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Two-dipole and three-dipole dispersion coefficients for interaction of alkaline-earth-metal atoms with alkaline-earth-metal atoms and alkaline-earth-metal ions

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Apropos of the growing interest in the study of long-range interactions for their applications in cold-atom physics, we perform theoretical calculations for the two-dipole C_6 and three-dipole C_9 dispersion coefficients involving alkaline-earth-metal atoms with alkaline-earth-metal atoms and alkaline-earth-metal ions. The C_6 and C_9 coefficients are expressed in terms of the dynamic dipole polarizabilities, which are calculated using relativistic methods. Thereafter, the calculated C_6 coefficients for the considered alkaline-earth-metal atoms are compared with previously reported values. Due to unavailability of any other earlier theoretical or experimental results, for the C_6 coefficients for alkaline-earth-metal atoms with alkaline-earth-metal ions and the C_9 coefficients we perform separate fitting calculations and compare the results. Our calculations match in an excellent manner with the fitting calculations. We also report the oscillator strengths for the leading transitions and static dipole polarizabilities for the ground states of the alkaline-earth-metal ions, i.e., Be^+, Mg^+, Ca^+, Sr^+, and Ba^+, as well as the alkaline-earth-metal atoms, i.e., Be, Mg, Ca, Sr, and Ba. These show good agreement when compared with the available experimental results.

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I. INTRODUCTION

Laser-cooled atoms and ions have been the subject of several recent investigations covering many aspects of ultracold-atom physics. Accurate knowledge of the long-range part of an interatomic interaction between cooled atoms and ions can be viewed as the cornerstone of research on atom-ion hybrid traps [1,2], experiments on photoassociation [3,4], determination of scattering lengths, fluorescence spectroscopy, analysis of Feshbach resonances, probing extra dimensions to accommodate Newtonian gravity in quantum mechanics, determination of stability of Bose-Einstein condensates, etc. [5–9]. The study of long-range interaction is of special interest for low-temperature collisions [2,10–18] and is quite important in the determination of collisional frequency shift. In various works it has been proposed that controlled ion-atom cold collisions can be used for future quantum information processing [19,20]. Further, the investigation of the long-range interaction yields vital information which helps in the understanding of the different aspects of the ion-atom bound state [21], charge-transfer processes [12,13,16,17,22], spin-exchange reactions, and formation of cold molecular ions [23,24].

The long-range interaction potential is mostly expressed in a power series of the inverse of the interatomic separation R. The leading R^{-6} term in this series representation is called the dispersion term, with coefficient C_6, which is of particular interest when the two atomic species are considered. In contrast, the term with coefficient C_9 is regarded as the main contributor to the nonadditive part of the interaction energy among three atomic species. The first theoretical study on ion-atom interactions goes back to the approach given by Langevin [25] and Margenau [26]. Since then, a number of theoretical approaches have been reported. In a recent review, Koutselos and Mason [27] summarized data on ion-atom dispersion C_6 coefficients using the Slater-Kirkwood formula. Ahlrichs *et al.* [28] also used the same method to calculate dispersion coefficients for Li^+, Na^+, K^+, P^-, and Cl^- ions interacting with He, Ne, and Ar atoms and found good agreement between the experimental and theoretical results. Koutselos *et al.* [29] determined interaction potentials from the universal interaction curves between the noble-gas–noble-gas, alkali-metal-ion–noble-gas, and halogen-ion–noble-gas interactions, which agree well with the experimentally determined potentials. They also successfully reproduced the measured diffusion coefficients and ion mobilities. Mitroy and Zhang [30] calculated long-range dispersion coefficients for Mg^+ and Ca^+ interacting with a number of atoms by using the sum rule. Tang *et al.* [31] evaluated C_6 coefficients for the ground and excited states of Li, Li^+, and Be^+ interacting with He, Ne, Ar, Kr, and Xe atoms in their ground states. They used the variational Hylleraas method to determine the necessary list of multipole matrix elements. Singh *et al.* [32] reported the long-range dispersion coefficients for the interaction of inert-gas atoms with alkali-metal atoms as well as alkaline-earth-metal and alkali-metal ions. They employed the relativistic coupled-cluster method to estimate the dynamic dipole and quadrupole polarizabilities of the alkali-metal atoms and singly ionized alkaline-earth-metal atoms, whereas a

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relativistic random-phase approximation approach was taken to determine these quantities for the closed-shell configured inert gas atom and singly ionized alkali-metal and doubly ionized alkaline-earth-metal ions. The accuracy of these results was checked by comparing their static polarizability values with the experimental results. Gould and Bucko [33] obtained a dispersion coefficient between rare-gas atoms and ions by implementing time-dependent density-functional theory with exchange kernels. They first calculated frequency-dependent dipole polarizabilities for atoms and ions and then integrated them over frequency to produce C_6 coefficients.

