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Relativistic calculations of C_6 and C_8 coefficients for strontium dimers

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The electric-dipole and quadrupole polarizabilities of the $5s5p\,^3P_1^o$ state and the C_6 and C_8 coefficients for the $^1S_0 + {}^1S_0$ and $^1S_0 + {}^3P_1^o$ dimers of strontium are calculated using a high-precision relativistic approach that combines configuration interaction and linearized coupled-cluster methods. Our recommended values of the long-range dispersion coefficients for the 0_u and 1_u energy levels are $C_6(0_u) = 3771(32)$ a.u. and $C_6(1_u) = 4001(33)$ a.u., respectively. They are in good agreement with recent results from experimental photoassociation data. We also calculate C_8 coefficients for Sr dimers, which are needed for precise determination of long-range interaction potential. We confirm the experimental value for the magic wavelength, where the Stark shift on the $^1S_0$-$^3P_1^o$ transition vanishes. The accuracy of calculations is analyzed and uncertainties are assigned to all quantities reported in this work.

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I. INTRODUCTION

The divalent alkaline-earth-metal element strontium is of interest for many applications of atomic, molecular, and optical physics. The atomic clock based on the $5s^2\,^1S_0$–$5s5p\,^3P_0^o$ transition in Sr has achieved a total systematic uncertainty of 6×10^{-18} [1], which is the smallest yet demonstrated. The architecture of this clock also provides capabilities for detailed studies of quantum many-body physics. The SU(N)-symmetric interactions of ^{87}Sr atoms in optical lattices provide a platform for quantum simulation of lattice gauge theories and a variety of quantum materials such as transition metal oxides, heavy fermion compounds, and exotic topological phases. Early demonstrations of this capability have been realized by high-resolution spectroscopy of SU(N)-symmetric interactions in Sr orbital magnetism [2].

All four stable isotopes of Sr have been brought to strong quantum degeneracy: Bose-Einstein condensation has been achieved in the bosonic isotopes 84, 86, and 88, and fermionic ^{87}Sr has been cooled to within 10% of its Fermi temperature [3]. The first isotope to be condensed [4], ^{84}Sr, is also distinctive in being the only atomic species to date which has been condensed by laser cooling alone [5]. Sr has also been used in ultracold gases of both homonuclear [6,7] and heteronuclear [8] molecules. A quantum degenerate gas mixture of Sr and Rb has been realized recently [9], as a prerequisite for the production of a quantum degenerate gas of polar molecules. Presently, there is much interest in Sr photoassociation spectroscopy due to its relevance for the production of ground-state ultracold molecules [6], coherent photoassociation [10], and search for time variation of the electron-proton mass ratio [11].

Understanding of the long-range interaction of the Sr atoms is needed for all of the applications mentioned above. In Ref. [2], we have provided recommended values of the C_6 long-range interaction coefficients for the $^1S_0$-$^1S_0$, $^1S_0$-$^3P_0^o$, and $^3P_0^o$-$^3P_0^o$ dimers for the determination of relevant interaction parameters for spin-orbital quantum dynamics.

Motivated by the diverse applications and particular interest in the $^1S_0$-$^3P_1^o$ intercombination line for the most recent photoassociation studies, we have calculated the C_6 and C_8 van der Waals coefficients for the Sr $^1S_0 + {}^1S_0$ and $^1S_0 + {}^3P_1^o$ dimers. The ground-state long-range interaction coefficients were previously studied in Refs. [12–14]; here we provide revised value of the C_8 coefficient that has been critically evaluated for its accuracy.

The energy levels of the $^1S_0$ + $^3P_1$ Sr^2 molecule were obtained for ^{88}Sr [15], ^{84}Sr [16], and ^{86}Sr [17]. In a recent paper, Borkowski *et al.* [17] provide a theoretical model based on recent state-of-the-art *ab initio* potential curves from [18,19] for the description of the long-range interactions in this excited state of the strontium dimer. They determined the van der Waals C_6 coefficients for the 0_u and 1_u bound states to be $C_6(0_u) = 3868(50)$ a.u. and $C_6(1_u) = 4085(50)$ a.u. [17]. Our recommended values of $C_6(0_u) = 3771(32)$ a.u. and $C_6(1_u) = 4001(33)$ a.u. provide further confidence in the fitting of precision photoassociation data.

In the course of our work, we also calculated a number of $E1$ transition amplitudes and the electric-dipole and quadrupole polarizabilities of the $5s5p\,^3P_1^o$ state of atomic Sr for use in other applications. We report recommended values of these quantities here.

This paper is organized as follows. In Sec. II we briefly describe the method of calculation and present the matrix elements of $E1$ transitions from the $^3P_1^o$ state to low-lying even-parity states. In Sec. III we discuss calculation of the scalar static $^3P_1^o$ polarizability. The $^1S_0$-$^3P_1^o$ magic wavelength is discussed in Sec. IV. Section V is devoted to calculation of the van der Waals $C_6(^1S_0 + {}^3P_1^o)$ coefficients. In Secs. VI and VII we present the results of calculation of the electric quadrupole $^3P_1^o$ polarizability and $C_8(^1S_0 + {}^3P_1^o)$ coefficients, respectively.

II. METHOD OF CALCULATION AND ELECTRIC-DIPOLE MATRIX ELEMENTS

We consider atomic Sr as an atom with frozen Ag-like Sr^{2+} core and two valence electrons. Interaction of the valence electrons is taken into account in the framework of the configuration interaction (CI) method (see, e.g., Ref. [20]) while core-core and core-valence correlations are treated in the framework of the many-body perturbation theory (MBPT) and the all-order single-double coupled-cluster method. Both CI+MBPT and CI+all-order methods were described in detail in a number of papers [21–24], so here we only briefly review their main features. While the CI+all-order method is more accurate, carrying out the calculations by both approaches allows us to estimate the accuracy of the final results.

Unless stated otherwise, we use atomic units (a.u.) for all matrix elements and polarizabilities throughout this paper: The numerical values of the elementary charge $|e|$, the reduced Planck constant, $\hbar = h/2\pi$, and the electron mass m_e are set equal to 1. The atomic unit for polarizability can be converted to SI units via $\alpha/h[\mathrm{Hz}/(\mathrm{V/m})^2] = 2.48832 \times 10^{-8}\alpha$ (a.u.), where the conversion coefficient is $4\pi\epsilon_0 a_0^3/h$ and the Planck constant h is factored out in order to provide direct conversion into frequency units; a_0 is the Bohr radius and ϵ_0 is the electric constant.

