]	32065.282[a]	–	1.266[C]	1.23[a]
			32100.309[D]	31957[b]		1.254[D]	1.262[b]
	$(7/2,\ 1/2)_4$	–	32346.703[C]	32273.597[a]	–	1.062[C,D]	1.064[b]
			32169.573[D]	32279[b]			
$4f^{14}6s7s$	$^3S_1$	57664.65[A]	32694.700[A]	32694.692[a]	2.002[A,B,C,D]	2.002[A,B]	2.01[a,c]
		40022.96[B,D]	32694.713[B]	32695[b]			2.00[b]
		32594.31[C]					
$4f^{14}6s7s$	$^1S_0$	59389.89[A]	34350.700[A]	34350.65[a]			
		43110.06[B,D]	34349.725[B]	34350[b]			
		34038.53[C]					
$4f^{13}(^2F^o_{7/2})6s^26p_{3/2}$	$(7/2,\ 3/2)_5$	–	35039.281[C]	35178.78[a]	–	1.20[C,D]	1.200[b]
			35163.035[D]	35172[b]			
	$(7/2,\ 3/2)_2$	–	35210.312[C]	35196.98[a]	–	1.060[C]	1.05[a]
			35397.304[D]	35199[b]		1.059[D]	1.059[b]
	$(7/2,\ 3/2)_3$	–	35826.279[C]	35807.52[a]	–	1.080[C]	1.08[a]
			35778.076[D]	35741[b]		1.093[D]	1.085[b]
	$(7/2,\ 3/2)_4$	–	36199.503[C]	36060.98[a]	–	1.202[C]	1.199[b]
			35977.204[D]	36041[b]		1.201[D]	
$4f^{14}6s6d$	$^3D_1$	46870.04[A]	39807.524[A]	39808.72[a]	0.499[A,B,C,D]	0.499[A,B]	0.50[a,b,c]
		47446.68[B,D]	39807.056[B]	39795[b]			
		51420.55[C]					
	$^3D_2$	46870.06[A]	39839.374[A]	39838.04[a]	1.167[A,B,C,D]	1.143[A]	1.16[a]
		47446.68[B,D]	39838.732[B]	39833[b]		1.142[B]	1.151[b]
		51421.52[C]					1.163[c]
	$^3D_3$	46870.09[A]	39965.998[A]	39966.09[a]	1.334[A,B,C,D]	1.334[A,B]	1.33[a]
		47446.68[B,D]	39967.809[B]	39952[b]			1.333[b]
		51422.53[C]					1.354[c]
$4f^{14}6s6d$	$^1D_2$	46877.79[A]	40061.204[A]	40061.51[a]	1.00[A,B,C,D]	1.024[A]	1.03[a]
		47452.23[B,D]	40057.109[B]	40094[b]		1.025[B]	1.016[b]
		51460.07[C]					1.020[c]
$4f^{14}6s8s$	$^3S_1$	47835.38[A]	41615.099[B]	41615.04[a]	2.002[A,B,D]	2.002[B]	2.02[a]
		58195.51[B,D]		41602[b]	2.001[C]		2.00[b]
		54228.50[C]					2.01[c]
$4f^{14}6s8s$	$^1S_0$	47843.59[A]	41919.359[B]	41939.90[a]			
		58900.12[B,D]		41955[b]			
		60105.46[C]					
$4f^{13}(^2F^o_{5/2})6s^26p_{1/2}$	$(5/2,\ 1/2)_3$	–	42253.692[C]	42413.58[a]	–	0.797[C]	0.801[b]
			42079.725[D]	42471[b]		0.814[D]	
	$(5/2,\ 1/2)_2$	–	42521.983[C]	42531.87[a]	–	0.973[C]	1.01[a]
			42361.895[D]	42578[b]		0.953[D]	0.976[b]

TABLE II (cont.)

