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Dynamic multipole polarizabilities and Rydberg states of the beryllium isoelectronic sequence

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Dynamic dipole, quadrupole, and octupole polarizabilities of the beryllium isoelectronic sequence up to $Z=10$ are calculated using time-dependent linear-response theory. Excitation energies and analytic representations of the singly excited Rydberg states of s, p, d, and f symmetries in their singlet configurations are also obtained for excitations up to principal quantum number $n=8$. The static limits $\alpha_{2^l}(\omega)_{\omega\to 0}$ obtained compare well with existing static results. Excitation energies compare favorably with the available spectroscopic values. The oscillator strengths for the dipolar and quadrupolar transitions are calculated and the effective quantum numbers are estimated using the complete screening model. Agreement is reasonably good with existing data wherever available.

I. INTRODUCTION

Knowledge of highly excited states of complex atoms having two electrons in the valence shell is relatively poor,[1] and its interpretation is also rather complicated because of the presence of perturbing near-degenerate configurations. The coupling between the highly excited orbital with the unpaired orbital in the ionic core further complicates the problem. Multichannel quantum-defect theory[2-6] (MQDT) was adopted to explain various features of these excited states quite successfully, although its practical application requires a large number of data. Recent experimental techniques using powerful lasers and ionic detection of resonances are providing extremely valuable information on these states. Because of the importance of highly excited states for studying superradiance,[7,8] laser isotope separation, microwave detection, and other physical processes,[1,9] a systematic theoretical study of such states is quite important. Another important topic for investigation is the excitation energies and radiative transition rates of highly stripped ions in their various excited states. These are needed for estimating the density and temperature of the solar corona and also for calculating the energy loss through impurity ions in plasmas and in high-temperature fusion plasma diagnostics.[10,11] The beryllium isoelectronic sequence of ions is particularly interesting because the effect of electron correlation effects due to the presence of real near-degenerate doubly excited configurations in the ground state is clearly recognized.[12-14]

In a recent series of papers,[15-19] the usefulness of time-dependent coupled Hartree-Fock (TDCHF) theory to calculate the excitation energies, oscillator strengths, quantum-defect values, and singly excited Rydberg states of different symmetries was clearly demonstrated. The success of the TDCHF theory, which is equivalent to the random-phase approximation[20,21] (RPA), lies mainly in the implicit inclusion of a certain class of correlation diagrams to all orders. The method particularly yields quite accurate oscillator strength values in spite of its computational simplicity.[18,19] There are quite a few number of theoretical calculations available for berylliumlike ions. Important calculations which include correlation and also relativistic effects in a consistent manner adopt many-body perturbation theory[22] (MBPT), Z-expansion methods,[23-25] large scale configuration-interaction (CI) calculations,[26-29] configuration mixing with relativistic wave functions,[30,31] variational configuration-interaction technique,[32] variational Bethe-Goldstone calculations,[33] model potential calculations,[34] multiconfiguration Hartree-Fock (MCHF) methods,[14,35,36] multiconfiguration Dirac-Fock methods,[13,37,38] MQDT methods,[6,39] polarization propagator method,[40] relativistic RPA (RRPA) methods,[41,42] and multiconfiguration RRPA (MCRRPA) methods.[42,43] However, most of these calculations are quite cumbersome, particularly for large scale applications.

In this paper we made a systematic study of the linear response properties of the berylliumlike systems ($Z=4,\ldots,10$) for single excitations, up to principal quantum number $n=8$ for the s, p, d, and f symmetries. The frequency-dependent dipolar, quadrupolar, and octupolar polarizabilities for all the ions have been evaluated along with the transition energies, oscillator strengths, etc., and analytic representations for the Rydberg states are obtained. We describe very briefly the salient features of the theory in Sec. II; the details may be found elsewhere.[15-19] By now several good reviews on the subject are available.[44,45] The results are discussed in Sec. III.

