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Determination of static dipole polarizabilities of Yb atom*

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We determine the static values of the scalar and tensor dipole polarizabilities of the ground, $6s6p\,^3P^o_0$, and $6s6p\,^3P^o_1$ states of the Yb atom. These results can be useful in many experiments undertaken using this atom. We employed a combined configuration interaction (CI) method and a second-order many-body perturbation theory (MBPT) to evaluate energies and electric dipole (E1) matrix elements of many low-lying excited states of the above atom. These values are compared with the other available theoretical calculations and experimental values. By combining these E1 matrix elements with the experimental excitation energies, we estimate the dominant valence correlation contributions to the dipole polarizabilities of the above states. The core contribution is obtained from the finite field approach. We also compare these values with the other theoretical results as there are no precise experimental values that are available for these properties.

Keywords: ytterbium atom, polarizabilities, configuration interaction, many-body perturbation

PACS: 31.10.+z, 31.15.am, 31.15.ap, 31.15.bw **DOI:** 10.1088/1674-1056/27/6/063101

1. Introduction

Static electric dipole polarizability (α) of an atomic system provides the information about the distortion of the electron cloud when the system is placed in an electric field. Accurate knowledge of this quantity is essential in many areas of physics. The ytterbium (Yb) atom is a special atom in the sense that its isotopes are rich in the earth and it has long-lived metastable $6s6p\,^3P^o_0$ and $^3P^o_1$ states and a number of allowed transitions with the wavelengths that are easily accessible by the lasers for cooling and trapping processes. The optically trapped Yb atoms provide a promising tool to study the degenerate quantum gases,[1] optical atomic clock,[2–4] quantum information processing,[5] search of the parity nonconservation,[6] CP-violation,[7] etc.

There are two transitions in Yb that are the most important. The first is the transition from the ground state $6s^2\,^1S_0$ to $6s6p\,^3P^o_0$, which is used for the clock transition of a Yb optical lattice clock.[8] The precision values of the static polarizabilities of $6s^2\,^1S_0$ and $6s6p\,^3P^o_0$ states are needed for the best evaluation of the uncertainty of the clock transition caused by the Stark shift and black-body radiation shift. The intercombination transition $6s^2\,^1S_0$–$6s6p\,^3P^o_1$ of Yb has a narrow linewidth around 181 kHz that could cool atoms down to the photon recoil temperature of 4.4 μK.[9] In order to gain a high-density trapping, a far-off resonant trap (FORT) for Yb atom was then adopted, which overlaps a magneto-optical trap (MOT) by using the $^1S_0$ to $^3P^o_1$ transition.[10–12] The high-density trapping and following achievement of Bose-Einstein condensation (BEC) of ^{174}Yb atoms using FORT experiments are expected to be important steps for the future investigation of new quantum phenomena.[1] There are no precise experimental α values available for the above states of Yb atom. A preliminary experimental result α of the ground state of Yb has been reported as 142(36) a.u. (The unit a.u. is short for atomic unit), that has a very large uncertainty.[13] There are also a number of calculations on these quantities, which have been carried out by employing the variants of many-body methods.[14–18] However, most of these calculations are not consistent with each other due to large electron correlation effects associated with this atom.

In this paper, we calculate the static α values of the $6s^2\,^1S_0$, $6s6p\,^3P^o_0$, and $6s6p\,^3P^o_1$ states of Yb by using the relativistic many-body methods. First, the energies and the electric dipole (E1) matrix elements are determined by employing a combined configuration interaction (CI) method and a lower-order many-body perturbation theory (MBPT) in the relativistic theory framework. We use these quantities later to estimate the dominant valence correlation contributions to α in the above states. The core contributions are estimated by using a relativistic coupled-cluster (RCC) method from the DIRAC package[19] in the finite field approach. These theories are described briefly in the next section. Throughout the paper, we use atomic units (a.u.) unless otherwise stated.

