High-precision study of Cs polarizabilities

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We present results of the first-principles calculation of Cs dipole static polarizabilities for the \( Ns \) \((N = 6 - 12)\), \( Np_j \) \((N = 6 - 10)\), and \( Nd_j \) \((N = 5 - 10)\) states using the relativistic all-order method. In our implementation of the all-order method, single and double excitations of Dirac-Fock wave functions are included to all orders in perturbation theory. Additional calculations are carried out for the dominant terms and the uncertainties of our final values are estimated for all states. A comprehensive review of the existing theoretical and experimental studies of the Cs polarizabilities is also carried out. Our results are compared with other values where they are available. These calculations provide a theoretical benchmark for a large number of Cs polarizabilities.

I. INTRODUCTION

Atomic and molecular polarizabilities are of great interest because various properties of matter can be expressed in terms of multipole moments and polarizabilities of the atoms or molecules in the system. Polarizabilities describe the response of a system to external electric fields. Therefore, atomic polarizabilities reflect the atomic structure and can be used to probe correlation and relativistic effects. On the other hand, atomic polarizabilities determine the long-range van der Waals interactions between the atoms and are used in describing atomic scattering processes. Atomic polarizabilities play an important role in high Rydberg state spectroscopy (e.g. [1]). The study of the alkali-metal atoms are of particular interest because they allow for very accurate comparison between the experiment and theory. The conclusions reached from such studies may also be useful for the understanding of more complicated systems. Cs is also of particular interest owing to the study of the parity nonconservation (PNC), designed to test the standard model of the electroweak interaction and to set limits on its possible extensions as well as to infer nuclear anapole moments. The highest accuracy of such an experiment was reached for cesium, where measurements of PNC amplitudes have reached an accuracy of 0.4% [2]. To make meaningful tests of the standard model, high-precision calculations of the PNC amplitudes must be carried out at a similar level of accuracy, and the uncertainty of the calculation has to be established.

In this work, we carry out a systematic study of a large number of Cs polarizabilities in order to provide recommended values for the \( Ns \) \((N = 6 - 12)\), \( Np_j \) \((N = 6 - 10)\), and \( Nd_j \) \((N = 5 - 10)\) states and evaluate their uncertainties. The best-set values for the 91 electric-dipole matrix elements used in our calculations are also provided with their uncertainties. These data are also useful for a number of other applications.

A. Experimental methods and studies of the atomic polarizabilities

In this section, we provide a summary of a variety of methods used to measure the atomic polarizabilities as well as describe the development in the experimental measurements of the electric-dipole polarizability of cesium ground state.

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In 2005, Gould and Miller [3] wrote a comprehensive review of the experimental methods to determine the static electric-dipole polarizabilities. Miller and Bederson’s earlier review from 1988 [4] concentrated on the bulk polarizability measurements and the atomic beam methods. Average bulk ground state static polarizabilities are measured by determining the dielectric constant of an atomic or molecular gas. The bulk dynamic polarizabilities are determined by measuring the refractive index of the gas, see [4]. The bulk methods are very accurate, but their limitation lies in the need to deal with atoms or molecules that are stable and gaseous at room temperature and the fact that the effect of the excited states can not be accounted for.

In 1974, Molof et al. [5] used the E-H-gradient balance technique to measure the static electric-dipole polarizabilities of alkali-metal atoms. They obtained the value \((59.6 \pm 1.2) \times 10^{-24} \text{ cm}^3\) for electric-dipole polarizability of the ground state of cesium. Hall and Zorn [6] measured the value \((63.3 \pm 4.6) \times 10^{-24} \text{ cm}^3\) for the electric-dipole polarizability of the ground state of cesium. They used the deflection of a velocity-selected atomic beam in inhomogeneous electric field. The technique is based on the fact that the deflection experienced by atoms moving through a region with known transverse electric field gradient is proportional to the dipole polarizability of the atoms. An important detail of this technique is that the precision with which the velocity of the atoms is known puts a limitation on the precision of the experiment. The short interaction time in the case of high velocity which leads to small deflection of the beam places another limitation on the accuracy of this method.

In 1995, Ekstrom et al. [7] designed an atomic interference experiment that allowed them to measure the ground state energy shifts with spectroscopic precision and determine the ground state dipole polarizability. In 2003, Amini and Gould [8] designed an experiment that avoids the problems associated with the measuring the deflection of a thermal beam in transverse electric-field gradient. They measure the effect of the electric-field gradient on the longitudinal velocity of the beam of cesium atoms in a magneto-optical trap (MOT). The cesium 6s scalar dipole polarizability is found from the time-of-flight of laser cooled and launched cesium atoms traveling through an electric field. The cited value is \((59.42 \pm 0.08) \times 10^{-24} \text{ cm}^3\). This is the most precise measurement of the ground state polarizability at this time.

Another group of experiments allows to infer the atomic polarizabilities by measuring the Stark shift of the cesium lines, e.g. [9]. In 1988, Tanner and Wiemann [10] measured the Stark shift in the \(6s_{1/2} \rightarrow 6p_{3/2}\) transition in Cs. The dc Stark shift of the cesium D1 line has been measured to 0.01% in Ref. [11]. The authors of this work [11] noted that it was the most precise Stark shift measurement ever reported. The Stark shifts of the \(6p_{3/2} - (10 - 13)s\) states in cesium were measured in Ref. [12]. The Stark shifts of cesium 11D states were measured with high precision by van Wijngaarden and Li in 1997 [13] using an electro-optically modulated laser beam. The authors note that the tensor polarizabilities reported in that work [13] were the most accurate yet determined for any atomic state. The dc Stark shift of the \(6s - 7s\) transition in atomic cesium was measured with high precision in 1999 [14] using laser spectroscopy. The result of this experiment disagrees with a previous measurement [14] but was within 0.3% of the value predicted by the \textit{ab initio} calculations [16, 17] removing the largest at that time outstanding disagreement between experiment and \textit{ab initio} theory of low-lying states in atomic cesium.

The atomic polarizabilities can be derived from measurements of the lifetimes of the corresponding levels. The contribution of the core electrons to the polarizability of the alkali atoms is small. Then, the main contribution to the ground s-state polarizability comes from the first low-lying excited P-states, i.e. dominant electric-dipole matrix elements are \(\langle Ns|D|np_{1/2,3/2}\rangle\); see [18, 19] for a detailed discussion and comparison of lifetime and polarizability measurements in cesium.

A large group of experiments makes use of the level-crossing of some hyperfine atomic levels at finite electric field. The first observation of the purely electric field level-crossing was reported in 1966 [20]. This type of measurements allows for experimental determination of the excited states tensor polarizabilities. Recent cesium measurements were reported by Auzinsh et al. [21, 22].
B. Theoretical studies of cesium polarizabilities

Since the alkali-metal atoms are monovalent systems, they represent an excellent opportunity to study the correlation effects. Heavy alkalis are of particular interest owing to the application to the study of fundamental symmetries. The polarizability of the alkali-metal atoms are essentially the same as the valence polarizability as the contribution of the ionic core was determined to be small. We summarize the theoretical studies of Cs polarizabilities below.

In his seminal paper, Dalgarno summarized the mathematical foundation of the theory of the atomic perturbation and discussed the methods of calculating the atomic polarizabilities and shielding factors. The polarizability of the cesium atom obtained by Dalgarno and Kingston using the oscillator-strength formula was \( (53.7 \pm 5.4) \times 10^{-24} \text{ cm}^3 \).

According to the oscillator-strength formula, the knowledge of the (reduced) electric-dipole matrix elements is crucial for calculation of the atomic polarizabilities. The reduced matrix elements can be computed in a number of approximations. Variety of theoretical methods are used, such as third-order many-body perturbation theory, multiconfiguration Hartree-Fock (MCHF), configuration interaction (CI) method, coupled-cluster (CC) method, and it relativistic linearized version referred to as the all-order method as well as others.

In 1970, Sternheimer used the Hartree-Fock wave functions to compute the quadrupole polarizability of some ions and alkali atoms. The cesium ground state value was calculated to be 71.31 \( 10^{-24} \text{ cm}^3 \). In 1971, Schmieder et al. calculated the scalar and quadrupole polarizabilities of cesium \( p_{3/2} \) states in the second order perturbation theory. The work by Kellö et al. contains a detailed investigation of the contracted Gaussian basis sets in the calculation of the electric-dipole polarizabilities of alkali-metal atoms. The calculations are performed using the complete-active-space self-consistent field and second order perturbation theory, CASSCF and CASPT2. Another group of Gaussian basis set methods use relativistic pseudopotentials (see 30 and the references there). Pseudopotential methods replace the core electrons by an effective, pseudopotential. The core polarization and the relativistic effects are incorporated as well. The Douglas-Kroll relativistic CCSD(T) method with the optimal basis set gives 58.09 \( 10^{-24} \text{ cm}^3 \) for the cesium ground state dipole polarizability.

Extensive calculation of the polarizabilities of cesium \( Ns, Np, Nd, \) and \( nF \) states was carried out by van Wijngaarden and Li using the Coulomb approximation. They also provided extensive comparison with other theoretical and experimental values.

Patil and Tang computed the multipolar polarizabilities, \( \alpha_q \), with \( q = 1, 2, \ldots, 12 \), for the alkali isoelectronic sequences. The ground state wave functions were taken to be the asymptotically correct wave functions, i.e. the two leading terms in the asymptotic expansion of the wave function are retained. The excited states are taken to be the Coulomb wave functions with a correction that makes sure the experimental energies of the low-lying states are reproduced correctly. The ground state electric-dipole polarizability of cesium was found to be 60.6 \( 10^{-24} \text{ cm}^3 \).