In addition to the above-mentioned theoretical studies for long-range ion-atom interactions, there are several experimental studies which have been performed on ion-atom interactions to understand the nature of force between ultracold atoms and ions in hybrid ion-atom traps and some of these are described here. Smith *et al.* [1] successfully constructed a hybrid ion-atom trap which was designed to cotrap laser-cooled Ca^+ ions along with cold Na atoms. The first experiment on ion-atom cold collisions was reported by Grier *et al.* [34] for an alkaline-earth-metal-like system, viz., Yb $+Yb^+$ at energies ranging from 35 mK to 45 K. Next, heteronuclear Yb^+-Ca collisions were investigated by Zipkes *et al.* [2,35] in the range of 0.2–5 K. Hall *et al.* [36,37] performed an experiment on cold reactive collisions among laser-cooled ions and atoms. Sullivan *et al.* [38] studied the collision of Ba^+ ions with Ca atoms, in which the charge-exchange process is energetically prohibited unless Ca is electronically excited by the cooling laser. Ravi *et al.* [39] investigated the cooling of the Rb^+ ion by Rb atoms, where they experimentally demonstrated that rubidium ions cool in contact with magneto-optically trapped rubidium atoms, unlike the general expectation of ion heating. The cooling process is described theoretically and justified with numerical simulations, which involves resonant charge exchange collisions. Lee *et al.* [40] also investigated the same system, i.e., $Rb^+ + Rb$, where the ions were produced directly from the atomic cloud by two-photon ionization. The use of such an alkaline-earth-metal molecular ionic system helps to examine the distinct processes that are essential for quantum information storage [41,42].

Besides the two-body dipole interaction, the three-body dipole interaction has also been of immense interest for the past few decades. The first few studies on three-dipole interactions were by Axilrod and Teller [43] and Muto [44]. Axilrod and Teller [43] predicted the order of magnitude of the C_9 coefficient and Muto [44] evaluated its value by using a simple atomic model. Later, Axilrod [45] also used a simplified atomic model to compute C_9 coefficients, which were in agreement with those of Muto [44]. Further, Marinescu and Starace [46] investigated the nonadditive part of the long-range interaction by implementing nondegenerate perturbation theory up to third order and calculated the dispersion coefficients C_9 for three alkali-metal atoms interacting through their electric dipole moments. Both the homonuclear and heteronuclear cases were studied in this work. Patil and Tang [47] studied two- and three-body dispersion coefficients for the alkali-metal isoelectronic sequence. They calculated multipolar matrix elements by using simple wave functions, which were based on the asymptotic behavior and binding energies of the valence electron. These matrix elements allowed them to evaluate polarizabilities and dispersion coefficients of heteronuclear and homonuclear interactions from C_6 to C_{24}. Anatole von Lilienfeld and Tkatchenko [48] presented a numerical estimation of the leading two- and three-body dispersion energy terms in van der Waals interactions for a broad range of molecules and solids. These calculations were based on Axilrod-Teller-Muto and London expressions where the required dispersion coefficients C_6 and C_9, are evaluated from the electron density. These coefficients were investigated by Huang and Sun [49] using a variational stable method of Gao and Starace [50], as well as the simple ground-state wave function of the valence electron previously suggested by Patil and Tang [47].

Ultracold alkaline-earth-metal atoms are widely used in precision measurements and quantum simulation studies. Due to their unique atomic structure, they can be used to investigate quantum many-body system problems, such as the simulation of synthetic gauge fields, Kondo physics, and $SU(N)$ physics. However, to thoroughly explore the potential of ultracold alkaline-earth-metal atoms, these systems need to be studied in detail [51]. Interestingly, recent developments in the experimental methods have opened the way for combining ultracold trapped ions and atoms in a single experimental setup [52,53]. Most of the ion-atom experiments use alkaline-earth-metal ions trapped and laser cooled in a Paul trap immersed in ultracold neutral alkali-metal or alkaline-earth-metal atoms trapped in magnetic, magneto-optical, or dipole traps [20,54–57].

Several cold atomic ion-atom combinations have already been experimentally investigated [55,57], including Ca atoms and Ba^+ ions, confined in a hybrid trap [38]. In addition, the interactions and chemical reactions between the neutral alkaline-earth metal (A) and ionic alkaline-earth metal (B) are also being studied for diatomic AB^+ and triatomic A_2B^+ systems [57,58]. Due to the recent developments in the research field, there is a growing interest worldwide in investigating these systems, both experimentally and theoretically. With this motivation, we have carried out a thorough theoretical study of the long-range (C_6 and C_9) atom-ion interactions between the alkaline-earth-metal atoms and their ions.