We start with the solutions of the Dirac-Fock equation,

$$H_0\,\psi_c = \varepsilon_c\,\psi_c, \tag{1}$$

where H_0 is the Dirac-Fock Hamiltonian [21,23] and ψ_c and ε_c are single-electron wave functions and energies. The calculations are carried out in the V^{N-2} potential, where N is the total number of electrons and an initial self-consistent Hartree-Fock procedure is applied to the $N - 2 = 36$ core electrons. The wave functions and the energy levels for the valence electrons are determined by solving the multiparticle relativistic equation [21],

$$H_{\mathrm{eff}}(E_n)\Phi_n = E_n\Phi_n, \tag{2}$$

with the effective Hamiltonian defined as

$$H_{\mathrm{eff}}(E) = H_{\mathrm{FC}} + \Sigma(E).$$

Here H_{FC} is the Hamiltonian in the frozen-core approximation and the operator $\Sigma(E)$, accounting for virtual core excitations, is constructed using second-order perturbation theory in the CI+MBPT method [21] and using a linearized coupled-cluster single-double method in the CI+all-order approach [23]. Since the valence space contains only two electrons, the CI can be made numerically complete. Our calculation of the energy levels was presented and discussed in detail in Ref. [25]. In analogy with the effective Hamiltonian we can construct effective electric-dipole and electric-quadrupole operators to account for dominant core-valence correlations [26–28].

In Ref. [25], we used the CI+all-order method to evaluate the static and dynamic polarizabilities of the $5s^2\,{}^1S_0$ and $5s5p\,{}^3P_0^o$ states of Sr. We found that the $E1$ matrix elements for the transitions that give dominant contributions to the ${}^3P_0^o$ polarizability are sensitive to the higher-order corrections to the wave functions and other corrections to the matrix elements beyond the random phase approximation (RPA). We included the higher-order corrections in an *ab initio* way using the CI+all-order approach and also calculated several other corrections beyond RPA. The resulting value for the dc Stark shift of the Sr ${}^1S_0$-${}^3P_0^o$ clock transition, 247.5 a.u., was found to be in excellent agreement with the experimental result 247.374(7) a.u. [29].

TABLE I. The CI+MBPT and CI+all-order results for absolute values of the reduced electric-dipole matrix elements for the transitions that give dominant contributions to the polarizabilities of the $5s5p\,{}^3P_0^o$ and $5s5p\,{}^3P_1^o$ states. The CI+MBPT and CI+all-order results including RPA corrections are given in columns labeled "CI+MBPT" and "CI+all", respectively. The relative differences between the CI+all-order and CI+MBPT results are given in the column labeled "HO" in %. The recommended values of the matrix elements are given in the last column (see text for details).

Transition	CI+MBPT	CI+all	HO	Recomm.
$5s5p\,{}^3P_0^o$–$5s4d\,{}^3D_1$	2.681	2.712	1.14%	2.675(13)[a]
$5s5p\,{}^3P_1^o$–$5s4d\,{}^3D_1$	2.326	2.354	1.19%	2.322(11)[a]
$5s5p\,{}^3P_1^o$–$5s4d\,{}^3D_2$	4.031	4.075	1.08%	4.019(20)
$5s5p\,{}^3P_0^o$–$5s6s\,{}^3S_1$	1.983	1.970	−0.66%	1.962(10)[a]
$5s5p\,{}^3P_1^o$–$5s6s\,{}^3S_1$	3.463	3.439	−0.70%	3.425(17)
$5s5p\,{}^3P_0^o$–$5s5d\,{}^3D_1$	2.474	2.460	−0.57%	2.450(24)[a]
$5s5p\,{}^3P_1^o$–$5s5d\,{}^3D_1$	2.065	2.017	−2.38%	2.009(20)
$5s5p\,{}^3P_1^o$–$5s5d\,{}^3D_2$	3.720	3.688	−0.87%	3.673(37)
$5s5p\,{}^3P_0^o$–$5p^2\,{}^3P_1$	2.587	2.619	1.22%	2.605(26)[a]
$5s5p\,{}^3P_1^o$–$5p^2\,{}^3P_0$	2.619	2.671	1.95%	2.657(27)
$5s5p\,{}^3P_1^o$–$5p^2\,{}^3P_1$	2.317	2.374	2.40%	2.362(24)
$5s5p\,{}^3P_1^o$–$5p^2\,{}^3P_2$	2.837	2.880	1.49%	2.865(29)

[a] Reference [25].

In order to predict the accurate values for the dynamic part of black-body radiation shift in the Sr clock, which is one of the largest sources of Sr clock systematic uncertainty, we have combined our theoretical calculations with the experimental measurements of the Stark shift [29] and magic wavelength [30] of the $5s^2\,{}^1S_0$–$5s5p\,{}^3P_0^o$ transition to determine very accurate recommended values for several relevant electric-dipole matrix elements [25]. Specifically, we were able to obtain accurate recommended values for the following most important transitions contributing to the ${}^3P_0^o$ polarizability: $5s5p\,{}^3P_0^o$–$5s4d\,{}^3D_1$, $5s5p\,{}^3P_0^o$–$5s6s\,{}^3S_1$, $5s5p\,{}^3P_0^o$–$5s5d\,{}^3D_1$, and $5s5p\,{}^3P_0^o$–$5p^2\,{}^3P_1$.

In this work, we use our previous results, supplemented with theoretical CI+all-order+RPA values of the reduced matrix element ratios, to obtain recommended values for eight transitions that give dominant contributions to the polarizability of the $5s5p\,{}^3P_1^o$ state. The results are summarized in Table I.

We assume that the transitions from even-parity states to the $5s5p\,{}^3P_1^o$ state are calculated in the CI+all-order+RPA approach with the same accuracy as similar transitions from even-parity states to the $5s5p\,{}^3P_0^o$ state, for which the recommended values were presented in Ref. [25]. Then, for example, the recommended value of the $\langle 5s4d\,{}^3D_2||D||5s5p\,{}^3P_1^o\rangle$ matrix element is obtained here from the CI+all-order+RPA ratio,

$$\frac{\langle 5s4d\,{}^3D_2||D||5s5p\,{}^3P_1^o\rangle}{\langle 5s4d\,{}^3D_1||D||5s5p\,{}^3P_0^o\rangle},$$

multiplied by the recommended value of the $\langle 5s4d\,{}^3D_1||D||5s5p\,{}^3P_0^o\rangle$ reduced matrix element. In a similar manner we find all other matrix elements listed in Table I. We assign the uncertainties to the new recommended values based on the uncertainties of the corresponding matrix element involving the $5s5p\,{}^3P_0^o$ state.

As an additional check, we also use a simple ratio between the relativistic and nonrelativistic reduced matrix element of the electric-dipole operator D valid in the LS coupling approximation. Since the dipole and spin operators commute, we obtain [31]

$$\begin{aligned}\langle \gamma J L S || D || \gamma' J' L' S' \rangle &= \delta_{SS'} \sqrt{(2J+1)(2J'+1)}\, (-1)^{S+L+J'+1} \\ &\quad \times \begin{Bmatrix} L & J & S \\ J' & L' & 1 \end{Bmatrix} \langle \gamma L S || D || \gamma' L' S \rangle, \end{aligned} \tag{3}$$

where S is the total spin momentum of the atomic state, L and J are the orbital and total angular momenta, and γ stands for all other quantum numbers.