The relativistic linearized version of the coupled-cluster singles-doubles method, i.e. all-order SD method, was used in to calculate the static dipole polarizabilities of the alkali-metal atoms. This method is discussed in more details in Section III. The value obtained for the ground state static dipole polarizability is 59.3(3) \( 10^{-24} \text{ cm}^3 \). In 33, Porsev and Derevianko computed the ground state quadrupole and octupole polarizabilities of the alkali-metal atoms using the relativistic MBPT.

In 2004, Safronova and Clark pointed out the inconsistencies between the lifetime and polarizability measurements in cesium. The dominant contribution to the \( 6p \) scalar polarizability comes from the \( 5d - 6p \) matrix elements. This allows for a check of the accuracy of the matrix elements. The authors compare the values of the \( 6p \) polarizabilities obtained using the relativistic all-order SD method and using the values of the matrix elements derived from the \( 5d \) lifetime experiment. They point out that the theoretical all-order values yield a polarizability result in agreement with the polarizability measurements but not with the lifetime measurements.

In a recent work, Gunawardena et al. report a precise measurement of the dc Stark shift of the \( 6s \rightarrow 8s \) transition in atomic cesium. The experiment makes use of the Doppler-free two-photon absorption measurement. The value of the static polarizability of \( 8s \) state in cesium, extracted from the experiment, is \( 38 \pm 0.3 \alpha_0 \). The authors present a theoretical value of \( 38 \pm 0.3 \alpha_0 \). The theoretical value of the polarizability is calculated using the relativistic all-order SD method.
II. METHOD

The energy shift of the $|\gamma jm\rangle$ atomic level in a dc electric field $E = \mathcal{E} \hat{z}$ is given by

$$\Delta E = -\frac{1}{2} \alpha_{\gamma jm} \mathcal{E}^2,$$

where $\alpha_{\gamma jm}$ defines the static polarizability of the corresponding atomic state $|\gamma jm\rangle$. The scalar and tensor static polarizabilities $\alpha_{0,\gamma jm}$ and $\alpha_{2,\gamma jm}$ are defined as

$$\alpha_{\gamma jm} = \alpha_{0,\gamma jm} + \alpha_{2,\gamma jm} \frac{3m^2 - j(j+1)}{j(2j-1)},$$

where $\alpha_{0,\gamma jm}$ and $\alpha_{2,\gamma jm}$ are the lowest values of the allowed electric-dipole transitions for Cs calculation. The sums over states $\beta$, respectively.

We separate the calculation of the scalar static polarizability into the calculation of the polarizability of the ionic core and the valence polarizability. The random-phase-approximation (RPA) calculation of the Cs core polarizability was carried out in Ref. [36] and yielded the value $(15.80 \pm 0.01)\alpha_0$, where $\alpha_0$ is the Bohr radius. Based on the evaluation of the accuracy of RPA approximation for the polarizabilities of the noble gases, this value is accurate to at least 5%. The core polarizability is small even in comparison with the valence polarizabilities of the lowest states such as $6p$ and $5d$. It is negligible for the higher states. For example, core polarizability contributes only 4% to the total value of the ground state polarizability and only 1% to the $6p_{1/2}$ polarizability. Therefore, the RPA value of the core polarizability is sufficiently accurate for this work. The separation of the scalar polarizability to the core and valence parts also produces a compensation term that accounts for the Pauli exclusion principle, i.e. in Cs it subtracts $1/2$ of the core polarizability contribution associated with the excitation to the valence shell. This term is only 2% of the core contribution [24] even for the ground state and, therefore, below the estimated uncertainty of the core term itself. It is negligible for all other states.

The valence scalar and tensor static polarizabilities of the atomic state $|\gamma j\rangle$ are expressed in lowest order as sums over unperturbed intermediate states $|\beta j\rangle$ of parity opposite to that of the state $|\gamma j\rangle$:

$$\alpha_0 = \frac{2}{3(2j+1)} \sum_{\beta} \frac{|\langle \gamma j | D | \beta j \rangle|^2}{E_\beta - E_\gamma},$$

$$\alpha_2 = 4 \sqrt{\frac{5j(2j-1)}{6(2j+3)(2j+1)(j+1)}} \sum_{\beta} (-1)^{j+j_\beta} \binom{j}{1} \binom{j}{2} \frac{|\langle \gamma j | D | \beta j \rangle|^2}{E_\beta - E_\gamma},$$

where $\langle \gamma j | D | \beta j \rangle$ is the reduced electric-dipole matrix element defined as

$$\langle \gamma jm | D_q | \gamma' j' m' \rangle = (-1)^{j' - m'} \left( j' \begin{array}{c} 1 \end{array} j \begin{array}{c} q \end{array} m \right) \langle \gamma j | D | \gamma' j' \rangle,$$

and the $D_q$ is the corresponding component of the electric-dipole operator in spherical coordinates.

The sums over states $\beta$ in Eqs. (3) separate into the two or three sums over the principal quantum number for each type of the allowed electric-dipole transitions for Cs calculation. The allowed values of $\beta$ are the following: $\beta = np_{1/2}$, $np_{3/2}$ for $Ns$ states, $\beta = ns, nd_{3/2}$ for the $np_{1/2}$ states, $\beta = ns, nd_{3/2}, nd_{5/2}$ for the $np_{3/2}$ states, $\beta = np_{1/2}, np_{3/2}, nf_{5/2}$ for the $nd_{5/2}$ states, $\beta = np_{3/2}, nf_{5/2}, nf_{7/2}$ for the $nd_{5/2}$ states. Here, $n$ and $N$ are principal quantum numbers. We note that there is no tensor contribution to the polarizability of the $Ns$ and $Np_{1/2}$ states.

In order to evaluate the sums over the principal quantum numbers $n$, we carry out all calculations in a finite B-spline basis set [37] constrained to a large spherical cavity and defined on a non-linear
The sums over the principal quantum numbers in Eqs. (3,4) converge very rapidly, with the exception of the sums involving the $5d_{3/2} - n f_{5/2}$ and $5d_{5/2} - f_{7/2}$ transitions which we will discuss separately in Section IV. In fact, each of the sum over the principal quantum number is dominated by one or two terms that correspond to the lowest possible values of the denominator $E_\beta - E_\gamma$ in Eqs. (3,4). A small number of other terms may also be significant for the precise calculation for some states. As a result, only a few terms from each sum have to be calculated accurately, allowing us to separate the calculation of the valence scalar and tensor polarizabilities into the two parts, the main term containing all significant contributions and the tail:

$$
a_{0,2} = a_{0,2}^{\text{main}} + a_{0,2}^{\text{tail}}.
$$

The separation of $\alpha$ into the main and tail parts is done independently for each of the two or three sums over the principal quantum number $n$ contributing to the polarizability of the specific state:

$$
\sum_n = \sum_{n_0}^{n_{\text{main}}} + \sum_{n_{\text{main}}+1}^{N_B},
$$

where the $n_0$ is the lowest possible value of principal quantum number for the particular set of $\beta$ states, $n_{\text{main}}$ is the cut-off that we select for the separation of the main and tail terms, and $N_B$ is the number of the finite basis set orbitals set to 70 in the present work. In general, $n_{\text{main}}$ may be selected differently for the specific state $\gamma$ and each $\beta$ sum, but we chose to use the same $n_{\text{main}}$ for all of the states considered in this work. We use $n_{\text{main}} = 12$ for $\beta = n s, n p_{1/2}, n p_{3/2}$, $n_{\text{main}} = 10$ for $\beta = n d_{5/2}, n d_{3/2}$, and $n_{\text{main}} = 8$ for $\beta = n f_{5/2}, n f_{7/2}$, respectively. The only exception is the addition of the $9f$ contributions to the calculation of the $10d$ polarizabilities.

Such high value of the cut-off principal quantum number also reduced the tail contribution and improved the accuracy of our calculations. The remaining tail contributions are evaluated using in the Dirac-Fock (DF) approximation, i.e. both energies and E1 matrix elements were calculated in the DF approximation.

In summary, we reduce the calculation of the polarizabilities to the calculation of the electric-dipole reduced matrix elements required for the evaluation of the main terms for each state. We use the experimental energies from Refs. [38, 39, 40] in the calculation of the main terms. Owing to the large number of states considered in this work, 317 transitions contribute to the main term and 102 transitions give dominant contributions. We calculated all of the 317 electric-dipole matrix elements using the relativistic all-order method and conducted additional calculation for the 102 transitions that involved the evaluation of the largest missing corrections and evaluation of the uncertainty of the final values. The calculation of the matrix elements is described in the next section.

