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Electric Dipole Transitions for Neutral Ytterbium (Z = 70)

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We have calculated the electric dipole transition parameters (wavelengths, weighted oscillator strengths, and transition probabilities) for some excited levels in neutral ytterbium (Yb I, Z = 70) by using two configuration interaction methods (the multiconfiguration Hartree-Fock (MCHF) method within the framework of Breit-Pauli relativistic corrections developed by Fischer and Cowan's relativistic Hartree-Fock (HFR) method). Results obtained have been compared with other calculations and experiments.

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I. INTRODUCTION

Lanthanide atoms and ions, because of the complexity of their spectra, are seldom the subject of intensive theoretical studies, despite vivid interest from astrophysicists, to whom the spectra of lanthanides are important for studies of the evolution of some young stars, *e.g.*, peculiar stars [1]. There is an increasing need for accurate spectroscopic data on rare-earth elements. Such data are essential in various fields: in nucleosynthesis processes of heavy elements in studies of chemically peculiar stars, in some problems in stellar structure and evolution, in the lighting-research community because of rich emission spectra, and in diagnostics and design of high-density discharge lamps in which the rare-earth salts were used.

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%). The structure of ytterbium has made it an important element for spectroscopic studies, as the ground state $4f^{14}6s^2\ ^1S_0$ configuration resembles that of the alkaline earths. However, the $4f$ subshell in ytterbium can be easily excited, which distinguishes its spectra from that of an alkaline earth, due to the near-energy degeneracy of the inner-shell and due to double excitation limits [2].

Cowan presented theoretical knowledge on the lanthanides [3]. The available theoretical and experimental works on energy levels and transition energies for ytterbium can be found in the literature [4–25]. These works were detailed in our previous works [26,27].

Radiative lifetimes and transitions of ytterbium have been studied by many authors. Kotochigova and Tupizin carried out calculations on the electronic level structure of rare earths by using the Hartree-Fock-Dirac method [28]. Rambow and Schearer measured radiative lifetimes and alignment depolarization cross sections for Yb I and Yb II [29]. Baumann and Wandel determined g_J factors and lifetimes of the excited states 6s6p $^1P^o_1$ and 6s6p $^3P^o_1$ of ytterbium [30, 31]. Baumann *et al.* performed time-resolved lifetime and quantum-beat measurements to determine lifetimes and $g_J$values in the D states of the $4f^{14}6s6d$ configuration and determined radiative lifetimes and g_J factors of low-lying even-parity levels in the Yb I spectrum [32,33]. They 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 [34]. Guo *et al.* measured both the lifetimes of the Rydberg levels of Yb I belonging to the perturbed series 6snp $^3P_2$ and the lifetimes of the perturbing $4f^{13}5d^26s\ ^3P_2$, $^1D_2$ levels [35]. The lifetimes of 21 excited states in atomic Yb were measured by Bowers *et al.* [36]. Radiative lifetimes of levels of Yb I and Yb II were compiled and analyzed by Blagoev and Komarovskii [37]. Model-potential oscillator strengths for $4f^n6s^2$-$4f^n6s6p$ transitions in Yb I were studied by Migdalek and Marcinek [38]. Migdalek and Baylis presented energies and the oscillator strength for the spin-allowed $6s^2\ ^1S_0$-6s6p $^1P^o_1$ transition in neutral ytterbium [39]. Later, they reported multiconfiguration Dirac-Fock calculations of the E1, E2, M1, and M2 transition probabilities and lifetimes for the low-lying levels of neutral ytterbium [40]. Discussions concerning the oscillator strengths and lifetimes for the resonance transitions in Yb I were presented by Doidge [41]. Bai and Mossberg performed lifetime and oscillator strength studies involving the 6s6p $^3P^o_1$–6s7s $^1S_0$ transition of atomic Yb [42]. Fang *et al.* measured the radiative lifetimes of the Ry-

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Table 1. Configurations for odd- and even-parity levels for electric dipole transitions (E1) in Yb I.

Levels	Configurations			
	A	B	C	D
For MCHF+BP calculations				
Even-parity	$4f^{14}6s^2$, $4f^{14}5dns$, $4f^{14}6snd$ (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), $4f^{14}6p5f$, $4f^{14}5f7p$, $4f^{14}5f^2$	$4f^{14}6s^2$, $4f^{14}5d6s$, $4f^{14}5d^2$, $4f^{14}6p^2$, $4f^{14}6sns$ (n = 7, 8), $4f^{14}6snd$ (n = 6, 7)	as in calculation A	$4f^{14}ns^2$, $4f^{14}5dns$, $4f^{14}np^2$ (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), $4f^{14}8s9s$, $4f^{14}8p9p$
Odd-parity	$4f^{14}6snp$ (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), $4f^{14}8p9s$, $4f^{14}9s9p$	$4f^{14}6snp$ (n = 6, 7), $4f^{14}6snf$ (n = 5, 6), $4f^{14}5f5g$	as in calculation B	$4f^{14}6snp$ (n = 6 - 9), $4f^{14}6snf$ (n = 5 - 9), $4f^{14}5dnp$ (n = 6, 7)
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), $4f^{14}5d6p$	$4f^{14}6s6p$, $4f^{13}5d6s^2$	$4f^{14}6s6p$, $4f^{13}5d6s^2$, $4f^{13}5d^26s$

dberg states of ytterbium for 6sns $^1S_0$ and 6snd $^1D_2$ (n = 21 - 27) [43]. 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 [44]. Jiang *et al.* measured the natural radiative lifetimes of ytterbium in the 6snd $^1D_2$ (n = 10 - 29) and 6snd $^3D_2$ (n = 10 - 20) Rydberg sequences [45]. They presented natural radiative lifetimes of ytterbium in the 6sns $^1S_0$ (n = 12 - 22) Rydberg sequence of Yb [46]. Jiang and Larsson studied perturbations in the np ^{1,3}P Rydberg sequences and lifetime measurements of Yb I [47]. The hyperfine structure and the isotope effects in neutral ytterbium have been investigated by different groups [48-53]. A list of energy levels for excited levels was compiled and presented by Sansonetti and Martin [54] and can be found on the NIST web site [55,56].