Levels		E [cm^{-1}]			Landé factors		
		This work		Other works	This work		Other works
Configuration	Term	MCHF+BP	HFR		MCHF+BP	HFR	
$4f^{14}6p^2$	$^3P_0$	43519.96^{A}	42511.300^{A}	42436.91^{a}			
		44243.37^{B,D}	42559.755^{B}	42429^{b}			
	$^3P_1$	44864.27^{A}	43835.200^{A}	43805.42^{a}	1.501^{A,B,D}	1.501^{A,B}	1.47^{a}
		45487.64^{B,D}	43534.913^{B}	43823^{b}			1.510^{b}
	$^3P_2$	46380.96^{A}	44540.599^{A}	44760.37^{a}	1.473^{A,B} 1.469^{D}	1.335^{A}	1.34^{a}
		46912.30^{B,D}	44393.023^{B}	44716^{b}		1.412^{B}	1.336^{b}
$4f^{14}6p^2$	$^1D_2$	51313.31^{A}	46531.601^{A}	47821.78^{a}?	0.984^{A} 0.986^{B,D}	1.154^{A}	1.04^{a}?
		51411.60^{B,D}	46780.665^{B}			1.027^{B}	
$4f^{14}6p^2$	$^1S_0$	56804.45^{A}	48324.000^{A}	48332^{b}			
		56732.09^{B,D}	48382.640^{B}				
$4f^{14}6s7d$	$^3D_1$	52760.91^{A}	44312.989^{A}	44311.38^{a}	0.498^{A,B,C,D}	0.499^{A,B}	0.500^{b}
		56843.28^{B,D}	44439.608^{B}	44316^{b}			0.508^{c}
		56267.91^{C}					
	$^3D_2$	52761.13^{A}	44313.811^{A}	44313.05^{a}	1.167^{A} 1.164^{B,C,D}	1.105^{A}	1.131^{b}
		56837.05^{B,D}	44441.300^{B}	44365^{b}		1.163^{B}	1.079^{c}
		56311.72^{C}					
	$^3D_3$	52761.49^{A}	44373.007^{A}	44380.82^{a}	1.334^{A,B,C,D}	1.334^{A,B}	1.32^{a}
		56831.76^{B,D}	44444.968^{B}	44386^{b}			1.333^{b}
		56355.86^{C}					1.338^{c}
$4f^{14}6s7d$	$^1D_2$	52994.07^{A}	44372.793^{A}	44357.60^{a}	0.990^{A}	1.074^{A}	1.10^{a}
		57051.98^{B,D}	44454.197^{B}	44298^{b}	1.017^{B,D}	1.052^{B}	1.080^{b}
		56038.55^{C}			1.002^{C}		1.111^{c}
$4f^{13}(^2F^o_{5/2})6s^26p_{3/2}$	$(5/2,\ 3/2)_1$	–	44624.702^{C}	44834.61^{a}	–	0.499^{C}	0.66^{a}
			44662.257^{D}	44797^{b}		0.561^{D}	0.610^{b}
	$(5/2,\ 3/2)_4$	–	45378.796^{C}	45497.62^{a}	–	1.037^{C}	1.033^{b}
			45118.924^{D}	45578^{b}		1.036^{D}	
	$(5/2,\ 3/2)_2$	–	45854.916^{C}	45913.86^{a}	–	0.800^{C}	0.826^{b}
			45619.503^{D}	45939^{b}		0.830^{D}	
	$(5/2,\ 3/2)_3$	–	46195.710^{C}	46262^{b}	–	1.024^{C}	1.167^{b}
			45915.795^{D}			1.037^{D}	
$4f^{14}5d^2$	$^3F_2$	53431.27^{A}	48528.773^{B}	47634.41^{a}?	0.720^{A}	0.666^{B}	–
		53410.63^{B,D}			0.713^{B,D}		
		57675.25^{C}			0.666^{C}		
	$^3F_3$	54260.26^{A}	48528.773^{B}	47860.28^{a}?	1.083^{A,B,C,D}	1.084^{B}	1.02^{a}?
		54258.23^{B,D}					
		57988.50^{C}					
	$^3F_4$	55599.91^{A}	48528.773^{B}	–	1.248^{A}	1.251^{B}	–
		55579.34^{B,D}			1.247^{B,D}		
		58390.82^{C}			1.249^{C}		
$4f^{14}5d^2$	$^1G_4$	63161.05^{A}	52118.913^{B}	–	1.002^{A,C}	1.000^{B}	–
		61382.83^{B,D}			1.014^{B,D}		
		62909.94^{C}					
$4f^{14}5d^2$	$^3P_0$	61975.96^{A}	52405.055^{B}	–			
		61232.57^{B,D}					
		66154.92^{C}					
	$^3P_1$	62496.21^{A}	52476.490^{B}	–	1.501^{A}	1.501^{B}	–
		62085.04^{B,D}			1.504^{B,D}		
		66312.61^{C}			1.500^{C}		
	$^3P_2$	63107.80^{A}	52914.805^{B}	–	1.475^{A}	1.494^{B}	–
		62423.09^{B,D}			1.379^{B,D}		
		66643.02^{C}			1.478^{C}		
$4f^{14}5d^2$	$^1D_2$	67568.86^{A}	56903.452^{B}	–	1.024^{A}	1.006^{B}	–
		64824.87^{B,D}			1.087^{B,D}		

TABLE II (cont.)