### III. CALCULATION OF THE E1 MATRIX ELEMENTS

We carry out the calculation of the electric-dipole reduced matrix elements using the relativistic SD all-order method where single and double excitations of the (frozen-core) Dirac-Fock wave function are included to all orders in perturbation theory [24, 41]. Triple excitations are also partially included for selected cases. The relativistic SD all-order method is a linearized coupled-cluster method restricted to single and double excitations. A comprehensive review of the coupled-cluster method and its applications in quantum chemistry is given in Ref. [42]. In the coupled-cluster method, the exact wave function of the monovalent atom in a state $v$ is represented as

$$
|\Psi_v\rangle = \exp(S)|\Phi_v\rangle,
$$

where $S$ is the single and double excitations matrix.
where $\Phi_v$ is the lowest-order atomic wave function for the state $v$, which taken to be a frozen core Dirac-Fock (DF) wave function in our calculations. The cluster operator $S$ is expressed as a sum of $n$-particle excitations $S_n$ of the lowest-order wave function

$$S = S_1 + S_2 + S_3 + \cdots. \quad (9)$$

The exponential function in Eq. (8) can be expanded to give

$$|\Psi_v \rangle = (1 + S + \frac{1}{2} S^2 + \cdots) |\Phi_v \rangle. \quad (10)$$

In the linearized single-double (SD) coupled-cluster method, only terms that are linear in the $S_i$ remain and all other terms, for example $S_1 \times S_2$ are omitted, i.e.

$$|\Psi_v \rangle = (1 + S_1 + S_2 + \cdots) |\Phi_v \rangle. \quad (11)$$

The contributions from the non-linear terms were recently investigated in Refs. [43, 44, 45]. We refer the reader to Ref. [45] for a complete list of the non-linear terms and detailed investigation of their contributions to the alkali-metal atom properties. The computational complexity of the calculations increases dramatically beyond the double excitations term $S_2$, and we include triple excitations partially in some of the calculations using a perturbative approach. We note that in this work very large ($N_B = 70$ for each partial wave) complete basis set is used to correctly reproduce necessary atomic properties for highly excited atomic states, requiring significant computational resources for the SD all-order calculations.

The expression for the single excitations is given by

$$S_1 = \sum_{ma} \rho_{ma} a_m^\dagger a_a + \sum_{m \neq v} \rho_{mv} a_m^\dagger a_v, \quad (12)$$

where the first term corresponds to single core excitations and the second term corresponds to single valence excitations. The expansion coefficients $\rho_{ma}$ and $\rho_{mv}$ are referred to as single core and valence excitation coefficients, and the $a_i^\dagger$ and $a_i$ are creation and annihilation operators for an electron in a state $i$. We use the letters from the beginning of the alphabet $a,b,...$ to designate core orbitals and letters from the middle of the alphabet, $m,n,...$ to designate excited states. For Cs, we include all 17 $a = 1s,...,5p\frac{3}{2}$ core shells in our calculations.

The double excitation term is given by

$$S_2 = \frac{1}{2} \sum_{mnab} \rho_{mnab} a_m^\dagger a_n^\dagger a_b a_a + \sum_{mnab} \rho_{mnab} a_m^\dagger a_n^\dagger a_b a_a + \sum_{m \neq v} \rho_{mv} a_m^\dagger a_v + \sum_{mna} \rho_{mnva} a_m^\dagger a_n^\dagger a_v a_a \quad (13)$$

and the quantities $\rho_{mnab}$ and $\rho_{mnva}$ are referred to as double core and valence excitation coefficients, respectively.

Therefore, the atomic wave function in the all-order SD method [41] is expressed via the single and double excitation coefficients as follows:

$$|\Psi_{v}^{SD} \rangle = \left(1 + \sum_{ma} \rho_{ma} a_m^\dagger a_a + \frac{1}{2} \sum_{mnab} \rho_{mnab} a_m^\dagger a_n^\dagger a_b a_a \right.$$ \hspace{1cm} \left.+ \sum_{m \neq v} \rho_{mv} a_m^\dagger a_v + \sum_{mna} \rho_{mnva} a_m^\dagger a_n^\dagger a_v a_a \right) |\Phi_v \rangle. \quad (14)$$

The equations for the excitations coefficients and the correlation energy are derived by substituting the SD all-order wave function given by the Eq. (14) into the Schrödinger equation

$$H |\Psi_v \rangle = E |\Psi_v \rangle, \quad (15)$$
where the Hamiltonian $H$ is the relativistic no-pair Hamiltonian \[46\], which can be written in second-quantized form as

$$H = \sum_i \epsilon_i a_i^\dagger a_i + \frac{1}{2} \sum_{ijkl} g_{ijkl} a_i^\dagger a_j^\dagger a_l a_k - \sum_{ij} U_{ij} a_i^\dagger a_j,$$

(16)

where $\epsilon_i$ are the one-body DF energies for the state $i$, $U_{ij}$ is taken to be frozen-core DF potential in our calculation, and $g_{ijkl}$ are the two-body Coulomb integrals:

$$g_{ijkl} = \int d^3r \int d^3r' \psi_i^\dagger(r) \psi_j^\dagger(r') \frac{1}{|r - r'|} \psi_k(r) \psi_l(r').$$

(17)

For example, the equation for the single valence excitation coefficients $\rho_{mv}$ is given by

$$(\epsilon_v - \epsilon_m + \delta E_v) \rho_{mv} = \sum_{bn} \tilde{\rho}_{mbvn} \rho_{nb} + \sum_{bnr} g_{mbnr} \rho_{nrvb} - \sum_{bcn} g_{bcvn} \rho_{mnvb},$$

(18)

where $\delta E_v$ is the correlation correction to the valence energy for the state $v$ given in terms of the excitation coefficients by

$$\delta E_v = \sum_{ma} \tilde{\rho}_{vamn} \rho_{nmva} + \sum_{mab} g_{abvm} \rho_{mvab} + \sum_{mna} g_{vbmn} \rho_{mnvb}.$$

(19)

We use the designation $\tilde{\rho}_{mnab} = \rho_{mnab} - \rho_{mnba}$ and $\tilde{\rho}_{mnab} = g_{mnab} - g_{mnba}$ in the equations above. The sum over the magnetic quantum numbers is carried out analytically and the resulting equations are solved iteratively for the excitation coefficients until the correlation energy converges. The excitation coefficients are then used for the calculation of the matrix elements as described below.

In general, the one-body operator $Z$ can be written in second quantization as $Z = \sum_{ijkl} z_{ijkl} a_i^\dagger a_j$.

The expression for SD matrix elements of operator $Z$ is obtained by substituting the SD wave function given by Eq. (14) into the expression

$$Z_{wv} = \frac{\langle \Psi_w | Z | \Psi_v \rangle}{\sqrt{\langle \Psi_w | \Psi_w \rangle \langle \Psi_v | \Psi_v \rangle}}.$$

(20)

The resulting SD matrix element is given by

$$Z_{wv} = \frac{z_{wv} + Z^{(a)} + \ldots + Z^{(t)}}{\sqrt{(1 + N_v)(1 + N_w)}},$$

(21)

where $z_{wv}$ is the DF matrix element, terms $Z^{(a)}, \ldots Z^{(t)}$ are linear or quadratic functions of the excitation coefficients, and $N_v$ and $N_w$ are normalization terms that are quadratic functions of the excitation coefficients. For most of the dominant transitions in our polarizability calculations, a single term

$$Z^{(c)} = \sum_m z_{wm} \rho_{mv} + \sum_m z_{mv} \rho_{mw}$$

(22)

gives the dominant contribution. Two other terms,

$$Z^{(a)} = \sum_{ma} z_{am} \tilde{\rho}_{wmva} + \sum_{ma} z_{ma} \tilde{\rho}_{vmwa}$$

(23)

and

$$Z^{(d)} = \sum_{mn} z_{mn} \rho_{mw} \rho_{nv}$$

(24)
may be dominant for selected important transitions. We note that both \( Z^{(c)} \) and \( Z^{d} \) terms contain only single valence excitations coefficients. The complete expression for the matrix elements is given in Ref. 47.

All sums over the excited state in the formulas above range over the basis set states. We truncated last five basis set orbitals for each partial wave since their contributions is negligible, i.e. 65/70 orbitals are included for each partial wave. All partial waves are included up to \( l_{\text{max}} = 6 \), and orbitals with \( j = l + 1/2 \) and \( j = l - 1/2 \) are considered separately since it is intrinsically relativistic calculation. The basis set is numerically stable, i.e. the increase of the number of the basis set orbitals does not change the results within the current accuracy. The numerical uncertainty associated with the truncation of the number of the partial waves at \( l_{\text{max}} = 6 \) is also negligible. We estimated the contribution from higher partial waves to be 0.1% for the 6s−6p\(_{j}\) transitions. The evaluation of the higher partial wave contribution is carried out by conducting the third-order perturbation theory calculation carried out as described in Ref. 47 with the same basis set and with higher number of the partial waves. We also verified that the use of the very large cavity did not affect the numerical accuracy of the atomic properties of the lower states by comparing the present results for the transitions between the lower states with all-order calculation carried out with the small cavity appropriate for the lower states. We note that large basis set size, \( N_{B} = 70 \), is necessary to reproduce the atomic properties correctly with such a large cavity. We found that the accuracy of the \( N_{B} = 50 \) B-spline basis set is not sufficient for such calculation.

As noted above, we have identified that the correlation correction for most of the dominant transitions in our polarizability calculation is essentially determined by a single term, \( Z^{(c)} \), that contains only single valence excitations. This term mostly corresponds to the Brueckner orbital correction as classified in the Ref. 47. It is established (16, 22, 48, 49) that it can be corrected by scaling the single excitation coefficients using the ratio of the “experimental” and theoretical correlation energies and redoing the matrix element calculation with modified excitation coefficients. The “experimental” correlation energies are determined as the differences of the experimental data and our lowest-order DF values. We carry out such scaling where appropriate and determine the uncertainty of our calculation of the matrix elements as the difference between the \textit{ab initio} and scaled data. In certain cases where this correction is particularly large, we also carried out \textit{ab initio} calculation of the limited triple excitations and conducted more accurate study of the uncertainty of the calculations. The limited inclusion of the triples was also aimed at correcting the \( p_{ma} \) excitation coefficients. Such calculations are described in detail in Refs. 22, 48, 49 and references therein. We note that term \( Z^{(d)} \) is also corrected by scaling as it contains only valence single excitation coefficients. We note that the scaling procedure allows to place an uncertainty on our theoretical data that is not derived from the comparison with the experiment. Our results are summarized in the next section.

