



Static dipole polarizabilities of atoms and ions from $Z = 1$ to 20 calculated within a single theoretical scheme

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Abstract. Static dipole polarizabilities for the first 20 atoms and ions of the Periodic Table are calculated within a single theoretical scheme: the coupled-cluster method with a Hartree–Fock reference wavefunction using an augmented-polarization-consistent and polarization-consistent basis set. The values of the atomic polarizabilities of neutral atoms obtained here agree extremely well with the experimentally measured values. For the ions, all the calculations are consistent with experimental values with the highest resolution so far, except for the monovalent calcium ion, probably due to strong relativistic effects. To the best of our knowledge, this is the first time, applying a single theoretical scheme successfully predicts static polarizabilities of all 20 consecutive elements across 8 columns and more than 3 full periods being consistent with the experimentally measured values both for neutrals and ions. The results clearly signal the universality of this theoretical scheme for the atomic polarizability calculation, and should be easy to extend to other elements with weak relativistic effects.

1 Introduction

The electric dipole polarizability of a system describes the lowest order moment of induced response to an external electric field [1]. As a fundamental quantity, the polarizability is essential for the study of atomic scattering [2], refractive indices [3], ion mobility in gases, van der Waals constants, dielectric constants [4] and investigations of clusters structures [5,6]. It is pressingly needed to acquire their values both experimentally and theoretically in the maximum precision [7]. Over a century, various techniques have been developed to measure electric polarizabilities of atoms, including f-sum rules technique [7–9], dielectric constant measurements [10–13], refractive index [14–17], deflection of an atom beam by electric fields [18–20], the E–H balance method [21–24], and atom interferometry [25–29]. For charged ions, there are not as many methods as neutral atoms to obtain the measurement. Up to now, accurate experimental values of monovalent and bivalent electron systems can be extracted through lifetime measurements [30] and reso-

nant excitation Stark ionization spectroscopy (RESIS) [31,32]. The accurate experimental values of ions for multivalent atom has not been available yet. Despite all this, several empirical and semi-empirical methods have been applied to acquire the polarizabilities of ions in condensed state, including refractive indexes or dielectric constants for ionic crystals [33,34]. However, for free atoms, theoretical calculations are the only option to get the accurate values of multivalence systems.

So far, many theoretical works have been conducted to obtain atomic polarizabilities, the applied theoretical schemes include the configuration interaction (CI) method [35,36], many-body perturbation theory (MBPT) [37,38] and the coupled-cluster (CC) method [39,40], but only a few works have been performed for ions [7]. Moreover, none of these theoretical frameworks have been applied to a large extent of the periodic table [41], which makes it difficult to fairly judge their universality and leaves their systematic errors unknown. This hinders the advance of the theoretical study of atomic polarizability. Self-consistent-field (SCF) methods based on coupled Hartree–Fock (CHF) approximation have been performed on the polarizabilities calculation of sodium, magnesium, noble gases [42–44] as well as some open-shell systems and $(ns)^2$ isoelectronic sequence [45,46]. The calculations on the static dipole polarizabilities of closed 1s, 2p, 3p, 3d,

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4p, 4d, and 5p shells ions also were conducted with the relativistic random-phase approximation, which can be considered as a relativistic version of CHF [47].

Other methods which directly account for electron correlation such as density functional theory (DFT), CC method (CI) and pseudo-potential also have been applied for the calculations. For instance, polarizability calculations of some free ions based on density functional theory with the hybrid potential B3LYP [48], the static dipole polarizabilities of positively charged alkali ions from Li^+ to 119^+ at the fully relativistic coupled-cluster level [49], the static polarizabilities for the ground states of neutral Na and four sodium isoelectronic ions Mg^+ , Al^{2+} , Si^{3+} and P^{4+} using a variation-perturbation method within a CI framework [50], the polarizabilities of the lithium-like systems from $Z=3$ to 50 based on the CI framework with a semi-empirical core potential (CICP) [51] as well as the polarizabilities of Al^+ and Si^{2+} based on CICP theory [52, 53]. From these references, it is noticeable that only a few ion polarizabilities have been calculated at high precision level. Most importantly, they have not been done with the same theoretical frame, which precludes an effective evaluation of theoretic methods against a large spectrum of atom sizes.

Regarding these challenges, in this work the highly accurate CCSD(T) method [54–56] with an augmented polarization consistent basis set—aug-PC-4 [57, 58] and PC-4 were found able to get the static dipole polarizabilities for the atoms H through Ca and ions in a great precision. Thus, this study presents systematic and accurate calculations of polarizabilities of the atoms and ions from $Z=1$ to 20 within a single theoretical framework, judged by its extraordinary performance over a large fraction of the stable elements, this shows the universality of its applicability for atomic polarizability calculations in general.