II. METHOD

We consider the ^1S state of berylliumlike systems to be described by the usual nonrelativistic Hamiltonian. The perturbing time-dependent multipolar field is described by

$$H'(\mathbf{r},t)=\lambda\sum_i r_i^l P_l(\cos\theta_i)e^{-i\omega t}+\text{c.c.} \quad (1)$$

Presently we consider specific multipolar excitations given by $l=0,1,2,3$. For $l=0$, i.e., excitations of the same symmetry as that of the ground state, r is chosen as the radial part of the perturbation.[19] In the presence of this multipolar perturbation, the zero-order function gets modified and the first-order corrections $\delta\psi_i^\pm$ to the ground orbital ψ_i are determined by optimizing a suitable variational functional described in detail earlier.[15-19] The multipolar polarizability is obtained from

$$\alpha_{2^l}(\omega)=\sum_i [\langle \delta\psi_i^- \mid r^l P_l(\cos\theta) \mid \psi_i \rangle + \langle \delta\psi_i^+ \mid r^l P_l(\cos\theta) \mid \psi_i \rangle] . \quad (2)$$

As usual, the frequency-dependent polarizability values increase monotonically with ω, with poles at certain frequencies. The positions of these poles give the excitation energies of the system and the excited-state wave functions are obtained by renormalizing appropriate $\delta\psi_i^-$. These are further used for calculating various properties connected with the transitions.

III. RESULTS AND DISCUSSIONS

In the present paper we studied the transitions $2\,^1S\rightarrow n\,^1S$ $(n=3,\ldots,8)$, $2\,^1S\rightarrow n\,^1P$ $(n=2,\ldots,8)$, $2\,^1S\rightarrow n\,^1D$ $(n=3,\ldots,8)$, and $2\,^1S\rightarrow n\,^1F$ $(n=4,\ldots,8)$ for the ions Be, B^+, C^{2+}, N^{3+}, O^{4+}, F^{5+}, and Ne^{6+}. The ground-state functions for all the ions have been taken from Clementi and Roetti,[46] while the radial parts of the perturbed orbitals are chosen as linear combinations of Slater bases,

$$\delta\psi_i^\pm(r)=\sum_q C_{iq}^\pm \chi_{iq}(r) , \quad (3)$$

where the bases χ_{iq}'s are chosen from physical considerations. $C_{iq}^\pm$'s are linear variation parameters to be determined variationally. In this calculation we have chosen a 12-parameter representation for all the excitations under study. The dynamic dipolar, quadrupolar, and octupolar polarizabilities are calculated from Eq. (2) and their static limits are obtained. In Table I we present the static limits along with other static results for comparison. Our results agree well with those obtained from similar calculations, except for the static limit of the octupolar polarizability for Be, where we get somewhat larger values than that of Arrighini *et al.*[47] and Markiewicz *et al.*[48] In order to check whether this is a basis-set effect we adopted different basis sets, but the results are the same. For the higher members of the sequence our results compare nicely with those of others listed in Table I. The effect of correlation is to lower the polarizability values, as has been reflected clearly for the Be atom in the calculations of Reinsch and Meyer,[49] Stevens and Billingsley,[50] Werner and Meyer,[51] and also of Chang *et al.*[52]

The dynamic dipole, quadrupole, and octupolar polarizability values (which are not listed here) increase monotonically in the normal-dispersion region and pass through poles at certain frequencies characteristic of the particular ion, and the overall behavior is identical with the figures plotted in our earlier papers.[18,19] The excitation energies obtained from the poles of the dynamic polarizability values for $2\,^1S\rightarrow n\,^1P$, $n\,^1D$, and $n\,^1F$ transitions and from the poles of an appropriate functional for $2\,^1S\rightarrow n\,^1S$ transitions are listed in Table II. They are compared with those listed by Bashkin and Stoner, Jr.[53] The maximum deviation is about 10%. These are also observed for other similar calculations. This is due to the effect of near-degenerate configurations in Be-like systems where a CI calculation[28,32] or MCRRPA calculation[12] yields much better results. The MCDF calculation of Cheng *et al.*[38] overshoots the transition energies considerably. As observed from Table II, other theoretical results are available mostly for the dipole-allowed transitions, the number of such calculations being maximum for Be. In Table II we have also listed the effective quantum number n^* of the Rydberg orbitals. Assuming complete screening, this is obtained by using the hydrogenic formula $n^*=1/\sqrt{2\varepsilon}$, where ε is the orbital ionization potential. These are compared with those obtained spectroscopically[53] and also with those of Stewart *et al.*[54] from a time-dependent Hartree-Fock (TDHF) calculation. We notice excellent agreement with those of Stewart *et al.*[54] wherever their data are available and reasonably good agreement with those obtained experimentally for the relatively lower principal quantum numbers. For the higher principal quantum numbers our results sometimes deviate considerably. This is probably due to the limited basis set used for representing the highly diffuse Rydberg orbitals, and also the use of ground orbital energies of Clementi and Roetti[46] may not be properly justified. One interesting feature is observed from the host of data collected here. For practically all the systems the quantum defect values $\Lambda=n-n^*$ remain constant over the different transitions. Experimental values corroborate this feature, but for $S\rightarrow P$ transitions for a number of ions like Be, B^+, etc., they tend to increase initially and gradually become constant at higher transitions. However, in quite a few cases data are not available.

