Relativistic calculations of $C_6$ and $C_8$ coefficients for strontium dimers

S. G. Porsev$^{1,2}$, M. S. Safronova$^{1,3}$, and Charles W. Clark$^3$

$^1$Department of Physics and Astronomy, University of Delaware, Newark, Delaware 19716, USA
$^2$Petersburg Nuclear Physics Institute, Gatchina, Leningrad District, 188300, Russia
$^3$Joint Quantum Institute, National Institute of Standards and Technology and the University of Maryland, Gaithersburg, Maryland, 20899, USA

(Dated: September 23, 2014)

The electric dipole and quadrupole polarizabilities of the $5s5p \, ^3P_1^o$ state and the $C_6$ and $C_8$ coefficients for the $\, ^{1}S_0 + \, ^{1}S_0$ and $\, ^{3}S_0 + \, ^{3}P_0$ 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 $\, ^1S_0 - ^3P_0^o$ transition vanishes. The accuracy of calculations is analyzed and uncertainties are assigned to all quantities reported in this work.

PACS numbers: 34.20.Cf, 32.10.Dk, 31.15.ac

I. INTRODUCTION

The divalent alkaline-earth element strontium is of interest for many applications of atomic, molecular and optical physics. The atomic clock based on the $5s^2 \, ^1S_0 - 5s5p \, ^3P_1^o$ transition in Sr has achieved a total systematic uncertainty of $6 \times 10^{-18}$ \cite{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 \cite{2}.

All four stable isotopes of Sr have been brought to strong quantum degeneracy: Bose-Einstein condensation have been achieved in the bosonic isotopes 84, 86 and 88, and fermionic $^{87}$Sr has been cooled to within 10\% of its Fermi temperature \cite{3}. The first isotope to be condensed $^{84}$Sr, is also distinctive in being the only atomic species to date which has been condensed by laser cooling alone \cite{4}. Sr has also been used in ultracold gases of both homonuclear $^4$Sr and heteronuclear $^{87}$Sr$^{85}$Sr molecules. A quantum degenerate gas mixture of Sr and Rb has been realized recently \cite{5}, 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 \cite{6}, coherent photoassociation \cite{7} and search for time-variation of the electron-proton mass ratio \cite{8}.

Understanding of long-range interaction of the Sr atoms is needed for all of the applications mentioned above. In Ref. \cite{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 $\, ^3P_0 - ^3P_0^o$ dimers for the determination of relevant interaction parameters for spin-orbital quantum dynamics.

Motivated by the diverse applications and particular interest of $\, ^1S_0 - ^3P_1^o$ intercombination line for 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. \cite{13,14}; here we provide revised values that have been critically evaluated for accuracy. In a recent paper, Borkowski et al. \cite{16} reported photoassociation spectroscopy of ultracold Sr atoms near the intercombination $\, ^1S_0 + ^3P_1^o$ line. They obtained the Coriolis mixing angles and linear Zee- man coefficients for all of the photoassociation lines and determined the van der Waals $C_6$ coefficients for the $0_u$ and $1_u$ bound state energies to be $C_6(0_u) = 3868(50)$ a.u. and $C_6(1_u) = 4085(50)$ a.u.. 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 Sections VI and VII we present the results of
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 configuration interaction (CI) method (see, e.g., [17]) while core-core and core-valence correlations are treated in the framework of many-body perturbation theory (MBPT) and all-order single-double coupled-cluster method. Both CI+MBPT and CI+all-order methods were described in detail in a number of papers [18–21], 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 $\alpha/h [\text{Hz}/(\text{V/m})^2] = 2.48832 \times 10^{-8} \alpha$ (a.u.), where the conversion coefficient is $4\pi \varepsilon_0 \alpha_0^2/h$ and the Planck constant $h$ is factored out in order to provide direct conversion into frequency units; $\alpha_0$ is the Bohr radius and $\varepsilon_0$ is the electric constant.

We start with the solutions of the Dirac-Fock equation

$$H_0 \psi_c = \varepsilon_c \psi_c,$$  \hspace{1cm} (1)

where $H_0$ is the Dirac-Fock Hamiltonian and $\psi_c$ and $\varepsilon_c$ 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 is 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 [18],

$$H_{\text{eff}}(E) \Phi_n = E_n \Phi_n,$$ \hspace{1cm} (2)

with the effective Hamiltonian defined as

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

Here $H_{\text{FC}}$ 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 [18] and using a linearized coupled-cluster single-double method in the CI+all-order approach [20]. 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. [22]. In analogy with the effective Hamiltonian we can construct effective electric-dipole and electric-quadrupole operators to account for dominant core-valence correlations [23–25].

In [22], we used the CI+all-order method to evaluate the static and dynamic polarizabilities of the 5$s^2$ $^1S_0$ and 5$s^5p^5$ $^1P_0$ states of Sr. We found that the $E1$ matrix elements for the transitions that give dominant contributions to the $\mu^2$ 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 $^1S_0$ − $^1P_0$ clock transition, 247.5 a.u., was found to be in excellent agreement with the experimental result 247.374(7) a.u. [26].