2 Computational approach

2.1 Finite-field polarizabilities

For a system in the presence of a homogeneous electric field with strength \mathbf{F} , which is weak compared to the inner field in the system, the total energy is given by

$$\begin{aligned} E(F) &= E(0) + \left. \frac{\partial E}{\partial F} \right|_{F=0} F + \frac{1}{2!} \left. \frac{\partial^2 E}{\partial F^2} \right|_{F=0} F^2 \\ &+ \frac{1}{3!} \left. \frac{\partial^3 E}{\partial F^3} \right|_{F=0} F^3 + \frac{1}{4!} \left. \frac{\partial^4 E}{\partial F^4} \right|_{F=0} F^4 + \dots \\ &\equiv E(0) - \mu_0 F - \frac{\alpha}{2} F^2 - \frac{\beta}{6} F^3 - \frac{\gamma}{24} F^4 - \dots \quad (1) \end{aligned}$$

where $E(0)$ denotes the energy without electric field, μ is the permanent dipole moment, α is the dipole polarizability

β is the first hyperpolarizability and γ is the second hyperpolarizability. If the systems are spherically symmetric (e.g., atoms), Eq. (1) can be written as [38, 39, 59]:

$$\begin{aligned} E(F) &= E(0) + \frac{1}{2!} \left. \frac{\partial^2 E}{\partial F^2} \right|_{F=0} F^2 + \frac{1}{4!} \left. \frac{\partial^4 E}{\partial F^4} \right|_{F=0} F^4 + \dots \\ &\equiv E(0) - \frac{1}{2} \alpha F^2 - \frac{1}{24} \gamma F^4 - \dots \quad (2) \end{aligned}$$

The polarizability α depends on the total angular momentum and azimuthal quantum numbers L and M . There is only a single, scalar polarizability α_0 , for S-state ($L = M = 0$) atoms. Mean polarizabilities for P states ($L = 1$) are defined by

$$\bar{\alpha} = (\alpha_{1,-1} + \alpha_{1,0} + \alpha_{1,1})/3 \quad (3)$$

Thus, given the energies of an atom perturbed by different homogeneous fields, the polarizability tensor can be expressed as partial derivatives in the limit of zero field as

$$\alpha_{ij} = - \left(\frac{\partial^2 E(F_i)}{\partial^2 F_i} \right)_{F=0} \quad (i, j = x, y, z) \quad (4)$$

In the finite-field method [38, 60], the polarizability can be calculated by using the following equation [61]:

$$\begin{aligned} \alpha_{ii} &= \frac{1}{12F_i^2} \{30E(0) - 16[E(F_i) + E(-F_i)] \\ &+ [E(2F_i) + E(-2F_i)]\} \quad (5) \end{aligned}$$

2.2 Energy calculations

The calculations of the finite-field energies started at the finite-field Hartree–Fock (HF) level. Then, the high-level CCSD(T) method was employed to include electron correlations with HF reference wavefunctions. Here, it is important to note that eventually all electrons are correlated to ensure the inclusion of inter-shell effects. The total electron correlation energy is defined as the difference between CCSD(T) calculated energy and the one at HF level.

In the calculation, the finite difference method is used to solve each component of polarizability. Theoretically, for the S-state atoms, the three components (α_{xx} , α_{yy} and α_{zz}) of the polarizability are the same, while only two components are the same for the P-state atoms. These properties are used to determine the convergence of the self-consistent process. In our calculations, the converge criteria of SCF energies is set to 10^{-9} Hartree. All calculations of the ionization potential and polarizability were carried out in the Gaussian 09 package [62] using the aug-PC-4 basis set, except Al for which the PC-4 was used.

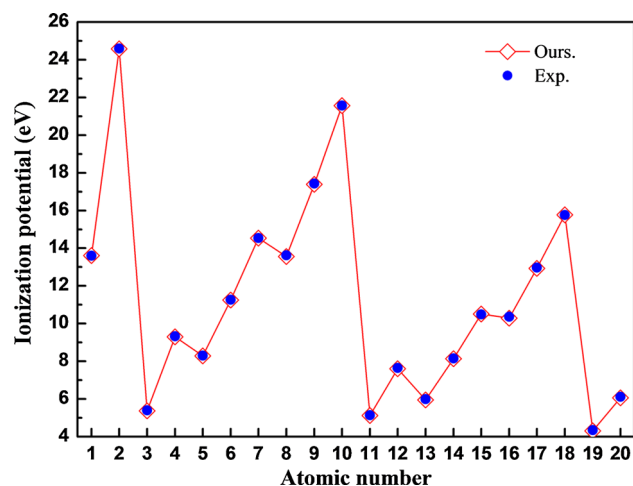


Fig. 1 Comparison of theoretical and experimental ionization potentials. The discrepancies between calculated and experimental values are within the size of the markers

3 Results and discussion

3.1 Test of calculation method

It is well known that the accuracy of calculated dipole polarizabilities is highly sensitive to the selection of the basis set. Therefore, in order to assess the appropriateness of the basis sets, the first ionization potentials of the top 20 atoms were calculated as benchmark using the high-level CCSD(T) method. They are compared with the experimental values, which are listed in Table 1 and plotted in Fig. 1. The deviations range from 0.02% (Ne) to 0.75% (Ca), the excellent agreement with the experimental values indicate the appropriateness of the selected basis set for these atoms.

