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Electric dipole polarizabilities at imaginary frequencies for hydrogen, the alkali–metal, alkaline–earth, and noble gas atoms

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ABSTRACT

The electric dipole polarizabilities evaluated at imaginary frequencies for hydrogen, the alkali–metal atoms, the alkaline–earth atoms, and the noble gases are tabulated along with the resulting values of the atomic static polarizabilities, the atom–surface interaction constants, and the dispersion (or van der Waals) constants for the homonuclear and the heteronuclear diatomic combinations of the atoms.

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Contents

1. Introduction

Dynamic electric dipole polarizability functions describe the response of atoms to applied oscillating and fluctuating electric fields and consequently they are necessary ingredients for many applications [1,2]. When evaluated as functions of imaginary frequencies they can be used for straightforward calculations of long-range interactions such as the dispersion (or van der Waals) and retarded (or Casimir–Polder) potentials between two atoms, the potential between an atom and a surface [3,4] or of an atom between two surfaces [5,6], and the dispersion (or Axilrod–Teller) potential between three atoms [7–9]. Other applications include evaluation of the Lifshitz formula for the free energy of macroscopic media at zero and non-zero temperature [10] and quantum reflection studies [11]. Numerical values of dynamic polarizabilities are useful tests for computations of atomic structure using wavefunction based methods [12] or density functional theory methods [13–15].

We have carried out a program of calculating the dynamic electric dipole polarizabilities of the alkali–metal atoms and of the alkaline–earth atoms for use in determining long-range dispersion coefficients [12,16–18] for photoassociation and ultra-cold atom scattering studies. For those papers it was not necessary to list the values of the polarizabilities as functions of imaginary frequencies. Since they are useful in a range of contexts, we present herein a set of values in readily usable form for these atoms as well as for hydrogen and the noble gases. For completeness, we also tabulate the corresponding static polarizabilities [19,20], dispersion coefficients, and atom–surface interaction coefficients.

2. The atomic dynamic electric dipole polarizability

The atomic dynamic electric dipole polarizability is given by the expression

$$\alpha(u) = \mathrm{S}'_n \frac{f_n}{\omega_n^2 - u^2}, \tag{1}$$

where f_n are the absorption oscillator strengths, ω_n the excitation energies, u the frequency of the applied electric field, and S′ a combined summation over final discrete states and integration over final continuum states excluding the initial state. The function $\alpha(i\omega)$ is defined by the replacement of u by $i\omega$ in Eq. (1) [7,21,8] and it can be constructed from calculated bound and continuum properties, or variationally, or obtained from fits to combinations of theoretical and empirical data. The function $\alpha(i\omega)$ is real and smooth. The static polarizability $\alpha(0)$ is the value of $\alpha(i\omega)$ at $\omega = 0$ and non-relativistically the oscillator strength sum rule dictates that $\alpha(i\omega) \sim N_e/\omega^2$ as $\omega \sim \infty$, where N_e is the number of electrons in the atom.

The dispersion (or van der Waals) constant $C_6(AB)$ enters in the interaction potential $-C_6(AB)/R^6$ between two ground state atoms A and B at large internuclear distances R; see, for example, Ref. [8]. The constant $C_6(AB)$ can be expressed as

$$C_6(AB) = \frac{3}{\pi}\int_0^\infty d\omega \alpha^A(i\omega)\alpha^B(i\omega), \tag{2}$$

where $\alpha^A(i\omega)$ and $\alpha^B(i\omega)$, respectively, correspond to atom A and atom B.

The potential between an atom and a perfectly conducting metal surface is given in terms of the normal distance z between the atom and the wall as $-C_3/z^3$, where the atom–surface interaction coefficient is

$$C_3 = \frac{1}{4\pi}\int_0^\infty d\omega \alpha(i\omega). \tag{3}$$

Integration of Eq. (3) for C_3 yields an alternate form in terms of the ground state atomic wavefunction $|0\rangle$,

$$C_3 = \frac{1}{12}\left\langle 0\left|\left(\sum_{i=1}^{N_e}\mathbf{r}_i\right)^2\right|0\right\rangle, \tag{4}$$

where $\mathbf{r}_i$ is the position vector of electron i from the nucleus.

3. Sources of polarizability data

3.1. Hydrogen and the alkali metals

The dynamic polarizability for hydrogen is known analytically, cf. [22]. It is also available in parameterized forms using pseudo-dipole oscillator strength distributions (or "pseudo-DOSDs") [23] as well as in tabulations at various imaginary frequencies [24]. For the present work, it was calculated to sufficient accuracy using direct summation over a relativistic B-spline basis for the Coulomb field.