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2. Theoretical method

We use the CI + MBPT method that is implemented in the package[20] in our calculations. This theory and implementation technique have been documented in Refs. [15] and [21]. The calculation method is based on a combination of a conventional configuration interaction (CI) method and many-body perturbation theory (MBPT). The former explicitly contains the interaction between valence electrons, while the latter includes core–core and core–valence correlations.[20] In the CI + MBPT method, the effective Hamiltonian for two valence electrons is written as

$$\hat{H}^{\rm eff} = \hat{h}_1(r_1) + \hat{h}_1(r_2) + \hat{h}_2(r_1, r_2), \tag{1}$$

where $\hat{h}_1$ and $\hat{h}_2$ are the single-electron and two-electron interaction terms of the relativistic Hamiltonian, respectively. In the implementation of the correlation operator $\hat{\Sigma}$, in addition to $\hat{\Sigma} = 0$ that corresponds to the standard CI method, both a single-electron operator $\hat{\Sigma}_1$ representing a correlation interaction of a particular valence electron with the atomic core, and a two electron operator $\hat{\Sigma}_2$ representing the screening of the Coulomb interaction between the two valence electrons by the core electrons are taken into account. In the CI + MBPT package, $\hat{\Sigma}_1$ and $\hat{\Sigma}_2$ are calculated in the second order of the MBPT. The basis set is constructed by using an "auto" generation regime that is provided in the CI + MBPT package.[20] The one-electron basis set includes 1s–23s, 2p–22p, 3d–22d, 4f–20f, and 5g–18g orbitals, where the core and 6s–9s, 6p–9p, 5d–8d orbitals are obtained from the Dirac–Hartree–Fock (DHF) method, while all the remaining orbitals are virtual ones. The V^{N-2} potential is used in the DHF calculation and the virtual orbitals are yielded numerically by using a recurrent relationship.[20]

Generally, the static polarizability α of the atomic state can be expressed as

$$\alpha = \alpha^{\rm S} + \frac{3M_J^2 - J(J+1)}{J(2J-1)}\alpha^{\rm T}, \tag{2}$$

where $\alpha^{\rm S}$ and $\alpha^{\rm T}$ are known as the scalar and tensor components of the polarizability, respectively. Both these components can be conveniently divided into three parts as expressed below.

$$\alpha^{\rm S/T} = \alpha_{\rm v}^{\rm S/T} + \alpha_{\rm c}^{\rm S/T} + \alpha_{\rm vc}^{\rm S/T}, \tag{3}$$

where the subscripts v, c, and vc represent the valence, core, and valence–core contributions, respectively. In the sum-over-states approach, the $\alpha_{\rm v}^{\rm S/T}$ parts of a state denoted by g are expressed as

$$\alpha_{\rm v}^{\rm S} = \frac{2}{3(2J_g+1)}\sum_i \frac{|\langle\psi_g\|D\|\psi_i\rangle|^2}{(E_i - E_g)}, \tag{4}$$

$$\alpha_{\rm v}^{\rm T} = 4\left[\frac{5J_g(2J_g-1)}{6(J_g+1)(2J_g+1)(2J_g+3)}\right]^{1/2} \times \sum_i (-1)^{J_g+J_i}\left\{\begin{array}{ccc} J_g & 1 & J_i \\ 1 & J_g & 2 \end{array}\right\}\frac{|\langle\psi_g\|D\|\psi_i\rangle|^2}{(E_i - E_g)}, \tag{5}$$

where $|\langle\psi_g\|D\|\psi_i\rangle|$ is the reduced matrix element of the electric dipole transition. The tensor component $\alpha_{\rm v}^{\rm T}$ only exists for states with $J_i > 1/2$. The core-valence contributions are generally small, so we neglect them in our work for reaching an accurate level of interest.