In order to predict the accurate values for the dynamic part of blackbody radiation shift in 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 [26] and magic wavelength [27] of the 5$s^2$ $^1S_0$ − 5$s^5p^5$ $^1P_0$ transition to determine very accurate recommended values for several relevant electric-dipole matrix elements [22]. Specifically, we were able to obtain accurate recommended values for the following most important transitions contributing to the $^1P_0$ polarizability: 5$s^5p$ $^3P_0$ − 5$s^4d$ $^3D_1$, 5$s^5p$ $^3P_0$ − 5$s^6s$ $^3S_1$, 5$s^5p$ $^3P_0$ − 5$s^5d$ $^3D_1$, and 5$s^5p$ $^3P_0$ − 5$p^2$ $^3P_1$.  

### Table I: The CI+MBPT and CI+all-order results for absolute values of the reduced electric dipole matrix elements

| Transition      | CI+MBPT    | CI+All    | HO | Recomm. |
|-----------------|------------|-----------|----|---------|
| 5$s^5p$ $^3P_0$ − 5$s^4d$ $^3D_1$ | 2.681      | 2.712     | 1.14% | 2.675(13)$^a$ |
| 5$s^5p$ $^3P_0$ − 5$s^4d$ $^3D_1$ | 2.326      | 2.354     | 1.19% | 2.322(11)$^a$ |
| 5$s^5p$ $^3P_0$ − 5$s^6s$ $^3S_1$ | 4.031      | 4.075     | 1.08% | 4.019(20)    |
| 5$s^5p$ $^3P_0$ − 5$s^6s$ $^3S_1$ | 1.983      | 1.970     | -0.66% | 1.962(10)$^a$ |
| 5$s^5p$ $^3P_0$ − 5$s^5d$ $^3D_1$ | 3.463      | 3.439     | -0.70% | 3.452(17)    |
| 5$s^5p$ $^3P_0$ − 5$s^5d$ $^3D_1$ | 2.474      | 2.460     | -0.57% | 2.450(24)$^a$ |
| 5$s^5p$ $^3P_0$ − 5$s^5d$ $^3D_1$ | 2.065      | 2.017     | -2.38% | 2.009(20)    |
| 5$s^5p$ $^3P_0$ − 5$s^5d$ $^3D_1$ | 3.720      | 3.688     | -0.87% | 3.673(37)    |
| 5$s^5p$ $^3P_0$ − 5$p^2$ $^3P_1$ | 2.587      | 2.619     | 1.22% | 2.605(26)$^a$ |
| 5$s^5p$ $^3P_0$ − 5$p^2$ $^3P_1$ | 2.619      | 2.671     | 1.95% | 2.657(27)    |
| 5$s^5p$ $^3P_0$ − 5$p^2$ $^3P_1$ | 2.317      | 2.374     | 2.40% | 2.302(24)    |
| 5$s^5p$ $^3P_0$ − 5$p^2$ $^3P_1$ | 2.837      | 2.880     | 1.49% | 2.865(29)    |

$^a$Reference [22].
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 8 transitions that give dominant contributions to the polarizability of the $5s5p \, ^3P_0$ state. The results are summarized in Table I.

We assume that the transitions from even-parity states to the $5s5p \, ^3P_0$ state are calculated in the CI+all-order+RPA approach with the same accuracy as similar transitions from even-parity states to the $5s5p \, ^3P_0$ state, for which the recommended values were presented in Ref. [22]. Then, for example, the recommended value of the $\langle 5s4d \, ^3D_2 \rangle |D| \langle 5s5p \, ^3P_0 \rangle$ matrix element is obtained here from the CI+all-order+RPA ratio

\[
\frac{\langle 5s4d \, ^3D_2 \rangle |D| \langle 5s5p \, ^3P_0 \rangle}{\langle 5s4d \, ^3D_1 \rangle |D| \langle 5s5p \, ^3P_0 \rangle}
\]
multiplied by the recommended value of the $\langle 5s4d \, ^3D_1 \rangle |D| \langle 5s5p \, ^3P_0 \rangle$ 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 $5s5p \, ^3P_0$ state.

As a additional check, we also use a simple ratio between 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

\[
\langle \gamma JLS || D || \gamma' J'L'S' \rangle = \delta SS' \sqrt{(2J + 1)(2J' + 1)} \times (-1)^{S + L + J + 1} \left\{ \begin{array}{ccc}
L & J & S \\
J' & L' & 1
\end{array} \right\} \langle \gamma LS || D || \gamma' L'S \rangle,
\]

where $S$ is the total spin momentum of the atomic state, $L$ and $J$ are the orbital and total angular momenta, and $\gamma$ 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 $5s5p \, ^3P_0 - 5s4d \, ^3D_J$ transitions give dominant contributions to the $5s5p \, ^3P_0$ 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 $5s5p \, ^3P_J$, $5s4d \, ^3D_J$, and $5s5d \, ^3D_J$ 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. [22], 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 expressed 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 $^3P_1$ STATE**

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

\[
\alpha(\omega) = \alpha^v(\omega) + \alpha^c(\omega) + \alpha^{vc}(\omega),
\]

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

The valence part of the polarizability is determined by solving the inhomogeneous equation in valence space,
which is approximated as [30]

\[(E_n - H_{\text{eff}})\langle \Psi(v, M') | \alpha | \Psi_0(v, J, M) \rangle = D_{\text{eff}} \langle \Psi_0(v, J, M) | \alpha | \Psi_0(v, J, M) \rangle \]

(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 \(\{v, J, M\}\) [30]. The effective dipole operator \(D_{\text{eff}}\) includes RPA corrections.