For alkali–metal atoms we employ dynamic polarizabilities calculated previously in Refs. [12,16,25]. In these works, dynamic polarizabilities were obtained by combining high-precision experimental data for matrix elements of principal transitions with several many-body methods of various accuracy. In particular, the relativistic linearized coupled-cluster method limited to single and double (SD) excitations from the reference state was used for calculation of oscillator strengths for the first several excited states. The results for SD matrix elements were presented in Ref. [26]. The relativistic random-phase approximation (RRPA) was employed for calculation of the contributions to the polarizabilities from core excitations, and, finally, the Dirac–Hartree–Fock (DHF) method was used to obtain less significant contributions.

The resulting static polarizabilities and dynamic polarizabilities at imaginary frequencies for hydrogen and the alkali–metal atoms are given in Table 1.

3.2. Alkaline–earth metals

To calculate the dynamic polarizabilities for alkaline–earth metal dimers, we employed several atomic relativistic many-body methods of varying accuracy [17,18]. The intermediate states in the sum appearing in Eq. (1) were formally separated into valence and core-excited states giving

$$\alpha(i\omega) = \alpha_v(i\omega) + \alpha_c(i\omega) + \alpha_{cv}(i\omega). \quad (5)$$

The valence contribution α_v, which gives the dominant contribution to C_6, was evaluated with the relativistic configuration interaction (CI) method coupled with many-body perturbation theory [27,28]. The smaller contributions of core-excited states α_c were estimated using RRPA for the atomic core. In this method excitations of core electrons are allowed into the occupied valence shell and we introduced the correction α_{cv} to remove these Pauli-exclusion-principle-violating excitations; this small correction was evaluated using the DHF method. The values of polarizabilities were further adjusted using accurate theoretical and experimental data for the electric dipole matrix elements and the energies of the principal transitions (see Refs. [17,18] for details). The resulting static polarizabilities and dynamic polarizabilities at imaginary frequencies for the alkaline–earth atoms are given in Table 2.

3.3. Noble gases

Dynamic polarizability data for the helium atom were obtained in the present work using an essentially exact relativistic CI method.

For the dynamic polarizabilities of Ne, Ar, Kr, and Xe, we used the semi-empirical dipole oscillator strength distributions constructed by Kumar and Meath [29] using constraints such as oscillator strength sum rules applied to certain available experimental data. The values in Table 3 constitute a different representation of the data presented by Kumar and Meath [29].

The resulting polarizabilities for the noble gases atoms are given in Table 3.

4. The tabulated data

The values of the static polarizability $\alpha(0)$ are given in the first line of Tables 1–3. Comparisons of values of $\alpha(0)$ from various sources for various atoms can be found in the literature (cf. [19,20]).

A typical application of dynamic polarizabilities involves integration of a product of $\alpha(i\omega)$ with a smoothly behaving function $f(\omega)$, $I = \int_0^\infty f(\omega)\alpha(i\omega)\,d\omega$. The integration over frequencies ranges from zero to infinite values. An economic and accurate method for evaluating such integrals is the method of Gaussian quadratures [24]. In this method the above integration is replaced by a finite sum $I = \sum_{k=1}^{N_g} w_k f(\omega_k)\alpha(i\omega_k)$ over values of $f(\omega_k)\alpha(i\omega_k)$ tabulated at certain frequencies ω_k yielding an N_g-point quadrature, where each term in the sum is weighted by factors w_k. In this work we use points and weights listed in Table A and $N_g = 50$.

Table A
Gaussian quadrature abscissas ω_k and weights w_k for a 50-pair integration, with $k = 1, \ldots, 50$.

k	ω_k	w_k	k	ω_k	w_k
1	0.00178065	0.00456886	26	2.10016	0.205361
2	0.00937463	0.0106185	27	2.31644	0.227799
3	0.0230068	0.0166378	28	2.55713	0.254343
4	0.042631	0.0225996	29	2.82683	0.286005
5	0.0681817	0.0284889	30	3.13128	0.324106
6	0.0995817	0.0342971	31	3.47776	0.370381
7	0.136748	0.0400227	32	3.87553	0.427154
8	0.179602	0.0456718	33	4.3366	0.497572
9	0.228071	0.0512592	34	4.87665	0.585976
10	0.282107	0.0568084	35	5.51655	0.698465
11	0.341686	0.0623519	36	6.28448	0.843785
12	0.406823	0.0679318	37	7.21927	1.03477
13	0.477579	0.0735998	38	8.37558	1.29076
14	0.554072	0.0794176	39	9.83228	1.64181
15	0.636488	0.085458	40	11.7066	2.13626
16	0.725091	0.0918056	41	14.179	2.85525
17	0.820235	0.0985589	42	17.5384	3.94176
18	0.922382	0.105832	43	22.2715	5.66354
19	1.03212	0.113758	44	29.2508	8.56095
20	1.15017	0.122493	45	40.168	13.8343
21	1.27743	0.132222	46	58.6667	24.5132
22	1.41501	0.143164	47	93.8285	49.7405
23	1.56425	0.155587	48	173.862	125.732
24	1.72679	0.169813	49	426.684	483.298
25	1.90461	0.18624	50	2246.37	5763.83

