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Relativistic coupled-cluster studies of dipole polarizabilities in closed-shell atoms

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We investigate the role of electron correlation effects in the electric-dipole polarizabilities of the ground states of the alkaline earth metals, helium, and ytterbium by employing the relativistic coupled-cluster (RCC) theory. These effects are incorporated via the residual Coulomb interaction to all orders in the RCC singles and doubles approximations. The perturbed wave functions used in the calculations of the polarizabilities are obtained by directly solving the first-order perturbed RCC equations, thereby avoiding the sum-over-states approach. Our results are compared with other calculations and available experimental data.

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I. INTRODUCTION

Knowledge of electric-dipole polarizabilities is necessary in many areas of physics and chemistry. In particular, it is required in studies of collisions involving atoms and molecules [1]. In recent years, the preeminent role of polarizabilities in the determination of interatomic interactions has assumed special significance in the context of research on ultracold atoms [2].

Calculations of atomic polarizabilities have come a long way since the classic work of Dalgarno and Lewis [3]. Following a series of calculations using the coupled Hartree-Fock method (see, for example, [4]), a number of state-of-the-art methods including the coupled-cluster (CC) theory have been used to calculate atomic and molecular polarizabilities [5–7]. A few calculations of the polarizabilities of heavy atomic systems have been performed in the past few years using the linearized [8] as well as the nonlinearized [9] relativistic coupled-cluster (RCC) theory. These are based on approaches that sum over a set of intermediate states. Liu and Kelly used a coupled-cluster linear-response-based approach to calculate the static and dynamic polarizabilities of He [10]. In contrast, we have obtained the first-order perturbed wave function by solving the first-order perturbed CC equation and used it to obtain the dipole polarizabilities of the closed-shell alkaline earth metals, helium (He), and ytterbium (Yb). Information on these quantities is useful for frequency standards experiments that have been proposed for Mg [11], Ca [12], Sr [13], and Yb [11,14] as well as the search for the electric-dipole moment [15] and parity nonconservation experiments [16–18] in Yb.

There has been considerable interest in accurate calculations of the dipole polarizabilities of alkaline earth metals, He, and Yb. The dipole polarizability of He is available to high precision both experimentally [19] and theoretically [20]. Sadlej *et al.* have calculated these quantities for Ca, Sr, and Ba using a quasirelativistic approach, but their treatment of correlation is rigorous [21]. Their calculations have been carried out at the finite-order many-body perturbation theory and CC levels. Porsev and Derevianko have performed calculations of the dipole polarizabilities of Mg, Ca, Sr, and Yb using a hybrid approach involving many-body perturbation theory and the configuration-interaction method [11]. A calculation of the dipole polarizability of Yb based on the time-dependent density functional theory (TDDFT) has been reported recently [22].

II. THEORY AND METHOD OF CALCULATIONS

In a uniform dc electric field $\mathbf{E}=\mathcal{E}\hat{\mathbf{z}}$, the energy shift ΔE of the ground state $|\Psi_0^{(0)}(\pi,J_0,M_0)\rangle$ with the parity eigenvalue π and angular momentum $J_0=0$ and its azimuthal value $M_0=0$ is given by

$$\Delta E=-\frac{1}{2}\alpha\mathcal{E}^2, \tag{2.1}$$

where α is the static polarizability and can be expressed as

$$\alpha=-2\sum_I\frac{|\langle\Psi_0^{(0)}(\pi,J_0,M_0)|D_z|\Psi_I^{(0)}(\pi',J_I,M_I)\rangle|^2}{E_0-E_I}, \tag{2.2}$$

where the subscripts 0 and I represent ground and excited states of the Dirac-Coulomb (DC) Hamiltonian ($H_0^{(\mathrm{DC})}$), respectively, the superscript (0) represents unperturbed wave functions, D_z is the zth component of the electric-dipole operator, J_I and M_I are the angular momentum quantum numbers of the intermediate states, π and π' are the parity quantum numbers for states of opposite parity, and E_0 and E_I are the energies of the ground and intermediate states, respectively.