Levels		E [cm^{-1}]			Landé factors		
		This work		Other works	This work		Other works
Configuration	Term	MCHF+BP	HFR		MCHF+BP	HFR	
For odd-parity:							
$4f^{14}6s6p$	$^3P^o_0$	18087.44[A]	17320.693[A]	17288.439[a]			
		18730.43[B]	17287.302[B]	17312[b]			
		17262.64[C]	17310.632[C]				
		18850.70[D]	17313.665[D]				
	$^3P^o_1$	18174.60[A]	17954.209[A]	17992.007[a]	1.501[A,B,D]	1.490[A,B]	1.49282[a]
		18817.59[B]	17917.397[B]	17962[b]	1.499[C]	1.492[C]	1.490[b]
		17567.98[C]	17963.859[C]			1.491[D]	
		18883.84[D]	17959.345[D]				
	$^3P^o_2$	18356.54[A]	19710.498[A]	19710.388[a]	1.501[A,B,C,D]	1.501[A,B,C,D]	1.50[a,b]
		18999.52[B]	19663.600[B]	19716[b]			
		18248.59[C]	19715.408[C]				
		18951.41[D]	19717.191[D]				
$4f^{14}6s6p$	$^1P^o_1$	24613.97[A]	25069.400[A]	25068.222[a]	1.000[A,B,C,D]	1.011[A,B]	1.035[a]
		25256.96[B]	25163.800[B]	25075[b]		1.065[C]	1.052[b]
		26667.25[C]	25063.101[C]			1.050[D]	
		24474.23[D]	25033.399[D]				
$4f^{13}(^2F^o_{7/2})5d_{3/2}6s^2$	$(7/2,\ 3/2)^o_2$	–	23341.506[C]	23188.518[a]	–	1.468[C]	1.45[a]
			23392.975[D]	23229[b]		1.462[D]	1.463[b]
	$(7/2,\ 3/2)^o_5$	–	25851.108[C]	25859.682[a]	–	1.021[C]	1.04[a]
			25757.722[D]	25847[b]		1.023[D]	1.022[b]
	$(7/2,\ 3/2)^o_3$	–	27562.712[C]	27445.638[a]	–	1.199[C]	1.22[a]
			27330.304[D]	27349[b]		1.213[D]	1.215[b]
	$(7/2,\ 3/2)^o_4$	–	28217.685[C]	28184.512[a]	–	1.163[C]	1.14[a]
			28136.414[D]	28128[b]		1.135[D]	1.139[b]
$4f^{13}(^2F^o_{7/2})5d_{5/2}6s^2$	$(7/2,\ 5/2)^o_6$	–	26980.996[C]	27314.919[a]	–	1.167[C,D]	1.16[a]
			27130.014[D]	27348[b]			1.167[b]
	$(7/2,\ 5/2)^o_2$	–	28583.678[C]	28195.960[a]	–	1.015[C]	1.02[a,b]
			28454.612[D]	28185[b]		1.023[D]	
	$(7/2,\ 5/2)^o_1$	–	28873.201[C]	28857.014[a]	–	1.215[C]	1.2635[a]
			28870.299[D]	28852[b]		1.222[D]	1.242[b]
	$(7/2,\ 5/2)^o_4$	–	29814.776[C]	29774.958[a]	–	1.063[C]	1.09[a]
			29908.595[D]	29788[b]		1.091[D]	1.087[b]
	$(7/2,\ 5/2)^o_3$	–	29854.112[C]	30207.380[a]	–	1.114[C]	1.08[a]
			30020.886[D]	30215[b]		1.102[D]	1.101[b]
	$(7/2,\ 5/2)^o_5$	–	30510.125[C]	30524.714[a]	–	1.175[C]	1.18[a]
			30545.679[D]	30621[b]		1.174[D]	1.174[b]
$4f^{13}(^2F^o_{5/2})5d_{5/2}6s^2$	$(5/2,\ 5/2)^o_0$	–	34574.884[C]	–			
			34824.108[D]				
	$(5/2,\ 5/2)^o_4$	–	36272.824[C]	–	–	0.830[C,D]	–
			36026.986[D]				
	$(5/2,\ 5/2)^o_1$	–	37223.407[C]	–	–	1.109[C]	–
			37349.998[D]			1.102[D]	
	$(5/2,\ 5/2)^o_2$	–	37651.594[C]	–	–	0.893[C]	–
			37314.388[D]			0.919[D]	
	$(5/2,\ 5/2)^o_5$	–	38207.585[C]	–	–	1.038[C]	–
			38293.284[D]			1.037[D]	
	$(5/2,\ 5/2)^o_3$	–	39384.583[C]	–	–	0.954[C]	–
			39216.304[D]			0.898[D]	
$4f^{13}(^2F_{5/2})5d_{3/2}6s^2$	$(5/2,\ 3/2)^o_1$	–	38855.484[C]	–	–	0.620[C]	–
			38550.804[D]			0.636[D]	
	$(5/2,\ 3/2)^o_2$	–	39281.239[C]	–	–	0.958[C]	–
			39249.622[D]			0.930[D]	
	$(5/2,\ 3/2)^o_3$	–	40406.723[C]	–	–	0.900[C]	–
			40422.239[D]			0.955[D]	