4.1. Applications to atom-atom dispersion coefficients

The dispersion coefficients are computed by evaluating Eq. (2) using the Gaussian quadrature method yielding

$$C_6(AB) = \frac{3}{\pi}\sum_{k=1}^{50} w_k \alpha^A(i\omega_k)\alpha^B(i\omega_k). \quad (6)$$

For comparisons listing various previous determinations of the van der Waals coefficients, see the work of Maeder and Kutzelnigg [30], and our previous papers [12,17]. The resulting coefficients for various pairs of alkali–metal, alkaline–earth, and noble gas atoms are listed in Tables B–G.

For the alkali–metals, the accuracy of calculation of the C_6 dispersion coefficients using Eq. (6) and presented in Table B was estimated using (i) experimental error bars for principal transitions and (ii) by comparison of the atom–wall interaction constant C_3 obtained as an integral of the dynamic polarizability, Eq. (3), with the SD *ab initio* calculation of Eq. (4) [31]. The estimated accuracy for the C_6 coefficients was at the level of 0.1% for Li, with less accurate results for heavier systems, reaching 1% for Cs and 1.5% for Fr.

Table B
Dispersion coefficients C_6 for alkali–metal atom pairs in atomic units.

	H	Li	Na	K	Rb	Cs	Fr
H	6.498	66.36(5)	73.83(9)	111.2(2)	124.3(3)	149.7(8)	142.3(1.2)
Li		1389(2)	1467(2)	2322(5)	2545(7)	3065(17)	2682(23)
Na			1556(4)	2447(6)	2683(7)	3227(18)	2842(24)
K				3897(15)	4274(13)	5159(30)	4500(39)
Rb					4690(23)	5663(34)	4946(44)
Cs						6846(74)	5968(60)
Fr							5256(89)

Table C
Dispersion coefficients C_6 and their estimated uncertainties (in parentheses) for alkaline–earth metal atom pairs in atomic units.

	Be	Mg	Ca	Sr	Ba
Be	214(3)	364(4)	652(7)	782(6)	992(9)
Mg		627(12)	1138(14)	1369(13)	1742(21)
Ca			2121(35)	2564(21)	3294(36)
Sr				3103(7)	3994(29)
Ba					5160(74)

Table D
Dispersion coefficients C_6 and their estimated uncertainties (in parentheses) for noble gas atom pairs in atomic units.

	He	Ne	Ar	Kr	Xe
He	1.461	3.03(2)	9.55(5)	13.42(7)	19.6(1)
Ne		6.38(6)	19.5(1)	27.3(2)	39.7(3)
Ar			64.3(6)	91.1(6)	134.5(9)
Kr				130(1)	192(2)
Xe					286(3)

Table E
Dispersion coefficients C_6 and their estimated uncertainties (in parentheses) for alkali–metal – alkaline–earth metal atom pairs in atomic units.

	Be	Mg	Ca	Sr	Ba
H	34.8(2)	57.4(6)	98.3(8)	117.5(1)	148(1)
Li	478(3)	853(8)	1660(14)	2022(3)	2637(19)
Na	521(4)	926(9)	1782(15)	2167(4)	2815(21)
K	790(6)	1411(14)	2756(23)	3362(8)	4396(33)
Rb	873(7)	1556(15)	3030(26)	3697(10)	4832(37)
Cs	1045(9)	1863(20)	3635(36)	4437(24)	5809(52)
Fr	963(11)	1701(22)	3265(39)	3974(34)	5170(57)

Table F
Dispersion coefficients C_6 and their estimated uncertainties (in parentheses) for alkaline–earth – noble gas pairs in atomic units.

	He	Ne	Ar	Kr	Xe
Be	13.23(9)	26.0(2)	97.9(8)	143(1)	221(2)
Mg	21.3(2)	41.9(5)	159(2)	234(3)	363(4)
Ca	35.7(3)	70.2(7)	268(3)	396(4)	617(6)
Sr	42.84(5)	84.2(4)	321(2)	474(2)	739(4)
Ba	53.7(4)	105.7(9)	403(4)	594(5)	927(8)

Agreement with subsequently determined experimental values for C_6 coefficients was excellent. For example, for Cs, the predicted value was found to be in an excellent agreement with the results from Feshbach resonance spectroscopy with ultracold atoms [16]. Similarly, in atomic units, our value 399.8 for the static polarizability of Cs listed in Table 1 is in 0.3% agreement with the experimental value [32] of 401.0(6).

For the alkaline–earth metals, in Table C, we present C_6 coefficients for homonuclear and heteronuclear dimers. The estimates of the uncertainties in these coefficients was discussed in detail in Ref. [18].