Relativistic and correlation effects play important roles in wave functions and total binding energies in particular heavy elements. Therefore, an incorporation of the relativistic and the correlation effects appears necessary in order to obtain reliable theoretical results for the energies. Correlation effects in atoms can often be conveniently split into intravalence, valence-core, and intracore contributions. In *ab-initio* calculations, these contributions can be evaluated by using multiconfiguration techniques [39].

The aim of this work is to determine the radiative properties, such as wavelengths, oscillator strengths and transition probabilities, for electric dipole transitions (E1) in Yb I (Z = 70). We made a similar study for La I (Z = 57) and Ac I (Z = 89) by using only the multiconfiguration Hartree-Fock (MCHF) method [57–62] and for Lu I (Z = 71) by using MCHF and relativistic Hartree-Fock (HFR) methods together [63]. Both of these methods are configuration interaction methods and include relativistic corrections. Because Yb is a heavy el-

ement, we considered the correlation and the relativistic effects, simultaneously. We performed atomic structure calculations for Yb I by using MCHF+BP [64] and HFR [65] codes. The ground-state level of neutral ytterbium is a $6s^2\ {}^1S_0$ closed shell formed by $4f^{14}$ electrons. We selected various configuration sets according to valence correlation for the correlation effects. In addition, we considered the core-valence correlation in the HFR calculation. We selected four configuration sets outside the core [Xe] in neutral ytterbium (Yb I), denoted by A, B, C, and D, for the MCHF+BP and the HFR calculations, and these configuration sets are presented in Table 1.

II. CALCULATION METHODS: MCHF AND HFR METHODS

In this work, the calculations were performed by using the MCHF method [66] and the HFR method [3]. The information on these methods can be found from Ref. 66 and Ref. 3. We will here introduce these methods briefly.

An electromagnetic transition between two states is characterized by the angular momentum and the parity of the corresponding photon. If the emitted or absorbed photon has angular momentum k and parity $\pi = (-1)^k$ then, the transition is an electric multipole transition (Ek). However, if the photon has parity $\pi = (-1)^{k+1}$ the transition is a magnetic multipole transition (Mk).

The transition rate (or probability) for emission due to a transition from an upper level to a lower level is given by

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

and emission oscillator strength is given by

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

where $C_k = (2k+1)(k+1)/k((2k+1)!!)^2$, and $g_{J'}$ denotes the statistical weight of the upper level, namely, $g_{J'} = 2J' + 1$. In addition, α is the fine structure constant, and γ denotes the configuration (seniority, configuration, coupling scheme, *etc.*). If each multipole is described by a transition operator $O_q^{\pi(k)}$ (a spherical operator of rank k and parity π), the line strength can be written as

$$S^{\pi k}(\gamma J, \gamma' J') = \sum_{M, M', q} \left| < \gamma J M | \, O_q^{\pi(k)} \, | \gamma' J' M' > \right|^2 . \tag{3}$$

The strongest transition rate (or probability) is for electric dipole (E1) radiation. For this reason, the E1 transitions are labelled 'allowed' whereas high-order transitions are referred to as 'forbidden'.

In the MCHF approximation within the framework of the Breit-Pauli Hamiltonian, wave functions are obtained as a linear combination of the form

$$\Psi(\gamma J M) = \sum_{i=1}^{M} c_i \Phi(\gamma_i L_i S_i J M), \tag{4}$$

where $\Phi(\gamma L S J M)$ are LSJ-coupled configuration state functions (CSFs), that is,

$$\Phi(\gamma L S J M) = \sum_{M_L M_S} \langle L M_L S M_S | L S J M \rangle \Phi(\gamma L M_L S M_S). \tag{5}$$

The orbital L_i and the spin S_i angular momenta are here coupled to give the total angular momentum J. The Breit-Pauli Hamiltonian is a first-order perturbation correction to the non-relativistic Hamiltonian. This Hamiltonian includes the non-relativistic Hamiltonian plus a relativistic shift operator including a mass correction, one-and two-body Darwin terms, a spin-spin contact term, an orbit-orbit term, and a fine structure operator, including spin-orbit, spin-other-orbit, and spin-spin terms.

The mixing (or expansion) coefficients c_i in Eq. (4) 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. The matrix eigenvalue problem becomes

$$\mathbf{H}\mathbf{c} = E\mathbf{c}, \tag{6}$$

where $\mathbf{H}$ is the Hamiltonian matrix with elements

$$H_{ij} = \langle \gamma_i L_i S_i J M | H_{BP} | \gamma_j L_j S_j J M \rangle. \tag{7}$$

and $\mathbf{c} = (c_1, \cdots, c_M)^t$ is the column vector of the expansion coefficients.

In the HFR method [3], the Hamiltonian is expanded as

$$\mathbf{H} = -\sum_i \nabla_i^2 - \sum_i \frac{2Z_0}{r_i} + \sum_{i>j} \frac{2}{r_{ij}} + \sum_i \xi_i(r_i) \mathbf{l}_i \mathbf{s}_i \tag{8}$$

in atomic units, with r_i being the distance of the i^{th} electron from the nucleus and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$. $\xi_i(R) = \frac{\alpha^2}{2} \frac{1}{r} \left(\frac{\partial V}{\partial r}\right)$ is the spin-orbit term, with α being the fine structure constant and V the mean potential field due to the nucleus and other electrons.

The wave function $|\gamma J M\rangle$ of the M sublevel of a level labelled γJ is expressed in terms of LS basis states $|\alpha L S J M\rangle$ by the formula

$$|\gamma J M\rangle = \sum_{\alpha L S} |\alpha L S J M\rangle \langle \alpha L S J | \gamma J \rangle. \tag{9}$$

If determinant wave functions are used for the atom, the total binding energy is given by

$$E = \sum_i (E_k^i + E_n^i + \sum_{j<i} E^{ij}) \tag{10}$$

Table 2. Wavelengths, λ (Å), for electric dipole (E1) transitions in Yb I.