TABLE II (cont.)

Levels		E [cm^{-1}]			Landé factors		
		This work		Other works	This work		Other works
Configuration	Term	MCHF+BP	HFR		MCHF+BP	HFR	
	$(5/2,\ 3/2)^o_4$	–	41120.079[C]	–	–	1.044[C,D]	–
			41059.367[D]				
$4f^{14}6s7p$	$^3P^o_0$	41425.37[A]	38071.599[A]	38090.71[a]			
		42068.36[B]	38064.690[B]	38073[b]			
		39035.66[D]					
	$^3P^o_1$	41425.46[A]	38204.902[A]	38174.17[a]	1.501[A,B,D]	1.495[A]	1.14[a]
		42068.45[B]	38198.014[B]	38199[b]		1.497[B]	1.468[b]
		39035.66[D]					
	$^3P^o_2$	41425.64[A]	38551.699[A]	38551.93[a]	1.501[A,B,D]	1.501[A,B]	1.50[a,b]
		42068.62[B]	38526.996[B]	38543[b]			
		39035.66[D]					
$4f^{14}6s7p$	$^1P^o_1$	41663.45[A]	40567.400[A]	40563.97[a]	1.000[A,B,D]	1.005[A]	1.01[a]
		42306.44[B]	40833.500[B]	40561[b]		1.004[B]	1.001[b]
		39045.72[D]					
$4f^{14}6s5f$	$^3F^o_2$	37628.69[A]	43510.488[A]	43433.85[a]	0.666[A,B,D]	0.685[A,B]	0.68[a]
		38271.68[B]	43579.210[B]	43419[b]			0.678[b]
		38159.19[D]					
	$^3F^o_3$	37628.71[A]	43137.729[A]	43292[b]	1.083[A,B,D]	1.061[A]	1.057[b]
		38271.70[B]	43284.921[B]			1.083[B]	
		38159.22[D]					
	$^3F^o_4$	37628.73[A]	43282.598[A]	43326[b]	1.251[A,B,D]	1.251[A,B]	1.250[b]
		38271.72[B]	43330.273[B]				
		38159.27[D]					
$4f^{14}6s5f$	$^1F^o_3$	37648.71[A]	43356.784[A]	43271[b]	1.000[A,B,D]	1.035[A]	1.029[b]
		38291.71[B]	43439.200[B]			1.001[B]	
		38189.29[D]					
$4f^{14}6s8p$	$^3P^o_0$	46387.38[C]	43298.721[B]	43614.27[a]			
		45073.77[D]					
	$^3P^o_1$	46387.37[C]	43303.371[B]	43659.38[a]	1.499[C] 1.501[D]	1.498[B]	1.48[a]
		45074.60[D]					
	$^3P^o_2$	46387.48[C]	43319.907[B]	43805.69[a]	1.501[C,D]	1.494[B]	1.49[a]
		45076.29[D]					
$4f^{14}6s8p$	$^1P^o_1$	46392.17[C]	43751.100[B]	44017.60[a]	1.001[C] 1.000[D]	1.004[B]	1.00[a]
		45620.30[D]					
$4f^{14}6s6f$	$^3F^o_2$	47110.44[A]	45915.530[A]	45956.27[a]	0.666[A,B,D]	0.674[A]	0.72[a]
		47753.43[B]	45887.198[B]	45942[b]	0.667[C]	0.675[B]	0.682[b]
		44519.06[C]					
		47630.87[D]					
	$^3F^o_3$	47111.81[A]	45944.761[A]	45942[b]	1.083[A,B,C,D]	1.079[A]	1.084[b]
		47754.80[B]	45925.308[B]			1.077[B]	
		44525.71[C]					
		47632.23[D]					
	$^3F^o_4$	47113.68[A]	46162.607[A]	46035[b]	1.251[A,B,C,D]	1.251[A,B]	1.214[b]
		47756.67[B]	46046.993[B]				
		44550.67[C]					
		47634.07[D]					
$4f^{14}6s6f$	$^1F^o_3$	47992.20[A]	45739.802[A]	45852[b]	1.000[A,B,C,D]	1.009[A]	1.001[b]
		48635.19[B]	45866.199[B]			1.010[B]	
		44430.22[C]					
		48492.69[D]					
$4f^{14}5d6p$	$^3F^o_2$	41693.28[C]	42827.805[A]	42720[b]	0.685[C]	0.695[A]	0.748[b]
			43003.005[B]			0.684[B]	
	$^3F^o_3$	42385.60[C]	44262.307[A]	44415[b]	1.084[C]	1.080[A]	1.093[b]
			44387.591[B]			1.083[B]	
	$^3F^o_4$	43153.30[C]	45623.205[A]	45725[b]	1.251[C]	1.251[A,B]	1.237[b]
			45482.101[B]				