For the noble gases, in Table D, we have indicated uncertainties of 1% for the tabulated values of C_6, as suggested by Kumar and Meath [29]. The analysis of the latest experimental data for noble gases by Bulanin and Kislyakov [33] is in excellent agreement with the results of Ref. [29] for values of the dynamic polarizability $\alpha(i\omega)$ below the first resonance. However, there are differences at the 1% level in the values of oscillator strength sums obtained in Ref. [29] and Ref. [33], supporting the estimate of a 1% level of accuracy for the C_6 coefficients obtained by Kumar and Meath [29].

Table G
Dispersion coefficients C_6 and their estimated uncertainties (in parentheses) for alkali–metal – noble gas pairs in atomic units.

	He	Ne	Ar	Kr	Xe
H	2.821	5.64(3)	19.8(1)	28.5(2)	42.8(2)
Li	22.44(2)	43.6(2)	173(1)	259(1)	409(2)
Na	25.51(3)	49.8(3)	195(1)	291(2)	458(2)
K	38.86(8)	76.1(4)	296(2)	440(3)	692(4)
Rb	44.07(11)	86.5(5)	334(2)	494(3)	776(4)
Cs	53.6(3)	105.4(8)	404(3)	598(4)	936(7)
Fr	52.4(4)	103(1)	390(4)	575(6)	896(9)

Table H
Coefficients C_3 for the atom–surface interaction in atomic units.

Group IA		Group IIA		Group VIII	
Atom	C_3	Atom	C_3	Atom	C_3
H	0.25			He	0.1881
Li	1.512	Be	1.01	Ne	0.4751
Na	1.871	Mg	1.666	Ar	1.096
K	2.896	Ca	2.744	Kr	1.542
Rb	3.426	Sr	3.382	Xe	2.164
Cs	4.268	Ba	4.293		
Fr	4.437				

For the heteronuclear atom pairs, the dispersion coefficient $C_6(AB)$ of the alkali–metals and the alkaline–earths are listed in Table E, the values for the alkaline–earths and the noble gases are listed in Table F, and those for the alkali–metals and the noble gases are listed in Table G.

The uncertainty $dC_6(AB)$ in $C_6(AB)$ was estimated using the expression

$$dC_6(AB)/C_6(AB) = \frac{1}{2}\left[\left(dC_6(AA)/C_6(AA)\right)^2 + \left(dC_6(BB)/C_6(BB)\right)^2\right]^{1/2}. \tag{7}$$

4.2. Applications to atom–surface interactions

The atom–surface interaction coefficients were computed with Eq. (3) using the Gaussian quadrature method yielding

$$C_3 = \frac{1}{4\pi}\sum_{k=1}^{50} w_k \alpha(i\omega_k). \tag{8}$$

The resulting values are given in Table H.

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Appendix A. Gauss–Legendre quadrature

We determine the tabulated grid points and weights in two steps. First we obtain the Gauss–Legendre abscissas x_k and weights g_k defined on the interval $(0,1)$ with $N_g = 50$ points. The weights and abscissas are generated by routine `gauleg` of Ref. [34]. Further we use the mapping function $\omega_k = 2\tan(\pi/2x_k)$, so that the resulting values of ω sample the entire integration range. The Gauss–Legendre weights are also properly redefined to incorporate the Jacobian of the coordinate transformation, $w_k = g_k\pi/\cos(\pi/2x_k)^2$. The final values are given in Table A.

Appendix B. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.adt.2009.12.002.

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Explanation of Tables

Table 1. Dynamic electric dipole polarizabilities of hydrogen and alkali–metal atoms at imaginary frequencies for use with the 50-point Gauss–Legendre quadrature method.

Column 1	Frequency: The value $\omega = 0$, yielding the static polarizability $\alpha(0)$ The value ω_k, corresponding to the index k in Table A
Columns 2–8	Value of $\alpha(0)$ or $\alpha(i\omega_k)$ for the chemical element listed

Table 2. Dynamic electric dipole polarizabilities of alkaline–earth metal atoms at imaginary frequencies for use with the 50-point Gauss–Legendre quadrature method.

Column 1	Frequency: The value $\omega = 0$, yielding the static polarizability $\alpha(0)$ The value ω_k, corresponding to the index k in Table A
Columns 2–6	Value of $\alpha(0)$ or $\alpha(i\omega_k)$ for the chemical element listed

Table 3. Dynamic electric dipole polarizabilities of noble gas atoms at imaginary frequencies for use with the 50-point Gauss–Legendre quadrature method.

Same as Table 2

Table 1
Dynamic electric-dipole polarizabilities of hydrogen and alkali–metal atoms at imaginary frequencies for use with the 50-point Gauss–Legendre quadrature method. See page 328 for Explanation of Tables.