The results produced by this formula for the transitions to $5s4d\,^3D_J$ states differ from recommended values listed in Table I by only 0.15% and 0.2%. These differences are substantially smaller than the quoted uncertainties of 0.5%. The $5s5p\,^3P_1^o$–$5s4d\,^3D_J$ transitions give dominant contributions to the $5s5p\,^3P_1^o$ polarizability. The differences between the use of Eq. (3) and the CI+all-order ratio for the other transitions range from 0.05% to 5.6%. This demonstrates that LS coupling works reasonably well for the $5s5p\,^3P_J^o$, $5s4d\,^3D_J$, and $5s5d\,^3D_J$ terms, as expected from the experimental splittings of the atomic terms.

We find that absolute values of all recommended matrix elements are slightly less than the *ab initio* CI+all-order results. The difference, as it was discussed in Ref. [25], can be attributed to the small corrections beyond RPA, such as the core-Brueckner, two-particle, structural radiation, and normalization corrections.

Along with the recommended values, we also give *ab initio* results of the CI+MBPT and CI+all-order calculations that include RPA corrections to the effective operator. The higher-order (HO) corrections may be estimated as the difference of the CI+all-order+RPA and CI+MBPT+RPA calculations. These contributions of the higher orders, listed in the "HO" column of Table I, provide a good estimate of the uncertainty and are larger than the more accurate final uncertainty estimate for most of the transitions. Since the basis set is numerically complete and the configuration space is saturated for two electrons, the contribution to the uncertainty budget coming from CI is negligible in comparison to the contributions arising from core-valence correlations.

III. POLARIZABILITY OF THE $^3P_1^o$ STATE

We calculated the static and dynamic polarizabilities of the Sr $5s5p\,^3P_1^o$ state using the high-precision CI+all-order method. The dynamic polarizability $\alpha(\omega)$ can be represented as a sum,

$$\alpha(\omega) = \alpha^v(\omega) + \alpha^c(\omega) + \alpha^{vc}(\omega), \tag{4}$$

where $\alpha^v(\omega)$ is the valence polarizability, α^c is the ionic core polarizability, and a small term α^{vc} compensates for Pauli-principle forbidden excitations to occupied valence shells and slightly modifies the ionic core polarizability.

TABLE II. Contributions to the $5s5p\,^3P_1^o$ static scalar polarizability of Sr in a.u. The dominant contributions to the valence polarizabilities are listed separately. The theoretical and experimental [32] transition energies are given in columns $\Delta E_{\rm th}$ and $\Delta E_{\rm expt}$. The remaining contributions to valence polarizability are given in row Other. The total of the core and α^{vc} terms is listed together in row Core + Vc. The dominant contributions to α_0, listed in columns α_0 (A) and α_0 (B), are calculated with the CI + all-order + RPA matrix elements and theoretical (A) and experimental (B) energies [32], respectively. The dominant contributions to α_0 listed in column α_0 (C) are calculated with experimental energies and our recommended values of the matrix elements given in Table I.

Contribution	$\Delta E_{\rm th}$	$\Delta E_{\rm expt}$	α_0 (A)	α_0 (B)	α_0 (C)
$5s5p\,^3P_1^o$–$5s4d\,^3D_1$	3589	3655	75.3	74.0	71.9
$5s5p\,^3P_1^o$–$5s4d\,^3D_2$	3656	3715	221.5	218.0	212.0
$5s5p\,^3P_1^o$–$5s6s\,^3S_1$	14484	14535	39.8	39.7	39.4
$5s5p\,^3P_1^o$–$5s5d\,^3D_1$	20472	20503	9.7	9.7	9.6
$5s5p\,^3P_1^o$–$5s5d\,^3D_2$	20488	20518	32.4	32.3	32.1
$5s5p\,^3P_1^o$–$5p^2\,^3P_0$	20807	20689	16.7	16.8	16.6
$5s5p\,^3P_1^o - 5p^2\,^3P_1$	21020	20896	13.1	13.2	13.0
$5s5p\,^3P_1^o$–$5p^2\,^3P_2$	21300	21171	19.0	19.1	18.9
$5s5p\,^3P_1^o$–$5s7s\,^3S_1$	22869	22920	1.8	1.8	1.8
Other			38.3	38.3	38.3
Core +Vc			5.55	5.55	5.55
Total			473.2	468.4	459.2
Recommended					459.2(3.8)

The valence part of the polarizability is determined by solving the inhomogeneous equation in valence space, which is approximated as [33]

$$(E_v - H_{\rm eff}) |\Psi(v,M')\rangle = D_{\rm eff} |\Psi_0(v,J,M)\rangle, \tag{5}$$

for the state v with total angular momentum J and magnetic quantum number M. The parts of the wave function $\Psi(v,M')$ with angular momenta of $J' = J, J \pm 1$ allow us to determine the scalar and tensor polarizabilities of the state $|v,J,M\rangle$ [33]. The effective dipole operator $D_{\rm eff}$ includes RPA corrections.

Small core terms α^c and α^{vc} are evaluated in the RPA. The latter is calculated by adding α^{vc} contributions from the individual electrons, i.e., $\alpha^{vc}(5s5p) = \alpha^{vc}(5s) + \alpha^{vc}(5p)$. The uncertainties of these terms are determined by comparing the Dirac-Fock and RPA values.

We use the sum-over-states formula for the scalar part of the dynamic valence polarizability [34] to establish the dominant contributions to the final value,

$$\alpha_0^v(\omega) = \frac{2}{3(2J+1)} \sum_n \frac{(E_n - E_v) |\langle v \| D \| n \rangle|^2}{(E_n - E_v)^2 - \omega^2}. \tag{6}$$

Here J is the total angular momentum of the state v and E_n is the energy of the state n. For the static polarizability, $\omega = 0$ in Eq. (6). Determination of the dominant contributions is essential for estimating the uncertainty of the final value.

We have carried out several calculations of the dominant contributions to the $5s5p\,^3P_1^o$ static scalar polarizability using different sets of the energies and $E1$ matrix elements. The results are presented in Table II. The theoretical and experimental [32] transition energies are given in columns $\Delta E_{\rm th}$ and $\Delta E_{\rm expt}$ in cm^{-1}. The dominant contributions to the polarizability listed in columns α_0 (A) and α_0 (B) are calculated with CI + all-order + RPA matrix elements and theoretical (A) and experimental

TABLE III. The dominant contributions to the Sr $5s5p\,^3P_1^o$ and $5s5p\,^3P_0^o$ scalar polarizabilities in a.u. and in percent. *Ab initio* (columns 2–5) and recommended (columns 6–9) values are given. Nonrelativistic term notation is used when the sum of relativistic contributions is given (see the main text for details). The results for the $5s5p\,^3P_0^o$ state are taken from Ref. [25]. Final (recommended) results for the scalar $5s5p\,^3P_1^o$ polarizability are given in the last column.