The $\alpha_{\rm c}^{\rm T}$ contribution vanishes and the $\alpha_{\rm c}^{\rm S}$ contributions are obtained through using the finite-field approach. First, we calculate energies considering the Dirac–Coulumn-Hartee ($H_{\rm DC}$) Hamiltonian. Then, we include the interaction potential energies induced by the external electric field and its gradient with $H_{\rm DC}$ and treat them perturbatively to estimate the $\alpha^{\rm E1}$ values, respectively. The energy of an atomic state $|\gamma JM_J\rangle$ in the presence of these interactions can be expressed as

$$E_0(\mathcal{E}_z) = E_0(0) - \frac{\alpha^{\rm E1}(\gamma JM_J)}{2}\mathcal{E}_z^2 - \cdots, \tag{6}$$

where $E_0(0)$ is the energy in the absence of the external field, and $\mathcal{E}_z$ is the electric field along the z direction. The scalar and tensor components of the electric dipole polarizability are then determined as

$$\alpha^{\rm S}(\gamma J) = \frac{1}{2J+1}\sum_{M_J}\alpha^{\rm E1}(\gamma JM_J) \tag{7}$$

and

$$\alpha^{\rm T}(\gamma J) = \alpha^{\rm E1}(\gamma JJ) - \alpha^{\rm S}(\gamma J). \tag{8}$$

This procedure is known as the finite-field approach to evaluating α. We have successfully used this method earlier to calculate α values of other atomic systems.[22,23] For achieving the numerical stability in the result, it would be necessary to repeat the calculations by considering a number of the electric fields as $\mathcal{E}_z = 0.0$, 0.0005, 0.001, and 0.002 a.u. This is accomplished by using the RCC method that is provided in the relativistic *ab initio* package DIRAC.[19] In this approach, the wave function of the doubled ionized Yb^{2+} with 68 electrons is expressed in the RCC theory formulation and the ground state energies are obtained by varying electric field strength. We verify the electron correlation arising from the internal core electrons and find that they have a negligible effect on α. Therefore, the atomic core $1s\cdots4d^{10}$ is frozen in this RCC calculation, while the 5s, 5p, 4f orbitals are only correlated. We use the Dyall's uncontracted correlated consistent double-, triple-, and quadruple-ζ GTO basis sets, which are referred to as $X\zeta$, where $X = 2$, 3, and 4, respectively.[24] Each shell is augmented by two additional diffuse functions (d-aug) and the exponential coefficient of the augmented function is calculated based on the following formula:

$$\zeta_{N+1} = \left[\frac{\zeta_N}{\zeta_{N-1}}\right]\zeta_N, \tag{9}$$

where ζ_N and ζ_{N-1} are the two most diffuse exponents for the respective atomic-shell in the original GTOs. The convergence of the results with the progressively larger basis set is verified. The final value is taken to be the α_c obtained by using the basis of 4ζ.

3. Results and discussion

First we give the results of the energies obtained by using the CI + MBPT method and compare our results with the previously available data. In Table 1, we present energies of the 17 even-parity $6s^2$, 6s7s, 6s8s, 5d6s, 6s6d, and $6p^2$, and 15 odd-parity 6s6p, 6s7p, and 6s8p low-lying states of Yb. We can find that our CI + MBPT results show good agreement with the experimental values listed in the National Institute of Standards and Technology (NIST) database[16] within an error of 1% except for the 5d6s, 6s7p, and $6p^2$ states, where the discrepancies are around 2%–5%. The reason for such a large discrepancy may be that the electron correlation arising from these states is not implemented sufficiently due to our limited configuration-state-function spaces.

Table 1. The excited energies (in unit cm^{-1}) of the low lying excited states of Yb, obtained by using the CI + MBPT method. The absolute difference in percentage between our CI + MBPT values and the NIST data[25] is denoted as "Diff.".