ω	H	Li	Na	K	Rb	Cs	Fr
0	4.5	164.0	162.6	290.2	318.6	399.8	317.8
ω_1	4.4997	1.6386[2]	1.625[2]	2.8996[2]	3.1832[2]	3.9938[2]	3.1752[2]
ω_2	4.4974	1.6094[2]	1.6025[2]	2.8329[2]	3.1076[2]	3.88[2]	3.1082[2]
ω_3	4.4857	1.4727[2]	1.4948[2]	2.5306[2]	2.7667[2]	3.3819[2]	2.8035[2]
ω_4	4.452	1.181[2]	1.2503[2]	1.934[2]	2.1035[2]	2.4771[2]	2.1973[2]
ω_5	4.3798	8.2483[1]	9.2082[1]	1.2835[2]	1.3939[2]	1.5921[2]	1.5244[2]
ω_6	4.252	5.3094[1]	6.1986[1]	8.0193[1]	8.7721[1]	9.9455[1]	1.0137[2]
ω_7	4.0561	3.355[1]	4.0336[1]	5.06[1]	5.627[1]	6.4749[1]	6.9056[1]
ω_8	3.7895	2.1584[1]	2.6414[1]	3.3376[1]	3.802[1]	4.5037[1]	4.9579[1]
ω_9	3.4624	1.4337[1]	1.7756[1]	2.326[1]	2.7268[1]	3.343[1]	3.7583[1]
ω_{10}	3.0959	9.8574	1.2345[1]	1.7106[1]	2.066[1]	2.6166[1]	2.9784[1]
ω_{11}	2.7157	7.0022	8.8866	1.3188[1]	1.6373[1]	2.1283[1]	2.4368[1]
ω_{12}	2.3453	5.1216	6.6142	1.0567[1]	1.3424[1]	1.776[1]	2.0363[1]
ω_{13}	2.0018	3.844	5.0767	8.7219	1.1272[1]	1.5058[1]	1.7246[1]
ω_{14}	1.6948	2.9512	4.0061	7.3564	9.6174	1.2886[1]	1.4729[1]
ω_{15}	1.4274	2.3111	3.2398	6.2984	8.2871	1.1086[1]	1.2648[1]
ω_{16}	1.1985	1.8417	2.6767	5.4454	7.1818	9.5655	1.0902[1]
ω_{17}	1.0049	1.4902	2.2523	4.7358	6.2421	8.2676	9.4258
ω_{18}	8.4223[−1]	1.2221	1.9245	4.1313	5.4316	7.1542	8.17
ω_{19}	7.06[−1]	1.0139	1.6651	3.6081	4.7265	6.1966	7.098
ω_{20}	5.9205[−1]	8.4974[−1]	1.4553	3.1504	4.1101	5.372	6.18
ω_{21}	4.9668[−1]	7.1822[−1]	1.2819	2.7476	3.5702	4.6611	5.3912
ω_{22}	4.1676[−1]	6.1136[−1]	1.1356	2.3919	3.097	4.0476	4.711
ω_{23}	3.4963[−1]	5.2334[−1]	1.0098	2.0774	2.6821	3.5171	4.1221
ω_{24}	2.9313[−1]	4.4989[−1]	8.9998[−1]	1.7993	2.3186	3.0576	3.61
ω_{25}	2.4546[−1]	3.8785[−1]	8.0261[−1]	1.5535	2.0004	2.6583	3.1623
ω_{26}	2.0515[−1]	3.3485[−1]	7.1525[−1]	1.3367	1.722	2.3104	2.7689
ω_{27}	1.7102[−1]	2.891[−1]	6.3608[−1]	1.1456	1.4788	2.0061	2.4215