Small core terms \(\alpha_c\) and \(\alpha_{vc}\) are evaluated in the RPA. The latter is calculated by adding \(\alpha_{vc}\) 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 [51] to establish the dominant contributions to the final value

\[\alpha_0^\text{v}(\omega) = \frac{2}{3(2J + 1)} \sum_n \frac{(E_n - E_\text{th})(\langle \psi || D || \psi \rangle)^2}{(E_n - E_V)^2 - \omega^2}.\]

(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 \(3P^o\) static scalar polarizability using different sets of the energies and \(E1\) matrix elements. The results are presented in Table III. The theoretical and experimental [29] transition energies are given in columns \(\Delta E_{\text{the}}\) and \(\Delta E_{\text{expt}}\) in cm\(^{-1}\). The dominant contributions to the polarizability listed in columns \(\alpha_0[A]\) and \(\alpha_0[B]\) are calculated with CI + all-order + RPA matrix elements and theoretical \([A]\) and experimental \([B]\) energies [29], respectively. The dominant contributions to \(\alpha_0\) listed in column \(\alpha_0[C]\) are calculated with experimental energies and recommended matrix elements. These results are taken as final. The remaining valence elements that are not listed separately are given in row labeled “Other”. The sum of the core and \(\alpha_{vc}\) terms is listed in row labeled “Core +Vc”.

A comparison of the main contributions to the 5s5p \(3P^o\) and 5s5p \(3P^o\) scalar polarizabilities is given in Table III. Two sets of calculations are presented. In the first calculation, we use the \textit{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 \(2D_1\) 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 \(\alpha_0(3P^o)\) means the sum of contributions of the 5s4d \(3D_1\) and 5s4d \(3D_2\) states, while in the case of the \(3P^o\) state the notation 5s4d \(3D\) means the contribution of the 5s4d \(3D_1\) state only.

The contribution of different terms to \(\alpha_0(3P^o)\) and \(\alpha_0(3P^o)\) 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 \(\alpha_0(3P^o)\) determined in [22]. Our final recommended result for the 5s5p \(3P^o\) scalar polarizability is 459.2(3.8) a.u.

**IV. MAGIC WAVELENGTH**

The magic wavelength \(\lambda^*\) at which \(\alpha_1(S_0, \lambda^*) = \alpha_{3P^o,1,|m, j|=1}(\lambda^*)\) and the quadratic Stark shift on the \(3S_0 - 3P^o_1\) transition vanishes, was experimentally determined by Ido and Katori [32] 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 \(\lambda^*\), and the experimental value of the matrix element \(|\langle 5s^21S_0 || D || 5s5p3P^o_1 \rangle| = 5.248(2)\) a.u. [33], \(\alpha_{3P^o}(\omega^*)\) was obtained in Ref. [34] to be 261.2(3) a.u. [35].

Solving inhomogeneous equation, Eq. (5), we found

---

**TABLE III:** The dominant contributions to the Sr 5s5p \(3P^o\) and 5s5p \(3P^o\) scalar polarizabilities in a.u. and in percent. \textit{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 \(3P^o\) state are taken from Ref. [22]. Final (recommended) results for the scalar 5s5p \(3P^o\) polarizability are given in the last column.

| State     | Theor. matrix elements and energies | Recomm. matrix elements and exp. energies | Recomm. matrix elements and exp. energies |
|-----------|-----------------------------------|------------------------------------------|------------------------------------------|
|           | \(\alpha_0(3P^o)\) | \(\alpha_0(3P^o)\) | \(\alpha_0(3P^o)\) | \(\alpha_0(3P^o)\) | \(\alpha_0(3P^o)\) | \(\alpha_0(3P^o)\) |
| 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) |
| 5p2 \(3P\) | 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) |
\( \omega' = 261.03 \) 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 \( \alpha_{J_0}^{+p} \) 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 \( C_6(1S_0 + 3P_1) \) coefficient is given by [35]

\[
C_6(\Omega_p) = \sum_{J=0}^{2} A_J(\Omega) X_J,
\]

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

\[
A_J(\Omega) = \frac{1}{3} \sum_{\mu=-1}^{1} \left\{ \frac{1}{\Omega} + \frac{1}{\mu} + J \right\}^{2}
\]

with the dipole weights \( w_{\mu}^{(1)} = 1 \) 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 \( 1S_0 + 3P_1 \) dimer are given by

\[
X_J = \frac{27}{2\pi} \int_0^\infty \alpha_1^A(\i) \alpha_1^B(\i) d\omega + \delta X_0 \delta X_0.
\]

where \( A \equiv 1S_0 \) and \( B \equiv 3P_1 \), possible values of the total angular momentum \( J \) are 0, 1, and 2, and the other quantities are defined below.