In a more explicit form, the above expression can be written as

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$$\begin{aligned}\alpha &= -2\sum_I \frac{\langle\Psi_0^{(0)}(\pi,J_0,M_0)|D_z|\Psi_I^{(0)}(\pi',J_I,M_I)\rangle\langle\Psi_I^{(0)}(\pi',J_I,M_I)|D_z|\Psi_0^{(0)}(\pi,J_0,M_0)\rangle}{E_0-E_I}\\ &= -\sum_I \frac{\langle\Psi_0^{(0)}(\pi,J_0,M_0)|D_z|\Psi_I^{(0)}(\pi',J_I,M_I)\rangle\langle\Psi_I^{(0)}(\pi',J_I,M_I)|D_z|\Psi_0^{(0)}(\pi,J_0,M_0)\rangle}{E_0-E_I}\\ &\quad -\sum_I \frac{\langle\Psi_I^{(0)}(\pi',J_I,M_I)|D_z|\Psi_0^{(0)}(\pi,J_0,M_0)\rangle\langle\Psi_I^{(0)}(\pi',J_I,M_I)|D_z|\Psi_0^{(0)}(\pi,J_0,M_0)\rangle}{E_0-E_I}\\ &= \langle\Psi_0^{(0)}(\pi,J_0,M_0)|D_z|\Psi_0^{(1)}(\pi',J',M')\rangle + \langle\Psi_0^{(1)}(\pi',J',M')|D_z|\Psi_0^{(0)}(\pi,J_0,M_0)\rangle = \langle\Psi_0|D_z|\Psi_0\rangle,\end{aligned} \tag{2.3}$$

where we define

$$|\Psi_0\rangle = |\Psi_0^{(0)}(\pi,J_0,M_0)\rangle + |\Psi_0^{(1)}(\pi',J',M')\rangle, \tag{2.4}$$

with $|\Psi_0^{(1)}(\pi',J',M')\rangle$ as the first-order correction with the angular momentum $J'(=1)$ and M' due to the operator D_z to the original unperturbed wave function, $|\Psi_0^{(0)}(\pi,J_0,M_0)\rangle$, in the presence of an external dc electric field and given by

$$|\Psi_0^{(1)}(\pi',J',M')\rangle = \sum_I |\Psi_I^{(0)}(\pi',J_I,M_I)\rangle \frac{\langle\Psi_I^{(0)}(\pi',J_I,M_I)|D_z|\Psi_0^{(0)}(\pi,J_0,M_0)\rangle}{E_0-E_I}\delta(J',J_I)\delta(M',M_I)\delta(M_0,M_I). \tag{2.5}$$

The first-order perturbed wave function $|\Psi_0^{(1)}(\pi',J',M')\rangle$ can be obtained using an approach that avoids explicitly summing over intermediate states.

A. Unperturbed wave function

Using the CC ansatz, the all-order unperturbed wave function $|\Psi_0^{(0)}(\pi,J_0,M_0)\rangle$ for closed-shell atoms can be expressed as [23]

$$|\Psi_0^{(0)}(\pi,J_0,M_0)\rangle = e^{T^{(0)}}|\Phi_0(\pi,J_0,M_0)\rangle, \tag{2.6}$$

where $|\Phi_0(\pi,J_0,M_0)\rangle$ are the Dirac-Fock (DF) wave functions determined using the mean-field approximation and $T^{(0)}$ are the electron excitation operators due to Coulomb interaction from the corresponding DF states.

In the present work, we have considered all possible single and double excitations (CCSD approach) in the calculations. We obtain the $T^{(0)}$ amplitudes by solving the following equations using the Jacobi iterative method:

$$\langle\Phi_0^*|\overline{H_N^{(\mathrm{DC})}}|\Phi_0\rangle = 0, \tag{2.7}$$

where $|\Phi_0^*\rangle$ represents the singly and doubly excited states with respect to $|\Phi_0\rangle$, the subscript N represents the normal-order form of the operators, and we have defined $\bar{H}=e^{-T^{(0)}}He^{T^{(0)}}=(He^{T^{(0)}})_{\mathrm{con}}$, with the subscript "con" representing connected terms.

B. First-order perturbed wave function

To obtain the $|\Psi_0^{(1)}(\pi',J',M')\rangle$, we proceed as follows.