ω_{28}	1.4207[−1]	2.4925[−1]	5.6376[−1]	9.7766[−1]	1.2664	1.739	2.113
ω_{29}	1.1751[−1]	2.1428[−1]	4.9735[−1]	8.3028[−1]	1.0812	1.5036	1.8379
ω_{30}	9.6682[−2]	1.834[−1]	4.3614[−1]	7.013[−1]	9.1991[−1]	1.2953	1.5914
ω_{31}	7.9029[−2]	1.5602[−1]	3.7966[−1]	5.8879[−1]	7.7965[−1]	1.1104	1.3701
ω_{32}	6.4103[−2]	1.3171[−1]	3.2757[−1]	4.9097[−1]	6.5784[−1]	9.4575[−1]	1.1712
ω_{33}	5.1524[−2]	1.1013[−1]	2.7968[−1]	4.0628[−1]	5.522[−1]	7.9902[−1]	9.9237[−1]
ω_{34}	4.0971[−2]	9.1031[−2]	2.3587[−1]	3.333[−1]	4.6071[−1]	6.683[−1]	8.3219[−1]
ω_{35}	3.2172[−2]	7.4209[−2]	1.9607[−1]	2.7077[−1]	3.8156[−1]	5.5221[−1]	6.8947[−1]
ω_{36}	2.4893[−2]	5.9517[−2]	1.6028[−1]	2.1753[−1]	3.1318[−1]	4.4973[−1]	5.6332[−1]
ω_{37}	1.8931[−2]	4.6826[−2]	1.2848[−1]	1.7253[−1]	2.5416[−1]	3.6009[−1]	4.5304[−1]
ω_{38}	1.4108[−2]	3.6019[−2]	1.0066[−1]	1.3479[−1]	2.0332[−1]	2.827[−1]	3.579[−1]
ω_{39}	1.0263[−2]	2.6979[−2]	7.6781[−2]	1.0341[−1]	1.5966[−1]	2.1698[−1]	2.7711[−1]
ω_{40}	7.2545[−3]	1.9581[−2]	5.6743[−2]	7.7582[−2]	1.2241[−1]	1.6227[−1]	2.0971[−1]
ω_{41}	4.9534[−3]	1.3686[−2]	4.0389[−2]	5.6563[−2]	9.0954[−2]	1.1779[−1]	1.5452[−1]
ω_{42}	3.2418[−3]	9.1389[−3]	2.7483[−2]	3.9715[−2]	6.4885[−2]	8.2549[−2]	1.1023[−1]
ω_{43}	2.0123[−3]	5.7691[−3]	1.7703[−2]	2.6512[−2]	4.3891[−2]	5.5437[−2]	7.5407[−2]
ω_{44}	1.1674[−3]	3.3923[−3]	1.0652[−2]	1.6525[−2]	2.7695[−2]	3.5233[−2]	4.8728[−2]
ω_{45}	6.1937[−4]	1.8183[−3]	5.8682[−3]	9.3754[−3]	1.5939[−2]	2.0733[−2]	2.9029[−2]
ω_{46}	2.9045[−4]	8.5884[−4]	2.8645[−3]	4.6648[−3]	8.0975[−3]	1.0867[−2]	1.535[−2]
ω_{47}	1.1357[−4]	3.3735[−4]	1.1666[−3]	1.919[−3]	3.4329[−3]	4.7421[−3]	6.7792[−3]
ω_{48}	3.3079[−5]	9.8504[−5]	3.5183[−4]	5.8509[−4]	1.0815[−3]	1.5266[−3]	2.2355[−3]
ω_{49}	5.4925[−6]	1.6372[−5]	5.9695[−5]	1.012[−4]	1.9126[−4]	2.7665[−4]	4.1737[−4]
ω_{50}	1.9816[−7]	5.9081[−7]	2.1693[−6]	3.7292[−6]	7.2051[−6]	1.0596[−5]	1.6446[−5]