### IV. RESULTS AND DISCUSSION

The results of the all-order calculation of the matrix elements are summarized in Table I. Owing to the very large number of the transitions involved in this calculation, we only listed the transitions that give dominant contributions to the polarizabilities of the states considered in this work. In order to provide a best set of known data for these transitions, we replaced all-order theoretical values by the experimental ones where high-precision values are available. The experimental values from Ref. 51 are used for the 6s−6p\(_{j}\) transitions, the values for the 6p\(_{j}\)−7s transitions are derived from the 7s lifetime measurement in 51, and the 6s−7p\(_{j}\) values are experimental values from 51. The 7s−7p\(_{j}\) values were derived from the 7s−6s Stark shift measurement 14. We are quoting these 7s−7p\(_{j}\) values in the present table as the most accurate values available, and we used them in the calculation of the 7p\(_{j}\) polarizabilities to provide recommended values for these states. However, we used our theoretical values in the calculation of the 7s polarizabilities for the evaluation of the accuracy of our calculation. Otherwise, the comparison of the 7s values with the experiment would have provided no information as we would have expected near exact agreement. Our theoretical values, 10.31(4) and 14.32(6), are in perfect agreement with values derived from the Stark shifts.

The values for the 5d−np and 6d−6p transitions are taken from the study of the inconsistencies
TABLE I: Absolute values of the selected reduced electric-dipole matrix elements $E_1$ in Cs and estimates of their uncertainties. Unless otherwise noted, these are all-order SD scaled values, including values from Refs. 22, 33. aExperimental values, Ref. 50. bSD all-order scaled values, previously published in Ref. 33. cexperimental values from Ref. 51. dderived from the $7s$ – $6s$ Stark shift value in Ref. 24. \(^e\) all-order values, Ref. 18. fSD all-order scaled values, previously published in Ref. 22. Units: $e a_0$. 

| Transition | $E_1$ | Transition | $E_1$ | Transition | $E_1$ |
|------------|-------|------------|-------|------------|-------|
| $6s - 6p_{1/2}$ | 4.489(7) | $6s - 7p_{1/2}$ | 9.313(65) | $10s - 9p_{1/2}$ | 24.50(10) |
| $6s - 7p_{1/2}$ | 0.276(2) | $6s - 8p_{1/2}$ | 17.78(7) | $10s - 10p_{1/2}$ | 38.31(10) |
| $6s - 6p_{3/2}$ | 6.324(7) | $6s - 7p_{3/2}$ | 14.07(7) | $10s - 9p_{3/2}$ | 36.69(10) |
| $6s - 7p_{3/2}$ | 0.586(5) | $6s - 8p_{3/2}$ | 24.56(10) | $10s - 10p_{3/2}$ | 52.67(16) |
| $7s - 6p_{1/2}$ | 4.236(21) | $7s - 8p_{1/2}$ | 16.06(8) | $11s - 10p_{1/2}$ | 34.64(12) |
| $7s - 7p_{1/2}$ | 10.308(10) | $7s - 9p_{1/2}$ | 27.10(8) | $11s - 11p_{1/2}$ | 51.42(11) |
| $7s - 6p_{3/2}$ | 6.473(32) | $7s - 8p_{3/2}$ | 24.12(8) | $11s - 10p_{3/2}$ | 51.77(12) |
| $7s - 7p_{3/2}$ | 14.320(14) | $7s - 9p_{3/2}$ | 37.33(13) | $11s - 11p_{3/2}$ | 70.58(19) |
| $12s - 11p_{1/2}$ | 46.49(15) | $5d_{3/2} - 6p_{1/2}$ | 9.06(16) | $5d_{2/2} - 6p_{3/2}$ | 9.66(20) |
| $12s - 12p_{1/2}$ | 66.43(13) | $5d_{3/2} - 6p_{3/2}$ | 3.19(8) | $5d_{2/2} - 4f_{5/2}$ | 1.93(30) |
| $12s - 11p_{3/2}$ | 69.37(15) | $5d_{3/2} - 4f_{5/2}$ | 7.1(5) | $5d_{2/2} - 4f_{7/2}$ | 8.6(6) |
| $12s - 12p_{3/2}$ | 91.1(2) | $6d_{5/2} - 6p_{3/2}$ | 6.01(26) | $7d_{3/2} - 7p_{1/2}$ | 6.56(2) |
| $6d_{3/2} - 7p_{1/2}$ | 18.0(2) | $6d_{5/2} - 7p_{3/2}$ | 24.3(3) | $7d_{3/2} - 8p_{1/2}$ | 32.0(2) |
| $6d_{3/2} - 6p_{3/2}$ | 2.05(9) | $6d_{5/2} - 4f_{5/2}$ | 6.60(5) | $7d_{3/2} - 7p_{3/2}$ | 3.52(2) |
| $6d_{3/2} - 7p_{3/2}$ | 8.01(7) | $6d_{5/2} - 5f_{5/2}$ | 1.11(15) | $7d_{3/2} - 8p_{3/2}$ | 14.35(8) |
| $6d_{3/2} - 4f_{5/2}$ | 24.6(2) | $6d_{5/2} - 4f_{7/2}$ | 29.5(2) | $7d_{3/2} - 4f_{5/2}$ | 13.0(2) |
| $6d_{3/2} - 5f_{5/2}$ | 3.9(6) | $6d_{5/2} - 5f_{7/2}$ | 4.96(67) | $7d_{3/2} - 5f_{5/2}$ | 43.4(3) |
| $7d_{5/2} - 7p_{3/2}$ | 9.64(4) | $8d_{3/2} - 8p_{1/2}$ | 9.18(5) | $8d_{3/2} - 8p_{3/2}$ | 13.65(7) |
| $7d_{5/2} - 8p_{1/2}$ | 4.3(2) | $8d_{3/2} - 9p_{1/2}$ | 49.3(2) | $8d_{3/2} - 9p_{3/2}$ | 66.6(2) |
| $7d_{5/2} - 5f_{5/2}$ | 11.66(7) | $8d_{3/2} - 8p_{3/2}$ | 4.7(1) | $8d_{3/2} - 5f_{5/2}$ | 6.85(4) |
| $7d_{5/2} - 4f_{7/2}$ | 15.3(2) | $8d_{3/2} - 9p_{3/2}$ | 22.13(7) | $8d_{3/2} - 6f_{5/2}$ | 17.54(8) |
| $7d_{5/2} - 5f_{7/2}$ | 52.2(3) | $8d_{3/2} - 5f_{5/2}$ | 26.1(2) | $8d_{3/2} - 5f_{7/2}$ | 30.6(2) |
| $9d_{3/2} - 9p_{1/2}$ | 12.2(2) | $9d_{3/2} - 9p_{3/2}$ | 18.3(2) | $10d_{3/2} - 10p_{1/2}$ | 15.6(2) |
| $9d_{3/2} - 10p_{1/2}$ | 70.0(2) | $9d_{3/2} - 10p_{3/2}$ | 94.5(2) | $10d_{3/2} - 11p_{1/2}$ | 94.1(2) |
| $9d_{3/2} - 9p_{3/2}$ | 6.33(6) | $9d_{3/2} - 7f_{5/2}$ | 24.36(9) | $10d_{3/2} - 10p_{3/2}$ | 8.16(7) |
| $9d_{3/2} - 10p_{3/2}$ | 31.45(8) | $9d_{3/2} - 6f_{7/2}$ | 49.3(3) | $10d_{3/2} - 11p_{3/2}$ | 42.30(9) |
| $9d_{3/2} - 6f_{5/2}$ | 40.4(4) | $9d_{3/2} - 7f_{7/2}$ | 108.9(4) | $10d_{3/2} - 7f_{5/2}$ | 61.0(2) |
| $9d_{3/2} - 7f_{5/2}$ | 90.5(4) | $9d_{3/2} - 6f_{7/2}$ | 65.2(4) | $10d_{3/2} - 8f_{5/2}$ | 119.4(4) |
| $10d_{3/2} - 10p_{3/2}$ | 23.5(3) | $10d_{3/2} - 8f_{5/2}$ | 32.2(1) | $10d_{3/2} - 8f_{7/2}$ | 143.8(5) |
| $10d_{3/2} - 11p_{3/2}$ | 127.1(3) | $10d_{3/2} - 7f_{7/2}$ | 71.7(3) | | |
TABLE II: The contributions to the scalar polarizability for the $9s$ state in cesium. The corresponding energy differences and the absolute values of the lowest-order $Z^{DF}$ and final all-order electric-dipole reduced matrix elements $Z^{SD}$ are also listed. The energy differences are given in cm$^{-1}$. Electric-dipole matrix elements are given in atomic units ($ea_0$), and polarizabilities are given in $10^3 a_0^3$, where $a_0$ is Bohr radius.