TABLE II (cont.)

Levels		E [cm^{-1}]			Landé factors		
		This work		Other	This work		Other
Configuration	Term	MCHF+BP	HFR	works	MCHF+BP	HFR	works
$4f^{14}5d6p$	$^3P^o_2$	49529.97^C	46840.765^A	48359^b	1.462^C	1.128^A	1.074^b
			47279.026^B			1.081^B	
	$^3P^o_1$	49353.89^C	47642.217^A	47847^b	1.456^C	1.142^A	1.373^b
			45891.904^B			1.384^B	
	$^3P^o_0$	49288.53^C	47438.195^A	47690^b			
			45848.693^B				
$4f^{14}5d6p$	$^1D^o_2$	43618.83^C	44980.704^A	45158^b	0.982^C	1.199^A	0.992^b
			45356.099^B			1.051^B	
$4f^{14}5d6p$	$^3D^o_1$	48458.61^C	46090.191^A	46281^b	0.544^C	0.863^A	1.00^b
			46214.203^B			0.787^B	
	$^3D^o_2$	48776.95^C	47883.425^A	47028^b	1.203^C	1.284^A	1.113^b
			46821.492^B			1.294^B	
	$^3D^o_3$	49357.19^C	47761.972^A	48167^b	1.320^C	1.279^A	1.286^b
			47681.701^B			1.254^B	
$4f^{14}5d6p$	$^1F^o_3$	53428.16^C	49417.315^A	–	1.002^C	1.042^A	–
			50600.200^B			1.006^B	
$4f^{14}5d6p$	$^1P^o_1$	64216.12^C	55353.600^A	55396^b	1.000^C	0.998^A	0.973^b
			55754.800^B			1.001^B	

[a]Ref. [47], [b]Ref. [10], [c]Ref. [31]

TABLE III

The radiative lifetimes for some excited levels in Yb I.