State	CI + MBPT	NIST	Diff./%
$6s^2\,^1S_0$	0	0	
$6s6p\,^3P^o_0$	17446	17288.439	0.9
$6s6p\,^3P^o_1$	18135	17992.007	0.8
$6s6p\,^3P^o_2$	19858	19710.388	0.8
$5d6s\,^3D_1$	25229	24489.102	3.0
$5d6s\,^3D_2$	25479	24751.948	2.9
$6s6p\,^1P^o_1$	25698	25068.222	2.5
$5d6s\,^3D_3$	25990	25270.902	2.8
$5d6s\,^1D_2$	28310	27677.665	2.3
$6s7s\,^3S_1$	32701	32694.692	0.02
$6s7s\,^1S_0$	34287	34350.65	0.2
$6s7p\,^3P^o_0$	38063	38090.71	0.04
$6s7p\,^3P^o_1$	38133	38174.17	0.1
$6s7p\,^3P^o_2$	38509	38551.93	0.1
$6s6d\,^3D_1$	39849	39808.72	0.1
$6s6d\,^3D_2$	39882	39838.04	0.1
$6s6d\,^3D_3$	40004	39966.09	0.1
$6s6d\,^1D_2$	40132	40061.51	0.2
$6s7p\,^1P^o_1$	38894	40563.97	4.1
$6s8s\,^3S_1$	41563	41615.04	0.1
$6s8s\,^1S_0$	41965	41939.90	0.06
$6p^2\,^3P_0$	43183	42436.91	1.8
$6s8p\,^3P^o_0$	43612	43614.27	<0.01
$6s8p\,^3P^o_1$	43618	43659.38	0.1
$6p^2\,^3P_1$	44471	43805.42	1.5
$6s8p\,^3P^o_2$	43797	43806.69	0.02
$6s8p\,^1P^o_1$	43861	44017.60	0.4
$6s7d\,^3D_1$	44611	44311.38	0.7
$6s7d\,^3D_2$	44496	44313.05	0.4
$6s7d\,^1D_2$	44583	44357.60	0.5
$6s7d\,^3D_3$	44569	44380.82	0.4
$6p^2\,^3P_2$	45768	44760.37	2.3

Table 2. Reduced electric-dipole transition matrix elements involving the $6s^2\,^1S_0$, $6s6p\,^3P^o_0$, and $6s6p\,^3P^o_1$ states (in unit a.u.) from the CI + MBPT method. Values from the CI+all-order calculation[16] and values deduced from the experimental measurements of lifetimes of atomic states are given wherever available.

Transition	CI + MBPT	CI + all-order	Exp.
$6s^2\,^1S_0$–$6s6p\,^3P^o_1$	0.58	0.571[16]	0.543(11)[26]
$6s^2\,^1S_0$–$6s6p\,^1P^o_1$	4.79	4.78[16]	4.148(2)[1]
$6s^2\,^1S_0$–$6s7p\,^3P^o_1$	0.08		
$6s^2\,^1S_0$–$6s7p\,^1P^o_1$	0.67	0.65[16]	
$6s^2\,^1S_0$–$6s8p\,^3P^o_1$	0.01		
$6s^2\,^1S_0$–$6s8p\,^1P^o_1$	0.21		
$6s^2\,^1S_0$–$4f^{13}5d6s^2\,(7/2,5/2)^o_1$			2.04(6)[27]
$6s6p\,^3P^o_0$–$5d6s\,^3D_1$	2.96	2.89[16]	
$6s6p\,^3P^o_0$–$6s6d\,^3D_1$	1.79	1.84[16]	
$6s6p\,^3P^o_0$–$6s7d\,^3D_1$	2.10		
$6s6p\,^3P^o_0$–$6s7s\,^3S_1$	1.95	1.95[16]	
$6s6p\,^3P^o_0$–$6s8s\,^3S_1$	0.62		
$6s6p\,^3P^o_0$–$6p^2\,^3P_1$	1.97		
$6s6p\,^3P^o_1$–$5d6s\,^3D_1$	2.57	2.51[34]	
$6s6p\,^3P^o_1$–$5d6s\,^3D_2$	4.45	4.35[34]	
$6s6p\,^3P^o_1$–$5d6s\,^1D_2$	0.46	0.453[34]	
$6s6p\,^3P^o_1$–$6s6d\,^3D_1$	1.57	1.62[34]	
$6s6p\,^3P^o_1$–$6s6d\,^3D_2$	2.72	2.78[34]	
$6s6p\,^3P^o_1$–$6s6d\,^1D_2$	0.53		
$6s6p\,^3P^o_1$–$6s7d\,^3D_1$	2.47		
$6s6p\,^3P^o_1$–$6s7d\,^3D_2$	1.67		
$6s6p\,^3P^o_1$–$6s7d\,^1D_2$	0.86		
$6s6p\,^3P^o_1$–$6s7s\,^3S_1$	3.47	3.46[34]	
$6s6p\,^3P^o_1$–$6s7s\,^1S_0$	0.24	0.243[34]	
$6s6p\,^3P^o_1$–$6s8s\,^3S_1$	1.00		
$6s6p\,^3P^o_1$–$6s8s\,^1S_0$	0.30		
$6s6p\,^3P^o_1$–$6p^2\,^3P_0$	2.59		
$6s6p\,^3P^o_1$–$6p^2\,^3P_1$	0.18		
$6s6p\,^3P^o_1$–$6p^2\,^3P_2$	2.92		