| Contribution | $\beta$ | $Z^{DF}_{Z,9s}$ | $Z^{SD}_{Z,9s}$ | $E_\beta - E_{8s}$ | $a_0(9s)$ |
|--------------|---------|-----------------|-----------------|-------------------|-----------|
| $\alpha^{\text{main}}(nP_{1/2})$ | $6p_{1/2}$ | 0.56 | 0.55 | -15732 | 0.00 |
| | $7p_{1/2}$ | 2.04 | 1.96 | -5145 | -0.05 |
| | $8p_{1/2}$ | 16.30 | 16.06 | -1209 | -15.7(2) |
| | $9p_{1/2}$ | 28.17 | 27.10 | 726 | 74.0(4) |
| | $10p_{1/2}$ | 2.67 | 2.76 | 1816 | 0.31 |
| | $11p_{1/2}$ | 1.01 | 1.08 | 2493 | 0.03 |
| | $12p_{1/2}$ | 0.56 | 0.60 | 2942 | 0.01 |
| $\alpha^{\text{tail}}(nP_{1/2})$ | | | | | 0.01 |
| $\alpha^{\text{main}}(nP_{3/2})$ | $6p_{3/2}$ | 0.79 | 0.77 | -15178 | 0.00 |
| | $7p_{3/2}$ | 2.86 | 2.73 | -4964 | -0.11 |
| | $8p_{3/2}$ | 24.31 | 24.12 | -1119 | -38.0(3) |
| | $9p_{3/2}$ | 38.99 | 37.33 | 771 | 132.3(9) |
| | $10p_{3/2}$ | 4.43 | 4.61 | 1843 | 0.85 |
| | $11p_{3/2}$ | 1.80 | 1.93 | 2510 | 0.11 |
| | $12p_{3/2}$ | 1.04 | 1.13 | 2954 | 0.03 |
| $\alpha^{\text{tail}}(nP_{3/2})$ | | | | | 0.04 |
| Total | | | | | 153.7(1.0) |

The measured $5d$ lifetimes values due to the inconsistencies of these values with the measured Stark shifts. The uncertainties of the $5d_{3/2} - 4f_{5/2}$ and $5d_{5/2} - 4f_{7/2}$ matrix elements are estimated as the differences of the SD scaled results and $ab$ initio SDpT values that partially include triple excitations.

The SD all-order values for the $8s - np$ and $7d_j - nlj$ transitions were previously published in Refs. [22, 35], respectively. In summary, the uncertainties of our calculations are generally small, ranging from 0.2% to about 1%. The only exceptions are the transitions involving the $5d$ states and some of the transition from the $6d$ states. We refer the reader to Ref. [18] for a detailed discussion of these transitions. We note that we may overestimate the uncertainty of our calculation for these transitions as our values for the $6p_{1/2}$ and $6p_{3/2}$ polarizabilities are in excellent agreement with the experiment [10, 11]. As a result, the actual accuracy of our values of $5d$ polarizabilities may be actually higher than we estimated.

As noted above, we used experimental energies for all of the main term calculations. Most of the energies values in this work are taken from the 1987 measurements by Weber and Sansonetti [39] and other values quoted in the same reference. The ionization potential value, required for the scaling procedure, is taken from the same work. The values of the several lower levels are taken from the NIST Handbook of Basic Atomic Spectroscopic Data [38]. The data for the $np_{3/2}$ levels are obtained by combining the $np_{1/2}$ values from [39] and fine-structure intervals from [40]. The data for the remaining few levels not given in either [38, 39] were taken from Ref. [40]. Since the energy denominators in the polarizability calculation are small for some of the higher states (below 100 cm$^{-1}$), we compiled the list of the most accurate known energies. As a result, the polarizability values quoted in this work for the $7d$, $9d$, and $10d$ states are slightly different from the ones quoted in Ref. [22] while the same matrix elements were used. We note that these differences are well within the uncertainties of the polarizability values. The uncertainties in the values of the energies can be neglected in all cases.
Next, we consider the examples of the polarizability calculation; one case is considered in detail for each of the \(nS\), \(Np_{1/2}\), \(Np_{3/2}\), \(Nd_{3/2}\), and \(Nd_{5/2}\) sequences of states. We consider the following sample cases: \(9s\), \(7p_{1/2}\), \(7p_{3/2}\), \(8d_{3/2}\), and \(8d_{5/2}\). In addition, we consider the \(5d_{3/2}\) and \(5d_{5/2}\) calculations separately as they do not follow the pattern of all other \(Nd\) state calculations. These are also the only cases where the tail contribution is significant and represent interesting exception among the states that we have considered.

We consider the \(9s\) case first. The detailed breakdown of the \(9s\) polarizability calculation is given in Table III. Each contribution to the main term, i.e. the contributions from the \(6p\), \(7p\), \(8p\), \(9p\), \(10p\), and \(11p\) and \(12p\) states are given separately, and the tail terms are group together for the \(np_{1/2}\) and \(np_{3/2}\) contributions. The corresponding main term energy differences and the absolute values of the lowest-order (DF) and final all-order electric-dipole reduced matrix elements are also listed. The lowest-order values are given to illustrate the size of the correlation corrections for these transitions. The energy differences are given in \(cm^{-1}\). Electric-dipole matrix elements are given in atomic units \((\text{ea}_0)\), and polarizabilities are given in \(10^3 \text{ } a_0^3\). The core contribution is negligible in this case (0.015 in the units of Table III) and is not listed. We find that two of the transitions, \(9s - 9p_{1/2}\) and \(9s - 9p_{3/2}\), give dominant contributions while two other, \(9s - 8p_{1/2}\) and \(9s - 8p_{3/2}\), are large and have to be calculated accurately. We note that there is rather significant cancellation between the \(9s - 9p_{j}\) and \(9s - 8p_{j}\) contributions. The dominant contribution is this case may have been easily predicted simply based on the size of the energy intervals listed in the fifth column of the table. We also find that all other contributions with the exception of the \(9s - 10p_{1/2}\) and \(9s - 10p_{3/2}\) contribution are very small and may be simply omitted without the loss of accuracy. The main uncertainty comes from the uncertainty in the \(9s - 9p_{3/2}\) transition. The precision our calculation in this case is expected to be very high as the correlation correction is small as illustrated by the comparison of the lowest-order and final values of the electric-dipole matrix elements. The final uncertainty is evaluated to be 0.7%. The breakdown of the calculation of the other \(Ns\) polarizabilities considered in this work is similar to the one for the

| Contribution | \(\beta\) | \(Z_{\alpha,7p_{1/2}}^{DF}\) | \(Z_{\alpha,7p_{1/2}}^{SD}\) | \(E_\beta - E_{7p_{1/2}}\) | \(\alpha_0(7p_{1/2})\) |
|--------------|---------|-----------------|-----------------|-----------------|----------------|
| \(\alpha_{\text{main}}(ns)\) | \(6s\) | 0.37 | 0.28 | -21765 | -0.000 |
| | \(7s\) | 11.01 | 10.31 | -3230 | -2.407(5) |
| | \(8s\) | 9.53 | 9.31 | 2552 | 2.487(35) |
| | \(9s\) | 2.04 | 1.97 | 5145 | 0.055 |
| | \(10s\) | 1.04 | 1.00 | 6535 | 0.011 |
| | \(11s\) | 0.68 | 0.65 | 7366 | 0.004 |
| | \(12s\) | 0.49 | 0.48 | 7904 | 0.002 |
| \(\alpha_{\text{tail}}(ns)\) | | | | | 0.012(12) |
| \(\alpha_{\text{main}}(nd_{3/2})\) | \(5d_{3/2}\) | 4.04 | 1.52 | -7266 | -0.023 |
| | \(6d_{3/2}\) | 19.62 | 17.99 | 824 | 28.74(70) |
| | \(7d_{3/2}\) | 4.03 | 6.56 | 4238 | 0.734(5) |
| | \(8d_{3/2}\) | 2.39 | 3.16 | 6046 | 0.121 |
| | \(9d_{3/2}\) | 1.63 | 2.00 | 7063 | 0.042 |
| | \(10d_{3/2}\) | 1.21 | 1.44 | 7703 | 0.020 |
| \(\alpha_{\text{tail}}(nd_{3/2})\) | | | | | 0.080(80) |
| Total | | | | | 29.89(70) |
9s state with the exception of the 6s state. For all other cases, the dominant contributions come from the $N_s - Np_{1/2}$ and the $Ns - Np_{3/2}$ matrix elements, while the other important contributions come from the $Ns - (N-1)p_{1/2}$ and the $Ns - (N-1)p_{3/2}$ matrix elements. The polarizability of the 6s state is overwhelmingly dominated by the contribution of the 6s−6p$_{1/2}$ and the 6s−6p$_{3/2}$ transitions. These two transitions add coherently and account for the 96% of the total value. The calculation of the 8s polarizability is described in detail in Ref. [35]. We limited this work by the 12s state as the 13p$_j$ states needed for the calculation of the 13s polarizability do not quite fit inside of our cavity and the basis set energies of the 13p states deviate from the DF energies.