In the present work we determine the two-dipole C_6 coefficients among Be, Mg, Ca, Sr, and Ba alkaline-earth-metal atoms and among Be^+, Mg^+, Ca^+, Sr^+, and Ba^+ alkaline-earth-metal ions. Also, the three-dipole C_9 coefficients for the interaction between three alkaline-earth-metal atoms, as well as two alkaline-earth-metal atoms with the alkaline-earth-metal ions, are evaluated. Despite their importance, the dispersion coefficients of these systems have not been explored experimentally or theoretically to date; therefore, we cannot compare our calculated data with the literature. To ascertain the reliability of our calculation procedure and the accuracy of the obtained results, we have calculated the dispersion coefficients C_6 for the homonuclear alkaline-earth-metal atoms and compared them with the previously available results [59–63].

In order to obtain these dispersion coefficients, we have employed relativistic methods to calculate dynamic dipole polarizabilities of atoms and ions. For this purpose, the oscillator strength of the leading transitions in alkaline-earth-metal ions and atoms are calculated and compared with data from the

National Institute of Standards and Technology (NIST) [64] as well as other [65–74] values. Results are also reported for ground-state polarizability and their comparison is presented with other calculations [60,75–78] and measurements [79–85] wherever available. Finally, C_6 coefficients for homonuclear dimers of alkaline-earth-metal atoms are compared with other results [62,63], whereas for C_6 and C_9 values of the remaining combinations we have used the approximate fitting models to verify our results.

The paper is organized as follows. In Sec. II we give a brief overview of the theoretical methodology employed in the present work. Our results are presented and discussed in Sec. III. Finally, a summary is given in Sec. IV. We have used atomic units (a.u.) throughout the paper unless stated otherwise.

II. THEORETICAL CALCULATION

A. Dispersion coefficients

The long-range van der Waals interaction among three atomic species in ground states is given by

$$\begin{aligned} V(\vec{R}_{12},\vec{R}_{23},\vec{R}_{31}) = &-\frac{C_6^{(12)}}{R_{12}^6}-\frac{C_8^{(12)}}{R_{12}^8}-\cdots-\frac{C_6^{(23)}}{R_{23}^6}-\frac{C_8^{(23)}}{R_{23}^8}\\ &-\cdots-\frac{C_6^{(31)}}{R_{31}^6}-\frac{C_8^{(31)}}{R_{31}^8}-\cdots\\ &+(1+3\cos\theta_1\cos\theta_2\cos\theta_3)\frac{C_9^{123}}{R_{12}^3R_{23}^3R_{31}^3}, \end{aligned} \tag{1}$$

where the $C_6^{(ij)}$ and $C_9^{(ijk)}$ parameters are the dispersion coefficients for two-body and three-body interactions, respectively, with $i, j, k = 1, 2, 3$, and R_{ij} is the interatomic distance between the ith and jth atomic systems. The angle θ_k is defined as $\cos\theta_k = -\hat{R}_{ik}\cdot\hat{R}_{kj}$. The leading contributor to the potential is from the C_6 terms, which are defined in terms of dipole polarizabilities $\alpha_i(i\omega)$ as

$$C_6^{(ij)} = \frac{3}{\pi}\int_0^\infty d\omega\,\alpha_i(i\omega)\alpha_j(i\omega). \tag{2}$$

The last term of Eq. (1) is the lowest order of the inverse powers to the internuclear distances in the third-order correction to the ground-state energy and it is a three-body interaction term which is given by [46]

$$C_9^{(ijk)} = \frac{3}{\pi}\int_0^\infty d\omega\,\alpha_i(i\omega)\alpha_j(i\omega)\alpha_k(i\omega). \tag{3}$$

Note that this term has a different sign from those of the other pair interaction terms in Eq. (1) and is thus called the nonadditive part of the long-range interaction potential. It is multiplied by an angle-dependent factor which is positive for $\max(\theta_1,\theta_2,\theta_3) < 117^\circ$ and negative for $\max(\theta_1,\theta_2,\theta_3) > 126^\circ$ [46]. In the present work, we determine the C_6 and C_9 coefficients using the *ab initio* methods as given by Eqs. (2) and (3).

In addition, we also calculate these coefficients using simple fitting formulas for comparison purposes. Since it is cumbersome to determine polarizabilities for a sufficiently large number of frequencies, instead of using the exact *ab initio* method, alternative fitting methods have been adopted to calculate the C_6 coefficients in the literature. Among these the Slater-Kirkwood formula [86] is one of the most frequently used methods in which the dispersion coefficients for the atom-ion system are approximated by

$$C_6^{(ij)} = \frac{3}{2}\frac{\alpha_i\alpha_j}{(\alpha_i/N_i)^{1/2}+(\alpha_j/N_j)^{1/2}}, \tag{4}$$

where N_i and N_j are the effective numbers of electrons in the ith and jth atomic systems, respectively; both can be determined using an empirical formula which assumes that the dominant contributions arise from the loosely bound electrons present in the outer shell of the systems

$$(N_i)^{1/2} = \tfrac{4}{3}C_6^{(ii)}\big/(\alpha_i)^{3/2}, \tag{5}$$

with the van der Waals coefficient C_6^{ii} of the homonuclear dimer and static polarizability α_i of the atom i. Substituting the above relation, we get

$$C_6^{(ij)} = \frac{2C_6^{(ii)}C_6^{(jj)}}{\big(\frac{\alpha_j}{\alpha_i}\big)C_6^{(ii)}+\big(\frac{\alpha_i}{\alpha_j}\big)C_6^{(jj)}}. \tag{6}$$