	Theor. matrix elements and energies				Recomm. matrix elements and expt. energies				Recomm.
State	$\alpha_0(^3P_1^o)$	$\alpha_0(^3P_0^o)$	$\alpha_0(^3P_1^o)$	$\alpha_0(^3P_0^o)$	$\alpha_0(^3P_1^o)$	$\alpha_0(^3P_0^o)$	$\alpha_0(^3P_1^o)$	$\alpha_0(^3P_0^o)$	$\alpha_0(^3P_1^o)$
$5s4d\,^3D$	296.8	285.0	62.7%	62.2%	283.9	272.6	61.8%	61.3%	283.9(3.4)
$5s6s\,^3S_1$	39.8	38.7	8.4%	8.4%	39.4	38.3	8.6%	8.6%	39.4(0.4)
$5s5d\,^3D$	42.1	42.9	8.9%	9.4%	41.7	42.5	9.1%	9.6%	41.7(0.8)
$5p^2\,^3P$	48.8	47.3	10.3%	10.3%	48.6	47.1	10.6%	10.6%	48.6(0.9)
$5p7s\,^3S_1$	1.81	1.70	0.4%	0.4%	1.81	1.69	0.4%	0.4%	1.81(0.05)
Other	38.3	36.9	8.1%	8.1%	38.2	36.9	8.3%	8.3%	38.2(1.1)
Core+Vc	5.6	5.6	1.2%	1.2%	5.6	5.6	1.2%	1.2%	5.55(0.06)
Total	473.2	458.1	100.0%	100.0%	459.2	444.6	100.0%	100.0%	459.2(3.8)

(B) energies [32], respectively. The dominant contributions to α_0 listed in column α_0 (C) are calculated with experimental energies and recommended matrix elements. These results are taken as final. The remaining valence contributions that are not listed separately are given in the row labeled "Other". The sum of the core and α^{vc} terms is listed in row labeled "Core +Vc".

A comparison of the main contributions to the $5s5p\,^3P_0^o$ and $5s5p\,^3P_1^o$ scalar polarizabilities is given in Table III. Two sets of calculations are presented. In the first calculation, we use the *ab initio* values of the matrix elements and energies, while in the second calculation the recommended matrix elements and the experimental energies are used. To simplify the comparison, we sum the contributions from the transitions to the ^3D_J and ^3P_J states and use ^3D and ^3P terms labels for the totals. For example, the contribution of the intermediate $5s4d\,^3D$ state to $\alpha_0(^3P_1^o)$ means the sum of contributions of the $5s4d\,^3D_1$ and $5s4d\,^3D_2$ states, while in the case of the $^3P_0^o$ state the notation $5s4d\,^3D$ means the contribution of the $5s4d\,^3D_1$ state only.

The contribution of different terms to $\alpha_0(^3P_1^o)$ and $\alpha_0(^3P_0^o)$ is very similar. Therefore, we are able to assign the uncertainties to these contributions based on the uncertainties of the matrix elements listed in Table I and on the uncertainties of the respective contributions to $\alpha_0(^3P_0^o)$ determined in Ref. [25]. Our final recommended result for the $5s5p\,^3P_1^o$ scalar polarizability is 459.2(3.8) a.u.

IV. MAGIC WAVELENGTH

The magic wavelength λ^* at which $\alpha_{^1S_0}(\lambda^*) = \alpha_{^3P^o_{1,|m_J|=1}}(\lambda^*)$ and the quadratic Stark shift on the $^1S_0$-$^3P_1^o$ transition vanishes, was experimentally determined by Ido and Katori [35] to be 914(1) nm. Note that $\alpha_{^3P^o_{1,|m_J|=1}}$ is the *total* polarizability, i.e., is the sum of the scalar and tensor parts. Using the magic frequency $\omega^* = 0.049851(5)$ a.u., corresponding to the magic wavelength λ^*, and the experimental value of the matrix element $|\langle 5s^2\,^1S_0||D||5s5p\,^1P_1^o\rangle| = 5.248(2)$ a.u. [36], $\alpha_{^1S_0}(\omega^*)$ was obtained in Ref. [37] to be 261.2(3) a.u.

Solving inhomogeneous equation (5), we found $\alpha_{^1S_0}(\omega^*) = 261.03$ a.u. in excellent agreement with the result 261.2(3). When this value was recalculated with the recommended matrix elements and the experimental energies we obtained 261.07 a.u. Similar calculations of the $\alpha_{^1P^o_{1,|m_J|=1}}(\omega^*)$ yield 264.3 a.u. and 261.0 a.u., respectively. Therefore, the use of the recommended matrix elements and the experimental energies yields the experimentally determined magic wavelength to within its stated uncertainty.

V. C_6 COEFFICIENTS

The expression for the $C_6(^1S_0 + {}^3P_1^o)$ coefficient is given by [38]

$$C_6(\Omega_p) = \sum_{J=0}^{2} A_J(\Omega) X_J, \tag{7}$$

where the angular dependence $A_J(\Omega)$ is represented by

$$A_J(\Omega) = \frac{1}{3}\sum_{\mu=-1}^{1}\left\{ w_\mu^{(1)} \begin{pmatrix} 1 & 1 & J \\ -\Omega & -\mu & \Omega+\mu \end{pmatrix}\right\}^2, \tag{8}$$

with the dipole weights $w_{\pm 1}^{(1)} = 1$ and $w_0^{(1)} = 2$ and $\Omega = 0,1$. The coefficients $A_J(\Omega)$ (and, consequently, the C_6 coefficients) do not depend on gerade/ungerade symmetry.

The quantities X_J for the $^1S_0 + {}^3P_1^o$ dimer are given by

$$X_J = \frac{27}{2\pi}\int_0^\infty \alpha_1^A(i\omega)\,\alpha_{1J}^B(i\omega)\,d\omega + \delta X_0\,\delta_{J,0}, \tag{9}$$

where $A \equiv {}^1S_0$ and $B \equiv {}^3P_1^o$, possible values of the total angular momentum J are 0, 1, and 2, and the other quantities are defined below.

The $\alpha_1^A(i\omega)$ is the electric-dipole dynamic polarizability of the $^1S_0$ state at the imaginary argument. The quantity $\alpha_{KJ}^\Phi(i\omega)$ is a part of the scalar electric-dipole ($K = 1$) or electric-quadrupole ($K = 2$) dynamic polarizability of the state Φ, in which the sum over the intermediate states $|n\rangle$ is restricted to the states with fixed total angular momentum $J_n = J$:

$$\alpha_{KJ}^\Phi(i\omega) \equiv \frac{2}{(2K+1)(2J_\Phi+1)} \times \sum_{\gamma_n} \frac{(E_n - E_\Phi)|\langle \gamma_n, J_n = J||T^{(K)}||\gamma_\Phi, J_\Phi\rangle|^2}{(E_n - E_\Phi)^2 + \omega^2}. \tag{10}$$

TABLE IV. A breakdown of the contributions to the $C_6(\Omega)$ coefficient for the $(^1S_0 + {}^3P_1^o)$ dimer. The CI+MBPT+RPA values for X_J are given in the column labeled "CI+MBPT". The explanation for two other calculations listed in "CI+all" and "Recomm." columns is given in the text. The δX_0 term is given separately in the second row; it is included in the $J = 0$ contribution.