Levels		Lifetimes [ns]						
		This work (HFR)					Other works	
Configuration	Term	A	B	C	D	E	Experimental	Theoretical
For even-parity:								
$4f^{14}5d6s$	$^3D_1$	247.0	246.0	–	202.0	227.0	380(30)^a	–
	$^3D_2$	306.0	301.0	–	243.0	277.0	460(30)^a	–
	$^3D_3$	480.0	461.0	–	379.0	429.0	–	–
$4f^{14}5d6s$	$^1D_2$	10500.0	12400.0	–	4360.0	10700.0	6700(500)^a	–
$4f^{14}6s7s$	$^3S_1$	16.0	15.3	–	–	13.1	15.9(19)^b	21^b
							12.5(1.5)^c	
$4f^{14}6s7s$	$^1S_0$	31.4	37.1	–	–	37.1	45.8(1.0)^d	–
$4f^{13}(^2F^o_{7/2})6s^26p_{1/2}$	$(7/2, 1/2)_3$	–	–	376.0	871.0	–	–	–
	$(7/2, 1/2)_4$	–	–	537.0	1220.0	–	–	–
$4f^{13}(^2F^o_{7/2})6s^26p_{3/2}$	$(7/2, 3/2)_5$	–	–	247.0	556.0	–	–	–
	$(7/2, 3/2)_2$	–	–	279.0	526.0	–	1120(50)^c	–
	$(7/2, 3/2)_3$	–	–	317.0	756.0	–	–	–
	$(7/2, 3/2)_4$	–	–	305.0	776.0	–	–	–
$4f^{13}(^2F^o_{5/2})6s^26p_{1/2}$	$(5/2, 1/2)_3$	–	–	626.0	1360.0	–	–	–
	$(5/2, 1/2)_2$	–	–	512.0	986.0	–	–	–
$4f^{13}(^2F^o_{5/2})6s^26p_{3/2}$	$(5/2, 3/2)_1$	–	–	227.0	573.0	–	–	–
	$(5/2, 3/2)_4$	–	–	309.0	792.0	–	–	–
	$(5/2, 3/2)_2$	–	–	334.0	804.0	–	–	–
	$(5/2, 3/2)_3$	–	–	375.0	856.0	–	–	–
$4f^{14}6s6d$	$^3D_1$	60.0	39.8	–	–	28.8	22.7(7)^{b,e}	12^b
	$^3D_2$	54.2	40.5	–	–	30.0	24.2(12)^{b,e}	24^b
	$^3D_3$	89.1	55.2	–	–	38.6	23.4(11)^b	35^b
							30.8(60)^e	
$4f^{14}6s6d$	$^1D_2$	44.6	52.5	–	–	43.4	35.2(10)^{b,e}	11^b
$4f^{14}6s8s$	$^3S_1$	–	32.0	–	–	34.4	34.3(42)^b	85^b
$4f^{14}6s8s$	$^1S_0$	–	42.6	–	–	18.9	37.9(42)^b	143^b
$4f^{14}6p^2$	$^3P_0$	3.76	3.97	–	–	4.15	–	–
	$^3P_1$	3.13	3.64	–	–	3.34	15(1)^c	–
	$^3P_2$	3.91	4.43	–	–	3.39	–	–

TABLE III (cont.)