Transitions		λ		
Upper Level	Lower Level	MCHF+BP	HFR	Other works
$4f^{14}6s6p\ ^1P^\circ_1$	$4f^{14}6s^2\ ^1S_0$	4079.50[A]	3988.9272[A]	3987.99[a]
		4052.49[B]	3973.9645[B]	
		3953.26[C]	3989.9337[C]	
		3757.65[D]	3994.7719[D]	
$4f^{14}6s6p\ ^3P^\circ_1$	$4f^{14}6s^2\ ^1S_0$	5483.41[B]	5569.7197[A]	5556.466[a]
		5303.30[C]	5581.1762[B]	
		5710.02[D]	5566.7341[C]	
			5568.3393[D]	
$4f^{14}6s7p\ ^1P^\circ_1$	$4f^{14}6s^2\ ^1S_0$	2396.61[B]	2465.0365[A]	2464.50[a]
		2361.55[C]	2448.9719[B]	
$4f^{14}6p^2\ ^3P_1$	$4f^{14}6s6p\ ^3P^\circ_0$	3759.63[A]	3771.5296[A]	-
		3743.27[B]	3809.8716[B]	
		3742.71[C]		
$4f^{14}6p^2\ ^3P_0$	$4f^{14}6s6p\ ^3P^\circ_1$	3949.30[A]	4072.1552[A]	-
		3955.21[B]	4058.0550[B]	
		3938.99[C]		
$4f^{14}6p^2\ ^3P_2$	$4f^{14}6s6p\ ^3P^\circ_2$	3581.37[A]	4027.3692[A]	3990.885[a]
		3576.26[B]	4043.7714[B]	
		3587.55[C]		
$4f^{14}6p^2\ ^3P_1$	$4f^{14}6s6p\ ^3P^\circ_2$	3773.92[A]	4145.1301[A]	-
		3781.36[B]	4189.1345[B]	
		3780.79[C]		
$4f^{14}6p^2\ ^3P_1$	$4f^{14}6s6p\ ^3P^\circ_1$	3764.32[A]	3863.8476[A]	3872.852[b]
		3755.53[B]	3903.5806[B]	
		3754.96[C]		
$4f^{14}6p^2\ ^3P_2$	$4f^{14}6s6p\ ^3P^\circ_1$	3553.14[B]	3761.3289[A]	3734.694[b]
		3564.28[C]	3777.0602[B]	
$4f^{14}6p^2\ ^1S_0$	$4f^{14}6s6p\ ^1P^\circ_1$	3103.73[A]	4300.2239[A]	4295.026[b]
		3181.01[C]	4306.8521[B]	
$4f^{14}6s6d\ ^3D_1$	$4f^{14}6s6p\ ^3P^\circ_0$	3501.72[A]	4447.0553[A]	-
		3481.85[B]	4440.5474[B]	
		3487.03[C]		
		2922.88[D]		
$4f^{14}6s6d\ ^3D_1$	$4f^{14}6s6p\ ^3P^\circ_1$	3505.79[A]	4575.9705[A]	-
		3492.45[B]	4568.3693[B]	
		3497.66[C]		
		2949.20[D]		

Transitions		λ		
Upper Level	Lower Level	MCHF+BP	HFR	Other works
$4f^{14}6s6d\ ^3D_2$	$4f^{14}6s6p\ ^3P^\circ_2$	3514.11[A]	4967.9823[A]	-
		3520.06[C]	4956.6053[B]	
		3008.65[D]		
$4f^{14}6s6d\ ^3D_2$	$4f^{14}6s6p\ ^3P^\circ_1$	3505.79[A]	4569.3107[A]	4576.209[a]
		3492.45[B]	4561.7679[B]	
		3497.67[C]		
		2949.12[D]		
$4f^{14}6s6d\ ^3D_3$	$4f^{14}6s6p\ ^3P^\circ_2$	3514.11[A]	4936.9154[A]	4935.500[a]
		3514.78[B]	4925.0950[B]	
		3520.06[C]		
		3009.43[D]		
$4f^{14}6s6d\ ^3D_1$	$4f^{14}6s6p\ ^3P^\circ_2$	3514.11[A]	4975.8561[A]	-
		3514.78[B]	4964.3998[B]	
		3520.06[C]		
		3009.61[D]		
$4f^{14}6s6d\ ^1D_2$	$4f^{14}6s6p\ ^3P^\circ_2$	3519.38[C]	4913.8190[A]	-
		3006.04[D]	4903.5289[B]	
$4f^{14}6s7d\ ^3D_1$	$4f^{14}6s6p\ ^3P^\circ_0$	2889.24[B]	3704.7699[A]	3699.514[b]
		2626.45[C]	3682.9295[B]	
		2560.15[D]		
$4f^{14}6s7d\ ^3D_1$	$4f^{14}6s6p\ ^3P^\circ_1$	2896.53[B]	3793.8099[A]	3798.402[b]
		2632.47[C]	3770.4262[B]	
		2580.32[D]		
$4f^{14}6s7d\ ^1D_2$	$4f^{14}6s6p\ ^3P^\circ_1$	2595.68[D]	3785.2214[A]	3791.741[b]
			3768.3532[B]	
$4f^{14}6s7d\ ^3D_1$	$4f^{14}6s6p\ ^3P^\circ_2$	2911.88[B]	4064.6303[A]	-
			4036.1683[B]	
$4f^{14}6s7d\ ^3D_2$	$4f^{14}6s6p\ ^3P^\circ_2$	2911.86[B]	4064.4941[A]	-
		2645.58[C]	4035.8924[B]	
		2623.43[D]		
$4f^{14}6s7d\ ^3D_3$	$4f^{14}6s6p\ ^3P^\circ_2$	2911.83[B]	4054.7393[A]	-
		2645.95[C]	4035.2949[B]	
		2620.40[D]		
$4f^{14}6s10d\ ^3D_3$	$4f^{14}6s6p\ ^3P^\circ_2$	-	3511.5585[B]	3488.855[b]
$4f^{14}6s10d\ ^1D_2$	$4f^{14}6s6p\ ^1P^\circ_1$	-	4313.5041[B]	4284.170[b]
$4f^{14}6s7s\ ^1S_0$	$4f^{14}6s6p\ ^3P^\circ_1$	4123.05[C]	6098.8906[A]	-
		6051.27[D]	6085.5692[B]	