Let us operate $(H_0^{(\mathrm{DC})}-E_0)$ on both sides of Eq. (2.5); i.e.,

$$\begin{aligned}(H_0^{(\mathrm{DC})}-E_0)|\Psi_0^{(1)}(\pi',J',M')\rangle &= \sum_I (H_0^{(\mathrm{DC})}-E_0)|\Psi_I^{(0)}(\pi',J_I,M_I)\rangle\frac{\langle\Psi_I^{(0)}(\pi',J_I,M_I)|D_z|\Psi_0^{(0)}(\pi,J_0,M_0)\rangle}{E_0-E_I}\\ &= \sum_I (E_I-E_0)|\Psi_I^{(0)}(\pi',J_I,M_I)\rangle\frac{\langle\Psi_I^{(0)}(\pi',J_I,M_I)|D_z|\Psi_0^{(0)}(\pi,J_0,M_0)\rangle}{E_0-E_I}\\ &= -\sum_I |\Psi_I^{(0)}(\pi',J_I,M_I)\rangle\langle\Psi_I^{(0)}(\pi',J_I,M_I)|D_z|\Psi_0^{(0)}(\pi,J_0,M_0)\rangle.\end{aligned} \tag{2.8}$$

Using the completeness principle of the atomic states of the DC Hamiltonian, $\Sigma_\alpha|\Psi_\alpha^{(0)}\rangle\langle\Psi_\alpha^{(0)}|=1$, we get

$$\sum_I |\Psi_I^{(0)}(\pi',J_I,M_I)\rangle\langle\Psi_I^{(0)}(\pi',J_I,M_I)| = 1 - \sum_{K\neq I}|\Psi_K^{(0)}(\pi,J_K,M_K)\rangle\langle\Psi_K^{(0)}(\pi,J_K,M_K)|. \tag{2.9}$$

Substituting Eq. (2.9) into Eq. (2.8), we get

$$
\begin{aligned}
(H_0^{(\mathrm{DC})} - E_0)|\Psi_0^{(1)}(\pi',J',M')\rangle &= - D_z|\Psi_0^{(0)}(\pi,J_0,M_0)\rangle + \sum_K |\Psi_K^{(0)}(\pi,J_K,M_K)\rangle\langle\Psi_K^{(0)}(\pi,J_K,M_K)|D_z|\Psi_0^{(0)}(\pi,J_0,M_0)\rangle \\
&= - D_z|\Psi_0^{(0)}(\pi,J_0,M_0)\rangle, \qquad (2.10)
\end{aligned}
$$

where the second term does not contribute since $|\Psi_K^{(0)}(\pi,J_K,M_K)\rangle$ and $|\Psi_0^{(0)}(\pi,J_0,M_0)\rangle$ have the same parity.

The above equation represents a first-order perturbed equation with D_z as the perturbation and the first-order energy equal to zero. The unperturbed wave function is represented by $|\Psi_0^{(0)}(\pi,J_0,M_0)\rangle$, and $|\Psi_0^{(1)}(\pi',J',M')\rangle$ is its first-order correction. In order to obtain the solution for $|\Psi_0^{(1)}(\pi',J',M')\rangle$, we solve Eq. (2.10) using the following (R)CC approach.

Using the above CC ansatz for closed-shell atoms, we can express the total wave function $|\Psi_0\rangle$, which is of mixed parity and angular momentum, by

$$|\Psi_0\rangle = e^{T}|\Phi_0(\pi,J_0,M_0)\rangle, \qquad (2.11)$$

where we define now

$$T = T^{(0)} + T^{(1)}, \qquad (2.12)$$

with $T^{(1)}$ representing the excitation operators containing all orders in the Coulomb interaction and one order in D_z. Substituting Eq. (2.12) into Eq. (2.11), we get

$$|\Psi_0\rangle = e^{T^{(0)}+T^{(1)}}|\Phi_0(\pi,J_0,M_0)\rangle = e^{T^{(0)}}(1 + T^{(1)})|\Phi_0(\pi,J_0,M_0)\rangle, \qquad (2.13)$$

where only terms up to linear in $T^{(1)}$—i.e., those terms up to one order in D_z—are retained.

It is clear from Eq. (2.13) that the first-order perturbed wave function can now be written as

$$|\Psi_0^{(1)}(\pi',J',M')\rangle = e^{T^{(0)}}T^{(1)}|\Phi_0(\pi,J_0,M_0)\rangle. \qquad (2.14)$$

The $T^{(1)}$ amplitudes are determined using the equations

$$\langle\Phi_0^{*}|\overline{H_0^{(\mathrm{DC})}}T^{(1)}|\Phi_0\rangle = - \langle\Phi_0^{*}|\overline{D_z}|\Phi_0\rangle, \qquad (2.15)$$

where have used the relation $\bar{O}=e^{-T^{(0)}}Oe^{T^{(0)}}=(Oe^{T^{(0)}})_{\mathrm{con}}$. A detailed description for evaluating these amplitudes and the corresponding Goldstone diagrams in the closed-shell and one valence systems are given elsewhere [24,25].