Levels		Lifetimes [ns]						
Configuration	Term	This work (HFR)					Other works	
		A	*B*	*C*	*D*	*E*	Experimental	Theoretical
$4f^{14}6p^2$	$^1D_2$	4.51	6.53	–	–	5.92	21.8(0.9)[f]	28.6[g]
$4f^{14}6p^2$	$^1S_0$	10.9	5.48	–	–	3.51	25.3(3.8)[f]	–
							27.5(16)[h]	
$4f^{14}6s7d$	$^1D_2$	45.2	24.1	–	–	74.6	49.8(20)[b]	38[b]
$4f^{14}6s7d$	$^3D_1$	32.8	61.8	–	–	49.0	38.4(17)[b]	34[b]
	$^3D_2$	37.1	57.0	–	–	53.9	66.5(36)[b]	63[b]
	$^3D_3$	40.1	80.7	–	–	63.1	43.1(12)[b]	93[b]
$4f^{14}5d^2$	$^3P_0$	–	7.21	–	–	4.60	–	–
	$^3P_1$	–	7.28	–	–	4.45	–	–
	$^3P_2$	–	5.67	–	–	4.03	–	–
$4f^{14}5d^2$	$^1D_2$	–	5.54	–	–	1.82	–	–
$4f^{14}5d^2$	$^1S_0$	–	2.76	–	–	0.629	–	–
For odd-parity:								
$4f^{14}6s6p$	$^3P^o_1$	366.9	374.7	419.1	396.2	323.6	850(50)[a]	1294[j]
							850(80)[c]	
							820(20)[i]	
							827(40)[k]	
							760(80)[l]	
$4f^{14}6s6p$	$^1P^o_1$	3.303	2.989	6.088	4.872	2.881	5.8(0.8)[c]	4.78[j]
							5.12(0.12)[i]	
							5.50(0.25)[k]	
$4f^{13}(^2F^o_{7/2})5d_{5/2}6s^2$	$(7/2,\ 5/2)^o_1$	–	–	3.806	5.266	–	15(1)[c]	–
							14.4(0.4)[i]	
$4f^{13}(^2F^o_{5/2})5d_{5/2}6s^2$	$(5/2,\ 5/2)^o_1$	–	–	4.655	7.198	–	–	–
$4f^{14}6s7p$	$^3P^o_0$	58.09	64.71	–	–	83.90	–	–
	$^3P^o_1$	54.54	61.34	–	–	77.74	120(30)[a]	–
	$^3P^o_2$	47.92	55.55	–	–	69.09	–	–
$4f^{14}6s7p$	$^1P^o_1$	29.28	27.81	–	–	25.15	9.8(0.6)[c]	–
							9.32(0.6)[i]	
$4f^{14}5d6p$	$^3F^o_2$	40.58	51.71	–	–	16.89	68(9)[a]	–
	$^3F^o_3$	10.86	10.31	–	–	10.28	22(7)[a]	–
	$^3F^o_4$	33.70	18.17	–	–	7.881	–	–
$4f^{14}5d6p$	$^3P^o_0$	5.031	11.17	–	–	5.757	–	–
	$^3P^o_1$	5.323	12.11	–	–	6.851	–	–
	$^3P^o_2$	10.04	11.37	–	–	11.76	–	–
$4f^{14}5d6p$	$^1D^o_2$	7.551	8.707	–	–	9.768	25(20)[a]	–
$4f^{14}5d6p$	$^3D^o_1$	6.509	10.80	–	–	14.01	–	–
	$^3D^o_2$	5.735	8.191	–	–	7.085	–	–
	$^3D^o_3$	6.531	8.619	–	–	9.214	–	–
$4f^{14}5d6p$	$^1F^o_3$	5.978	8.309	–	–	10.07	–	–
$4f^{14}5d6p$	$^1P^o_1$	0.716	1.820	–	–	5.551	–	–
$4f^{14}6s5f$	$^1F^o_3$	41.82	45.96	–	–	38.20	62(9)[a]	–
$4f^{14}6s5f$	$^3F^o_2$	11.84	11.37	–	–	23.55	26(7)[a]	–
	$^3F^o_3$	180.8	93.92	–	–	59.86	88(10)[a]	–
	$^3F^o_4$	52.18	57.59	–	–	49.14	–	–
$4f^{14}6s6f$	$^3F^o_2$	38.36	35.38	–	–	47.60	53(9)[a]	–
	$^3F^o_3$	29.33	36.87	–	–	40.89	–	–
	$^3F^o_4$	8.585	14.59	–	–	822.9	–	–
$4f^{14}6s6f$	$^1F^o_3$	226.0	99.73	–	–	78.05	–	–
$4f^{14}6s8p$	$^3P^o_0$	–	89.20	–	–	141.9	–	–
	$^3P^o_1$	–	93.06	–	–	120.5	140(20)[a]	–
	$^3P^o_2$	–	109.6	–	–	99.84	140(20)[a]	–
$4f^{14}6s8p$	$^1P^o_1$	–	80.36	–	–	82.32	50(20)[a]	
							47(4)[c]	
							39.1(3.5)[i]	–

[a]Ref. [34], [b]Ref. [31], [c]Ref. [35], [d]Ref. [37], [e]Ref. [30], [f]Ref. [32], [g]Ref. [39],
[h]Ref. [41], [i]Ref. [27], [j]Ref. [45], [k]Ref. [29], [l]Ref. [42]