Next, in Table 2 we also give reduced E1 matrix elements (RME) of all the possible transitions among these states. We compare our CI + MBPT data of E1 matrix elements with the literature data. We find that our data are consistent with previously reported CI + all-order values[16] within an error of 2%. But, the large difference is found for the $6s^2\,^1S_0$–$6s6p\,^1P^o_1$ transition. From the lifetime measurement of the $6s6p\,^1P^o_1$ state, the RME of $6s^2\,^1S_0$–$6s6p\,^1P^o_1$ can be deduced very precisely. The experimental value is reported to be 4.184(2) a.u.,[16,17] while our CI + MBPT and also the CI + all-order values[16] are obtained to be about 4.78 a.u.–4.79 a.u. This difference is about 16% and has also been noted earlier.[15–17] The $4f^{13}nln'l'n''l''$ configurations are missed in the configuration-state-function space due to the limit of the computation model. The importance of the $4f^{13}nln'l'n''l''$ configurations has been discussed by Dzuba *et al.*,[15] who suggested that the large theory–experiment disagreement for the E1 matrix elements of the $6s^2\,^1S_0$–$6s6p\,^1P^o_1$ transition is due to the high mixing of the $6s6p\,^1P^o_1$ state with the core-excited state $4f^{13}5d6s^2\,(7/2,5/2)^o_1$. The $4f^{13}nln'l'n''l''$ configurations have been ruled out from the computational model space of

the divalence system that is used in our CI + MBPT method and the previous CI+all-order calculations. The considered $6s^2\,{}^1S_0$–$6s6p\,{}^1P^o_1$ transition contributes about 90% to the polarizability of the $6s^2\,{}^1S_0$ state, thus we decide to use the experimental value of the E1 matrix element for the $6s^2\,{}^1S_0$–$6s6p\,{}^1P^o_1$ transition instead of the results obtained by the CI + MBPT method, and at the same time we include the contribution of the $4f^{13}5d6s^2\,(7/2,5/2)^o_1$ states. The RME of $6s^2\,{}^1S_0$–$4f^{13}5d6s^2\,(7/2,5/2)^o_1$ is estimated in a similar way to that in Ref. [27] where the weighted mean of the E1 matrix element contribution to the lifetimes of five states[28] is determined.

Table 3. Breakdown of the contributions of static scalar polarizability α^S for $6s^2\,{}^1S_0$ state of Yb atom.