This formula has been extensively tested by Kramer and Herschbach [87] and found to give a quite good estimate of the C_6 coefficients. Similarly, the nonadditive C_9 coefficients for the atomic three-dipole dispersion coefficient can be obtained by using an approximate fitting through the expression derived by Midzuno and Kihara [88],

$$C_9^{(iii)} = \tfrac{3}{4}\alpha_i(0)C_6^{(ii)}, \tag{7}$$

and for the general case of three different atoms they obtain

$$C_9^{(ijk)} = \frac{2Q^iQ^jQ^k(Q^i+Q^j+Q^k)}{(Q^i+Q^j)(Q^j+Q^k)(Q^k+Q^i)}, \tag{8}$$

where [89]

$$Q^i = \frac{\alpha_j(0)\alpha_k(0)}{\alpha_i(0)}C_6^{(ii)}. \tag{9}$$

Nevertheless, both the above fitting formulas (6) and (8) are only valid and suitable for the qualitative description of the ion-atom dispersion coefficients, but it is imperative to use more accurate values of polarizabilities for the precise description of the ion-atom dispersion coefficients. In the present work, we determine these quantities for the alkaline-earth-metal ions and alkaline-earth-metal atoms using the *ab initio* methods as given by Eqs. (2) and (3) and further compare these coefficients with the values obtained using the Slater-Kirkwood formula (6) and with the approximations (7) and (8) used by Midzuno and Kihara [88], which we refer to as the fitted values in our discussion. Moreover, we also determine the oscillator strengths of the leading transition and static dipole polarizabilities of the ground states of the alkaline-earth-metal ions and atoms and compare them with the available experimental values and other precise calculations.

B. Dipole polarizability

It follows that calculation of the dispersion coefficients require knowledge of the dipole $\alpha^v(i\omega)$ dynamic polarizabilities for the atom and ion in ground state v. Following [90], $\alpha^v(i\omega)$ can be categorized into three parts,

$$\alpha^v(i\omega) = \alpha_c^v(i\omega) + \alpha_{\rm val}^v(i\omega) + \alpha_{vc}^v(i\omega), \tag{10}$$

with c and val representing the contributions due to the core and valence effects, respectively, and α_{vc}^v the compensation term, which accounts for the contribution from the excitation to the occupied valence shell that is forbidden by the Pauli exclusion principle. In the sum-over-states approach the valence correlation contributions to the ground state can be estimated using the expression

$$\alpha_{\rm val}^v(i\omega) = \sum_{p\neq v} \frac{f_{vp}}{(E_v - E_p)^2 + \omega^2}, \tag{11}$$

where f is the oscillator strength from state v to excited intermediate states p and the E are the corresponding energies of the states. The oscillator strengths f for the corresponding transitions can be deduced using the relation [91]

$$f_{vp} = -\frac{303.756}{g_v\lambda}|\langle j_p||D||j_v\rangle|^2. \tag{12}$$

Here λ is the transition wavelength expressed in angstroms, g_v denotes the statistical weight, and $\langle j_p||D||j_v\rangle$ represents the reduced dipole matrix element in a.u. It is required to calculate a sufficient number of atomic states so that ample oscillator strengths can be evaluated to estimate contributions to the $\alpha_{\rm val}^v$ values.

We have evaluated as many transitions as possible for accurate calculation of the valence contribution by using the all-order method and the multiconfigurational Dirac-Fock (MCDF) approximation for ions and atoms, respectively, as discussed in the next section. For better accuracy in the calculation of polarizabilities, instead of using our calculated energy values, we use experimental energies from the NIST database [64], where the best compiled values are given.

The core contributions $\alpha_c^v(i\omega)$ have been calculated using a random-phase approximation as described in Refs. [92–94]. The core-valence contributions $\alpha_{vc}^v(i\omega)$ are typically extremely small in magnitude and are ignored in the present study.

C. Evaluation of matrix elements

The approach we use here to evaluate the dispersion coefficients is based on the use of accurately calculated dipole

TABLE I. Comparison of our calculated oscillator strengths f of the leading transitions with the previous available values. Numbers in square brackets denote multiplication by powers of 10.