3.2 Polarizabilities of neutral atoms ($Z \leq 20$)

The HF and CCSD(T) calculated values for the polarizabilities of the atoms H through Ca are listed in Table 2 and plotted in Fig. 2 together with previously calculated and experimental values. Our basis set yields HF values of all the atoms from He through Ca that are quite close to the existing Numerical Hartree–Fock (NHF) values [64] in Table 2, meanwhile our HF values of Li^+ , Be^+ , B^{3+} , B^{2+} , B^+ , C^{4+} , C^{3+} , C^{2+} , N^{5+} , N^{4+} , N^{3+} , O^{6+} , O^{5+} , O^{4+} , F^{7+} , F^{6+} , F^{5+} , Ne^{8+} , Ne^{6+} , Mg^{2+} , Mg^+ , Al^{3+} , Al^{2+} , Al^+ , Si^{4+} , Si^{3+} , Si^{2+} , P^{5+} , P^{4+} , P^{3+} , S^{6+} , S^{5+} , S^{4+} , Cl^{7+} , Cl^{6+} , Cl^- , Ar^{8+} , Ar^{3+} , Ar^{2+} , Ar^+ , K^+ and Ca^{2+} agree well with the reported CHF values [42–47] or Uncoupled Hartree–Fock (UHF) values [104], which again clearly indicate the appropriateness of the basis set selection. Up to now, no experimental values are available for the atoms H, Be, B, C, F, Si, P, S and Cl, while our results closely match previously calculated values [39, 65, 68, 69, 76, 93]. Agreement with the known polarizabilities of He [72, 73], Li [21], Ne [3, 86] and Ar [72, 98] are very good. Also, the values for

N, O, Na, Mg, K and Ca all lie within the experimental error bounds [19, 21, 81, 91, 103].

For the aluminum atom, the calculated polarizability is 56.6 a.u. by using the aug-PC-4 basis set, which lies considerably outside of the experimentally measured value of 46 ± 2 a.u. [19]. This is mainly due to the high sensitivity of the calculations to the selection of d-type functions in the basis set, more detailed analysis can be found in our recent work [105]. Then, accordingly, the PC-4 basis was chosen for the calculations of the Al atom, which yield a value of 47.69 a.u., which perfectly reproduced the experimental value.

Electron correlation effects tend to lower the HF value of metal atoms (Li, Be, Na, Mg, Al, K, Ca), and raise it for nonmetal atoms (H, He, C, N, O, F, Ne, S, Cl, Ar). Electron correlation has rather little effect on the HF value of Li, C, N, P, S, Cl and Ar of about 2.2%, 2.9%, 1.0%, 2.0%, 1.2%, 2.4% and 3.0%, respectively, while it largely influences Be, Na, Mg, K and Ca of about 17.5%, 13.6%, 13.3%, 30.0% and 13.2%, respectively.

3.3 Polarizabilities of ions ($Z \leq 20$)

The polarizabilities of ions are reported in Table 3 with the existing theoretical and experimental values, and the calculated ones are plotted in Fig. 3.

In Table 3, our results of Li^+ , Na^+ , Mg^{2+} , Mg^+ , Al^+ , Si^{3+} , Si^{2+} , K^+ and Ca^{2+} almost exactly match the experimental values [32, 53, 107–111], and previously calculated values [49, 50, 52, 112–114, 125]. There are no measured values for He^+ , Be^+ , B^{2+} , B^+ , C^{3+} , C^{2+} , N^{5+} , N^{4+} , N^{3+} , O^{6+} , O^{5+} , F^{7+} , F^+ , Ne^{8+} , Ne^+ , Al^{2+} , P^{4+} , P^{3+} and S^{4+} , but our calculations agree closely (to within 1%) with the previously calculated values [50, 51, 68, 112, 114–117, 122, 124, 132, 133, 135]. There are no results that come from higher-level methods for O^{4+} , F^{6+} , F^{5+} , Ne^{6+} , S^{5+} and Cl^{6+} , except for existing CHF [42, 46] or UHF [104] method, but our HF values match well with the corresponding CHF or UHF values, which strongly signals the reliability of our CCSD(T) results.

From Table 3, our results of B^{3+} , C^{4+} , Al^{3+} , Si^{4+} , P^{5+} , S^{6+} , Cl^{7+} and Ar^{8+} are close to previously calculated values [44, 47, 48, 126, 133, 134] but have large discrepancies with the corresponding experimental values [118, 119]. This indicates that these theoretical schemes may be limited to the low charge ions only. The previously obtained values of B^{3+} , C^{4+} , Al^{3+} extracted from the measured spectra using the Born–Heisenberg model [118] far overestimated the polarizabilities of ions, while, those of Na^+ , Mg^{2+} , Al^{3+} , Si^{4+} , P^{5+} , S^{6+} , Cl^{7+} and Ar^{8+} based on the semiempirical methods [118, 119] underestimate the values.