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

\[
\alpha_1^B(\i) \equiv \frac{2}{(K+1)(2J_0+1)} \times \sum_{\gamma_n} \frac{(E_n - E_\Phi)|\langle \gamma_n | J_n = J | T(K) | \gamma_\Phi, J_\Phi \rangle|^2}{(E_n - E_\Phi)^2 + \omega^2} \tag{10}
\]

Here \( \gamma_n \) stands for all quantum numbers of the intermediate states except \( J_n \).

The correction \( \delta X_0 \) to the \( X_0 \) term in Eq. (9) arises due to a downward \( 3P_1 \rightarrow 1S_0 \) transition and is given by the following expression:

\[
\begin{align*}
\delta X_0 &= 2 |\langle 3P_1 | D | 1S_0 \rangle|^2 \sum_{n \neq 3P_0} \frac{(E_n - E_{1S_0}) |\langle n | D | 1S_0 \rangle|^2}{(E_n - E_{1S_0})^2 - \omega_0^2} \\
&+ \frac{|\langle 3P_0 | D | 1S_0 \rangle|^4}{2\omega_0} \tag{11}
\end{align*}
\]

where \( \omega_0 = E_{3P_0} - E_{1S_0} \). A breakdown of the \( C_6(\Omega) \) contributions for the \( Sr(1S_0 + 3P_1) \) dimer is given in Table IV. Two calculations were carried out:

- In the first calculation (labeled "CI+All" in Table IV) the CI+all-order+RPA values of matrix elements and energies were used for \( \alpha_1(3P_0)(i\omega) \). For \( \alpha_1(1S_0)(i\omega) \) we used the experimental \( 1S_0 - 3P_0 \) electric dipole matrix element and experimental transition energy for all frequencies.

- 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 \( \alpha_1(3P_0)(i\omega) \).

We list in Table IV the quantities \( X_J \) and coefficients \( J \) given by Eqs. (8) and (9) for allowed \( J = 0, 1, 2 \). The \( \delta X_0 \) 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 \( \delta C_6 \) for the A + B dimer may be expressed via fractional uncertainties in the scalar static dipole polarizabilities of the atomic states A and B [36],

\[
\delta C_6 \approx \sqrt{(\delta \alpha_1^A(0))^2 + (\delta \alpha_1^B(0))^2}. \tag{12}
\]

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. [22]; its recommended value is \( \alpha_0(1S_0) = 197.14(20) \) a.u.. The uncertainty of the scalar \( 3P_1 \) polarizability was determined in this work to be 0.8%. The uncertainty of the tensor part of the static \( 3P_1 \) 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 \( C_6(\Omega)(1S_0 + 3P_1) \) 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 \( 5s5p 3P_1 \) states. There are three contributions to \( \alpha_2(3P_1) \) coming from the intermediate states with \( J = 1, 2, 3 \).
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 column labeled “CI+MBPT”. The explanation for two other calculations listed in “CI+All” and “Recomm.” columns is given in the text. The $\delta X_0$ term is given separately in the second row; it is included in the $J = 0$ contribution.

| $J$ | $\Omega = 0$ | $\Omega = 1$ | CI+MBPT | CI+All | Recomm. | $C_6$ [CI+All] | $C_6$ [Recomm.] |
|-----|--------------|--------------|----------|--------|---------|---------------|----------------|
|     | $A_J$        |              |          |        |         | $\Omega = 0$ | $\Omega = 1$   |
| 0   | 4/9          | 1/9          | 1473     | 1494   | 1486    | 664           | 166            |
| $\delta X_0$ | 4/9          | 1/9          | 22.8     | 23.7   | 23      | 11            | 3              |
| 1   | 1/9          | 5/18         | 6406     | 6395   | 6320    | 711           | 1776           |
| 2   | 11/45        | 19/90        | 9981     | 10007  | 9853    | 2446          | 2113           |
| Sum |              |              |          |         |         | 3821          | 4055           |

Recommended

4001(33)

TABLE V: The $5s^2\,1S_0$, $5s5p\,3P_1^0$, and $5s5p\,3P_1^o$ electric-dipole, $\alpha_1$, 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 $3P_1^0$ state the scalar $(\alpha_{1s})$ and tensor $(\alpha_{1tt})$ parts of the polarizabilities are presented. $C_6(\Omega_{2/9,3/9})$ 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 $\alpha_1(3P_1^0)(i\omega)$ 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. |
|-------|----------|----------|--------|----|---------|
| $5s^2\,1S_0$ | $\alpha_1$ | 195.4 | 197.8 | 1.2% | 197.14(20)$^+$ |
| $5s5p\,3P_1^0$ | $\alpha_1$ | 482.1 | 458.1 | -5.2% | 444.51(20)$^+$ |
| $5s5p\,3P_1^o$ | $\alpha_{1s}$ | 499.1 | 473.2 | -5.2% | 459.2(3.8) |
|        | $\alpha_{1tt}$ | 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) |

$^+$From Ref. [22].