Ion	Upper level	Lower level	Term	$f_{\rm present}$	$f_{\rm previous}$
Be^+	$2p$	$2s$	$^2S_{1/2} \to {}^2P_{1/2}$	0.166[0]	0.166[0][a]
Be^+	$2p$	$2s$	$^2S_{1/2} \to {}^2P_{3/2}$	0.332[0]	0.332[0][a]
Mg^+	$3p$	$3s$	$^2S_{1/2} \to {}^2P_{1/2}$	0.303[0]	0.303[0][b]
Mg^+	$3p$	$3s$	$^2S_{1/2} \to {}^2P_{3/2}$	0.609[0]	0.608[0][b]
Ca^+	$4p$	$4s$	$^2S_{1/2} \to {}^2P_{1/2}$	0.321[0]	0.330[0][c]
Ca^+	$4p$	$4s$	$^2S_{1/2} \to {}^2P_{3/2}$	0.648[0]	0.682[0][c]
Sr^+	$5p$	$5s$	$^2S_{1/2} \to {}^2P_{1/2}$	0.344[0]	0.341[0][d]
Sr^+	$5p$	$5s$	$^2S_{1/2} \to {}^2P_{3/2}$	0.710[0]	0.703[0][d]
Ba^+	$6p$	$6s$	$^2S_{1/2} \to {}^2P_{1/2}$	0.342[0]	0.348[0][e]
Ba^+	$6p$	$6s$	$^2S_{1/2} \to {}^2P_{3/2}$	0.739[0]	0.690[0][e]
Atom	Upper level	Lower level	Term	$f_{\rm present}$	$f_{\rm previous}$
Be	$2s2p$	$2s^2$	$^1S_0 \to {}^3P_1$	0.204[−9]	0.390[−8][f]
Be	$2s2p$	$2s^2$	$^1S_0 \to {}^1P_1$	0.137[1]	0.137[1][g]
Mg	$3s3p$	$3s^2$	$^1S_0 \to {}^3P_1$	0.309[−6]	0.238[−5][h]
Mg	$3s3p$	$3s^2$	$^1S_0 \to {}^1P_1$	0.175[1]	0.180[1][i]
Ca	$4s4p$	$4s^2$	$^1S_0 \to {}^3P_1$	0.825[−3]	0.510[−4][j]
Ca	$4s4p$	$4s^2$	$^1S_0 \to {}^1P_1$	0.175[1]	0.175[1][j]
Sr	$5s5p$	$5s^2$	$^1S_0 \to {}^3P_1$	0.351[−3]	0.100[−2][d]
Sr	$5s5p$	$5s^2$	$^1S_0 \to {}^1P_1$	0.199[1]	0.192[1][d]
Ba	$6s6p$	$6s^2$	$^1S_0 \to {}^3P_1$	0.836[−2]	0.840[−2][e]
Ba	$6s6p$	$6s^2$	$^1S_0 \to {}^1P_1$	0.162[1]	0.164[1][e]

[a] Reference [65].
[b] Reference [66].
[c] Reference [67].
[d] Reference [68].
[e] Reference [69].
[f] Reference [70].
[g] Reference [71].
[h] Reference [72].
[i] Reference [73].
[j] Reference [74].

matrix elements for the two atomic states. The wave functions required for the evaluation of matrix elements for alkaline-earth-metal ions are obtained considering the single- and double-excitation approximation in the all-order (SD) method as described in Refs. [92,95]. In the SD method, the wave function of the state with the closed core with a valence electron v is represented as an expansion

$$|\Psi_v\rangle_{\mathrm{SD}} = \left[1 + \sum_{ma} \rho_{ma} a_m^\dagger a_a + \frac{1}{2} \sum_{mnab} \rho_{mnab} a_m^\dagger a_n^\dagger a_b a_a + \sum_{m \neq v} \rho_{mv} a_m^\dagger a_v + \sum_{mna} \rho_{mnva} a_m^\dagger a_n^\dagger a_a a_v \right] |\Phi_v\rangle, \quad (13)$$

where $|\Phi_v\rangle$ is the Dirac-Hartree-Fock wave function of the state. In the above expression, $a_i^\dagger$ and a_i are the creation and annihilation operators, the indices $\{m, n\}$ and $\{a, b\}$ designate the virtual and core orbitals of $|\Phi_v\rangle$, ρ_{ma} and ρ_{mv} are the corresponding single core and valence excitation coefficients, and ρ_{mnab} and ρ_{mnva} are the double core and valence excitation coefficients, respectively. To construct the single-particle orbitals for the SD method, we have used a total of 70 B-spline functions with a cavity of radius $R = 220$ a.u.