Transitions		λ		
Upper Level	Lower Level	MCHF+BP	HFR	Other works
$4f^{14}6s7s\ ^3S_1$	$4f^{14}6s6p\ ^3P^\circ_0$	4731.79[A]	6504.4801[A]	-
		4705.01[C]	6490.3864[B]	
		6499.17[D]		
$4f^{14}6s7s\ ^3S_1$	$4f^{14}6s6p\ ^3P^\circ_1$	4739.22[A]	6784.0229[A]	6799.60[a]
		2536.28[B]	6767.1333[B]	
		4724.38[C]		
		6630.76[D]		
$4f^{14}6s7s\ ^3S_1$	$4f^{14}6s6p\ ^3P^\circ_2$	4754.44[A]	7701.6249[A]	7699.49[a]
		2548.04[B]	7673.9616[B]	
		4765.34[C]		
		6944.14[D]		
$4f^{13}(^2F^\circ_{5/2})5d6s^2$ $(5/2,5/2)^\circ_1$	$4f^{14}6s^2\ ^1S_0$	-	2573.6410[C]	-
			2594.0224[D]	
$4f^{13}(^2F^\circ_{5/2})5d6s^2$ $(5/2,3/2)^\circ_1$	$4f^{14}6s^2\ ^1S_0$	-	2686.4828[C]	-
			2677.4208[D]	
$4f^{13}(^2F^\circ_{7/2})5d6s^2$ $(7/2,5/2)^\circ_1$	$4f^{14}6s^2\ ^1S_0$	-	3463.4175[C]	3464.37[a]
			3463.8424[D]	
$4f^{13}5d6s6p\ (^4F^\circ_{7/2})$ $(7/2,7/2)_0$	$4f^{14}6s6p\ ^3P^\circ_1$	-	3562.6755[D]	3559.032[b]
$4f^{13}5d6s6p(^2D^\circ_{5/2})$ $(7/2,5/2)_2$	$4f^{14}6s6p\ ^3P^\circ_1$	-	3605.7863[D]	3655.729[b]
$4f^{13}5d6s6p\ (^2D^\circ_{3/2})$ $(7/2,3/2)_2$	$4f^{14}6s6p\ ^1P^\circ_1$	-	4265.3038[D]	4333.909[b]
$4f^{13}(^2F^\circ_{5/2})6s^26p_{3/2}$ $(5/2,3/2)_3$	$4f^{13}(^2F^\circ_{7/2})5d6s^2$ $(7/2,3/2)^\circ_2$	-	4375.5526[C]	4337.599[b]
			4439.9485[D]	

[a]Ref. 56, [b]Ref. 52

where E^i_k is the kinetic energy, E^i_n is the electron-nuclear Coulomb energy, and E^{ij} is the Coulomb interaction energy between electrons i and j averaged over all possible magnetic quantum numbers. This method calculates one-electron radial wave functions for each of any number of specified electron configurations by using the Hartree-Fock or any of several other approximate methods. The center-of-gravity energy of each configuration and the radial Coulomb and spin-orbit integrals required to calculate the energy levels for the configuration are obtained. After the wave functions are obtained, they are used to calculate the configuration interaction Coulomb integrals between each pair of interacting configurations. Then, energy matrices are set up for each possible value of J, and each matrix is dioganalized to get eigenvalues (energy levels) and eigenvectors. In this method, relativistic corrections have been limited to calculations to the mass-velocity and the Darwin corrections by using the relativistic correction to total binding energy

$$E_r = \sum_i E^i_r = \sum_i (E^i_m + E^i_D). \tag{11}$$

where

$$E_m^i = -\frac{1}{4}\alpha^2\langle i|(\varepsilon^i - V^i(r))^2|i\rangle, \quad (12)$$

$$E_D^i = -\frac{1}{4}\alpha^2\left\langle i\left|\left(\frac{dV^i}{dr}\frac{d}{dr}\right)\right|i\right\rangle. \quad (13)$$

III. RESULTS AND DISCUSSION

We here calculate the radiative parameters (wavelengths, weighted oscillator strengths and transition rates) for electric dipole (E1) transitions in Yb I (Z = 70) by using MCHF+BP [64] and HFR [65] codes. In the MCHF+BP calculation, four calculations are performed to obtain configuration state functions (CSFs) according to the valence-valence correlation. The configuration sets considered for investigating the correlation effect are given in Table 1. We have tried to use various correlations (core-core and core-valence correlation) other than valence-valence correlation. However, in this case, the computer constraints occur due to the large configuration state function expansions including open subshells and optimization of the orbitals. Therefore we generally restrict our calculations to the valence-valence correlation. In the HFR calculation, we consider the core-valence correlation, as well as the valence-valence correlation. However, we do not perform MCHF+BP core-valence calculations because of the optimization constraints of these levels belong to large configuration state functions from open inner subshells. The optimization procedure in the MCHF+BP calculation is not executed in this case. In the columns including the results obtained from the HFR calculation in Table 1, A and B indicate the valence-valence correlation calculations whereas C and D indicate the core-valence correlation calculations.

The wavelengths, λ (in Å), and the weighted oscillator strengths, *gf*, as well as the transition rates (or probabilities), A_{ki} (in s^{-1}), for $4f^{14}6s6p$-$4f^{14}6s^2$, $4f^{14}6s7p$-$4f^{14}6s^2$, $4f^{14}6p^2$-$4f^{14}6s6p$, $4f^{14}6s6d$-$4f^{14}6s6p$, $4f^{14}6s7d$-$4f^{14}6s6p$, $4f^{14}6s10d$-$4f^{14}6s6p$, $4f^{14}6s7s$-$4f^{14}6s6p$, $4f^{13}5d6s^2$-$4f^{14}6s^2$, $4f^{13}5d6s6p$-$4f^{14}6s6p$, and $4f^{13}6s^26p$-$4f^{13}5d6s^2$ electric dipole transitions are reported in Table 2 and in Table 3, respectively. These tables include only some of the large-scale transition calculations. In these tables, the calculations for the various configuration sets are represented by A, B, C, and D for both the MCHF+BP and the HFR calculations. 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}".