Table 2
Dynamic electric-dipole polarizabilities of alkaline–earth metal atoms for use with the 50-point Gauss–Legendre quadrature method. See page 328 for Explanation of Tables.

ω	Be	Mg	Ca	Sr	Ba
0	37.76	71.26	157.1	197.2	273.5
ω_1	3.7761[1]	7.126[1]	1.5713[2]	1.9717[2]	2.7346[2]
ω_2	3.7678[1]	7.1031[1]	1.5605[2]	1.9555[2]	2.7034[2]
ω_3	3.7253[1]	6.9862[1]	1.5063[2]	1.8758[2]	2.5527[2]
ω_4	3.6068[1]	6.6665[1]	1.3683[2]	1.6778[2]	2.2011[2]
ω_5	3.3715[1]	6.0587[1]	1.1414[2]	1.3662[2]	1.704[2]
ω_6	3.008[1]	5.184[1]	8.768[1]	1.0236[2]	1.2209[2]
ω_7	2.5525[1]	4.1845[1]	6.3831[1]	7.319[1]	8.5059[1]
ω_8	2.0729[1]	3.2325[1]	4.5563[1]	5.1843[1]	5.9832[1]
ω_9	1.6321[1]	2.4354[1]	3.2695[1]	3.7271[1]	4.3314[1]
ω_{10}	1.2635[1]	1.8193[1]	2.3915[1]	2.7517[1]	3.2474[1]
ω_{11}	9.7285	1.3632[1]	1.7939[1]	2.0939[1]	2.5192[1]
ω_{12}	7.5094	1.0315[1]	1.3817[1]	1.6407[1]	2.0129[1]
ω_{13}	5.8375	7.9115	1.0916[1]	1.3194[1]	1.6469[1]
ω_{14}	4.5801	6.1592	8.8202	1.0842[1]	1.3718[1]
ω_{15}	3.6298	4.8683	7.2655	9.0627	1.1576[1]
ω_{16}	2.9053	3.9049	6.0798	7.6742	9.8569
ω_{17}	2.3471	3.1759	5.1505	6.5592	8.4461
ω_{18}	1.9124	2.6161	4.4038	5.6421	7.2685
ω_{19}	1.57	2.1803	3.79	4.8731	6.274
ω_{20}	1.2974	1.836	3.2758	4.2187	5.4271
ω_{21}	1.0782	1.5604	2.8384	3.6559	4.7019
ω_{22}	9.0039[−1]	1.3366	2.4616	3.1682	4.078
ω_{23}	7.548[−1]	1.1527	2.1343	2.7435	3.5396
ω_{24}	6.3468[−1]	9.9944[−1]	1.8481	2.3725	3.0734
ω_{25}	5.3487[−1]	8.7016[−1]	1.5969	2.0478	2.6686
ω_{26}	4.5139[−1]	7.5976[−1]	1.3759	1.7634	2.3161
ω_{27}	3.8116[−1]	6.6437[−1]	1.1812	1.5144	2.0081
ω_{28}	3.2178[−1]	5.8102[−1]	1.0098	1.2964	1.7382
ω_{29}	2.7133[−1]	5.0746[−1]	8.5909[−1]	1.1059	1.5008
ω_{30}	2.2829[−1]	4.4195[−1]	7.2678[−1]	9.397[−1]	1.2913
ω_{31}	1.9145[−1]	3.8318[−1]	6.1095[−1]	7.9489[−1]	1.1058
ω_{32}	1.5981[−1]	3.3015[−1]	5.0991[−1]	6.6906[−1]	9.4128[−1]
ω_{33}	1.3258[−1]	2.8215[−1]	4.2213[−1]	5.5999[−1]	7.9502[−1]
ω_{34}	1.0911[−1]	2.3865[−1]	3.4627[−1]	4.657[−1]	6.6503[−1]
ω_{35}	8.888[−2]	1.993[−1]	2.8111[−1]	3.8439[−1]	5.4976[−1]
ω_{36}	7.1473[−2]	1.639[−1]	2.2553[−1]	3.1446[−1]	4.4807[−1]
ω_{37}	5.6557[−2]	1.323[−1]	1.7851[−1]	2.5446[−1]	3.591[−1]
ω_{38}	4.3871[−2]	1.0445[−1]	1.391[−1]	2.0311[−1]	2.8221[−1]
ω_{39}	3.3206[−2]	8.0308[−2]	1.0641[−1]	1.593[−1]	2.1681[−1]
ω_{40}	2.4388[−2]	5.9819[−2]	7.961[−2]	1.2211[−1]	1.6226[−1]
ω_{41}	1.7262[−2]	4.2895[−2]	5.7918[−2]	9.0832[−2]	1.1783[−1]
ω_{42}	1.1673[−2]	2.9376[−2]	4.0634[−2]	6.4943[−2]	8.258[−2]
ω_{43}	7.4569[−3]	1.9017[−2]	2.7154[−2]	4.4068[−2]	5.544[−2]
ω_{44}	4.4315[−3]	1.1476[−2]	1.6976[−2]	2.7905[−2]	3.5224[−2]
ω_{45}	2.3965[−3]	6.3285[−3]	9.6727[−3]	1.6113[−2]	2.0737[−2]
ω_{46}	1.1397[−3]	3.0887[−3]	4.835[−3]	8.2051[−3]	1.0887[−2]
ω_{47}	4.4978[−4]	1.2589[−3]	1.9961[−3]	3.4837[−3]	4.7639[−3]
ω_{48}	1.3169[−4]	3.8074[−4]	6.0959[−4]	1.0995[−3]	1.5374[−3]
ω_{49}	2.1915[−5]	6.4812[−5]	1.056[−4]	1.9486[−4]	2.7913[−4]
ω_{50}	7.9107[−7]	2.3589[−6]	3.8988[−6]	7.3492[−6]	1.0706[−5]

Table 3
Dynamic electric-dipole polarizabilities of noble gas atoms for use with the 50-point Gauss–Legendre quadrature method. See page 328 for Explanation of Tables.