The breakdown of the contributions to the $7p_{1/2}$ and $7p_{3/2}$ polarizabilities is given in Tables III and IV respectively. All tables illustrating the contributions to polarizabilities are structured in the same way. In the case of the $7p_{1/2}$ polarizability, the dominant contribution comes from a single transition, $7p_{1/2} - 6d_{3/2}$, as none of the other levels are as close to the $7p_{1/2}$ levels as the $6d_{3/2}$ level. The contribution from the next transition, $7p_{1/2} - 7d_{3/2}$, is significantly smaller, only 2% of the dominant contribution. Interestingly, the contributions of the $7p_{1/2} - 7s$ and $7p_{1/2} - 8s$ transitions, while being 10% of the main contribution, cancel out nearly exactly. We note that while significant cancellation is present for all other $Np_{1/2}$ cases, it is the most severe in the case of the $7p_{1/2}$ state. The tail contribution is larger than for the $N$s calculation but is still very small, 0.3%. We assume

| Contribution | $\beta$ | $Z_{\beta}^{DF}_{7p_{3/2}}$ | $Z_{\beta}^{SD}_{7p_{3/2}}$ | $E_{\beta} - E_{7p_{3/2}}$ | $\alpha_0(7p_{3/2})$ | $\alpha_2(7p_{3/2})$ |
|--------------|--------|-----------------|-----------------|-----------------|----------------|----------------|
| $\alpha_{\text{main}}(ns)$ | 6s | 0.69 | 0.59 | -21946 | -0.001 | 0.001 |
| | 7s | 15.35 | 14.32 | -3411 | 2.199(4) | 2.199(4) |
| | 8s | 14.28 | 14.07 | 2371 | 3.05(3) | -3.05(3) |
| | 9s | 2.86 | 2.73 | 4964 | 0.055 | -0.055 |
| | 10s | 1.44 | 1.38 | 6354 | 0.111 | -0.011 |
| | 11s | 0.93 | 0.89 | 7185 | 0.004 | -0.004 |
| | 12s | 0.68 | 0.65 | 7722 | 0.002 | -0.002 |
| $\alpha_{\text{tail}}(ns)$ | | | | 0.01(1) | -0.01(1) |
| $\alpha_{\text{main}}(nd_{3/2})$ | 5d$_{3/2}$ | 1.69 | 0.58 | -7447 | -0.002 | -0.0013 |
| | 6d$_{3/2}$ | 8.86 | 8.07 | 642 | 3.71(10) | 2.97(8) |
| | 7d$_{3/2}$ | 2.11 | 3.32 | 4102 | 0.098(1) | 0.079(1) |
| | 8d$_{3/2}$ | 1.19 | 1.54 | 5865 | 0.015 | 0.012 |
| | 9d$_{3/2}$ | 0.79 | 0.96 | 6882 | 0.005 | 0.004 |
| | 10d$_{3/2}$ | 0.58 | 0.68 | 7522 | 0.002 | 0.002 |
| $\alpha_{\text{tail}}(nd_{3/2})$ | | | | 0.009(9) | 0.007(7) |
| $\alpha_{\text{main}}(nd_{5/2})$ | 5d$_{5/2}$ | 5.02 | 1.87 | -7350 | -0.017 | 0.004 |
| | 6d$_{5/2}$ | 26.61 | 24.35 | 685 | 31.6(7) | -6.33(15) |
| | 7d$_{5/2}$ | 6.30 | 9.64 | 4122 | 0.825(6) | -0.165(1) |
| | 8d$_{5/2}$ | 3.55 | 4.52 | 5877 | 0.127 | -0.025 |
| | 9d$_{5/2}$ | 2.37 | 2.83 | 6889 | 0.042 | -0.009 |
| | 10d$_{5/2}$ | 1.75 | 2.02 | 7527 | 0.020 | -0.004 |
| $\alpha_{\text{tail}}(nd_{5/2})$ | | | | 0.08(8) | -0.02(2) |
| Total | | | | 37.52(75) | -4.41(17) |
TABLE V: The contributions to the scalar and tensor polarizabilities for the $8d_{3/2}$ state in cesium. The corresponding energy differences and the absolute values of the lowest-order (DF) and final all-order electric-dipole reduced matrix elements are also listed. The energy differences are given in cm$^{-1}$. Electric-dipole matrix elements are given in atomic units ($e\alpha_0$), and polarizabilities are given in $10^3 a_0^3$, where $a_0$ is Bohr radius.

| Contribution | $\beta$ | $Z_{\beta,8d_{3/2}}^{DF}$ | $Z_{\beta,8d_{3/2}}^{SD}$ | $E_\beta - E_{8d_{3/2}}$ | $\alpha_0(8d_{3/2})$ | $\alpha_2(8d_{3/2})$ |
|--------------|--------|----------------|----------------|-----------------|----------------|----------------|
| $\alpha_{\text{main}}(np_{1/2})$ | 6$p_{1/2}$ | 1.11 | 1.30 | -16633 | 0.00 | 0.00 |
| | 7$p_{1/2}$ | 2.39 | 3.16 | -6046 | -0.06 | 0.06 |
| | 8$p_{1/2}$ | 5.55 | 9.18 | -2102 | -1.47(2) | 1.47(2) |
| | 9$p_{1/2}$ | 50.96 | 49.29 | -174 | -510(3) | 510(3) |
| | 10$p_{1/2}$ | 20.43 | 14.02 | 916 | 7.85 | -7.85 |
| | 11$p_{1/2}$ | 5.84 | 4.50 | 1592 | 0.46 | -0.46 |
| | 12$p_{1/2}$ | 3.07 | 2.44 | 2041 | 0.11 | -0.11 |
| $\alpha_{\text{tail}}(np_{1/2})$ | | | | 0.2(2) | -0.2(2) |
| $\alpha_{\text{main}}(np_{3/2})$ | 7$p_{3/2}$ | 1.19 | 1.54 | -5865 | -0.01 | -0.01 |
| | 8$p_{3/2}$ | 2.97 | 4.71 | -2020 | -0.40 | -0.32 |
| | 9$p_{3/2}$ | 23.02 | 22.13 | -130 | -138.3(9) | -110.6(7) |
| | 10$p_{3/2}$ | 8.43 | 5.53 | 942 | 1.18 | 0.95 |
| | 11$p_{3/2}$ | 2.49 | 1.83 | 1610 | 0.08 | 0.06 |
| | 12$p_{3/2}$ | 1.32 | 1.00 | 2053 | 0.02 | 0.01 |
| $\alpha_{\text{tail}}(np_{3/2})$ | | | | 0.04(4) | 0.03(3) |
| $\alpha_{\text{main}}(nf_{5/2})$ | 4$f_{5/2}$ | 2.34 | 2.49 | -3339 | -0.07 | -0.01 |
| | 5$f_{5/2}$ | 19.18 | 26.06 | -840 | -29.6(4) | 5.9(1) |
| | 6$f_{5/2}$ | 70.91 | 65.22 | 518 | 300(3) | -60.0(6) |
| | 7$f_{5/2}$ | 8.74 | 0.33 | 1337 | 0.00 | 0.00 |
| | 8$f_{5/2}$ | 5.71 | 1.28 | 1868 | 0.03 | -0.01 |
| $\alpha_{\text{tail}}(nf_{5/2})$ | | | | 1(1) | -0.2(2) |
| Total | | | | -369(5) | 339(4) |

100% uncertainty in the tail contributions in all of our calculations for consistency. It is still negligible for all of the cases with the exception of the $5d$ calculation.

As noted above, there are three types of the transitions contributing to the polarizabilities of the $np_{3/2}$ states. The dominant contribution comes from the single transition as in the case of the $7p_{1/2}$ polarizabilities, $7p_{3/2} - 6d_{5/2}$. The contribution of the $7p_{3/2} - 6d_{3/2}$ transition is 10 times as small as the dominant one. Again, the contributions from the $7p_{3/2} - 7s$ and $7p_{3/2} - 8s$ partially cancel, but the cancellation is not as complete as in the case of the $7p_{1/2}$ states.

While the calculations of the scalar and tensor polarizabilities use the same matrix elements and energies and only differ by the angular factors, the uncertainty of the $7p_{3/2}$ tensor polarizability calculation (4%) is twice as high as that of the scalar polarizability owing to the significant cancellation of the terms contributing to the tensor polarizability. The relative accuracy of the calculation of the tensor polarizability calculation gradually improves to 1% for the $10p_{3/2}$ state but this uncertainty is still more than twice as high as the uncertainty of the corresponding scalar polarizability calculation (0.4%). The breakdown of all other $np_{1/2}$ and $np_{3/2}$ polarizabilities parallels the one of the $7p_{1/2}$ and $7p_{3/2}$ states.

The contributions to scalar and tensor polarizabilities for the $8d_{3/2}$ and $8d_{5/2}$ states in cesium are given by Tables VI and VII. For the $8d_{3/2}$ states, three contributions are dominant, $8d_{3/2} - 9p_{1/2}$, $8d_{3/2} - 9p_{1/2}$, and $8d_{3/2} - 6f_{5/2}$ for both scalar and tensor polarizabilities. Unlike the case of the $Np_{3/2}$
TABLE VI: The contributions to the scalar and tensor polarizabilities for the $8d_{5/2}$ state in cesium. The corresponding energy differences and the absolute values of the lowest-order (DF) and final all-order electric-dipole reduced matrix elements are also listed. The energy differences are given in cm$^{-1}$. Electric-dipole matrix elements are given in atomic units ($a_0$), and polarizabilities are given in $10^3 a_0^3$.