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 structures. In particular, we tried to select a configuration including the $5g$ subshell although that complicated the calculations. In addition, highly excited levels of such atoms may need to be considered. Therefore, although this provides useful information for understanding the correlation effect, computer constraints occur. Therefore, we increasingly varied some parameters 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 could reasonably be made. In the atomic structure calculation and in an accurate prediction of radiative atomic properties for heavy atoms such as Yb I, complex configuration interaction and relativistic effects must be considered simultaneously, but this may result in some constraints related to the method and some computer-usage limitations.

In the MCHF+BP calculations, we studied the various configuration sets displayed in Table 1. We used the MCHF atomic-structure package for the calculations [64]. The contribution of the other configurations listed in Table 1 to the ground level are 0.02%, 0.025%, 0.02%, and 0.07% only from $4f^{14}6p^2$ in the A, B, C, and D calculations, respectively. The contribution for first excited level is only from $4f^{14}6s6p$ (100%) in all calculations. We obtained the 9136, 349, 3254 and 5734 possible E1 transitions for the levels selected in the calculations A, B, C, and D, respectively. For $4f^{14}6s6p$-$4f^{14}6s^2$, $4f^{14}6s7p$-$4f^{14}6s^2$, and $4f^{14}6p^2$-$4f^{14}6s6p$ electric dipole transitions for calculations denoted with A, B, C and D, the wavelengths were often in agreement with other works (Table 2), but good agreement for transitions between highly-excited levels ($4f^{14}6s6d$-$4f^{14}6s6p$, $4f^{14}6s7d$-$4f^{14}6s6p$, and $4f^{14}6s7s$-$4f^{14}6s6p$) is not seen. Comparing $\Delta\lambda = \lambda_{\text{MCHF+BP}} - \lambda_{\text{others}}$ of others to our MCHF+BP results, we find differences of $34 < \Delta\lambda < 68$ for the transitions $4f^{14}6s6p\ {}^1P_1^o$, ${}^3P_1^o$-$4f^{14}6s^2\ {}^1S_0$, and $4f^{14}6s7p\ {}^1P_1^o$-$4f^{14}6s^2\ {}^1S_0$, $100 < \Delta\lambda < 1000$ for the transitions $4f^{14}6p^2\ {}^3P_{2,1}$-$4f^{14}6s6p\ {}^3P_{2,1}^o$, $4f^{14}6s7d\ {}^3D_1$-$4f^{14}6s6p\ {}^3P_{0,1}^o$, $4f^{14}6s7s\ {}^3S_1$-$4f^{14}6s6p\ {}^3P_{1,2}^o$, and $\Delta\lambda > 1000$ for the transitions $4f^{14}6p^2\ {}^1S_0$-$4f^{14}6s6p\ {}^1P_1^o$, $4f^{14}6s6d\ {}^3D_{2,3}$-$4f^{14}6s6p\ {}^3P_{1,2}^o$, $4f^{14}6s7d\ {}^1D_2$-$4f^{14}6s6p\ {}^3P_1^o$. The *gf* and the A_{ki} values for these transitions are presented in Table 3, but there are a few values for *gf* and A_{ki} in the literature. Therefore, we only compare the *gf* and the A_{ki} values for $4f^{14}6s6p$-$4f^{14}6s^2$, $4f^{14}6s7p$-$4f^{14}6s^2$, and $4f^{14}6s7s$-$4f^{14}6s6p$ transitions. The agreement is seen to be good (except for $4f^{14}6s6p\ {}^3P_1^o$-$4f^{14}6s^2\ {}^1S_0$). Especially, the *gf* values obtained from the B and the D calculations for the transition $4f^{14}6s6p\ {}^1P_1^o$-$4f^{14}6s^{21}S_0$ are in agreement with those in Ref. 38 whereas the *gf* values from the A and the C calculations are in agreement with those in Refs. 31, 39, and 41. The A_{ki} values obtained from our calculations for this transition, in particular those for the A, C and D calculations, are also in agreement with those of other works [40,56]. The agreement for the

Table 3. Weighted oscillator strengths, *gf*, and transition probabilities, $A_{ki}(s^{-1})$, for electric dipole (E1) transitions in Yb I.