	A_J		X_J			C_6 (CI+all)		C_6 (Recomm.)	
J	$\Omega = 0$	$\Omega = 1$	CI+MBPT	CI+all	Recomm.	$\Omega = 0$	$\Omega = 1$	$\Omega = 0$	$\Omega = 1$
0	4/9	1/9	1473	1494	1486	664	166	660	165
δX_0	4/9	1/9	22.8	23.7	23	11	3	10	3
1	1/9	5/18	6406	6395	6320	711	1776	702	1756
2	11/45	19/90	9981	10007	9853	2446	2113	2409	2080
Sum						3821	4055	3771	4001
Recommended								3771(32)	4001(33)

Here $T^{(K)}$ is the electric-multipole operator of rank K (in particular, $T^{(1)} \equiv D$ and $T^{(2)} \equiv Q$) and γ_n stands for all quantum numbers of the intermediate states except J_n.

The correction δX_0 to the X_0 term in Eq. (9) arises due to a downward ${}^3P_1^o \to {}^1S_0$ transition and is given by the following expression:

$$\delta X_0 = 2\left|\langle {}^3P_1^o||D||{}^1S_0\rangle\right|^2 \sum_{n\neq {}^3P_1^o} \frac{(E_n - E_{{}^1S_0})\,|\langle n||D||{}^1S_0\rangle|^2}{\left(E_n - E_{{}^1S_0}\right)^2 - \omega_0^2} + \frac{\left|\langle {}^3P_1^o||D||{}^1S_0\rangle\right|^4}{2\omega_0}, \tag{11}$$

where $\omega_0 = E_{{}^3P_1^o} - E_{{}^1S_0}$.

A breakdown of the $C_6(\Omega)$ contributions for the Sr $(^1S_0 + {}^3P_1^o)$ dimer is given in Table IV. Two calculations were carried out.

(1) In the first calculation (labeled "CI+all" in Table IV) the CI+all-order+RPA values of matrix elements and energies were used for $\alpha_1({}^3P_1^o)(i\omega)$. For $\alpha_1({}^1S_0)(i\omega)$ we used the experimental ${}^1S_0$-${}^1P_1^o$ electric-dipole matrix element and experimental transition energy for all frequencies.

(2) In the second calculation (labeled "Recomm." in Table IV) the CI+all-order matrix elements and energies were replaced by the recommended matrix elements and the experimental energies for *all* frequencies in the evaluation of $\alpha_1({}^3P_1^o)(i\omega)$.

We list in Table IV the quantities X_J and coefficients A_J given by Eqs. (8) and (9) for allowed $J = 0,1,2$. The δX_0 term is given separately in the second row to illustrate the magnitude of this contribution. It is very small, 0.3% of the total for $\Omega = 0$ and 0.07% for $\Omega = 1$.

The fractional uncertainty δC_6 for the $A + B$ dimer may be expressed via fractional uncertainties in the scalar static dipole polarizabilities of the atomic states A and B [39],

$$\delta C_6 \approx \sqrt{\left(\delta\alpha_1^A(0)\right)^2 + \left(\delta\alpha_1^B(0)\right)^2}. \tag{12}$$

The polarizabilities and their absolute uncertainties are presented in Table V. The uncertainty of the electric-dipole static ${}^1S_0$ polarizability was discussed in detail in Ref. [25]; its recommended value is $\alpha_0({}^1S_0) = 197.14(20)$ a.u. The uncertainty of the scalar static ${}^3P_1^o$ polarizability was determined in this work to be 0.8%. The uncertainty of the tensor part of the static ${}^3P_1^o$ polarizability was determined as the difference of the CI+all-order+RPA and CI+MBPT+RPA values. Using the uncertainties of the scalar polarizabilities and Eq. (12) we are able to determine the fractional uncertainty of the $C_6(\Omega)(^1S_0 + {}^3P_1^o)$ coefficients to be 0.83%. The final recommended values are presented in Table IV.

VI. ELECTRIC QUADRUPOLE POLARIZABILITIES

In this section we discuss the calculation of the static electric quadrupole polarizabilities for the $5s^2\,{}^1S_0$ and $5s5p\,{}^3P_1^o$ states. There are three contributions to $\alpha_2({}^3P_1^o)$ coming from the intermediate states with $J = 1,2,3$.

Using Eq. (10), we find for the valence part of the reduced dynamic scalar electric quadrupole polarizability $\alpha_2(i\omega)$ of the state $|\gamma_0, J_0\rangle \equiv |0\rangle$ with the energy E_0,

$$\alpha_{2J}^v(i\omega) = \frac{2}{5(2J_0+1)} \sum_n \frac{(E_n - E_0)|\langle \gamma_n J_n = J||Q||0\rangle|^2}{(E_n - E_0)^2 + \omega^2}. \tag{13}$$

To correctly include the core contributions for all projections J we use the equation,

$$\alpha_{2J} = \alpha_{2J}^v + \frac{2J+1}{5(2J_0+1)}\left(\alpha_2^c + \alpha_2^{vc}\right),$$

TABLE V. The $5s^2\,{}^1S_0$, $5s5p\,{}^3P_0^o$, and $5s5p\,{}^3P_1^o$ electric-dipole, α_1, static polarizabilities in the CI+MBPT+RPA and CI+all-order+RPA approximations are given in columns labeled "CI+MBPT" and "CI+all". For the ${}^3P_1^o$ state the scalar (α_{1s}) and tensor (α_{1t}) parts of the polarizabilities are presented. $C_6(\Omega_{u/g})$ coefficients for the $A + B$ dimers are listed in the bottom part. The values of C_6, given in column "CI+all", were obtained with the CI+all-order+RPA values of $\alpha_{1s}({}^3P_1^o)(i\omega)$ and CI+all-order+RPA values of $\alpha_1({}^1S_0)(i\omega)$ (adjusted for the experimental ${}^1P_1^o$–${}^1S_0$ matrix element and transition energy).

Level	Property	CI+MBPT	CI+all	HO	Recomm.
$5s^2\,{}^1S_0$	α_1	195.4	197.8	1.2%	197.14(20)[a]
$5s5p\,{}^3P_0^o$	α_1	482.1	458.1	−5.2%	444.51(20)[a]
$5s5p\,{}^3P_1^o$	α_{1s}	499.1	473.2	−5.2%	459.2(3.8)
	α_{1t}	27.9	25.7	−8.6%	26(2)
${}^1S_0 + {}^3P_1^o$	$C_6(0_{u/g})$	3806	3821	0.4%	3771(32)
	$C_6(1_{u/g})$	4050	4055	0.1%	4001(33)

[a] From Ref. [25].

TABLE VI. Contributions to the $5s^2\,{}^1S_0$ and $5s5p\,{}^3P_1^o$ quadrupole scalar polarizabilities. The experimental transition energies [32] are given in column $\Delta E_{\rm expt}$. Theoretical transition energies, absolute values of electric quadrupole reduced matrix elements Q, and the dominant contributions to α_2 are given for the CI+MBPT+RPA and CI+all-order+RPA approximations in columns labeled $\Delta E_{\rm th}$ (in cm^{-1}), Q (in a.u.), and α_2 (in a.u.). The remaining contributions to valence polarizability are grouped together in row Other. The contributions from the core and vc terms are listed together in row Core + Vc. The recommended values of the dominant contributions to α_2, listed in column α_2(Recomm.), are calculated with the CI+all-order+RPA values of Q and the experimental energies.