C. (R)CC expression for α

Using Eqs. (2.6) and (2.14), the expression for the polarizabilities using the (R)CC operators can be expressed as

$$
\begin{aligned}
\alpha &= \frac{\langle\Phi_0|e^{T^{\dagger}}D_z e^{T}|\Phi_n\rangle}{\langle\Phi_0|e^{T^{\dagger}}e^{T}|\Phi_0\rangle} \\
&= \frac{\langle\Phi_0|(T^{(1)^{\dagger}}\overbrace{D_z^{(0)}} + \overbrace{D_z^{(0)}}T^{(1)})|\Phi_0\rangle}{\mathcal{N}_0}, \qquad (2.16)
\end{aligned}
$$

where for computational simplicity we define $\overbrace{D_z^{(0)}}=e^{T^{(0)^{\dagger}}}D_z e^{T^{(0)}}$ and $\mathcal{N}_0=\langle\Phi_0|e^{T^{(0)^{\dagger}}}e^{T^{(0)}}|\Phi_0\rangle$. We compute these terms by expressing them as effective one-body and two-body terms using the generalized Wick's theorem [26].

III. RESULTS AND DISCUSSIONS

In Table I, we present our results of electric-dipole polarizabilities and compare them with those available in the literature. The error bars in the experimental results are large for all the systems except in He, and our results lie within them. The results of the calculations that are given in Table I are obtained using a variety of many-body theories. Our results are in reasonable agreement with most of them. We have also estimated the contributions from the important triple excitations in addition to the CCSD contributions and taken them as the upper limits of the errors associated in our calculations. They are mentioned in the parentheses next to our results presented in Table I.

There are several calculations of the ground-state He polarizability available using different methods, and some of them have also included certain QED contributions [20]. Similarly, a number of precise measurements are listed in [20] among which the latest result is reported in [19]. It is therefore desirable to calculate He polarizability using our method. A linear response approach derived from time-dependent CC theory was also earlier used by Liu and Kelly

TABLE I. Static dipole polarizabilities in divalent atoms He, Be, Mg, Ca, Sr, Ba, and Yb (in a.u.). Results from this work are based on the CCSD method and contributions from important triple excitations given as error bars in the parentheses.

Atoms	Expt.	Others	This work
He	1.383746(7)[a]	1.383193,[b] 1.389[c]	1.382(1)
Be		37.755,[d] 37.69,[e] 37.9[f]	37.80(47)
Mg	71.5(3.1)[g]	71.35,[e] 72.0,[f] 71.3(7)[h]	73.41(2.32)
Ca	169(17)[g]	159.4,[e] 152.7,[g] 157.1(1.3),[h] 152,[i] 158.0[j]	154.58(5.42)
Sr	186(15)[g]	201.2,[e] 193.2,[f] 197.2(2),[h] 190,[i] 198.9[j]	199.71(7.28)
Ba	268(22)[k]	264,[l] 273,[i] 273.9[j]	268.19(8.74)
Yb	142(36)[m]	111.3(5),[h] 141.7,[n] 157.30[o]	144.59(5.64)

[a] Reference [19].
[b] Reference [20].
[c] Reference [10].
[d] Reference [33].
[e] Reference [27].
[f] Reference [34].
[g] Reference [35].
[h] Reference [11].
[i] Reference [21].
[j] Reference [30].
[k] Reference [36].
[l] Reference [29].
[m] Reference [37].
[n] Reference [31].
[o] Reference [22].

TABLE II. Contributions from DF and important perturbed CC terms (in a.u.) for the dipole polarizabilities.

Atoms	DF	$(\overline{D}_zT_1^{(1)}$+c.c.)-DF	$\overline{D}_zT_2^{(1)}$+c.c.	$\mathcal{N}_0$
He	1.495	1.376	0.005	-0.1×10^{-4}
Be	45.82	−7.94	−0.09	0.02
Mg	82.44	−8.77	−0.21	0.03
Ca	184.14	−29.23	−0.07	−0.26
Sr	234.41	−34.46	−0.17	−0.08
Ba	328.32	−61.18	0.09	0.81
Yb	183.32	−39.86	0.032	1.10