Transitions		*gf*			A_{ki}		
Upper Level	Lower Level	MCHF+BP	HFR	Other works	MCHF+BP	HFR	Other works
$4f^{14}6s6p\ ^1P_1^\circ$	$4f^{14}6s^2\ ^1S_0$	1.06431^{A}	2.16663^{A}	1.818^{b}	1.4219×10^{8A}	3.027×10^{8A}	1.92×10^{8a}
		1.73756^{B}	2.37646^{B}	1.36^{c}	2.3524×10^{8B}	3.346×10^{8B}	2.91×10^{8g1}
		1.16198^{C}	1.17606^{C}	1.30^{d}	1.6531×10^{8C}	1.643×10^{8C}	2.09×10^{8g2}
		1.98381^{D}	1.47337^{D}	1.50^{e}	3.1238×10^{8D}	2.053×10^{8D}	
$4f^{14}6s6p\ ^3P_1^\circ$	$4f^{14}6s^2\ ^1S_0$	0.00018^{B}	0.03803^{A}	0.0159^{c}	0.1342×10^{5B}	2.725×10^{6A}	1.15×10^{6a}
		0.00009^{C}	0.03739^{B}	0.0167^{d}	0.7151×10^{4C}	2.668×10^{6B}	7.55×10^{5g1}
		0.00223^{D}	0.03326^{C}		0.1526×10^{6D}	2.387×10^{6C}	7.71×10^{5g2}
			0.03520^{D}			2.524×10^{6D}	
$4f^{14}6s7p\ ^1P_1^\circ$	$4f^{14}6s^2\ ^1S_0$	0.32074^{B}	0.00588^{A}	-	$1.2416 \times 10^{8\ B}$	0.2151×10^{7A}	1.00×10^{8a}
		1.26039^{C}	0.00367^{B}		5.0249×10^{8C}	0.1362×10^{7B}	
$4f^{14}6p^2\ ^3P_1$	$4f^{14}6s6p\ ^3P_0^\circ$	0.38228^{A}	0.78922^{A}	-	$0.6013 \times 10^{8\ A}$	1.233×10^{8A}	-
		0.43528^{B}	0.68260^{B}		0.6907×10^{8B}	1.046×10^{8B}	
		0.42802^{C}			0.6794×10^{8C}		
$4f^{14}6p^2\ ^3P_0$	$4f^{14}6s6p\ ^3P_1^\circ$	0.34641^{A}	0.66105^{A}	-	$1.4815 \times 10^{8\ A}$	2.66×10^{8A}	-
		0.40521^{B}	0.60985^{B}		1.7278×10^{8B}	2.47×10^{8B}	
		0.39444^{C}			1.6957×10^{8C}		
$4f^{14}6p^2\ ^3P_2$	$4f^{14}6s6p\ ^3P_2^\circ$	1.38625^{A}	1.78403^{A}	-	$1.4418 \times 10^{8\ A}$	1.467×10^{8A}	-
		1.58958^{B}	1.88076^{B}		1.6580×10^{8B}	1.534×10^{8B}	
		1.54255^{C}			1.5989×10^{8C}		
$4f^{14}6p^2\ ^3P_1$	$4f^{14}6s6p\ ^3P_2^\circ$	0.47584^{A}	0.85923^{A}	-	$0.7428 \times 10^{8\ A}$	1.112×10^{8A}	-
		0.53859^{B}	0.77339^{B}		0.8375×10^{8B}	0.979×10^{8B}	
		0.52945^{C}			0.8235×10^{8C}		
$4f^{14}6p^2\ ^3P_1$	$4f^{14}6s6p\ ^3P_1^\circ$	0.28637^{A}	0.56668^{A}	-	$4.4933 \times 10^{7\ A}$	8.44×10^{7A}	-
		0.32526^{B}	0.48952^{B}		5.1275×10^{7B}	7.14×10^{7B}	
		0.31989^{C}			5.0445×10^{7C}		
$4f^{14}6p^2\ ^3P_2$	$4f^{14}6s6p\ ^3P_1^\circ$	0.53935^{B}	0.91937^{A}	-	$5.6993 \times 10^{7\ B}$	8.66×10^{7A}	-
		0.52407^{C}	0.74353^{B}		5.5032×10^{7C}	6.95×10^{7B}	
$4f^{14}6p^2\ ^1S_0$	$4f^{14}6s6p\ ^1P_1^\circ$	0.65791^{A}	0.15087^{A}	-	$4.5555 \times 10^{8\ A}$	0.54×10^{8A}	-
		0.73318^{C}	0.50331^{B}		4.8331×10^{8C}	1.81×10^{8B}	
$4f^{14}6s6d\ ^3D_1$	$4f^{14}6s6p\ ^3P_0^\circ$	0.07874^{A}	0.08449^{A}	-	1.4278×10^{7A}	0.950×10^{7A}	-
		0.12632^{B}	0.12802^{B}		2.3167×10^{7B}	1.443×10^{7B}	
		0.15205^{C}			2.7805×10^{7C}		
		0.01376^{D}			0.3582×10^{7D}		
$4f^{14}6s6d\ ^3D_1$	$4f^{14}6s6p\ ^3P_1^\circ$	0.05871^{A}	0.05826^{A}	-	1.0621×10^{7A}	0.6186×10^{7A}	-
		0.09402^{B}	0.08974^{B}		1.7139×10^{7B}	0.9560×10^{7B}	
		0.11315^{C}			2.0566×10^{7C}		
		0.01072^{D}			0.2740×10^{7D}		

Transitions		gf			A_{ki}		
Upper Level	Lower Level	MCHF+BP	HFR	Other works	MCHF+BP	HFR	Other works
$4f^{14}6s6d\ ^3D_2$	$4f^{14}6s6p\ ^3P^\circ_2$	0.05862^A	0.04073^A	-	$6.3332 \times 10^{6\,A}$	$2.20 \times 10^{6\,A}$	-
		0.11232^C	0.06471^B		$1.2093 \times 10^{7\,C}$	$3.51 \times 10^{6\,B}$	
		0.01077^D			$1.5861 \times 10^{6\,D}$		
$4f^{14}6s6d\ ^3D_2$	$4f^{14}6s6p\ ^3P^\circ_1$	0.17565^A	0.20342^A	-	$1.9067 \times 10^{7\,A}$	$1.299 \times 10^{7\,A}$	-
		0.28159^B	0.29035^B		$3.0799 \times 10^{7\,B}$	$1.861 \times 10^{7\,B}$	
		0.33881^C			$3.6947 \times 10^{7\,C}$		
		0.03037^D			$0.4658 \times 10^{7\,D}$		
$4f^{14}6s6d\ ^3D_3$	$4f^{14}6s6p\ ^3P^\circ_2$	0.32539^A	0.27685^A	-	$2.5109 \times 10^{7\,A}$	$1.08 \times 10^{7\,A}$	-
		0.51936^B	0.45068^B		$4.0061 \times 10^{7\,B}$	$1.77 \times 10^{7\,B}$	
		0.62477^C			$4.8046 \times 10^{7\,C}$		
		0.05649^D			$0.5943 \times 10^{7\,D}$		
$4f^{14}6s6d\ ^3D_1$	$4f^{14}6s6p\ ^3P^\circ_2$	0.00386^A	0.00327^A	-	$6.9664 \times 10^{5\,A}$	$2.93 \times 10^{5\,A}$	-
		0.00618^B	0.00530^B		$1.1113 \times 10^{6\,B}$	$4.77 \times 10^{5\,B}$	
		0.00743^C			$1.3334 \times 10^{6\,C}$		
		0.00076^D			$1.8618 \times 10^{5\,D}$		
$4f^{14}6s6d\ ^1D_2$	$4f^{14}6s6p\ ^3P^\circ_2$	0.00124^C	0.00866^A	-	$1.3403 \times 10^{5\,C}$	$4.78 \times 10^{5\,A}$	-
		0.00218^D	0.01555^B		$3.2210 \times 10^{5\,D}$	$8.62 \times 10^{5\,B}$	
$4f^{14}6s7d\ ^3D_1$	$4f^{14}6s6p\ ^3P^\circ_0$	0.08644^B	0.10081^A	-	$2.3022 \times 10^{7\,B}$	$1.633 \times 10^{7\,A}$	-
		0.00340^C	0.05024^B		$0.1095 \times 10^{7\,C}$	$0.823 \times 10^{7\,B}$	
		0.00645^D			$0.2188 \times 10^{7\,D}$		
$4f^{14}6s7d\ ^3D_1$	$4f^{14}6s6p\ ^3P^\circ_1$	0.06432^B	0.07263^A	-	$1.7045 \times 10^{7\,B}$	$1.123 \times 10^{7\,A}$	-
		0.00254^C	0.03537^B		$0.8155 \times 10^{6\,C}$	$0.553 \times 10^{7\,B}$	
		0.00602^D			$2.0099 \times 10^{6\,D}$		
$4f^{14}6s7d\ ^1D_2$	$4f^{14}6s6p\ ^3P^\circ_1$	0.00157^D	0.00736^A	-	$0.3105 \times 10^{6\,D}$	$0.686 \times 10^{6\,A}$	-
			0.09121^B			$0.856 \times 10^{7\,B}$	
$4f^{14}6s7d\ ^3D_1$	$4f^{14}6s6p\ ^3P^\circ_2$	0.00422^B	0.00473^A	-	$1.1071 \times 10^{6\,B}$	$0.6370 \times 10^{6\,A}$	-
			0.00215^B			$0.2937 \times 10^{6\,B}$	
$4f^{14}6s7d\ ^3D_2$	$4f^{14}6s6p\ ^3P^\circ_2$	0.06325^B	0.00632^A	-	$9.9509 \times 10^{6\,B}$	$0.510 \times 10^{6\,A}$	-
		0.00249^C	0.00543^B		$0.4753 \times 10^{6\,C}$	$0.445 \times 10^{6\,B}$	
		0.00742^D			$1.4391 \times 10^{6\,D}$		
$4f^{14}6s7d\ ^3D_3$	$4f^{14}6s6p\ ^3P^\circ_2$	0.35302^B	0.39839^A	-	$3.9675 \times 10^{7\,B}$	$2.31 \times 10^{7\,A}$	-
		0.01305^C	0.18092^B		$0.1777 \times 10^{7\,C}$	$1.06 \times 10^{7\,B}$	
		0.02872^D			$0.3986 \times 10^{7\,D}$		
$4f^{14}6s10d\ ^3D_3$	$4f^{14}6s6p\ ^3P^\circ_2$	-	0.02070^B	-	-	$0.1600 \times 10^{7\ B}$	-
$4f^{14}6s10d\ ^1D_2$	$4f^{14}6s6p\ ^1P^\circ_1$	-	0.18184^B	-	-	$1.3036 \times 10^{7\,B}$	-