Comparing our results of Li^+ , Na^+ , Mg^{2+} to previously calculated values using DFT at B3LYP/6-311++g(3df,3pd) level [48] clearly show that DFT calculations tend to underestimate the polarizabilities of ions, the great match of our results to the experimental ones further imply the reliability of these results for F^- , Al^{3+} , S^{2-} and Cl^- .

Table 1 The first ionization potentials (eV) of the top 20 atoms in the periodic table calculated at CCSD(T)/ aug-PC-4 level (Calc.) and experimentally measured values (Exp.)

	H	He	Li	Be	B	C	N
Calc.	13.606	24.577	5.375	9.301	8.281	11.249	14.538
Exp ^a .	13.598	24.587	5.391	9.322	8.298	11.260	14.534
	O	F	Ne	Na	Mg	Al	Si
Calc.	13.563	17.389	21.570	5.127	7.612	5.953	8.132
Exp ^a .	13.618	17.422	21.565	5.139	7.646	5.985	8.152
	P	S	Cl	Ar	K	Ca	
Calc.	10.504	10.287	12.928	15.774	4.313	6.067	
Exp ^a .	10.487	10.360	12.968	15.760	4.341	6.113	

^a From Ref. [63]**Table 2** Dipole polarizabilities (in atomic units) of the atoms H through Ca. The Hartree–Fock (HF) and CCSD(T) values are compared with Numerical Hartree–Fock (NHF), other higher-level calculations (Calc.) and experimental values (Expt.). ECC are electron correlation terms

Atom	HF	NHF ^a	CCSD(T)	Calc.	ECC	Expt.
H	4.4960		4.4962	4.5 ^b 4.49975 ^c	0.0002	
He	1.3207	1.3222	1.3821	1.38319 ^d 1.38376 ^e	0.0614	1.383746 ± 0.000007 ^f
Li	169.93	170.1	166.18	164.05 ^g 164.11 ^h	− 3.75	164.0 ± 3.4 ⁱ
Be	45.598	45.616	37.632	37.755 ^j 37.69 ^k	− 7.966	
B	22.184	22.020	20.304	20.47 ^l 20.59 ^m 20.43 ± 0.11 ⁿ	− 1.880	
C	11.966	12.033	11.638	11.39 ^o 11.67 ± 0.07 ⁿ	0.328	
N	7.173	7.358	7.246	7.43 ^l 7.26 ± 0.05 ⁿ 7.41 ^p	0.073	7.6 ± 0.4 ^q
O	4.78	4.73	5.21	5.4 ^o 5.24 ± 0.04 ⁿ	0.43	5.2 ± 0.4 ^r
F	3.30	3.284	3.68	3.76 ^l 3.70 ± 0.03 ⁿ	0.38	
Ne	2.376	2.377	2.662	2.666 ^s 2.663 ^t	0.286	2.663 ^u 2.66110 ± 0.00003 ^v
Na	189.877	190.50	164.104	162.6 ± 0.3 ^w 162.88 ± 0.60 ^x	− 25.773	162.7 ± 0.5 ^y 161 ± 7.5 ^z
Mg	81.65	81.594	70.76	71.7 ^{aa} 71.4 ^{bb} 70.90 ^{cc}	− 10.89	59 ± 16 ^z 75.0 ± 3.5 ^{dd}
Al	60.22	62.05	47.69	56.27 ^{ee} 55.5 ^m 57.74 ^{ff}	− 12.53	46 ± 2 ^{gg}
Si	38.240	38.81	36.896	36.32 ^{ee} 37.17 ± 0.21 ^{ff} 37.4 ^{hh}	− 1.344	
P	25.462	25.469	24.946	24.7 ± 0.5 ^{ee} 24.93 ± 0.15 ^{ff} 24.9 ^p	− 0.516	
S	19.162	19.131	19.38	19.60 ^{ee} 19.37 ± 0.12 ^{ff}	0.22	
Cl	14.246	14.238	14.593	14.71 ^{ee} 14.57 ± 0.10 ^{ff} 14.73 ⁱⁱ	0.347	
Ar	10.762	10.758	11.084	11.10 ^{ee} 11.085 ± 0.060 ^{jj}	0.322	11.083 ± 0.002 ^{kk} 11.070 ± 0.007 ^{ll}
K	421.65	417.8	295.34	290.2 ^{mmm} 291.1 ± 1.5 ⁿⁿ	− 126.31	292.9 ± 6.1 ⁱ 290.6 ± 1.4 ^z
Ca	183.88	185.44	159.60	176.6 ^{ee} 160 ^{oo} 160.77 ^{pp}	− 24.28	169 ± 17 ^{qq}