Polariz.	Contrib.	$\lvert\langle g\rVert D\rVert m\rangle\rvert$	α_i
$\alpha^S({}^1S_0)$	$6s6p\,{}^1P^o_1$	4.148(2)[26]	100.4(1)
	$6s6p\,{}^3P^o_1$	0.543(11)[1]	2.4(1)
	$6s7p\,{}^1P^o_1$	0.67	1.62
	$6s7p\,{}^3P^o_1$	0.08	0.021
	$6s8p\,{}^1P^o_1$	0.21	0.15
	$6s8p\,{}^3P^o_1$	0.014	0.0007
$4f^{13}5d6s^2(7/2,5/2)^o_1$		2.04(6)[27]	21.1(1.2)
	All others		2.04
	α_{core}		7.27(4)
	Total		135(3)
	Refs.		118(45),[17] 144.59,[18] 141(6),[15] 139(15),[29] 141(2),[16]
		$134.4\pm1.0<\alpha^S<144.2\pm1.0$[27]	

Table 4. Breakdown of the contributions of static scalar polarizabilities α^S for $6s6p\,{}^3P^o_0$ state of Yb atom.

Polariz.	Contrib.	$\lvert\langle g\rVert D\rVert m\rangle\rvert$	α_i
$\alpha^S({}^3P^o_0)$	$5d6s\,{}^3D_1$	2.96	177.95
	$6s6d\,{}^3D_1$	1.79	20.83
	$6s7d\,{}^3D_1$	2.10	23.86
	$6s7s\,{}^3S_1$	1.95	36.21
	$6s8s\,{}^3S_1$	0.62	2.28
	$6p^2\,{}^3P_1$	1.97	21.33
	All others		15.23
	α_{core}		7.27(4)
	Total		305(19)
	Refs.		302(14),[15] 293(10),[16]
		$280.1\pm1.0<\alpha^S<289.9\pm1.0$[27]	

In Tables 3, 4, and 5, we give the contributions from the intermediate states, respectively, to the static polarizabilities of the $6s^2\,{}^1S_0$, $6s6p\,{}^3P^o_0$, and $6s6p\,{}^3P^o_1$ states of the Yb atom. The energies are cited from the NIST data. The values of RMEs are cited from our CI + MBPT calculation except the RMEs of $6s^2\,{}^1S_0$–$6s6p\,{}^1P^o_1$, $6s^2\,{}^1S_0$–$6s6p\,{}^3P^o_1$, and $6s^2\,{}^1S_0$–$4f^{13}5d6s^2(7/2,5/2)^o_1$ are replaced with the experimental values as cited. Each contribution is given under "α_i" for the dominant valence states. The contribution from the core is given by "α_{core}". Again as argued by Dzuba *et al.*, due to the missing of the $4f^{13}nln'l'n''l''$ configurations discussed above it is necessary to include a more accurate core contribution than the random phase approximation (RPA) as in this case the excitation from the $4f_{7/2}$ to $5d_{5/2}$ states is important. Therefore, instead of the RPA result for 6.39 a.u.[15] for α_c, we have taken it as 7.27±0.04 a.u. from our finite field calculation of the polarizability in Yb^{2+}. The RCC theory automatically captures the correlation contribution for $4f_{7/2}\rightarrow 5d_{5/2}$. Our RCC value of α_c is about 15% larger than the previously reported RPA value, but it is in agreement with another RCC calculation obtained from the perturbative formulation.[33]

Table 5. Breakdown of the contributions of static scalar polarizability α^S and tensor polarizability α^T for $6s6p\,{}^3P^o_1$ state of Yb atom.