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 $E_0$

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

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

$$\alpha_{2,J} = \alpha_{2,J}^{\gamma} + \frac{2J + 1}{5(2J_0 + 1)}(\alpha_{2}^{x} + \alpha_{2}^{y})$$

from [35], where we assume that the factor $(2J + 1)/(5(2J_0 + 1))$ is the same for both $\alpha_2^{x}$ and $\alpha_2^{y}$. This is correct for the $1S_0$ state. For the $3P_1^o$ state, the $\alpha_2^{x}$ 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 $5s5d\,2D_2$ states, which give together 84% of total. The main contribution to the scalar part of the $3P_1^o$ static quadrupole polarizability comes from the $5s5p\,3P_2^o$ state. This intermediate state gives 94% of total. This is due to a very small energy interval $\Delta E = E(3P_1^o) - E(3P_2^o)$ of only 394.2 cm$^{-1}$. We note that we obtained very close results for $\Delta E$, 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:

$$C_8 = 15\int_0^{\infty} \alpha_1^A(i\omega) \alpha_2^A(i\omega) d\omega.$$  

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 [VII]. 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
TABLE VI: Contributions to the $5s^2$ $^1S_0$ and $5s5p$ $^3P_1^o$ quadrupole scalar polarizabilities. The experimental transition energies [29] are given in column $\Delta E_{\text{expt}}$. Theoretical transition energies, absolute values of electric quadrupole reduced matrix elements $Q$, and the dominant contributions to $\alpha_2$ are given for the CI+MBPT+RPA and CI+all-order+RPA approximations in columns labeled $\Delta E_{\text{th}}$ (in cm$^{-1}$), $Q$ (in a.u.), and $\alpha_2$ (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 $\alpha_2$, listed in column $\alpha_2[\text{Recom}]$ are calculated with the CI+all-order+RPA values of $Q$ and the experimental energies.

| State          | Contribution                        | $\Delta E_{\text{expt}}$ | $\Delta E_{\text{th}}$ | $Q$ | $\alpha_2$ | $\Delta E_{\text{th}}$ | $Q$ | $\alpha_2$ | $\alpha_2[\text{Recom}]$ |
|----------------|-------------------------------------|---------------------------|-------------------------|-----|------------|-------------------------|-----|------------|-------------------------|
| $5s^2$ $^1S_0$ | $5s^2$ $^1S_0 - 5s4d$ $^3D_2$       | 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                    |
|                | $5s^2$ $^1S_0 - 5s5d$ $^3D_2$       | 34958                     | 35092                   | 17.39| 757       | 34727                   | 17.26| 749        | 754                     |
|                | $5s^2$ $^1S_0 - 5s5d$ $^1D_2$       | 35226                     | 35387                   | 0.52| 1         | 35022                   | 0.54| 1          | 1                       |
|                | Other                               |                           |                         |     |            |                         |     |            | 689                     |
|                | Core + Vc                           | 17                        |                         |     |            |                         |     |            | 697                     |
|                | 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                   |
|                | $5s5p$ $^3P_1^o - 4d5p$ $^3P_2^o$  | 18763                     | 18724                   | 15.51| 376       | 18909                   | 16.17| 404        | 408                     |
|                | $5s5p$ $^3P_1^o - 4d5p$ $^3P_0^o$  | 19085                     | 19095                   | 25.46| 994       | 19264                   | 26.26| 1048       | 1057                    |
|                | $5s5p$ $^3P_1^o - 5s6p$ $^3P_2^o$  | 19364                     | 19260                   | 9.89 | 149       | 19332                   | 10.07| 154        | 153                     |
|                | $5s5p$ $^3P_1^o - 5s6p$ $^3P_0^o$  | 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) $\times 10^5$|

TABLE VII: The $X_{J_k}^{p_J}$ 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 $\delta X_{J_1}^{11}$ is included in $X_{J_1}^{11}$ and the contribution of $\delta X_{J_2}^{20}$ is included in $X_{J_2}^{20}$. 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.