^aFrom Ref. [64]. ^bFrom Ref. [65–67]. ^cFrom Ref. [65,68,69]. ^dFrom Ref. [67,70].^eFrom Ref. [71]. ^fFrom Ref. [72,73]. ^gFrom Ref. [74,75]. ^hFrom Ref. [67]ⁱFrom Ref. [21]. ^jFrom Ref. [74]. ^kFrom Ref. [76]. ^lFrom Ref. [77].^mFrom Ref. [78]. ⁿFrom Ref. [39]. ^oFrom Ref. [79]. ^pFrom Ref. [80].^qFrom Ref. [22,81]. ^rFrom Ref. [81]. ^sFrom Ref. [82–84]. ^tFrom Ref. [85].^uFrom Ref. [3]. ^vFrom Ref. [86]. ^wFrom Ref. [87]. ^xFrom Ref. [88].^yFrom Ref. [25]. ^zFrom Ref. [19]. ^{aa}From Ref. [38]. ^{bb}From Ref. [89].^{cc}From Ref. [90]. ^{dd}From Ref. [91]. ^{ee}From Ref. [92]. ^{ff}From Ref. [93].^{gg}From Ref. [19,94]. ^{hh}From Ref. [95]. ⁱⁱFrom Ref. [96]. ^{jj}From Ref. [93,97].^{kk}From Ref. [72]. ^{ll}From Ref. [98]. ^{mmm}From Ref. [99]. ⁿⁿFrom Ref. [100].^{oo}From Ref. [101]. ^{pp}From Ref. [102]. ^{qq}From Ref. [103]

Table 3 Comparison of calculated and experimental (Expt.) polarizabilities of free ions. HF and Ours. represent our calculated results by using Hartree-Fock method and coupled-cluster method, respectively. CHF, UHF and Calc. are previous results by using coupled Hartree-Fock, uncoupled Hartree-Fock, and other higher-level calculations (Calc.), respectively. ECC are electron correlation terms. The uncertainties in the last digits are given in parentheses

	He ⁺	Li ⁺	Be ²⁺	Be ⁺	B ³⁺	B ²⁺	B ⁺
HF	0.2811	0.1863	0.0478	24.9036	0.0195	7.9445	11.3802
Ours.	0.2811	0.1931	0.0488	24.7039	0.0197	7.8818	9.6601
ECC	0.0000	0.0068	0.0010	- 0.1997	0.0002	- 0.0627	- 1.7201
CHF		0.1895 ^a 0.1894 ^c	0.05186 ^a 0.05182 ^c		0.01955 ^a 0.01953 ^c		11.38 ^b
UHF ^d		0.1851	0.05123	24.82	0.01941	7.972	11.6
Calc.	0.28119 ^e	0.15 ^f 0.1924 ⁱ	0.0523 ^g 0.05227 ^l	24.48 ^h 24.495 ^j	0.0197 ^k 0.0196 ^l	7.847 ^h 7.81 ^m	9.6501 ^k 9.67 ⁿ
Expt.		0.1930 ^o	0.0472 ^p		0.0223 ^p		
	C ⁴⁺	C ³⁺	C ²⁺	C ⁺	N ⁵⁺	N ⁴⁺	N ³⁺
HF	0.00893	3.4897	4.5085	6.3124	0.00464	1.8328	2.2372
Ours.	0.00891	3.4706	3.8452	5.7714	0.00463	1.8254	1.9108
ECC	- 0.00002	- 0.0191	- 0.6633	- 0.5410	- 0.00001	0.0074	- 0.3264
CHF	0.008935 ^a 0.008919 ^c		4.508 ^b	6.033 ^u	0.004645 ^a 0.004633 ^c		2.237 ^b
UHF ^d	0.00891	3.504	4.41		0.004628	1.839	2.12 1.8895 ^r
Calc.	0.00896 ⁱ 0.00895 ⁱ	3.456 ^h 3.44 ^m	3.846 ⁿ	5.6079 ^k 5.651 ⁿ	0.0046555 ^g 0.004655 ^l	1.802 ^q	
Expt.	0.0101 ^p						
	N ²⁻	N ³⁻	O ⁶⁺	O ⁵⁺	O ⁴⁺	O ³⁺	O ²⁻
HF	388.93	625.962	268.6	1.07925	1.2709	18.727	
Ours.	78.59	233.100	975.6	1.07601	1.0836	27.575	
ECC	- 310.34	- 392.862	702.0	- 0.00324	- 0.1873	8.848	
CHF				0.002648 ^a 0.002639 ^c	1.271 ^b		
UHF ^d				0.002641	1.18		
Calc.				0.002645 ⁱ 0.002653 ^s			35.66 ⁿ 17.40 ^t
Expt.				1.082			
				1.0595 ^q			