Polariz.	Contrib.	$\lvert\langle g\rVert D\rVert m\rangle\rvert$	α_i
$\alpha^S({}^3P^o_1)$	$6s^2\,{}^1S_0$	0.543(11)[1]	-0.80
	$5d6s\,{}^3D_1$	2.57	49.44
	$5d6s\,{}^3D_2$	4.45	142.96
	$5d6s\,{}^1D_2$	0.46	1.04
	$6s6d\,{}^3D_1$	1.57	5.54
	$6s6d\,{}^3D_2$	2.72	16.46
	$6s6d\,{}^1D_2$	0.53	0.62
	$6s7d\,{}^3D_1$	2.47	11.33
	$6s7d\,{}^3D_2$	1.67	5.14
	$6s7d\,{}^1D_2$	0.86	1.36
	$6s7s\,{}^3S_1$	3.47	39.91
	$6s7s\,{}^1S_0$	0.24	0.17
	$6s8s\,{}^3S_1$	1.00	2.06
	$6s8s\,{}^1S_0$	0.29	0.18
	$6p^2\,{}^3P_0$	2.59	13.43
	$6p^2\,{}^3P_1$	0.18	0.06
	$6p^2\,{}^3P_2$	2.92	15.59
	all others		16.87
	α_{core}		7.27(4)
	total		329(20)
	Refs.	278(15),[15] 315(11)[34]	
$\alpha^T({}^3P^o_1)$			24.0(1.5)
	Refs.	24.3(1.5),[17] 24.06(1.37),[30] 24.26(84),[31] 23.33(52)[32]	

In our calculations, the main uncertainty arises from the contributions from the neglected high-lying excited states and citations in the above table as "all others", which is estimated based on the known contributions of all other terms except the dominant ones, as given in previous CI + all-order calculations.[16,34] We assign the error caused by "all others" to be 50%. Such an assignment should be reasonable because the difference in the E1 matrix element between the CI + MBPT and CI + all-order methods is less than 2% for the excited states we calculated. Besides, through the comparison of our calculated E1 matrix element values with previous CI + all-order ones,[16,34] we include the additional 2% errors to the E1 matrix elements of the $6s^2\,{}^1S_0$–$6s6p\,{}^1P^o_1$, $6s^2\,{}^1S_0$–$6s6p\,{}^3P^o_1$, $6s^2\,{}^1S_0$–$4f^{13}5d6s^2\,(7/2,5/2)^o_1$ transitions. The errors in the "all others" contributions and our calculated E1 matrix elements are translated into the net uncertainties of the α^S values.

Finally, the values of α^S for the $6s^2\,{}^1S_0$, $6s6p\,{}^3P^o_0$, and $6s6p\,{}^3P^o_1$ states are determined to be 135(3) a.u., 305(19) a.u., and 329(20) a.u. respectively. Similarly, the tensor polarizability α^T for the $6s6p\,{}^3P^o_1$ state is determined to be 24.0(1.5) a.u. The ground state result agrees quite well with the other recent RCC calculation by using the perturbative approach.[7] It can be noted that the discussion about the static polarizability of the ground state of Yb is whether the electronic correlation arising from the $4f^{13}nln'l'n''l''$ configurations is important. In this work, our calculation with the contribution of $6s^2\,{}^1S_0$–$4f^{13}5d6s^2\,(7/2,5/2)^o_1$ transition added is just consistent with the RCC result.[7] This proves the importance of the electronic correlation from the $4f^{13}nln'l'n''l''$ configurations.

4. Conclusions

We have determined the scalar and tensor dipole polarizabilities of the $6s^2\,{}^1S_0$, $6s6p\,{}^3P^o_0$, and $6s6p\,{}^3P^o_1$ states of the ytterbium atom by a sum-over-states approach. These results will be quite useful for the theoretical and experimental studies using this atom. Accuracies of these results can be tested when the corresponding experimental results are available. We have estimated these quantities by the sum-over-states approach through dividing the total contributions into three major categories, i.e., valence–, core–, and valence–core correlation contributions. The dominant valence correlation contributions are evaluated using the accurate values of E1 matrix elements and experimental energies, and the core contributions are estimated by the finite field approach in the relativistic coupled-cluster theory. Our ground state result is in good agreement with other recent relativistic coupled-cluster theory calculations in the perturbative framework. We also compare our results for the excited states with previous theoretical results and find that they are in reasonable agreement with each other.

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