| Contribution  | $\beta$ | $Z_{\beta,8d_{5/2}}^{DF}$ | $Z_{\beta,8d_{5/2}}^{SD}$ | $E_\beta - E_{8d_{5/2}}$ | $\alpha_0(8d_{5/2})$ | $\alpha_2(8d_{5/2})$ |
|---------------|---------|----------------------------|-----------------------------|---------------------------|-----------------------|-----------------------|
| $a_{\text{main}}(nP_{3/2})$ | 6$p_{3/2}$ | 1.59 | 1.81 | -16091 | 0.00 | 0.00 |
| | 7$p_{3/2}$ | 3.55 | 4.52 | -5877 | -0.08 | 0.08 |
| | 8$p_{3/2}$ | 8.82 | 13.65 | -2031 | -2.24(2) | 2.24(2) |
| | 9$p_{3/2}$ | 69.07 | 66.57 | -141 | -765(5) | 765(5) |
| | 10$P_{3/2}$ | 25.43 | 17.30 | 931 | 7.84 | -7.84 |
| | 11$P_{3/2}$ | 7.51 | 5.68 | 1598 | 0.49 | -0.49 |
| | 12$P_{3/2}$ | 3.98 | 3.10 | 2041 | 0.11 | -0.11 |
| $a_{\text{tail}}(nP_{3/2})$ | | | | | 0.2(2) | -0.2(2) |
| $a_{\text{main}}(nF_{5/2})$ | 4$f_{5/2}$ | 0.62 | 0.67 | -3350.4 | 0.00 | 0.00 |
| | 5$f_{5/2}$ | 5.11 | 6.85 | -851.3 | -1.34(2) | -1.53(2) |
| | 6$f_{5/2}$ | 18.97 | 17.54 | 506.6 | 14.8(1) | 16.9(2) |
| | 7$f_{5/2}$ | 2.37 | 0.04 | 1325.1 | 0.00 | 0.00 |
| | 8$f_{5/2}$ | 1.54 | 0.42 | 1855.9 | 0.00 | 0.00 |
| $a_{\text{tail}}(nF_{5/2})$ | | | | | 0.05(5) | 0.05(5) |
| $a_{\text{main}}(nF_{7/2})$ | 4$f_{7/2}$ | 2.79 | 2.99 | -3350.7 | -0.06 | 0.02 |
| | 5$f_{7/2}$ | 22.82 | 30.60 | -851.6 | -26.8(4) | 9.6(1) |
| | 6$f_{7/2}$ | 84.82 | 78.43 | 506.5 | 296(3) | -106(1) |
| | 7$f_{7/2}$ | 10.61 | 0.19 | 1325.0 | 0.00 | 0.00 |
| | 8$f_{7/2}$ | 6.89 | 1.86 | 1855.8 | 0.05(5) | -0.02 |
| $a_{\text{tail}}(nF_{7/2})$ | | | | | 1(1) | -0.4(4) |
| Total | | | | | -475(5) | 678(5) |

states, significant cancellations are observed between terms for both scalar and tensor polarizabilities. We would like to specifically note interesting problem with the $8d_{3/2} - 7f_{5/2}$ transition. While the DF value for the transition is 8.74, the final all-order number is very small, 0.33 owing to extremely large correlation correction that essentially cancels the lowest order. We also note that the $ab\ initio$ all-order value for this transition (0.73) significantly differs from the scaled values. While we assigned this value 100% uncertainty, the resulting uncertainty in the polarizability value is negligible.

We observe similar problem with the $8d_{5/2} - 7f_{7/2}$ transition as well as similar transitions for other values of $N$ and $n$ with the exception of the $5d - 4f$ transitions. For the case of the $6d - 5f$ transition, the cancellation of the lowest order and the correlation correction is less severe. We note that the correlation correction to the previous transition in the sequence, $8d_{3/2} - 6f_{5/2}$ is small, only 8%. Similar issue exists for the next in line transition, $8d_{3/2} - 8f_{5/2}$, but its contribution was too small to warrant its more accurate consideration.

The $8d_{3/2} - 7f_{5/2}$ and $8d_{5/2} - 7f_{7/2}$ transitions are two of the very few transitions for which we conducted the scaling but did not list the values in the Table II of the recommended matrix elements as the uncertainties of these values are very high. In general, if the main term transition was not listed in Table II we used $ab\ initio$ SD value and did not conduct the evaluation of the uncertainty. The contributions of these terms are small enough so their contribution to the total uncertainties would be negligible. Again, significant cancellations are observed between the terms. The polarizability calculation of the all other $Nd$ is similar to the $8d$ examples with the exception of the $5d$ scalar.
TABLE VII: The contributions to the scalar and tensor polarizabilities for the 5d\textsubscript{3}/2 and 5d\textsubscript{5}/2 states in cesium. The corresponding energy differences and the absolute values of the lowest-order (DF) and final all-order electric-dipole reduced matrix elements are also listed. The energy differences are given in cm\textsuperscript{-1}. Electric-dipole matrix elements are given in atomic units (ea\textsubscript{0}), and polarizabilities are given in 10\textsuperscript{3} a\textsubscript{0}\textsuperscript{3}, where a\textsubscript{0} is Bohr radius.

| Contribution | \(\beta\) | \(Z_{\beta,5d_{3/2}}^{\text{DF}}\) | \(Z_{\beta,5d_{5/2}}^{\text{DF}}\) | \(E_{\beta} - E_{5d_{3/2}}\) | \(\alpha_0(5d_{3/2})\) | \(\alpha_2(5d_{3/2})\) |
|--------------|-----------|-----------------|-----------------|-----------------|----------------|----------------|
| \(\alpha_{\text{main}}(np_{1/2})\) | 6p\textsubscript{1/2} | 8.98 | 7.06 | -3321 | -0.550(24) | 0.550(24) |
| | 7p\textsubscript{1/2} | 4.04 | 1.52 | 7266 | 0.012 | -0.012 |
| \(\alpha_{\text{tail}}(np_{1/2})\) | | | | 0.002 | -0.002 |
| \(\alpha_{\text{main}}(np_{3/2})\) | 6p\textsubscript{3/2} | 4.06 | 3.19 | -2767 | -0.134(6) | -0.107(5) |
| | 7p\textsubscript{3/2} | 1.69 | 0.58 | 7447 | 0.002 | 0.001 |
| \(\alpha_{\text{tail}}(np_{3/2})\) | | | | 0.000 | 0.000 |
| \(\alpha_{\text{main}}(nf_{5/2})\) | 4f\textsubscript{5/2} | 10.66 | 7.11 | 9973 | 0.186(27) | 0.037(5) |
| | 5f\textsubscript{5/2} | 4.72 | 3.34 | 12472 | 0.033 | -0.007 |
| | 6f\textsubscript{5/2} | 2.90 | 2.24 | 13830 | 0.013 | -0.003 |
| | 7f\textsubscript{5/2} | 2.04 | 1.66 | 14649 | 0.007 | -0.001 |
| | 8f\textsubscript{5/2} | 1.55 | 1.30 | 15180 | 0.004 | -0.001 |
| \(\alpha_{\text{tail}}(nf_{5/2})\) | | | | 0.059(59) | -0.012(12) |
| Total | | | | -0.352(69) | 0.370(28) |

| Contribution | \(\beta\) | \(Z_{\beta,5d_{5/2}}^{\text{DF}}\) | \(Z_{\beta,5d_{5/2}}^{\text{SD}}\) | \(E_{\beta} - E_{5d_{5/2}}\) | \(\alpha_0(5d_{5/2})\) | \(\alpha_2(5d_{5/2})\) |
|--------------|-----------|-----------------|-----------------|-----------------|----------------|----------------|
| \(\alpha_{\text{main}}(np_{3/2})\) | 6p\textsubscript{3/2} | 12.19 | 9.66 | -2865 | -0.794(33) | 0.794(33) |
| | 7p\textsubscript{3/2} | 5.02 | 1.87 | 7350 | 0.012 | -0.012 |
| \(\alpha_{\text{tail}}(np_{3/2})\) | | | | 0.002 | -0.002 |
| \(\alpha_{\text{main}}(nf_{5/2})\) | 4f\textsubscript{5/2} | 2.84 | 1.93 | 9876 | 0.009(3) | 0.011(3) |
| | 4f\textsubscript{5/2} | 1.26 | 0.91 | 12375 | 0.002 | 0.002 |
| \(\alpha_{\text{tail}}(nf_{5/2})\) | | | | 0.004(3) | 0.004(3) |
| \(\alpha_{\text{main}}(nf_{7/2})\) | 4f\textsubscript{7/2} | 112.70 | 8.62 | 9875 | 0.184(24) | -0.066(9) |
| | 5f\textsubscript{7/2} | 5.64 | 4.08 | 12375 | 0.033 | -0.012 |
| | 6f\textsubscript{7/2} | 3.46 | 2.73 | 13733 | 0.013 | -0.005 |
| | 7f\textsubscript{7/2} | 2.44 | 2.01 | 14551 | 0.007 | -0.002 |
| | 8f\textsubscript{7/2} | 1.86 | 1.57 | 15082 | 0.004 | -0.001 |
| \(\alpha_{\text{tail}}(nf_{7/2})\) | | | | 0.056(56) | -0.020(20) |
| Total | | | | -0.453(70) | 0.691(40) |

Polarizability calculation, which is anomalous and is discussed separately below. The calculation of the 7d, 9d, and 10d polarizabilities was discussed in detail in Ref. 22.