Transitions		gf			A_{ki}		
Upper Level	Lower Level	MCHF+BP	HFR	Other works	MCHF+BP	HFR	Other works
$4f^{14}6s7s\ ^1S_0$	$4f^{14}6s6p\ ^3P^\circ_1$	0.00686[C]	0.01924[A]	0.0024[f]	2.6905×10^{6}[C]	3.451×10^{6}[A]	-
		0.00349[D]	0.01363[B]		0.6363×10^{6} [D]	2.454×10^{6}[B]	
$4f^{14}6s7s\ ^3S_1$	$4f^{14}6s6p\ ^3P^\circ_0$	0.88909[A]	0.18502[A]	-	8.8291×10^{7}[A]	0.973×10^{7}[A]	-
		1.13533[C]	0.19152[B]		1.1403×10^{8}[C]	1.011×10^{7}[B]	
		0.21494[D]			1.1314×10^{7}[D]		
$4f^{14}6s7s\ ^3S_1$	$4f^{14}6s6p\ ^3P^\circ_1$	2.66325[A]	0.51472[A]	-	2.6364×10^{8}[A]	0.2486×10^{8}[A]	-
		0.08688[B]	0.53418[B]		0.3003×10^{8}[B]	0.2593×10^{8}[B]	
		3.38861[C]			3.3756×10^{8}[C]		
		0.61408[D]			0.3105×10^{8}[D]		
$4f^{14}6s7s\ ^3S_1$	$4f^{14}6s6p\ ^3P^\circ_2$	4.42608[A]	0.74723[A]	-	4.3535×10^{8}[A]	0.2800×10^{8}[A]	-
		0.14238[B]	0.77995[B]		0.4876×10^{8}[B]	0.2944×10^{8}[B]	
		5.59391[C]			5.4770×10^{8}[C]		
		0.92929[D]			0.4285×10^{8}[D]		
$4f^{13}(^2F^\circ_{5/2})5d6s^2$	$4f^{14}6s^2\ ^1S_0$	-	0.27421[C]	-	-	9.20×10^{7}[C]	-
$(5/2,5/2)^\circ_1$			0.21176[D]			6.99×10^{7}[D]	
$4f^{13}(^2F^\circ_{5/2})5d6s^2$	$4f^{14}6s^2\ ^1S_0$	-	0.69733[C]	-	-	2.15×10^{8} [C]	-
$(5/2,3/2)^\circ_1$			0.44461[D]			1.38×10^{8}[D]	
$4f^{13}(^2F^\circ_{7/2})5d6s^2$	$4f^{14}6s^2\ ^1S_0$	-	1.41743[C]	-	-	2.627×10^{8} [C]	0.683×10^{8}[a]
$(7/2,5/2)^\circ_1$			1.02472[D]			1.898×10^{8}[D]	
$4f^{13}5d6s6p\ (^4F^\circ_{7/2})$	$4f^{14}6s6p\ ^3P^\circ_1$	-	0.00467[D]	-	-	2.454×10^{6}[D]	-
$(7/2,7/2)_0$							
$4f^{13}5d6s6p(^2D^\circ_{5/2})$	$4f^{14}6s6p\ ^3P^\circ_1$	-	0.00011[D]	-	-	0.1081×10^{5}[D]	-
$(7/2,5/2)_2$							
$4f^{13}5d6s6p(^2D^\circ_{3/2})$	$4f^{14}6s6p\ ^1P^\circ_1$	-	0.00018[D]	-	-	0.1297×10^{5}[D]	-
$(7/2,3/2)_2$							
$4f^{13}(2F5/2)6s^26p_{3/2}$	$4f^{13}(^2F^\circ_{7/2})5d6s^2$	-	0.00089[C]	-	-	0.4433×10^{5}[C]	-
$(5/2,3/2)_3$	$(7/2,3/2)^\circ_2$		0.00265[D]			1.2804×10^{5}[D]	