| $^1S_0 + ^1S_0$ | $C_8$ | 361454 | 370965 | 2.4% | 371455 | 3.7(1) $\times 10^5$ |
| $^1S_0 + ^3P_1^o$ | $\delta X_{J_1}^{11}$ | 126234 | 128515 | 1.8% | 126515 |
|                  | $X_{J_1}^{11}$ | 186311 | 189088 | 1.5% | 189088 |
|                  | $X_{J_1}^{12}$ | 704597 | 713986 | 1.3% | 711015 |
|                  | $X_{J_1}^{13}$ | 425433 | 429976 | 1.1% | 429976 |
|                  | $\delta X_{J_2}^{20}$ | 863  | 890   | 3.0% | 900      |
|                  | $X_{J_2}^{20}$ | 57407  | 59132  | 2.9% | 59202   |
|                  | $X_{J_2}^{21}$ | 247138 | 249097 | 0.8% | 249812  |
|                  | $X_{J_2}^{22}$ | 383908 | 387224 | 0.9% | 388487  |
|                  | $X_{J_1}^{1}$ | 90     | 90     |       |         |
|                  | $X_{J_2}^{1}$ | 154    | 154    |       |         |
|                  | $C_8(2u)$ | 555172 | 561944 | 1.2% | 562406 | 5.624(73) $\times 10^5$ |
|                  | $C_8(1u)$ | 724902 | 733370 | 1.2% | 732694 | 7.327(86) $\times 10^5$ |
|                  | $C_8(0u)$ | 554954 | 561727 | 1.2% | 562187 | 5.622(73) $\times 10^5$ |
|                  | $C_8(1g)$ | 724829 | 733297 | 1.2% | 732621 | 7.326(86) $\times 10^5$ |
TABLE VIII: The values of the $A_{J_1J_2}^{J_3J_4}(\Omega_p)$ 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           |
| $A_1^{12}$    | 1/15          |
| $A_1^{13}$    | 43/105        |
| $A_1^{20}$    | 3/5           |
| $A_1^{21}$    | 1/5           |
| $A_1^{22}$    | 9/25          |
| $A_1^{31}$    | (-1)$^p$ 3/5  |
| $A_1^{32}$    | (-1)$^p$ 9/25 |

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 $C_8(5s^2 S_0 \pm 5s5p^3P_0^o)$ coefficient can be written in a general form: \( C_8(\Omega_p) = \sum_{J_1J_2J_3J_4}(\Omega_p)X_{J_1J_2J_3J_4} \).

The non-zero angular factors $A_{J_1J_2}^{J_3J_4}(\Omega_p)$ are listed in Table VIII. A derivation of the corresponding quantities $X_{J_1J_2J_3J_4}$ was discussed in detail in Ref. 33, therefore, we give only the final formulas:

\[
X_4^{11} = \frac{45}{2\pi} \int_0^\infty \alpha_1^A(\omega) \alpha_2^B(\omega) d\omega + \delta X_4^{11} \delta_{J_1J_1} \tag{16}
\]

\[
\delta X_4^{11} = \frac{3}{2} |\langle 3P_1^o||Q||3P_1^o \rangle|^2 \alpha_1^A(0),
\]

where $J = 1, 2, 3$.

\[
X_4^{2J} = \frac{45}{2\pi} \int_0^\infty \alpha_2^A(\omega) \alpha_1^B(\omega) d\omega + \delta X_4^{20} \delta_{J_0J_0} \tag{17}
\]

\[
\delta X_4^{20} = 5 |\langle 3P_1^o||D||1S_0 \rangle|^2 \alpha_2^B(\omega_0),
\]

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

\[
X_4^{11} = \sum_{n,k} \langle 1S_0||D||n \rangle \langle n||Q||3P_1^o \rangle \langle 3P_1^o||Q||k\rangle \langle k||D||1S_0 \rangle \frac{E_n - E_{1S_0} + E_k - E_{3P_1^o}}{E_n - E_{1S_0} + E_k - E_{3P_1^o}}.
\]

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

A complete calculation of the $X_4^{11}$ 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 $X_4^{11}$ and $X_4^{22}$ only a few first terms arriving at the following approximate expressions:

\[
X_4^{11} \approx \langle 3P_1^o||Q||5s5p^3P_1^o \rangle \langle 5s5p^3P_1^o||D||1S_0 \rangle \sum_n \frac{\langle 1S_0||D||n \rangle \langle n||Q||3P_1^o \rangle}{E_n - E_{1S_0}} \frac{E_n - E_{1S_0} + E_k - E_{3P_1^o}}{E_n - E_{1S_0} + E_k - E_{3P_1^o}}.
\]

\[
X_4^{22} \approx \langle 1S_0||Q||5s4d^3D_2 \rangle \langle 5s4d^3D_2||D||3P_1^o \rangle \sum_{k,j_0=2} \frac{\langle 3P_1^o||D||k \rangle \langle k||Q||1S_0 \rangle}{E_k - E_{3P_1^o} + E(5s4d^3D_2) - E_{1S_0}} \frac{E_k - E_{3P_1^o} + E(5s4d^3D_2) - E_{1S_0}}{E_k - E_{3P_1^o} + E(5s4d^3D_2) - E_{1S_0}}.
\]
The $X^{J_aJ_b}$ values and $C_8(\Omega_{J_a/J_b})$ coefficients for the \textit{5}s\textit{5}p\textit{3}P\textit{0} \textit{Sr} dimer are given in Table VII. The contributions of the $X^{11}_3$ and $X^{22}_4$ 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 \textit{Sr} and, correspondingly, $X^{11}_3$ and $X^{22}_4$ are four orders of magnitude smaller than the main contributions coming from $X^{1J}_1$ and $X^{2J}_2$ 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 $X^{11}_3$ and $X^{22}_4$. Then, designating

$$C_1 \equiv \sum_{J=1}^{3} A_1^{1J} X_1^{1J},$$

$$C_2 \equiv \sum_{J=0}^{2} A_2^{2J} X_2^{2J},$$  \hspace{1cm} (20)