Table 3 continued

	O^{2-}	F^{7+}	F^{6+}	F^{5+}	F^{4+}	F^{-}	Ne^{8+}
HF	83.7	0.001618	0.68826	0.7907	1.72	10.1078	0.001043
Ours.	122.6	0.001616	0.68655	0.6748	1.77	14.5334	0.001042
ECC	38.9	-0.000002	-0.00171	-0.1159	0.05	4.4256	-0.000001
CHF		0.001618 ^v		0.7907 ^w		10.66 ^v	0.001044 ^v
							0.001038 ^x
UHF ^y		0.001611 ^x					
Calc.		0.001615	0.6898	0.719	1.771 ^{bb}	12.1 ^z	0.001042
		0.001619 ^{aa}			1.72 ^{dd}	16.38 ^{bb}	0.001045 ^{ee}
Expt.							
	Ne^{6+}	Ne^{3+}	Ne^{2+}	Ne^{+}	Na^{+}	Mg^{2+}	Mg^{+}
HF	0.5251	0.71444	0.8305	1.2417	0.9285	0.4585	38.8002
Ours.	0.4500	0.68325	0.8373	1.3110	1.0054	0.4814	35.4595
ECC	-0.0751	-0.03119	0.0068	0.0693	0.0769	0.0229	-3.3407
CHF	0.5251 ^w				0.9454 ^v	0.4701 ^v	38.897 ^{ff}
					0.9457 ^x	0.4698 ^x	
UHF ^y	0.471		0.82 ^{dd}	1.33 ^{dd}	0.98 ^z	0.45 ^z	35.66 ^{hh}
Calc.				1.306 ^{gg}	1.00(4) ^{cc}	0.4814 ^{jj}	35.05 ^{mm}
						0.489 ^{ll}	
Expt.					1.0015(15) ⁿⁿ	0.486(7) ^{oo}	35.04(3) ^{mm}
					0.998 ^{ss}	0.469 ^{ss}	34.62(26) ^{pp}
							35.00(5) ^{uu}
	Al^{3+}	Al^{2+}	Al^{+}	Si^{4+}	Si^{3+}	Si^{2+}	Si^{+}
HF	0.2631	15.4464	26.461	0.1605	7.943	12.6007	19.5286
Ours.	0.2719	14.4291	24.317	0.1644	7.532	11.7955	18.4832
ECC	0.0088	-1.0173	-2.144	0.0039	-0.411	-0.8052	-1.0454
CHF	0.2652 ^v	15.4509 ^{ff}	26.44 ^v	0.1627 ^v	7.931 ^{ff}	12.59 ^{ff}	
	0.2649 ^x		26.38 ^{vv}	0.1624 ^x		12.57 ^{vv}	
Calc.	0.26 ^z	14.44 ^{hh}	24.14(12) ⁱⁱ	0.1626 ^{tt}	7.50 ^{hh}	11.688 ^{xx}	
					7.419 ^{mm}	11.75 ^{kk}	
			24.1 ^{kk}				
Expt.	3.577 ^{rr}		24.3 ^{qq}	0.15 ^{xx}	7.433(25) ^{mm}	11.669(9) ^{xx}	
	0.253 ^{ss}		24.20(75) ^{ww}		7.426(12) ^{yy}	11.666(4) ^{zz}	

Table 3 continued

	P⁵⁺	P⁴⁺	P³⁺	P⁻	P²⁻	P³⁻	S⁶⁺
HF	0.1045	4.6951	7.1667	86.585	265.43	402.77	0.07121
Ours.	0.1064	4.4924	6.7703	95.179	337.99	500.60	0.07110
ECC	0.0019	-0.2027	-0.3964	8.594	72.56	97.83	-0.00011
CHF	0.1060 ^{ccc}	0.1057 ^{eee}	7.155 ^{bbb}	7.164 ^{ddd}			0.07235 ^{ccc}
Calc.		4.51 ^{ggg}	6.73 ^{hhh}				0.07205 ^{eee}
Expt.	0.0948 ⁱⁱⁱ						0.0631 ⁱⁱⁱ
	S⁵⁺	S⁴⁺	S⁻	S²⁻	Cl⁷⁺	Cl⁶⁺	Cl⁻
HF	3.0299	4.5235	48.01	151.53	0.0504	2.0789	30.477
Ours.	2.9178	4.2969	55.09	206.03	0.0509	2.0115	34.449
ECC	-0.1121	-0.2266	7.08	54.50	0.0005	-0.0674	3.972
CHF	3.0300 ^{aaa}	4.522 ^{ddd}			0.0512 ^{ccc}	2.0785 ^{aaa}	31.55 ^{ccc}
Calc.		4.26 ^{hhh}	47.84 ^{jjj}	127 ^{fff}			33.7 ^{fff}
Expt.					0.0438 ⁱⁱⁱ		
	Ar⁸⁺	Ar³⁺	Ar²⁺	Ar⁺	K⁺	Ca²⁺	Ca⁺
HF	0.03674	3.713	4.806	6.807	5.455	3.258	98.00
Ours.	0.03706	3.549	4.747	6.834	5.586	3.283	77.47
ECC	0.00032	-0.164	-0.059	0.027	0.131	0.025	-20.53
CHF	0.03732 ^{ccc}	3.60 ^{rrr}	4.78 ^{rrr}	6.84 ^{rrr}	5.461 ^{ccc}	3.261 ^{ccc}	3.254 ^{eee}
Calc.			4.69 ^{jjj}	6.85 ^{jjj}	5.53 ^{fff}	3.28 ^{fff}	76.1(1.1) ^{mmm}
Expt.	0.0313 ⁱⁱⁱ			7.2(3) ^{qqq}	5.47 ^{ooo}	3.12 ^{ooo}	74.11 ⁿⁿⁿ