The wave functions required for the computation of matrix elements for alkaline-earth-metal atoms in their initial and final states are obtained through the MCDF approach using the GRASP2K code [96]. In this approximation an atomic state function (ASF) is considered as a linear combination of various configurational state functions (CSFs) which have same total angular momentum and parity, i.e.,

$$|\Psi_v\rangle_{\mathrm{MCDF}} = \sum_{n=1}^{N} a_n |\Phi_n\rangle, \quad (14)$$

where n denotes the number of CSFs, a_n is the mixing coefficient of the CSF $|\Phi_n\rangle$ in representation of the state $|\Psi_v\rangle$. The single-particle orbital radial functions and expansion coefficients are obtained first by multiconfiguration self-consistent-field calculations using the Dirac-Coulomb Hamiltonian. Further, relativistic configuration-interaction calculations are performed including Breit and quantum electrodynamic corrections. In order to increase the accuracy of the ASF we consider the maximum number of CSFs in the linear contribution and finally retain only those which have a mixing coefficient of value greater than 10^{-3}. It is important to mention here that in the present work we have used the all-order method for ions as this method is suitable for the monovalent system and gives an accurate result for them as compared to the MCDF method. Since for the two-valence-electron alkaline-earth-metal atoms it is difficult to apply the all-order method and also at present we do not have a suitable code developed, we have used the MCDF approach and utilized the available GRASP2K code [96], which gives equally accurate results for divalent systems.

After obtaining wave functions for the aforementioned ions and atoms, we determine the dipole-allowed ($E1$) matrix element for a transition. It is relatively straightforward to make use of the generated list of matrix elements to evaluate oscillator strengths and dipole polarizabilities which are

TABLE II. Comparison of our calculated static dipole polarizabilities $\alpha^v(0)$ (in a.u.) for the considered alkaline-earth-metal ions and alkaline-earth-metal atoms in their ground states with the available measurements and other theoretical calculations.

Ion	State	Present calculations	Other calculations	Measurements
Be^+	$2s$	24.5	24.5[a]	
Mg^+	$3s$	35.0		
Ca^+	$4s$	76.1	75.88[b]	75.3(4)[c]
Sr^+	$5s$	91.7	91.10[b], 93.3(9)[d]	86(11)[e]
Ba^+	$6s$	125.5	123.07[b]	123.88(5)[f]
Atom	State	Present calculations	Other calculations	Measurements
Be	$2s^2$	36.6	38.1[g], 37.76(22)[h]	
Mg	$3s^2$	71.9	71.3(7)[h]	71.5(3.1)[i]
Ca	$4s^2$	158.2	157.1(1.3)[h]	168.7(13.5)[j]
Sr	$5s^2$	214.5	197.2(2)[h]	186(15)[k]
Ba	$6s^2$	276.2	273.5(2.0)[h]	268(22)[l]

[a] Reference [75].
[b] Reference [76].
[c] Reference [79].
[d] Reference [77].
[e] Reference [80].
[f] Reference [81].
[g] Reference [78].
[h] Reference [60].
[i] Reference [82].
[j] Reference [83].
[k] Reference [84].
[l] Reference [85].

TABLE III. Dispersion coefficients C_6 for the interaction between two homonuclear alkaline-earth-metal atoms in the ground state.

Interaction	Present calculation	Other calculations	Measurements
Be-Be	196	213.1[a], 214[b], 248[c]	
Mg-Mg	636	629.5[a], 627(12)[b], 648[c]	683(35)[d]
Ca-Ca	2138	2188[a], 2121(35)[b], 2002[c]	2080(7)[e]
Sr-Sr	3654	3250[a], 3103(7)[b], 2849[c]	
Ba-Ba	5324	5160(74)[b], 4479[c]	

[a] Reference [59].
[b] Reference [60].
[c] Reference [61].
[d] Reference [62].
[e] Reference [63].

further used to calculate the dispersion coefficients as described in the theory earlier.

III. RESULTS

A. Oscillator strengths

We have calculated the first few oscillator strengths having dominant contributions to the dipole polarizability as given by Eq. (11). Table I presents a comparison between the present calculations and other previously reported results [65–74], which are also available from the NIST database [64]. We find excellent agreement between the two results for ions. However, for atoms, the calculated oscillator strengths agree well with the previous data for the $^1S_0 \rightarrow {}^1P_1$ transition, while for $^1S_0 \rightarrow {}^3P_1$ transitions a slight discrepancy of the order of $\sim 10^{-6}$ can be observed. This difference can be conveniently ignored as the small value of the oscillator strength will have an insignificant contribution to the determination of polarizability. Thus, our results for oscillator strengths are precise enough to predict the reliable values of the polarizability of the ionic and atomic systems considered.

B. Static dipole polarizabilities

The calculated oscillator strengths are used to determine the static dipole polarizabilities of the alkaline-earth-metal ions and atoms concerned. As described previously in the theoretical method, we use a sum-over-states approach to calculate the polarizability in this work. It should however be noted that for the ground-state polarizability, only the first few low-lying transitions contribute the most. Note that the error introduced due to the truncation of the summation was not more than 1.5% for ions and even smaller for the atoms.