[10] to determine static and dynamic polarizabilities of the ground state of He. This is different from our approach where an expectation value of the electric-dipole operator is evaluated using first-order electric-dipole perturbed wave functions. Our formulation as described earlier is based on the time-independent coupled-cluster theory. From Table I, it is evident that our result is in good agreement with both high-precision calculations and measurements. Mitroy and Bromley [27] have used oscillator strengths from a semiempirical approach to obtain the polarizabilities. Some results based on an *ab initio* method that combines the configuration-interaction (CI) method and many-body perturbation theory (MBPT) are available [11,28,29]. In these calculations, the valence-electron correlation effects are evaluated by the CI method, whereas the core-electron correlation effects are calculated using the MBPT method. However, these calculations consider the core-polarization effects in the framework of finite-order MBPT, while our CC method takes them into account to all orders. Lim and Schwerdtfeger employed the scalar-relativistic Douglas-Kroll Hamiltonian to determine some of these quantities [30]. In these calculations, they showed the importance of relativistic effects. There are also a few calculations available for the Yb polarizabilities using the CC method [31,32], where the atomic orbitals are evaluated using the molecular symmetries. Recently TDDFT was used for calculating the same quantities [22], but this method treats exchange and correlation effects via local potentials. The main difference between the methods on which all these calculations are based and ours is that we calculate both the unperturbed and the first-order perturbed wave functions using a RCC approach that implicitly takes into consideration all the intermediate states.

To emphasize the importance of correlation effects in these calculations, we present the DF and the leading RCC contributions in Table II for the electric-dipole polarizabilities. For all the cases that have been considered, the DF results are larger than the total results. From the individual RCC contributions, we find that only the terms arising from $\overline{D}_zT_1^{(1)}$ and its conjugate (c.c.) are significant. Given that these terms include the DF, leading core-polarization, and other important correlation effects to all orders, it is not surprising that they should collectively make up the largest contribution. In Fig. 1, we give the breakdown of $\overline{D}_zT_1^{(1)}$ in terms of the DF, random phase approximation (RPA), and other diagrams. All the above-mentioned calculations where these terms have been evaluated are based on finite-order MBPT, but in our present method, we treat them to all orders in the residual Coulomb interaction. The $^3P_1$ and $^1P_1$ configurations are of crucial importance for the leading term of $\overline{D}_zT_1^{(1)}$ and its conjugate.

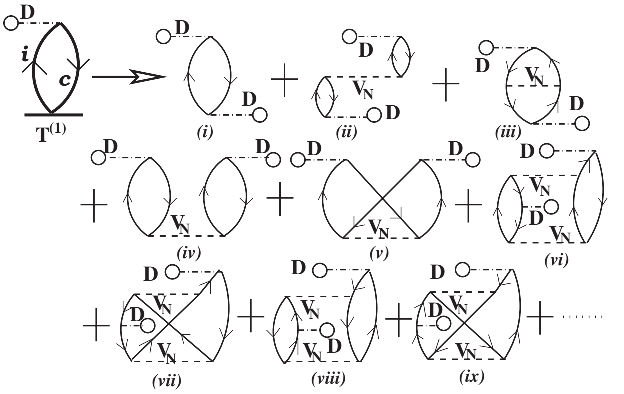

FIG. 1. Breakdown of the $\overline{D}_zT_1^{(1)}$ CC diagram in terms of lower-order MBPT and RPA diagrams that contribute significantly to the polarizability calculations. Here, D_z and V_N represent the dipole and normal-order Coulomb interaction operators which are shown as single dotted and dashed lines, respectively. The notations c and i represent the occupied and unoccupied orbitals, respectively, of the considered systems.

IV. CONCLUSION

We have carried out calculations of electric-dipole polarizabilities for many alkaline earth metals, helium, and ytterbium using the RCC method and highlighted the importance of the correlation effects. These calculations avoid the sum-over-states approach in determining polarizabilities and implicitly consider all the intermediate states by solving the perturbed RCC wave function to first order in the dipole and all orders in the residual Coulomb interaction.

Note added. We recently became aware of a recent calculation of the polarizability of the ground state of Yb [38]. It was performed using full and approximate relativistic *ab initio* methods, and the result is in good agreement with ours.

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[1] T. M. Miller and B. Bederson, Adv. At. Mol. Phys. **13**, 1 (1977).

[2] C. J. Pethick and H. Smith, *Bose-Einstein Condenstaion in Dilute Gases* (Cambridge University Press, Cambridge, England, 2002).

[3] A. Dalgarno and J. T. Lewis, Proc. R. Soc. London, Ser. A **233**, 70 (1955).

[4] A. Dalgarno and H. A. J. McIntyre, Proc. Phys. Soc. **85**, 47 (1965).

[5] B. Kundu and D. Mukherjee, Chem. Phys. Lett. **179**, 468 (1991).