^a Ref. [44]. ^b Ref. [46]. ^c Ref. [47]. ^d Ref. [104]. ^e Ref. [68]. ^f Ref. [48].
^g Ref. [133]. ^h Ref. [51]. ⁱ Ref. [112]. ^j Ref. [115]. ^k Ref. [116]. ^l Ref. [134].
^m Ref. [120]. ⁿ Ref. [132]. ^o Ref. [107]. ^p Ref. [118]. ^q Ref. [122]. ^r Ref. [117].
^s Ref. [123, 134]. ^t Ref. [96]. ^u Ref. [121].
^v Ref. [44]. ^w Ref. [46]. ^x Ref. [47]. ^y Ref. [104]. ^z Ref. [48]. ^{aa} Ref. [124].
^{bb} Ref. [132]. ^{cc} Ref. [49]. ^{dd} Ref. [96]. ^{ee} Ref. [112, 133]. ^{ff} Ref. [42]. ^{gg} Ref. [135].
^{hh} Ref. [50]. ⁱⁱ Ref. [52]. ^{jj} Ref. [113]. ^{kk} Ref. [114]. ^{ll} Ref. [125]. ^{mm} Ref. [32].
ⁿⁿ Ref. [108]. ^{oo} Ref. [109]. ^{pp} Ref. [30]. ^{qq} Ref. [110]. ^{rr} Ref. [118]. ^{ss} Ref. [119, 137]. ^{tt} Ref. [126]. ^{uu} Ref. [37]. ^{vv} Ref. [43]. ^{ww} Ref. [128]. ^{xx} Ref. [53]. ^{yy} Ref. [127].
^{zz} Ref. [129].
^{aaa} Ref. [42]. ^{bbb} Ref. [43]. ^{ccc} Ref. [44]. ^{ddd} Ref. [46]. ^{eee} Ref. [47]. ^{fff} Ref. [48].
^{ggg} Ref. [49]. ^{hhh} Ref. [114]. ⁱⁱⁱ Ref. [119, 137]. ^{jjj} Ref. [96]. ^{kkk} Ref. [136]. ^{lll} Ref. [125].
^{mmm} Ref. [130]. ⁿⁿⁿ Ref. [30]. ^{ooo} Ref. [110]. ^{ppp} Ref. [111]. ^{qqq} Ref. [131]. ^{rrr} Ref. [45]

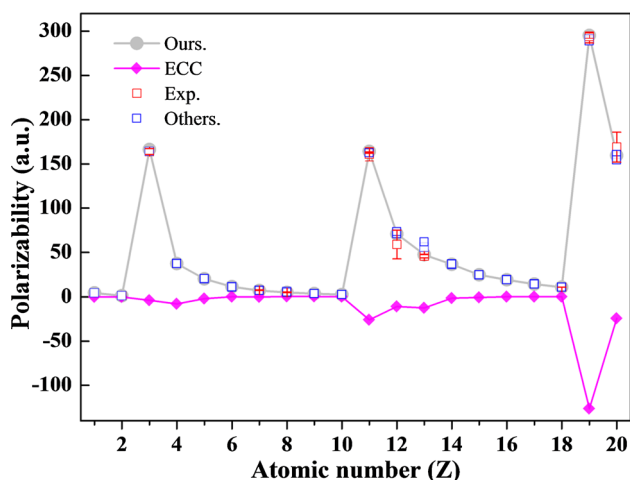


Fig. 2 Comparison of the results of previous higher-level calculations (open blue squares), measured values (open red squares), and calculated values in this work (gray filled circles). The magenta filled diamonds are the electron correlation terms

Based on the performance of aug-PC-4 on Be, Be⁺, C⁴⁺, C³⁺, C²⁺, C, Ar⁸⁺, Ar²⁺, Ar⁺ and Ar, it is reasonable to trust results of Be²⁺, C⁺ and Ar³⁺ based on HF even though they have a large discrepancies (8.4%, 4.8% and 3.0%) with previously calculated polarizabilities by using CHF and UHF.

For O⁻, Ne²⁺, S⁻ and Ar²⁺, our CCSD(T) values are larger than the previous calculated ones at complete-active-space perturbation-theory (CASPT) levels [96]. However, to case of Ne²⁺ and Ar²⁺ CASPT yields similar value with CCSD(T) due to the underestimation of ECC, which indicates the better performance of CCSD(T)

Although there are no calculated and experimental values for N⁻, N²⁻, O²⁻, Ne³⁺, Si⁺, P⁻, P²⁻, it is reasonable to trust the reliability of those numbers based on the performance of the method on N^{5+,4+,3+,0}, O^{6+,5+,4+,0}, Ne^{8+,0}, Si^{4+,3+,2+,0}, P^{5+,4+,3+,0} ions.

For Ca⁺ with a single 4s electron, our result (77.4711 a.u.) agrees well with the nonrelativistic value (77.71 a.u.) calculated by Ivan S. Limand *et al.*, but it is larger than the relativistic value of 75.88 a.u. [136] and 74.11 a.u. [30]. The overestimation is due to ignoring the 4s valence shell relativistic contraction which lowers the polarizability. The same consideration of relativistic effects have been applied to the calculation of positively charged alkali ions from Li⁺ to 119⁺ [49].