1. Alkaline-earth-metal ions

Our results for static dipole polarizability of alkaline-earth-metal ions are presented and compared in Table II with other theoretical calculations of [75–77] as well as different precise measurements [79–81]. One can readily see that present results are in good agreement with the theoretical results [76] that are obtained using the relativistic coupled-cluster method in the finite field gradient technique along with the optimized Gaussian-type basis set. However, in our calculation, we have used a sum-over-states approach which permits us to use accurate experimental energy data wherever available. This justifies the good agreement of the present calculations with the measurements. For example, the static dipole polarizability value of the Ca^+ ion, measured by Chang [79], is in very close agreement with our evaluated value, whereas for other ions, i.e., Sr^+ [80] and Ba^+ [81], the agreement is within 2%. Unfortunately, for the Mg^+ ion we did not find any data in the literature to compare with our result. However, based on our results of Be^+, Ca^+, Sr^+, and Ba^+ ions, we believe our value for the Mg^+ ion should also be reliable.

2. Alkaline-earth-metal atoms

The present results of static dipole polarizability of alkaline-earth-metal atoms are given in Table II, where these are compared with the previously reported calculation of Porsev and Derevianko [60] and other experimental results [82–85]. Porsev and Derevianko calculated their static dipole polarizabilities by using available reported experimental energies and theoretically calculated matrix elements. Close agreement between our results for Be, Mg, Ca, and Ba atoms with theoretical calculations [60] and other experimental measurements [82–85] can be seen from Table II. However, for the Sr atom, we observe that our value of static dipole polarizability is somewhat higher as compared to the available calculation [60] and the experimental value [84]. This could be due to our slightly higher value of oscillator strength as

TABLE IV. Dispersion coefficients C_6 for the interaction between two heteronuclear alkaline-earth-metal atoms and their comparison with the fitted result obtained by Eq. (6).

Interaction	Present calculation	Fitted
Be-Mg	351	364
Be-Ca	626	663
Be-Sr	814	786
Be-Ba	969	977
Mg-Ca	1150	1160
Mg-Sr	1494	1380
Mg-Ba	1784	1727
Ca-Sr	2793	2652
Ca-Ba	3360	3367
Sr-Ba	4403	4032

TABLE V. Dispersion coefficients C_6 for the alkaline-earth-metal ions interacting with the alkaline-earth-metal atoms and their comparison with the fitted value obtained using Eq. (6).

	Be		Mg		Ca		Sr		Ba	
Ion	Present calc.	Fitted	Present calc.	Fitted	Present calc.	Fitted	Present calc.	Fitted	Present calc.	Fitted
Be^+	115	105	208	188	379	377	493	453	589	587
Mg^+	173	188	312	310	564	574	733	682	876	853
Ca^+	322	377	587	584	1082	1105	1413	1317	1698	1664
Sr^+	388	453	706	702	1302	1335	1699	1593	2044	2016
Ba^+	511	587	930	930	1719	1770	2247	2112	2708	2673

compared to the NIST [64] value for the leading transition $^1S_0 \rightarrow {}^1P_1$.

C. The C_6 coefficients

Using our calculations for dipole polarizabilities, we further calculate the C_6 dispersion coefficients for the combination of interactions between two homonuclear alkaline-earth-metal atoms, two heteronuclear alkaline-earth-metal atoms, and alkaline-earth-metal atoms with their ions in their ground state. We have taken the calculation of C_6 for homonuclear alkaline-earth-metal atom dimers simply for comparison purposes in order to check the reliability of our calculations and to see how these match with the other available results. These coefficients are presented in Table III, where we have also compared our calculations with the available previous theoretical [59–61] and experimental [62,63] results. We find that our calculated value of C_6 for Ca-Ca dimer shows excellent agreement with the experimental result while it deviates from measurements by ~7% for the Mg-Mg dimer. Also, one can see from Table III that there is significant disagreement among the reported theoretical values from Mitroy and Bromley [59], Porsev and Derevianko [60], and Patil [61] for all homonuclear alkaline-earth-metal-atom dimers. This difference among these results can be attributed to different methodologies adopted in the theoretical approaches. We also observe that with an increase in the atomic size of the homonuclear dimer the C_6 dispersion coefficients also increase. The same trend can also be seen in the other reported theoretical and experimental results.

Further, we have calculated C_6 dispersion coefficients for the interaction between the two heteronuclear alkaline-earth-metal atoms in their ground state; these are shown in Table IV. There are no other results reported for these C_6 coefficients with which we can compare our results. However, for the sake of comparison, we have also obtained C_6 using the Slater-Kirkwood formula given by Eq. (6) using experimental values of static dipole polarizabilities of each atom as well as C_6 coefficients as reported by Porsev and Derevianko [60] for homonuclear alkaline-earth-metal-atom dimers. These calculated values are also presented for comparison in Table IV and are referred to as the fitted calculations. Results determined using this approach show close agreement with the present C_6 values, except for the dimer, which is combined with the Sr atom, i.e., Be-Sr, Mg-Sr, Ca-Sr, and Sr-Ba dimers. This could be due to our calculated dipole polarizability of the Sr atom being higher than the experimental value, as can be seen from Table II. Agreement between results from both methods clearly confirms the validity of our method of calculation of C_6 dispersion coefficients for heteronuclear alkaline-earth-metal atoms. Similar to the previous case, we again find that the value of C_6 increases with the increasing size of interacting atoms.