			CI+MBPT+RPA			CI+all-order+RPA			
State	Contribution	$\Delta E_{\rm expt}$	$\Delta E_{\rm th}$	Q	α_2	$\Delta E_{\rm th}$	Q	α_2	α_2 (Recomm.)
$5s^2\,{}^1S_0$	$5s^2\,{}^1S_0 - 5s4d\,{}^3D_2$	18394	18298	1.20	7	18219	1.18	7	7
	$5s^2\,{}^1S_0 - 5s4d\,{}^1D_2$	20441	20428	26.00	2905	20150	26.54	3026	3069
	$5s^2\,{}^1S_0 - 5s5d\,{}^1D_2$	34958	35092	17.39	757	34727	17.26	749	754
	$5s^2\,{}^1S_0 - 5s5d\,{}^3D_2$	35226	35387	0.52	1	35022	0.54	1	1
	Other				689			697	697
	Core +Vc				17			17	17
	Total				4375			4496	4545
	Recommended								4545(120)
$5s5p\,{}^3P_1^o$	$5s5p\,{}^3P_1^o - 5s5p\,{}^3P_2^o$	394.2	404.3	36.30	95397	403.2	36.46	96487	98680
	$5s5p\,{}^3P_1^o - 4d5p\,{}^3F_2^o$	18763	18724	15.51	376	18909	16.17	404	408
	$5s5p\,{}^3P_1^o - 4d5p\,{}^3F_3^o$	19085	19095	25.46	994	19264	26.26	1048	1057
	$5s5p\,{}^3P_1^o - 5s6p\,{}^3P_1^o$	19364	19260	9.89	149	19332	10.07	154	153
	$5s5p\,{}^3P_1^o - 5s6p\,{}^3P_2^o$	19469	19370	16.03	388	19395	18.61	522	521
	Other				4596			4482	4482
	Core +Vc				17			17	17
	Total				101917			103114	105317
	Recommended								$1.053(12)\times10^5$

from [38], where we assume that the factor $(2J+1)/(5(2J_0+1))$ is the same for both α_2^c and α_2^{vc}. This is correct for the ${}^1S_0$ state. For the ${}^3P_1^o$ state, the α_2^{vc} term is negligibly small.

The breakdown of the contributions to the $5s^2\,{}^1S_0$ $E2$ and $5s5p\,{}^3P_1^o$ $E2$ scalar polarizabilities obtained using the CI+MBPT and CI+all-order methods is given in Table VI. The RPA corrections to the quadrupole operator were also included. The recommended values obtained by replacing the theoretical transition energies by the experimental ones are given in the last column of the table. The uncertainties were determined as the differences of the CI+all-order+RPA and CI+MBPT+RPA results.

The main contribution to the ground-state quadrupole polarizability comes from the $5s4d\,{}^1D_2$ and $5s5d\,{}^1D_2$ states, which give together 84% of the total. The main contribution to the scalar part of the ${}^3P_1^o$ static quadrupole polarizability

TABLE VII. The $X_k^{J_aJ_b}$ for different J_a, J_b, and k and C_8 coefficients obtained in the CI+MBPT+RPA and CI+all-order+RPA approximations are given in columns labeled "CI+MBPT" and "CI+all". The recommended values, given in column labeled "Recomm.", are calculated with CI+all-order+RPA values of Q and the experimental transition energies to the mainly contributing intermediate states listed in Table VI. The contribution of δX_1^{11} is included in X_1^{11} and the contribution of δX_2^{20} is included in X_2^{20}. The (rounded) recommended values are taken as final. Higher-order contributions, defined as relative differences of the "CI+all" and "CI+MBPT" values, are listed in column labeled "HO" in %. Determination of uncertainties, given in parenthesis, is discussed in the text. All quantities are given in a.u.

		CI+MBPT	CI+all	HO	Recomm.	Final
${}^1S_0+{}^1S_0$	C_8	361454	370965	2.4%	371455	$3.7(1)\times10^5$
${}^1S_0+{}^3P_1^o$	δX_1^{11}	126234	128515	1.8%	128515	
	X_1^{11}	186311	189088	1.5%	189088	
	X_1^{12}	704597	713986	1.3%	711015	
	X_1^{13}	425433	429976	1.1%	429976	
	δX_2^{20}	863	890	3.0%	920	
	X_2^{20}	57407	59132	2.9%	59202	
	X_2^{21}	247138	249097	0.8%	249812	
	X_2^{22}	383908	387224	0.9%	388487	
	X_3^{11}		90		90	
	X_4^{22}		154		154	
	$C_8(0_u)$	555172	561944	1.2%	562406	$5.624(73)\times10^5$
	$C_8(1_u)$	724902	733370	1.2%	732694	$7.327(86)\times10^5$
	$C_8(0_g)$	554954	561727	1.2%	562187	$5.622(73)\times10^5$
	$C_8(1_g)$	724829	733297	1.2%	732621	$7.326(86)\times10^5$

TABLE VIII. The values of the $A_l^{J_a J_b}(\Omega_p)$ coefficients. The parameter $p = 0$ for ungerade symmetry and $p = 1$ for gerade symmetry.

	$\Omega_p = 0$	$\Omega_p = 1$
A_1^{11}	3/5	1/5
A_1^{12}	1/15	7/15
A_1^{13}	43/105	31/105
A_2^{20}	3/5	1/5
A_2^{21}	1/5	2/5
A_2^{22}	9/25	8/25
A_3^{11}	$(-1)^p\ 3/5$	$(-1)^p\ 1/5$
A_4^{22}	$(-1)^p\ 9/25$	$(-1)^p\ 3/25$

comes from the $5s5p\,{}^3P_2^o$ state. This intermediate state gives 94% of the total. This is due to a very small energy interval $\Delta E = E({}^3P_2^o) - E({}^3P_1^o)$ of only 394.2 cm^{-1}. We note that we obtained very close results for ΔE, 404 and 403 cm^{-1}, at the CI+MBPT and CI+all-order stages, respectively. At the same time these values are 2.5% larger than the experimental transition energy $\Delta E = 394.2$ cm^{-1}. This difference is taken into account in the recommended values of the quadrupole polarizabilities, where the experimental energies are used for the dominant transitions.

VII. C_8 COEFFICIENTS

The C_8 dispersion coefficient for the ${}^1S_0 + {}^1S_0$ dimer can be found as the quadrature of the electric-dipole $\alpha_1^A(i\omega)$ and the electric-quadrupole $\alpha_2^A(i\omega)$ dynamic polarizabilities of the $A \equiv {}^1S_0$ state:

$$C_8 = \frac{15}{\pi}\int_0^\infty \alpha_1^A(i\omega)\,\alpha_2^A(i\omega)\,d\omega. \tag{14}$$

The results of calculation of the C_8 coefficient in the CI+MBPT+RPA and CI+all-order+RPA approximations are presented in Table VII. The recommended value is obtained with the CI+all-order+RPA matrix elements of the Q operator and the experimental transition energies for the intermediate states listed in Table VI. The recommended value is taken as final.