The influence of electron correlation effects varies with specific atoms. It is noticeable from our HF and CCSD(T) results that electron correlation is strong in B⁺, C²⁺, N³⁺, N⁻, N²⁻, N³⁻, O⁴⁺, O⁻, O²⁻, F⁵⁺, F⁻, Ne⁶⁺, P²⁻, P³⁻, S⁻, S²⁻, Cl⁻ and Ca⁺, which changes of about -15.11%, -14.71%, -14.59%, -79.79%, -62.76%, 261.36%, -14.74%, 47.25%, 46.48%, -14.66%, 43.78%, -14.30%, 27.34%, 24.29%, 14.75%, 35.97% and -20.95%, respectively, meanwhile, it has rather diminished influence (within about 1%)

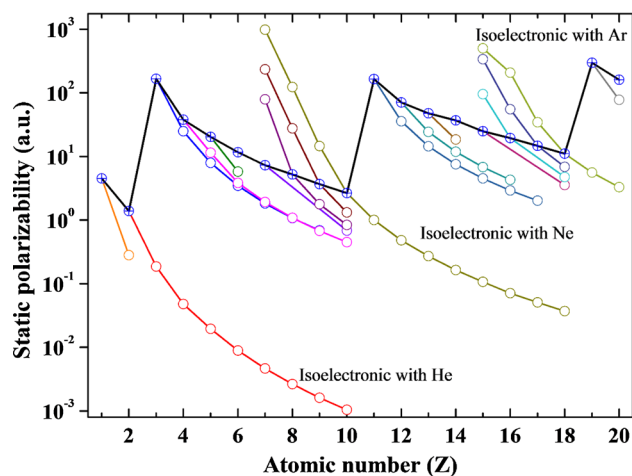


Fig. 3 Semi-logarithm plot of calculated static polarizabilities of neutral atoms (filled circles, black line) and ions (open circles). The colored lines join isoelectronic species

on He⁺, B³⁺, C⁴⁺, C³⁺, N⁵⁺, N⁴⁺, O⁶⁺, O⁵⁺, F⁷⁺, F⁶⁺, Ne⁸⁺, Ne²⁺, S⁶⁺, Cl⁷⁺, Ar²⁺, Ar⁺ and Ca²⁺ at HF level, which explains why the previously calculated CHF or UHF values of corresponding ions match well with our HF and CCSD(T) values.

All the calculated values in this work are plotted together in Fig. 3. It is noticeable that the trends resemble a self-similar fractal-like structure.

3.4 Uncertainty estimates

To estimate the uncertainties of the present results, some important sources have been identified. The sources of errors are mainly from three aspects, the neglect of relativistic effects, higher-order excitations when using CCSD(T) theory, and the incompleteness of the basis set.

Considering the results from Ref. [75, 84, 136], the relativistic effect on the polarizability of H, Li, Ne, Na, Ar and Ca atoms are 0.0056%, 0.0344%, 0.148%, 0.60%, 0.178% and 1.244%, respectively. So, in this work we take 0.034%, 0.148%, 0.60% and 1.244% as the upper bound on the uncertainty caused by relativistic effects for the first, second, third and fourth period atoms, respectively.

In order to estimate the influence of higher order excitations in CC theory on the polarizability, the contribution from triple excitation is used as the upper bound on the uncertainty. According to the previous calculations [75, 84, 136], for Li, Ne, Na, Ar and Ca atoms, the polarizability calculated using CCSD(T) method can produce 1.12% correction compare to using CCSD method on average. Therefore, 1.12% is a rational upper bound on the uncertainty associated the neglect of higher order excitations.

Considering the case of Ar atom which has accurate experimental values 11.083 ± 0.002 a.u. [72], the up-bound given by aforementioned source of error is

0.1906, which apparently guarantee the reliability of this method. Therefore, it is reasonable to only include the above two error estimates and ignore the error of incomplete basis set. Combining all these sources, the uncertainty of our results for the first, second, third and fourth period atoms to be below 1.15%, 1.27%, 1.72% and 2.36%, respectively.

4 Conclusion

To summarize, the static dipole polarizability of atoms and ions from H to Ca using HF and CCSD(T) methods have been calculated with a large basis set. Our CCSD(T)/aug-PC-4 scheme performs extremely well on computing the mean dipole polarizabilities of corresponding atoms and ions. The only discrepancy observed in the case of the singly ionized calcium is probably due to the strong relativistic effects. In the case of Al, the best results were obtained with the PC-4 basis instead of the aug-PC-4. More importantly, this signals that the calculation of polarizability could be used as a probe to assess the appropriateness of a basis set for a particular atom and further can be reliably used for the calculation of systems composed by those atoms. The successful application of this single theoretical scheme over the first 20 elements of the periodic table points to its universality and suggests it could be safely extended to other elements including neutral, anions and cations. The success of a single consistent theoretical framework in the calculation of atomic polarizability is a triumph of the advent of the modern quantum methods.

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