[a]Ref. 56, [b]Ref. 38, Converted from f, [c]Ref. 41, Converted from$f$, [d]Ref. 31, Converted from f, [e]Ref. 39, Converted from f, [f]Ref. 42, Converted from f, [g1,g2]Ref. 40

gf values from the transition $4f^{14}6s6p\ ^3P^o_1$-$4f^{14}6s^2\ ^1S_0$ is poor. The A_{ki} values for this transition are also somewhat poor. For the transition $4f^{14}6s7s\ ^1S_0$-$4f^{14}6s6p\ ^3P^o_1$, the gf value is in agreement with that in Ref. 42. The agreement for the A_{ki} value from B calculation for the transition $4f^{14}6s7p\ ^1P^o_1$-$4f^{14}6s^2\ ^1S_0$ is good. We think, as mentioned above, that these results obtained within the MCHF+BP approximation can be improved when configurations including more unfilled d and f subshells and the levels excited from $4f^{14}$ are considered, but a huge number of levels arise from these configurations, so an optimization procedure was not run.

In the HFR calculations, we again studied four configuration sets. These configuration sets selected for considering correlation effects in the HFR calculations performed using Cowan's computer code [65] are also

given in Table 1. This approach, although based on the Schrödinger equation, includes relativistic effects like the mass-velocity corrections and Darwin contribution, in addition to 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 the configuration interaction integrals (R^k), not optimized in the least-squares fitting, were chosen to be equal to 0.75 while the spin-orbit parameters were left at their *ab-initio* values. This low value of 0.75 for the scaling factors was suggested by Cowan for neutral heavy elements [3].

In the HFR calculations, the contributions of the other configurations listed in Table 1 to the ground level are 0.3% $4f^{14}6p^2$, 2.3% $4f^{14}6p^2$ and 0.4% $4f^{14}5d^2$, only $4f^{14}6s^2$, and 2.0% $4f^{13}5d6s6p$ in the A, B, C, and D calculations, respectively. The contributions for the first excited level are 1.5% $4f^{14}5d6p$ and 0.3% $4f^{14}6s7p$, 1.3% $4f^{14}5d6p$ and 0.3% $4f^{14}6s7p$, only $4f^{14}6s6p$, and 0.1% $4f^{13}5d^2(^1G)6s$ and 0.1% $4f^{13}5d^2(^3F)6s$ in the A, B, C, and D calculations, respectively. We obtained 345, 3074, 151 and 19485 possible E1 transitions for the levels in the calculations A, B, C, and D, respectively. For the $4f^{14}6s6p$-$4f^{14}6s^2$, $4f^{14}6s7p$-$4f^{14}6s^2$, $4f^{14}6p^2$-$4f^{14}6s6p$, $4f^{14}6s6d$-$4f^{14}6s6p$, $4f^{14}6s7d$-$4f^{14}6s6p$, $4f^{14}6s10d$-$4f^{14}6s6p$, $4f^{14}6s7s$-$4f^{14}6s6p$, $4f^{13}5d6s^2$-$4f^{14}6s^2$, $4f^{13}5d6s6p$-$4f^{14}6s6p$, and $4f^{13}6s^26p$-$4f^{13}5d6s^2$ electric dipole transitions, the wavelengths were in very good agreement with those of other works (Table 2). Again, we investigated $\Delta\lambda = \lambda_{\rm HFR} - \lambda_{\rm others}$, the difference was about $0.5 < \Delta\lambda < 70$. In addition, our *gf* and A_{ki} values for the transitions $4f^{14}6s6p$-$4f^{14}6s^2$, $4f^{14}6s7p$-$4f^{14}6s^2$, $4f^{14}6s7s$-$4f^{14}6s6p$, and $4f^{13}5d6s^2$-$4f^{14}6s^2$ are compared with those of others in Table 3. The *gf* value obtained from the A calculation for the transition $4f^{14}6s6p\ {}^1P^o_1$-$4f^{14}6s^2\ {}^1S_0$ is in agreement with the value in Ref. 38 and the *gf* values obtained from the C and D calculations are in agreement with those in Refs. 31, 39, and 41. For this transition, the A_{ki} values, in particular those from the A, C, and D calculations, are in agreement with those in other works [40, 56]. For the transition $4f^{14}6s6p\ {}^3P^o_1$-$4f^{14}6s^2\ {}^1S_0$, the *gf* values are good when compared to those in Refs. 31 and 41. Only the *gf* value for the transition $4f^{14}6s7s\ {}^1S_0$-$4f^{14}6s6p\ {}^3P^o_1$ appears to be somewhat poor when compared with that in another work [42]. The A_{ki} value for the transition $4f^{14}6s7p{}^1P^o_1$-$4f^{14}6s^2\ {}^1S_0$ is also poor. We expect the HFR results to be better than the MCHF+BP results. Because the levels obtained from the HFR calculations are fitted with their experimental values and include a core-valence correlation, as well as a valence-valence correlation.

IV. CONCLUSION

The main purpose of this paper was to perform MCHF+BP and HFR calculations to obtain 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. The present results provide an extensive set of radiative parameters for Yb I. Experiments are known to be extremely expensive and difficult, and the theoretical methods are known to need huge computing facilities or a long computing time for a heavy element such as ytterbium. It may be mentioned that the results from the two configuration interaction methods (MCHF and HFR) are good. Of course, in this work, the HFR calculation results are generally better than MCHF+BP calculation results. We think that this is due to the fact that a fitting procedure using available experimental values was used in the HFR calculation. However, it is noted that there are a few experimental or theoretical oscillator strengths (*gf*) and transition probabilities (A_{ki}) values for this atom in literature. For this reason, the MCHF+BP results are also valuable.

In summary, reliable atomic data are needed in the study of astrophysical problems. In spectrum synthesis work, particularly for CP stars, accurate data for transition probabilities and oscillator strengths for lanthanide atoms are needed to establish reliable abundances for these species. Consequently, we hope that our results obtained using the MCHF and the HFR methods will be useful for other future works on the Yb I spectrum.

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