In analogy to the C_6 coefficient the fractional uncertainty of $C_8({}^1S_0 + {}^1S_0)$ can be expressed via fractional uncertainties of the electric-dipole and quadrupole static polarizabilities of the $A \equiv {}^1S_0$ state as

$$\delta C_8({}^1S_0 + {}^1S_0) \approx \sqrt{\left(\delta\alpha_1^A(0)\right)^2 + \left(\delta\alpha_2^A(0)\right)^2}. \tag{15}$$

Now taking into account that $\delta\alpha_1^A(0)$ is negligible in comparison to $\delta\alpha_2^A(0)$, we arrive at $\delta C_8 \approx \delta\alpha_2^A(0) \approx 2.6\%$.

The $C_8(5s^2\,{}^1S_0 + 5s5p\,{}^3P_1^o)$ coefficient can be written in a general form [38]:

$$C_8(\Omega_p) = \sum_{l=1}^{4}\sum_{J_\alpha J_\beta} A_l^{J_\alpha J_\beta}(\Omega_p)\,X_l^{J_\alpha J_\beta}.$$

The nonzero angular factors $A_l^{J_\alpha J_\beta}(\Omega_p)$ are listed in Table VIII. A derivation of the corresponding quantities $X_l^{J_\alpha J_\beta}$ was discussed in detail in Ref. [38], therefore, we give only the final formulas:

$$\begin{aligned} X_1^{1J} &= \frac{45}{2\pi}\int_0^\infty \alpha_1^A(i\omega)\,\alpha_{2J}^B(i\omega)\,d\omega + \delta X_1^{11}\,\delta_{J1},\\ \delta X_1^{11} &= \frac{3}{2}\left|\langle {}^3P_1^o||Q||{}^3P_1^o\rangle\right|^2 \alpha_1^A(0), \end{aligned} \tag{16}$$

where $J = 1,2,3$.

$$\begin{aligned} X_2^{2J} &= \frac{45}{2\pi}\int_0^\infty \alpha_2^A(i\omega)\,\alpha_{1J}^B(i\omega)\,d\omega + \delta X_2^{20}\,\delta_{J0},\\ \delta X_2^{20} &= 5\left|\langle {}^3P_1^o||D||{}^1S_0\rangle\right|^2 \alpha_2^A(\omega_0), \end{aligned} \tag{17}$$

where $J = 0,1,2$ and $\omega_0 \equiv E_{{}^3P_1^o} - E_{{}^1S_0}$.

$$X_3^{11} = \sum_{n,k}\frac{\langle {}^1S_0||D||n\rangle\langle n||Q||{}^3P_1^o\rangle\langle {}^3P_1^o||Q||k\rangle\langle k||D||{}^1S_0\rangle}{E_n - E_{{}^1S_0} + E_k - E_{{}^3P_1^o}},$$

$$X_4^{22} = \sum_{n,k}\frac{\langle {}^1S_0||Q||n\rangle\langle n||D||{}^3P_1^o\rangle\langle {}^3P_1^o||D||k\rangle\langle k||Q||{}^1S_0\rangle}{E_n - E_{{}^1S_0} + E_k - E_{{}^3P_1^o}}.$$

A complete calculation of the X_3^{11} and X_4^{22} terms is rather difficult due to double summations over intermediate states n and k. However, these expressions can be simplified if we note that the main contributions to the static electric-dipole and quadrupole ${}^1S_0$ polarizabilities come from a few low-lying intermediate states. Thus, we can leave in the sums over index k in X_3^{11} and X_4^{22} only a few first terms arriving at the following approximate expressions:

$$\begin{aligned} X_3^{11} \approx{}& \langle {}^3P_1^o||Q||5s5p\,{}^3P_1^o\rangle\langle 5s5p\,{}^3P_1^o||D||{}^1S_0\rangle \sum_n \frac{\langle {}^1S_0||D||n\rangle\langle n||Q||{}^3P_1^o\rangle}{E_n - E_{{}^1S_0}}\\ &+\langle {}^3P_1^o||Q||5s5p\,{}^1P_1^o\rangle\langle 5s5p\,{}^1P_1^o||D||{}^1S_0\rangle \sum_n \frac{\langle {}^1S_0||D||n\rangle\langle n||Q||{}^3P_1^o\rangle}{E_n - E_{{}^1S_0} + E_{(5s5p\,{}^1P_1^o)} - E_{{}^3P_1^o}}\\ &+\langle {}^3P_1^o||Q||5s6p\,{}^3P_1^o\rangle\langle 5s6p\,{}^3P_1^o||D||{}^1S_0\rangle \sum_n \frac{\langle {}^1S_0||D||n\rangle\langle n||Q||{}^3P_1^o\rangle}{E_n - E_{{}^1S_0} + E_{(5s6p\,{}^3P_1^o)} - E_{{}^3P_1^o}}\\ &+\langle {}^3P_1^o||Q||5s6p\,{}^1P_1^o\rangle\langle 5s6p\,{}^1P_1^o||D||{}^1S_0\rangle \sum_n \frac{\langle {}^1S_0||D||n\rangle\langle n||Q||{}^3P_1^o\rangle}{E_n - E_{{}^1S_0} + E_{(5s6p\,{}^1P_1^o)} - E_{{}^3P_1^o}}. \end{aligned} \tag{18}$$

$$\begin{aligned}
X_4^{22} \approx\ & \langle {}^1S_0||Q||5s4d\,{}^3D_2\rangle\langle 5s4d\,{}^3D_2||D||{}^3P_1^o\rangle \sum_{k,J_k=2} \frac{\langle {}^3P_1^o||D||k\rangle\langle k||Q||{}^1S_0\rangle}{E_k - E_{{}^3P_1^o} + E_{(5s4d\,{}^3D_2)} - E_{{}^1S_0}} \\
&+ \langle {}^1S_0||Q||5s4d\,{}^1D_2\rangle\langle 5s4d\,{}^1D_2||D||{}^3P_1^o\rangle \sum_{k,J_k=2} \frac{\langle {}^3P_1^o||D||k\rangle\langle k||Q||{}^1S_0\rangle}{E_k - E_{{}^3P_1^o} + E_{(5s4d\,{}^1D_2)} - E_{{}^1S_0}} \\
&+ \langle {}^1S_0||Q||5s5d\,{}^1D_2\rangle\langle 5s5d\,{}^1D_2||D||{}^3P_1^o\rangle \sum_{k,J_k=2} \frac{\langle {}^3P_1^o||D||k\rangle\langle k||Q||{}^1S_0\rangle}{E_k - E_{{}^3P_1^o} + E_{(5s5d\,{}^1D_2)} - E_{{}^1S_0}} \\
&+ \langle {}^1S_0||Q||5s5d\,{}^3D_2\rangle\langle 5s5d\,{}^3D_2||D||{}^3P_1^o\rangle \sum_{k,J_k=2} \frac{\langle {}^3P_1^o||D||k\rangle\langle k||Q||{}^1S_0\rangle}{E_k - E_{{}^3P_1^o} + E_{(5s5d\,{}^3D_2)} - E_{{}^1S_0}}. \qquad (19)
\end{aligned}$$

The $X_l^{J_a J_b}$ values and $C_8(\Omega_{g/u})$ coefficients for the $5s^2\,{}^1S_0 + 5s5p\,{}^3P_1^o$ dimer are given in Table VII. The contributions of the X_3^{11} and X_4^{22} are very small, which is expected since these terms contain intercombination transition matrix elements for both D and Q operators. Such matrix elements are equal to zero in nonrelativistic approximation. Relativistic corrections are small for Sr and, correspondingly, X_3^{11} and X_4^{22} are four orders of magnitude smaller than the main contributions coming from the X_1^{1J} and $X_2^{2J'}$ terms.