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

$$\Delta C_8^{AB} \approx \sqrt{\Delta C_1^2 + \Delta C_2^2}. \hspace{1cm} (21)$$

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

$$\delta C_1 \approx \sqrt{(\delta \alpha_A(0))^2 + (\delta \alpha_B(0))^2},$$

$$\delta C_2 \approx \sqrt{(\delta \alpha_A(0))^2 + (\delta \alpha_B(0))^2}. \hspace{1cm} (22)$$

We note that $X^{11}_3$ includes the additional term $\delta X^{11}_3$ (see Eq. (10)). Nevertheless the equation above for $\delta C_1$ is valid if we assume that the uncertainty of $\langle |3P_o^5||Q||3P_f^5\rangle|^2 \text{ is approximately the same as the uncertainty of the scalar part of } \alpha_2(3P_f^5)$. This assumption is based on that the $5s5p\textit{3}P_0$ state contributes $\sim 94\%$ to the scalar $\alpha_2(3P_f^5)$, i.e., the uncertainty of $\alpha_2(3P_f^5)$ is mostly determined by the uncertainty of the matrix element $\langle |3P_o^5||Q||3P_f^5\rangle$. The latter is assumed to be the same as the absolute uncertainty of the matrix element $\langle |3P_o^5||Q||3P_f^5\rangle = 20.9$ a.u.

The term $\delta X^{20}_3$ contributing to $X^{20}_3$ 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.

| Property | This work | Other results |
|----------|-----------|--------------|
| $1S_0 + 1S_0$ | $C_6$ | 3107(4)$^b$ |
|         |         | 3103(7)$^b$ |
|         |         | 2890$^d$ |
| $C_8$ |         | $3.7(1) \times 10^5$ |
|         |         | $3.792(8) \times 10^5$ |
|         |         | $3.854 \times 10^5$ |
| $1S_0 + 3P_0^o$ | $C_6$ | 5360(200)$^c$ |
|         |         | 5260(500)$^c$ |
| $3P_0^o + 3P_0^o$ | $C_6$ | 3880(80)$^c$ |
| $1S_0 + 3P_1^o$ | $C_6(0_{u/g})$ | 3771(32) |
|         | $C_6(1_{u/g})$ | 4001(33) |
|         |         | 4085(50)$^f$ |
| $C_8(0_{u})$ |         | $5.624(73) \times 10^5$ |
| $C_8(1_{u})$ |         | $7.327(86) \times 10^5$ |
| $C_8(0_{g})$ |         | $5.622(73) \times 10^5$ |
| $C_8(1_{g})$ |         | $7.326(86) \times 10^5$ |

$^a$Reference 22.$^b$Reference 15.$^c$Reference 4.$^d$Reference 1.$^e$Reference 3.$^f$Reference 16.

VIII. SUMMARY

In Table IX we summarize the results obtained for the van der Waals coefficients in this work. We also include 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 provided in Ref. 2. Comparing our results with other data, where available, we see very good agreement for all quantities listed in the table.

To conclude, we evaluated $E1$ transition amplitudes from the $5s5p\textit{3}P_1^o$ state to the low-lying even-parity states and the electric dipole and quadrupole static polarizabilities of the $5s5p\textit{3}P_1^o$ state of atomic Sr. We also calculated $C_6$ and $C_8$ coefficients for the Sr $1S_0 + 1S_0$ and $1S_0 + 3P_1^o$ dimers. 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 $C_6(0_{u}) = 3868(50)\text{ a.u.}$ and $C_6(1_{u}) = 4085(50)\text{ a.u.}$ obtained in Ref. 16. We confirm 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.

IX. ACKNOWLEDGEMENT*

We thank P. Julienne, M. Borkowski, and R. Ciurylo for helpful discussions. This research was performed un-
under the sponsorship of the US Department of Commerce, National Institute of Standards and Technology, and was supported by the National Science Foundation under Physics Frontiers Center Grant No. PHY-0822671 and by the Office of Naval Research. The work of S.G.P. was supported in part by US NSF Grant No. PHY-1212442.