[6] J. F. Stanton and R. J. Bartlett, J. Chem. Phys. **99**, 5178 (1993).

[7] M. Kallay and J. Gauss, J. Mol. Struct.: THEOCHEM **768**, 71 (2006).

[8] U. I. Safronova, W. R. Johnson, and M. S. Safronova, Phys. Rev. A **76**, 042504 (2007).

[9] B. K. Sahoo, B. P. Das, R. K. Chaudhuri, D. Mukherjee, R. G. E. Timmermans and K. Jungmann, Phys. Rev. A **76**, 040504(R) (2007).

[10] Z. W. Liu and H. P. Kelly, Theor. Chim. Acta **80**, 307 (1991).

[11] S. G. Porsev and A. Derevianko, Phys. Rev. A **74**, 020502(R) (2006).

[12] C. Degenhardt *et al.*, Phys. Rev. A **72**, 062111 (2005).

[13] M. M. Boyd, A. D. Ludlow, S. Blatt, S. M. Foreman, T. Ido, T. Zelevinsky, and J. Ye, Phys. Rev. Lett. **98**, 083002 (2007).

[14] Z. W. Barber, C. W. Hoyt, C. W. Oates, L. Hollberg, A. V. Taichenachev, and V. I. Yudin, Phys. Rev. Lett. **96**, 083002 (2006).

[15] Y. Takahashi *et al.* (unpublished).

[16] D. DeMille, Phys. Rev. Lett. **74**, 4165 (1995).

[17] C. J. Bowers, D. Budker, S. J. Freedman, G. Gwinner, J. E. Stalnaker, and D. DeMille, Phys. Rev. A **59**, 3513 (1999).

[18] K. Tsigutkin, J. E. Stalnaker, D. Budker, S. J. Freedman, and V. V. Yashchuk, in *From Parity Violation to Hadronic Structure and more …*, edited by K. de Jager *et al.* (Springer-Verlag, Berlin, 2007).

[19] K. Grohman and H. Luther, *Temperature—Its Measurement and Control in Science and Industry* (AIP, New York, 1992), Vol. 6, p. 21.

[20] M. Masili and A. F. Starace, Phys. Rev. A **68**, 012508 (2003), and references therein.

[21] A. J. Sadlej, M. Urban, and O. Gropen, Phys. Rev. A **44**, 5547 (1991).

[22] X. Chu, A. Dalgarno, and G. C. Groenenboom, Phys. Rev. A **75**, 032723 (2007).

[23] J. Cizek, J. Chem. Phys. **45**, 4256 (1966).

[24] B. K. Sahoo, B. P. Das. R. K. Chaudhuri, and D. Mukherjee, J. Comput. Methods Sci. Eng. **7**, 57 (2007).

[25] B. K. Sahoo, Chem. Phys. Lett. **448**, 144 (2007).

[26] I. Lindgen and J. Morrison, in *Atomic Many-Body Theory*, edited by G. Ecker, P. Lambropoulos, and H. Walther (Springer-Verlag, Berlin, 1985).

[27] J. Mitroy and M. W. J. Bromley, Phys. Rev. A **68**, 052714 (2003).

[28] S. G. Porsev, Y. G. Rakhlina, and M. G. Kozlov, Phys. Rev. A **60**, 2781 (1999).

[29] M. G. Kozlov and S. G. Porsev, Eur. Phys. J. D **5**, 59 (1999).

[30] I. S. Lim and P. Schwerdtfeger, Phys. Rev. A **70**, 062501 (2004).

[31] A. A. Buchachenko, M. M. Szczesniak, and G. Chalasinski, J. Chem. Phys. **124**, 114301 (2006).

[32] Y. Wang and M. Dolg, Theor. Chem. Acc. **100**, 124 (1998).

[33] J. Komasa, Phys. Rev. A **65**, 012506 (2001).

[34] S. H. Patil, J. Phys. D **10**, 341 (2000).

[35] T. M. Miller, *Atomic and Molecular Polarizabilities* (CRC Press, Boca Raton, FL, 1995), Vol. 76, p. 10.

[36] H. L. Schwartz, T. M. Miller, and B. Bederson, Phys. Rev. A **10**, 1924 (1974).

[37] T. M. Miller, in *CRC Handbook of Chemistry and Physics*, 77th ed., edited by D. R. Lide (CRC Press, Boca Raton, FL, 1996).

[38] P. Zhang and A. Dalgarno, J. Phys. Chem. A **111**, 12471 (2007).