The recommended values are calculated with the CI+all-order+RPA values of Q and the experimental transition energies for the main intermediate states listed in Table VI. The (rounded) recommended values are taken as final. Higher-order contributions were defined as relative differences of the CI+all-order+RPA and CI+MBPT+RPA values.

To estimate the uncertainties of the C_8 coefficients we neglect small quantities X_3^{11} and X_4^{22}. Then, designating

$$\begin{aligned}
C_1 &\equiv \sum_{J=1}^{3} A_1^{1J} X_1^{1J}, \\
C_2 &\equiv \sum_{J=0}^{2} A_2^{2J'} X_2^{2J'},
\end{aligned} \qquad (20)$$

we can express the absolute uncertainty of C_8^{AB} via absolute uncertainties of C_1 and C_2 as

$$\Delta C_8^{AB} \approx \sqrt{\Delta C_1^2 + \Delta C_2^2}. \qquad (21)$$

The fractional uncertainties in C_1 and C_2 can be expressed via corresponding fractional uncertainties in the scalar static polarizabilities,

$$\begin{aligned}
\delta C_1 &\approx \sqrt{\left(\delta\alpha_1^A(0)\right)^2 + \left(\delta\alpha_2^B(0)\right)^2}, \\
\delta C_2 &\approx \sqrt{\left(\delta\alpha_2^A(0)\right)^2 + \left(\delta\alpha_1^B(0)\right)^2}.
\end{aligned} \qquad (22)$$

We note that X_1^{11} includes the additional term δX_1^{11} [see Eq. (16)]. Nevertheless the equation above for δC_1 is valid if we assume that the uncertainty of $|\langle {}^3P_1^o||Q||{}^3P_1^o\rangle|^2$ is approximately the same as the uncertainty of the scalar part of $\alpha_2({}^3P_1^o)$. This assumption is based on the $5s5p\,{}^3P_2^o$ state contributing ~94% to the scalar $\alpha_2({}^3P_1^o)$, i.e., the uncertainty of $\alpha_2({}^3P_1^o)$ is mostly determined by the uncertainty of the matrix element $|\langle {}^3P_1^o||Q||{}^3P_2^o\rangle|$. The latter is assumed to be the same as the uncertainty of the matrix element $|\langle {}^3P_1^o||Q||{}^3P_1^o\rangle| = 20.9$ a.u.

The term δX_2^{20} contributing to X_2^{20} gives only 0.25% of total C_2 and, respectively, its contribution to the uncertainty budget is negligible.

Using these formulas and knowing the fractional uncertainties of the polarizabilities we assign the uncertainties to the final values of the C_8 coefficients presented in Table VII. It is worth noting that if we estimate the uncertainties of the C_8 coefficients as the difference of the CI+all-order+RPA and CI+MBPT+RPA values, we obtain very close results.

VIII. SUMMARY

In Table IX we summarize the results for the Sr van der Waals coefficients obtained in the present work and

TABLE IX. The C_6 and C_8 coefficients for the Sr ${}^1S_0 + {}^1S_0$, ${}^1S_0 + {}^3P_0^o$, ${}^3P_0^o + {}^3P_0^o$, and ${}^1S_0 + {}^3P_1^o$ dimers (in a.u.). The uncertainties are given in parenthesis.

	Property	This work	Other results	Ref.
${}^1S_0 + {}^1S_0$	C_6		3103(7)	[14]
			3250	[13]
			3164(10)	[40]
			3131(41)	[41]
			3142	[18]
	C_8	$3.7(1)\times 10^5$	$3.792(8)\times 10^5$	[14]
			3.854×10^5	[13]
${}^1S_0 + {}^3P_0^o$	C_6		3880(80)	[2]
${}^3P_0^o + {}^3P_0^o$	C_6		5360(200)	[2]
			5260(500)	[42]
			5102	[43]
${}^1S_0 + {}^3P_1^o$	$C_6(0_{u/g})$	3771(32)	3868(50)	[17]
			3951[a]	[18]
	$C_6(1_{u/g})$	4001(33)	4085(50)	[17]
			4220[a]	[18]
	$C_8(0_u)$	$5.624(73) \times 10^5$		
	$C_8(1_u)$	$7.327(86) \times 10^5$		
	$C_8(0_g)$	$5.622(73) \times 10^5$		
	$C_8(1_g)$	$7.326(86) \times 10^5$		

[a] Calculated via $C_6(0_u) = C_6(c\,{}^3\Pi_u)$ and $C_6(1_u) = (C_6(a\,{}^3\Sigma_u^+) + C_6(c\,{}^3\Pi_u))/2$ [17,44] from Hund's case (a) values of Ref. [18].

other studies [2,13,14,17,18,40–43]. The *ab initio* molecular calculations carried out using the multireference configuration interaction (MRCI) method [18] give the ground-state C_6 coefficient with excellent agreement with the recommended value of Ref. [40]. The MRCI results for the excited state $^1S_0$-$^3P_1^o$ Sr dimer agree well, to 5%, with our values for C_6 coefficients. The difference between the present values and MRCI results is significantly larger for the C_8 coefficients. Our recommended values of the long-range dispersion coefficients $C_6(0_u) = 3771(32)$ a.u. and $C_6(1_u) = 4001(33)$ a.u. are in a good agreement with the experimental results $C_6(0_u) = 3868(50)$ a.u. and $C_6(1_u) = 4085(50)$ a.u. obtained in Ref. [17].

To conclude, we evaluated $E1$ transition amplitudes from the $5s5p\,^3P_1^o$ state to the low-lying even-parity states and the electric-dipole and quadrupole static polarizabilities of the $5s5p\,^3P_1^o$ state of atomic Sr. We also calculated the C_6 and C_8 coefficients for the Sr $^1S_0 + {^1S_0}$ and $^1S_0 + {^3P_1^o}$ dimers and confirmed the experimental value for the $^1S_0$-$^3P_1^o$ magic wavelength. We have analyzed the accuracy of calculations and assigned the uncertainties to all presented quantities.

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