The calculated C_6 dispersion coefficients for the alkaline-earth-metal ions interacting with the alkaline-earth-metal atoms are shown in Table V. In this case, there are again no other previously reported theoretical or experimental results to compare with our results. Consequently, we performed calculations using the fitting approach using Eq. (6) and compared these in Table V. We observe good agreement between the present results with our fitting calculations for all the dimers of alkaline-earth-metal ions with the alkaline-earth-metal atoms except when the neutral Sr atom is involved. The possible reason can again be the higher value of our calculated dipole polarizability. The close agreement between these two

TABLE VI. Dispersion coefficients C_9 for the interaction among three alkaline-earth-metal atoms. Fitted values are obtained from Eq. (7).

Atom	Calculation	Be-Be	Mg-Mg	Ca-Ca	Sr-Sr	Ba-Ba
Be	present	5368	18310	66608	115009	169600
Be	fitted	6051	18830	72683	104765	175036
Mg	present	9893	34024	125721	217665	322323
Mg	fitted	10644	33482	131571	190085	319626
Ca	present	18503	64768	248117	432498	647488
Ca	fitted	20459	65779	267852	388883	663115
Sr	present	24160	84848	327456	571661	858017
Sr	fitted	24439	78724	322681	468843	801218
Ba	present	28978	102290	399639	699526	1054803
Ba	fitted	31021	100814	420111	611823	1052640

TABLE VII. Dispersion coefficients C_9 for the interaction between two alkaline-earth-metal atoms and alkaline-earth-metal ions. The fitted values are obtained using Eq. (8).

Ion	Calculation	Be-Be	Mg-Mg	Ca-Ca	Sr-Sr	Ba-Ba
Be^+	present	3264	11261	41903	72644	107799
Be^+	fitted	3466	11457	49331	72185	125948
Mg^+	present	4840	16634	61381	106248	157285
Mg^+	fitted	5261	16537	64896	93742	157547
Ca^+	present	9276	32308	122618	213393	318658
Ca^+	fitted	10167	32420	130467	189086	320800
Sr^+	present	11091	38619	146658	255303	381479
Sr^+	fitted	12292	39314	159066	230705	392236
Ba^+	present	14571	50859	194466	339068	508069
Ba^+	fitted	16297	52133	210998	306040	520380

approaches justifies the accuracy of our method of obtaining C_6 coefficients.

D. The C_9 coefficients

After calculating the value of C_6 for dimers, we have determined the C_9 dispersion coefficients for the interaction between three alkaline-earth-metal atoms. The calculated results are shown in Table VI. Due to unavailability of other results for comparisons, we have again evaluated C_9 using fitting equations, i.e., Eqs. (7) and (8). In order to solve these equations, we have used C_6 coefficients for homonuclear alkaline-earth-metal-atom dimers by Porsev and Derevianko [60] and used experimental static dipole polarizability from Schwerdtfeger and Nagle [97]. One can see from Table VI that both sets of values for C_9 dispersion coefficients of the systems concerned show close agreement. The maximum difference between the two results can be seen for the systems which have the Sr atom in their combinations for the reason stated earlier.

Finally, we have calculated the values of C_9, as given in Table VII, for the interaction between two alkaline-earth-metal atoms and alkaline-earth-metal ions. In addition to a calculation by our method, we have determined these coefficients with fitting equations, i.e., Eqs. (7) and (8). To solve these equations experimental values [97] of the static dipole polarizability Ca^+, Sr^+, and Ba^+ are used. In the case of Be^+ and Mg^+ our calculated result for dipole polarizability is utilized due to unavailability of the corresponding measurements. From this table we find close agreement between both sets of calculations, excluding the systems with the Sr atom. This is consistent with our other results for C_6 and C_9. The C_9 coefficients also show trends similar to C_6 with respect to the size of the interacting atomic systems.

IV. CONCLUSION

In the present work, we have studied the nature of the interaction coefficients for the alkaline-earth-metal atoms interacting among themselves and with the alkaline-earth-metal ions and obtained the values of the two-body C_6 and three-body C_9 dispersion coefficients. To determine these coefficients, oscillator strengths for leading transitions and static dipole polarizability of atoms and ions in their ground states were determined using relativistic methods. These results were compared with corresponding data from other theoretical calculations, measurements, and the NIST database and overall good agreement was found. Apart from C_6 values for alkaline-earth-metal homonuclear dimers, the C_6 and C_9 coefficients were reported here. Therefore, we have performed fitting calculations, for the sake of comparison, using measured values of dipole polarizability and other available parameters. Good agreement between values from our and fitting methods indicates the reliability of our calculations for C_6 and C_9 dispersion coefficients. We hope our results will induce more theoretical and experimental studies in this direction and help to make progress in quantum information processing, quantifying molecular potentials for ultracold collision investigation, and designing better atomic clocks.

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