The contributions to the scalar and tensor polarizabilities for the 5d\textsubscript{3}/2 and 5d\textsubscript{5}/2 states in cesium are given in Table VII. We grouped small contributions of the 5d – np\textsubscript{j} and 5d – nf\textsubscript{j} transitions together with the tail in this table. Comparison of the 5d\textsubscript{3}/2 and 8d\textsubscript{5/2} tables (as well as all the other nd\textsubscript{5/2} contribution breakdowns) shows the 5d\textsubscript{3}/2 scalar polarizability case to be anomalous. In this case, none of the 5d – nf energy denominators are small, and the largest contribution from nf\textsubscript{j} states is still a third of the one from the dominant 5d\textsubscript{3}/2 – 6p\textsubscript{1/2} transition. There is also no damping of the
TABLE VIII: Comparison of the Cs scalar polarizabilities with other theory and experiment. All values are given in \(10^3 \alpha_0\). \(^a\)Recommended value from Ref. \[23\]. \(^b\)\textit{ab initio} all-order value from Ref. \[21\]. \(^c\)Ref. \[32\], \(^d\)Ref. \[8\]. \(^e\)derived from the Ref. \[14\] 7s–6s Stark shift measurement and the 6s result from \[8\]. \(^f\)Ref. \[35\]. \(^g\)Refs. \[12, 31\]. \(^h\)derived from Ref. \[11\] D1 line Stark shift measurement and the 6s result from \[8\]. \(^i\)Ref. \[52\], \(^j\)derived from Ref. \[10\] D2 line Stark shift measurement and the 6s result from \[8\]. \(^k\)Ref. \[53\]. \(^l\)Ref. \[54\]. \(^m\)Ref. \[55\].

| State | 6s | 7s | 8s | 9s | 10s | 11s |
|-------|----|----|----|----|-----|-----|
| Present | 0.3984(7) | 6.238(41) | 38.27(28) | 153.7(1.0) | 478(3) | 1246(8) |
| Ref. \[31\] | 0.394 | 6.14 | 37.9 | 153 | 475 | 1240 |
| Theory | 0.3999(19) \(^a\) | 6.272 \(^b\) | 4.909 \(^c\) | 0.4010(6) \(^d\) | 6.238(6) \(^e\) | 38.06(25) \(^f\) | 479(1) \(^g\) | 1246(1) \(^g\) |
| Expt. | \(6p_{1/2}\) | \(7p_{1/2}\) | \(8p_{1/2}\) | \(9p_{1/2}\) | \(10p_{1/2}\) | 2871(2) \(^g\) |
| Present | 1.338(54) | 29.9(7) | 223(2) | 1021(7) | 3499(19) | 2866(30) |
| Ref. \[31\] | 1.29 | 29.4 | 221 | 1020 | 3490 | 2840 |
| Expt. | 1.3284(6) \(^h\) | 29.6(6) \(^i\) | 37.9(8) \(^j\) | 1246 \(^k\) | 4522(19) |
| Present | 1.648(56) | 37.5(8) | 284(3) | 1312(7) | 4522(19) |
| Ref. \[31\] | 1.60 | 36.9 | 282 | 1310 | 4510 |
| Expt. | 1.641(2) \(^j\) | 37.9(8) \(^k\) | 1246(1) \(^k\) |
| State | \(5d_{3/2}\) | \(6d_{3/2}\) | \(7d_{3/2}\) | \(8d_{3/2}\) | \(9d_{3/2}\) | \(10d_{3/2}\) |
| Present | -0.352(69) | -5.68(45) | -66.7(1.7) | -369(5) | -1402(13) | -4234(32) |
| Ref. \[31\] | -0.418 | -5.32 | -65.2 | -366 | -1400 | -4220 |
| Expt. | -60(8) \(^j\) | -1450(120) \(^m\) | -4185(4) \(^n\) |
| State | \(5d_{5/2}\) | \(6d_{5/2}\) | \(7d_{5/2}\) | \(8d_{5/2}\) | \(9d_{5/2}\) | \(10d_{5/2}\) |
| Present | -0.453(70) | -8.37(55) | -88.8(2.0) | -475(5) | -1777(14) | -5316(38) |
| Ref. \[31\] | -0.518 | -7.95 | -87.1 | -472 | -1770 | -5300 |
| Expt. | -76(8) \(^j\) | -2050(100) \(^m\) | -5303(8) \(^n\) |

remaining \(5d_{3/2} - n f_{5/2}\) contributions observed for the higher \(8d_{3/2} - n f_{5/2}\) transitions. Therefore, there is basis to assume that the DF tail is substantially overestimated. It may be overestimated by about 15-20% based on the comparison of the DF and the all-order matrix element values. As a result, the tail contribution is 25% of the total contribution of the \(5d_{3/2} - n f_{5/2}\) sum and its uncertainty gives the dominant contribution to the uncertainty of the \(5d_{3/2}\) scalar polarizability. We note that the \(5d_{3/2} - n f_{5/2}\) tensor polarizability tail is small with comparison to the dominant \(5d_{3/2} - 6p_{1/2}\) contribution, and its contribution to the total uncertainty is small. As a result, the \(5d_{3/2}\) tensor polarizability calculation is similar to the \(8d_{3/2}\) one. Its reduced accuracy is due to much larger correlation correction to the \(5d_{3/2} - 6p_{1/2}\) matrix element in comparison to the \(8d_{3/2} - 9p_{1/2}\) one as illustrated by the comparison of the lowest-order and the all-order \(5d_{3/2} - 6p_{1/2}\) and \(8d_{3/2} - 9p_{1/2}\) data. The analysis of the \(5d_{5/2}\) polarizability is similar to that of the \(5d_{3/2}\) one. The main contribution to the uncertainty of the scalar polarizability comes from the \(5d_{5/2} - n f_{7/2}\) tail and the uncertainties of the dominant terms are substantially larger than the uncertainties for the other \(Nd\) states for both scalar and tensor polarizabilites owing to large correlation correction of the corresponding transitions.
TABLE IX: Comparison of the Cs tensor polarizabilities with other theory and experiment. All values are given in $10^3 a_0^3$.

| State | $6p_{3/2}$ | $7p_{3/2}$ | $8p_{3/2}$ | $9p_{3/2}$ | $10p_{3/2}$ |
|-------|------------|------------|------------|------------|------------|
| Present | -0.261(13) | -4.41(17)  | -30.6(6)   | -135(2)    | -451(5)    |
| Ref. [31] | -0.223     | -4.28      | -30.2      | -134       | -449       |
| Expt. | -0.2624(15)$^a$ | -4.43(12)$^b$ | -30.7(1.2)$^c$ | -4.33(17)$^d$ | -4.00(8)$^e$ |

| State | $5d_{3/2}$ | $6d_{3/2}$ | $7d_{3/2}$ | $8d_{3/2}$ | $9d_{3/2}$ | $10d_{3/2}$ |
|-------|------------|------------|------------|------------|------------|------------|
| Present | 0.370(28)  | 8.77(36)   | 71.1(1.2)  | 339(4)     | 1189(10)   | 3416(26)   |
| Ref. [31] | 0.380      | 8.62       | 70.4       | 336        | 1190       | 3410       |
| Expt. | 74.5(2.0)$^f$ | 333(16)$^c$ | 1183(35)$^f$ | 3401(4)$^g$ |           |            |

| State | $5d_{5/2}$ | $6d_{5/2}$ | $7d_{5/2}$ | $8d_{5/2}$ | $9d_{5/2}$ | $10d_{5/2}$ |
|-------|------------|------------|------------|------------|------------|------------|
| Present | 0.691(40)  | 17.33(50)  | 142(2)     | 678(5)     | 2386(13)   | 6869(34)   |
| Ref. [31] | 0.703      | 17.00      | 140        | 675        | 2380       | 6850       |
| Expt. | 129(4)$^h$ | 734(4)$^c$ | 2660(140)  | 6815(36)   | 7140(36)$^c$ |           |

V. COMPARISON WITH OTHER THEORY AND EXPERIMENT

Our final results for the scalar and tensor Cs polarizabilities and their uncertainties are compared with other theoretical and experimental values in Tables VIII and IX respectively. As we noted above, the theory values for the $8s$, $7d$, $9d$, and $10d$ polarizabilities from Refs. [22, 35] differ very slightly from the present values since they are obtained using the same values of the matrix elements but more accurate energies. Therefore, we do not quote theory values from Refs. [22, 35] separately in Tables VIII and IX. The experimental values for the $7s$, $6p_{1/2}$, and $6p_{3/2}$ states are obtained by combining the most accurate measurements of the $7s$−$6s$ [14], $6p_{1/2}$−$6s$ [11], and $6p_{3/2}$−$6s$ [10] Stark shifts with the recent measurement of the $6s$ polarizability [3] respectively. We find excellent agreement of our values with high-precision measurements of Refs. [8, 10, 11, 12, 21, 35, 56]. Disagreements with older values for the $Nd$ states are discussed in detail in Ref. [22]. In all cases where the new measurements are available, our data support most precise measurements. In particular, we find that our method works very well for even such highly-excited states as $12s$ and $10d$.

We also compare our values with the van Wijngaarden and Li [31] work where the extensive calculations of the polarizabilities of cesium $Ns$, $Np$, $Nd$, and $Nf$ states were carried out using the Coulomb approximation. Our values are in excellent agreement with those results for higher excited states where the method of Ref. [31] is expected to work well.

VI. CONCLUSION

We have carried out a systematic study of the Cs electric-dipole static polarizabilities for the $Ns$ ($N = 6 − 12$), $Np_j$ ($N = 6 − 10$), and $Nd_j$ ($N = 5 − 10$) states using the relativistic all-order method. The recommended values for the polarizabilities of all these states are given and their uncertainties are estimated. This work involved the calculation of 317 electric-dipole transition in Cs. Recommended values for the 91 transitions that give the dominant contributions to the polarizabilities are presented together with their uncertainties. Our polarizability values are compared with other theory and experiment. Our data are found to be in excellent agreement with the high-precision measurements. These
calculations provide a theoretical benchmark for a large number of Cs electric-dipole matrix elements and polarizabilities.

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