ω	He	Ne	Ar	Kr	Xe
0	1.383	2.669	11.08	16.79	27.16
ω_1	1.3832	2.6693	1.1082[1]	1.679[1]	2.7156[1]
ω_2	1.3831	2.669	1.1079[1]	1.6786[1]	2.7145[1]
ω_3	1.3824	2.6678	1.1067[1]	1.6761[1]	2.7088[1]
ω_4	1.3804	2.6641	1.1031[1]	1.6689[1]	2.6923[1]
ω_5	1.3761	2.656	1.0954[1]	1.6534[1]	2.6571[1]
ω_6	1.3681	2.6412	1.0814[1]	1.6256[1]	2.5947[1]
ω_7	1.355	2.617	1.0591[1]	1.5819[1]	2.4986[1]
ω_8	1.3355	2.5811	1.0269[1]	1.5202[1]	2.367[1]
ω_9	1.3081	2.5315	9.8423	1.4405[1]	2.2034[1]
ω_{10}	1.2721	2.4671	9.3171	1.3454[1]	2.0164[1]
ω_{11}	1.227	2.3878	8.7097	1.2392[1]	1.8172[1]
ω_{12}	1.1732	2.2948	8.044	1.1269[1]	1.6165[1]
ω_{13}	1.1117	2.19	7.3471	1.0136[1]	1.4233[1]
ω_{14}	1.0439	2.0762	6.6443	9.0318	1.2437[1]
ω_{15}	9.7176[−1]	1.9562	5.9571	7.9877	1.0809[1]
ω_{16}	8.9716[−1]	1.8327	5.3018	7.0221	9.3621
ω_{17}	8.2198[−1]	1.7081	4.6893	6.1444	8.0938
ω_{18}	7.4784[−1]	1.5844	4.1258	5.3569	6.9925
ω_{19}	6.7605[−1]	1.4632	3.6139	4.6573	6.0419
ω_{20}	6.0757[−1]	1.3456	3.1534	4.0403	5.2242
ω_{21}	5.4303[−1]	1.2325	2.7424	3.4989	4.5216
ω_{22}	4.8284[−1]	1.1244	2.3777	3.0256	3.9179
ω_{23}	4.2714[−1]	1.0215	2.0555	2.6129	3.3983
ω_{24}	3.7596[−1]	9.2402[−1]	1.7719	2.2535	2.9499
ω_{25}	3.2919[−1]	8.3201[−1]	1.5229	1.9409	2.5615
ω_{26}	2.8667[−1]	7.4541[−1]	1.3049	1.6691	2.2239
ω_{27}	2.4818[−1]	6.6416[−1]	1.1142	1.4329	1.9291
ω_{28}	2.135[−1]	5.8814[−1]	9.4788[−1]	1.2276	1.6705
ω_{29}	1.8237[−1]	5.1726[−1]	8.0296[−1]	1.0493	1.4427
ω_{30}	1.5457[−1]	4.5142[−1]	6.7699[−1]	8.9435[−1]	1.2414
ω_{31}	1.2987[−1]	3.9052[−1]	5.6773[−1]	7.5977[−1]	1.0627
ω_{32}	1.0804[−1]	3.345[−1]	4.7325[−1]	6.4289[−1]	9.0391[−1]
ω_{33}	8.8889[−2]	2.833[−1]	3.9181[−1]	5.4141[−1]	7.6262[−1]
ω_{34}	7.2211[−2]	2.3685[−1]	3.2189[−1]	4.5327[−1]	6.3702[−1]
ω_{35}	5.7821[−2]	1.9512[−1]	2.6211[−1]	3.7666[−1]	5.2567[−1]
ω_{36}	4.5539[−2]	1.5804[−1]	2.1123[−1]	3.1002[−1]	4.2747[−1]
ω_{37}	3.5189[−2]	1.2553[−1]	1.6814[−1]	2.5197[−1]	3.4156[−1]
ω_{38}	2.6598[−2]	9.7463[−2]	1.3181[−1]	2.0141[−1]	2.673[−1]
ω_{39}	1.9593[−2]	7.3682[−2]	1.0136[−1]	1.5751[−1]	2.0416[−1]
ω_{40}	1.4001[−2]	5.3982[−2]	7.6035[−2]	1.1976[−1]	1.5163[−1]
ω_{41}	9.648[−3]	3.8104[−2]	5.5247[−2]	8.7897[−2]	1.0912[−1]
ω_{42}	6.3624[−3]	2.573[−2]	3.8541[−2]	6.1803[−2]	7.5839[−2]
ω_{43}	3.9735[−3]	1.6472[−2]	2.5547[−2]	4.1315[−2]	5.0763[−2]
ω_{44}	2.316[−3]	9.8772[−3]	1.5877[−2]	2.6037[−2]	3.2591[−2]
ω_{45}	1.2329[−3]	5.4433[−3]	9.0623[−3]	1.5259[−2]	1.9829[−2]
ω_{46}	5.795[−4]	2.6642[−3]	4.5722[−3]	8.0494[−3]	1.1001[−2]
ω_{47}	2.2691[−4]	1.0845[−3]	1.9[−3]	3.5374[−3]	5.073[−3]
ω_{48}	6.614[−5]	3.2458[−4]	5.7452[−4]	1.1184[−3]	1.6545[−3]
ω_{49}	1.0985[−5]	5.458[−5]	9.7061[−5]	1.9243[−4]	2.8817[−4]
ω_{50}	3.9634[−7]	1.9807[−6]	3.5573[−6]	7.0524[−6]	1.0532[−5]