In addition, we have presented some lifetimes results from HFR calculation. Again, we have studied with configuration sets displayed in Table I for A, B, C and D calculations. We have also taken into account $4f^{14}6s^2$, $4f^{14}5d6s$, $4f^{14}6p^2$, $4f^{14}5d^2$, $4f^{14}6snd$ ($n = 6$–20), $4f^{14}6sns$ ($n = 7$–12), $4f^{14}6sng$ ($n = 5$–8), $4f^{14}6snp$ ($n = 6$–20), $4f^{14}6snf$ ($n = 5$–18) and $4f^{14}5d6p$ configurations outside the core [Xe] represented by E. This set includes also the configurations with g orbitals. The energy and the Landé factor results are rather the same as results from A and B calculations. But, the lifetime results are somewhat different. We have, therefore, also presented the lifetime results obtained from E calculation in Table III. In this calculation, the scaling factors, not optimized in the least-squares fitting, were chosen equal to 0.85. The lifetimes (in ns) for $4f^{14}5d6s$, $4f^{13}6s^26p$, $4f^{14}6sns$ ($n = 7$, 8), $4f^{14}6snd$ ($n = 6$, 7), $4f^{14}6p^2$ and $4f^{14}5d^2$ even-parity levels of $4f^{14}6snp$ ($n = 6$–8), $4f^{13}5d6s^2$, $4f^{14}6snf$ ($n = 5$, 6), and $4f^{14}5d6p$ odd-parity levels of Yb are given and compared with the literature in Table III. This table contains the lifetime calculations according to the formula (3) for these levels considering all possible transitions to lower levels. As seen from Table III, the lifetime results obtained from our calculations are in agreement with others, generally. Only the lifetimes of $4f^{13}(^2F^{\mathrm{o}}_{7/2})6s^26p_{3/2}$, $4f^{14}6s6p\ ^3P^{\mathrm{o}}_1$ and some highly excited levels are somewhat poor. But it is noted that there is no agreement between experimental [27, 29, 35, 34, 42] and other theoretical [45] results for first excited $4f^{14}6s6p\ ^3P^{\mathrm{o}}_1$ level. In our calculations, it was seen that, among admixing configurations, the most contribution for the wave function of this level is 1.9% from $4f^{14}6s6p\ ^1P^{\mathrm{o}}$ and 1.6% from $4f^{14}5d6p\ ^3P^{\mathrm{o}}$, 1.9% from $4f^{14}6s6p\ ^1P^{\mathrm{o}}$ and 1.4% from $4f^{14}5d6p\ ^3P^{\mathrm{o}}$, 1.7% from $4f^{14}6s6p\ ^1P^{\mathrm{o}}$ and 0.1% $4f^{13}5d(^3F)6s^2\ ^1P^{\mathrm{o}}$, 1.9% from $4f^{14}6s6p\ ^1P^{\mathrm{o}}$ and 0.1% from $4f^{13}5d^2(^1G)6s\ ^3P^{\mathrm{o}}$, and 2.4% from $4f^{14}6s6p\ ^1P^{\mathrm{o}}$ and 0.4% from $4f^{14}5d6p\ ^3P^{\mathrm{o}}$ in A, B, C, D, and E calculations, respectively. The energy for this level agrees with others. When the core–valence contribution on the levels is investigated, the lifetime value for $4f^{14}6s6p\ ^1P^{\mathrm{o}}_1$ is in agreement with other. But the lifetimes agreement of $4f^{13}(^2F^{\mathrm{o}}_{7/2})5d_{5/2}6s^2$ $(7/2, 5/2)^{\mathrm{o}}_1$ and $4f^{14}6s7p\ ^3P^{\mathrm{o}}$ is somewhat good. Also, in E calculation including 5g orbital, the agreement for highly excited levels is good, especially $4f^{14}6snf\,^3F^{\mathrm{o}}_2$ ($n = 5$, 6) and $4f^{14}6snp\ ^3P^{\mathrm{o}}_{1,2}$ ($n = 7$, 8). For even-parity according to this calculation the agreement is good. An agreement except for some levels is seen when our results are compared with other works. The lifetimes of some levels will probably be improved because more configurations include levels excited from core. This case is restricted by computer limitations.

4. Conclusion

The main purpose of this paper was to perform MCHF+BP and HFR calculations for obtaining a description of the Yb I spectrum. We have here reported new data including valence–valence and core–valence correlation (only in HFR calculation) effects and relativistic corrections in Yb I. We have also presented the Landé factors of the energy levels. The Landé factor is a measure of the magnetic sensitivity of atomic level. It is known that the experimental values for Landé factors of rare-earth elements are far from being complete. Somewhat poor agreement between theory and experiment which is showed for some of the levels calculated in the present work requires further consideration. The energy data and Landé factors presented for Yb I in this work can be useful to investigations for some radiative parameters. It is known that the experiments are extremely expensive and difficult and the theoretical methods need huge computing facilities or along time to be worked out for a heavy element such as ytterbium. Consequently, we hope that our results obtained using MCHF and HFR methods will be useful for the other works in the future for Yb I spectrum.

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