[1] B. J. Bloom, T. L. Nicholson, J. R. Williams, S. L. Campbell, M. Bishof, X. Zhang, W. Zhang, S. L. Bromley, and J. Ye, Nature (London) 506, 71 (2014).
[2] X. Zhang, M. Bishof, S. L. Bromley, C. V. Kraus, M. S. Safronova, P. Zoller, A. M. Rey, and J. Ye, Science 345, 1467 (2014).
[3] S. Stellmer, R. Grimm, and F. Schreck, Phys. Rev. A 87, 013611 (2013).
[4] S. Stellmer, M. K. Tey, B. Huang, R. Grimm, and F. Schreck, Phys. Rev. Lett. 103, 200401 (2009).
[5] S. Stellmer, B. Pasquoiu, R. Grimm, and F. Schreck, Phys. Rev. A 85, 043414 (2012).
[6] W. Skomorowski, R. Moszynski, and C. P. Koch, Phys. Rev. A 88, 043414 (2012).
[7] G. Reinaudi, C. B. Osborn, M. McDonald, S. Kotochigova, and T. Zelevinsky, Phys. Rev. Lett. 109, 115303 (2012).
[8] M. Tomza, F. Pawlowski, M. Jeziorska, C. P. Koch, and R. Moszynski, Phys. Chem. Chem. Phys. 13, 18893 (2011).
[9] B. Pasquoiu, A. Bayerle, S. M. Tzanova, S. Stellmer, J. Szczepkowsi, M. Parigger, R. Grimm, and F. Schreck, Phys. Rev. A 88, 023601 (2013).
[10] W. Skomorowski, R. Moszynski, and C. P. Koch, Phys. Rev. Lett. 111, 150402 (2013).
[11] M. Yan, B. J. DeSalvo, Y. Huang, P. Naidon, and T. C. Killian, Phys. Rev. Lett. 111, 150402 (2013).
[12] S. Kotochigova, T. Zelevinsky, and J. Ye, Phys. Rev. A 79, 021504 (2009).
[13] S. G. Porser and A. Derevianko, Phys. Rev. A 65, 020701(R) (2002).
[14] J. Mitroy and M. W. J. Bromley, Phys. Rev. A 68, 052714 (2003).
[15] S. G. Porser and A. Derevianko, Zh. Eksp. Teor. Fiz. 129, 227 (2006). [Sov. Phys. JETP 102, 195 (2006)].
[16] M. Borkowski, P. Morzyński, R. Ciuryło, P. S. Julienne, M. Yan, B. J. DeSalvo, and T. C. Killian, Phys. Rev. A 90, 032713 (2014).
[17] S. A. Kotochigova and I. I. Tupitsyn, J. Phys. B 20, 4759 (1987).
[18] V. A. Dzuba, V. V. Flambaum, and M. G. Kozlov, Phys. Rev. A 54, 3948 (1996).
[19] M. G. Kozlov, Int. J. Quant. Chem. 100, 336 (2004).
[20] M. S. Safronova, M. G. Kozlov, W. R. Johnson, and D. Jiang, Phys. Rev. A 80, 012516 (2009).
[21] M. S. Safronova, M. G. Kozlov, and C. W. Clark, Phys. Rev. Lett. 107, 143006 (2011).
[22] M. S. Safronova, S. G. Porser, U. I. Safronova, M. G. Kozlov, and C. W. Clark, Phys. Rev. A 87, 012509 (2013).
[23] V. A. Dzuba, M. G. Kozlov, S. G. Porser, and V. V. Flambaum, JETP 87, 885 (1998).
[24] S. G. Porser, Yu. G. Rakhлина, and M. G. Kozlov, Phys. Rev. A 60, 2781 (1999).
[25] S. G. Porser, Yu. G. Rakhлина, and M. G. Kozlov, J. Phys. B 32, 1113 (1999).
[26] T. Middelmann, S. Falke, C. Lisdat, and U. Sterr, Phys. Rev. Lett. 109, 263004 (2012).
[27] A. D. Ludlow, T. Zelevinsky, G. K. Campbell, S. Blatt, M. M. Boyd, M. H. G. de Miranda, M. J. Martin, J. W. Thomsen, S. M. Foreman, J. Ye, et al., Science 319, 1805 (2008).
[28] I. I. Sobelman, Atomic Spectra And Radiative Transitions (Springer-Verlag, Berlin, Heidelberg, New York, 1979).
[29] Kramida, A., Ralchenko, Yu., Reader, J. and NIST ASD Team (2013). NIST Atomic Spectra Database (version 5.1). Available at [http://physics.nist.gov/asd]. National Institute of Standards and Technology, Gaithersburg, MD.
[30] M. G. Kozlov and S. G. Porser, Eur. Phys. J. D 5, 59 (1999).
[31] J. Mitroy, M. S. Safronova, and C. W. Clark, J. Phys. B 43, 202001 (2010).
[32] T. Ido and H. Katori, Phys. Rev. Lett. 91, 053001 (2003).
[33] M. Yasuda, T. Kishimoto, M. Takamoto, and H. Katori, Phys. Rev. A 73, 011603R (2006).
[34] S. G. Porser, A. D. Ludlow, M. M. Boyd, and J. Ye, Phys. Rev. A 78, 032508 (2008).
[35] S. G. Porser, M. S. Safronova, A. Derevianko, and C. W. Clark, Phys. Rev. A 89, 012711 (2014).
[36] S. G. Porser and A. Derevianko, J. Chem. Phys. 119, 844 (2003).
[37] R. Santra, K. V. Christ, and C. H. Greene, Phys. Rev. A 69, 042510 (2004).