In Table III we have listed the dipole and quadrupole oscillator strengths for the transitions studied here. The oscillator strengths have been found out using the formulas given in our earlier papers.[55,19] There are several calculations including many experimental data available for the dipole oscillator strengths, although the calculations are mostly confined to $2\,^1S\rightarrow 2\,^1P$ transitions. From the host of data collected we find that for the first few transitions the results of our calculations agree well with other theoretical values. As compared with the experimental results, our values are slightly higher. For a given transition the dipolar oscillator strength value usually diminishes gradually for the higher members of the isoelectronic sequence. Also for the same ion it diminishes with increasing principal quantum number. For the quadrupolar oscillator strengths, as far as the authors knowledge goes, no other results are available for comparison. Here also the same general trend is followed for the variation of oscillator strength against principal quantum number. But the variation along the isoelectronic sequence is not monotonic.

We obtained analytic representations for all the wave functions under the present discussion (the list may be obtained on request from the authors). In many of the

TABLE I. Static limits $\alpha_d(\omega)_{\omega\to 0}$, $\alpha_q(\omega)_{\omega\to 0}$, and $\alpha_o(\omega)_{\omega\to 0}$ for the dynamic dipole, quadrupole, and octupole polarizabilities, respectively.

Atom or ion	Dipole polarizability (a_0^3) Static limit	Dipole polarizability (a_0^3) Other theoretical values	Quadrupole polarizability (a_0^5) Static limit	Quadrupole polarizability (a_0^5) Other theoretical values	Octupole polarizability (a_0^7) Static limit	Octupole polarizability (a_0^7) Other theoretical values
Be	45.678	45.62[a–h], 30.64[i], 64.11[j], 36.58[k], 64.32[l], 37.9[m], 44.86[n], 36.51[o], 37.84[p], 39.44[p], 46.77[q,r], 37.05[s], 38.14[t], 47.17[u], 42.11[v], 45.44[w], 45.03[x]	344.98	342.6[a], 342.2[b], 343.4[f], 342.4[g], 224.1[i], 363.9[j], 342.5[y], 301.8[z]	5765	5624[a], 5635[g]
B^{+}	11.409	11.40[a,b], 11.39[c], 11.35[d], 11.405[e,f], 11.38[g], 11.409[h], 13.23[l], 9.65[m]	28.68	28.68[a], 28.2[b,y], 28.44[f], 28.28[g]	186.5	185.1[a], 179.1[g]
C^{2+}	4.511	4.512[a], 4.522[b,e,f], 4.506[c], 4.49[d], 4.508[g], 4.511[h], 3.645[k], 4.407[l], 5.412[u],	5.250	5.250[a], 5.302[b,f,y], 5.224[g]	17.99	17.99[a], 17.70[g]
N^{3+}	2.238	2.22[d], 2.237[e,g], 2.238[h], 1.89[l]	1.437	1.433[g,y]	3.062	3.035[g]
O^{4+}	1.271	1.27[d], 1.271[e,g,h], 1.03[k], 0.945[l]	0.501	0.4995[g], 0.4996[y]	0.732	0.7251[g]
F^{5+}	0.791	0.784[d], 0.790[e], 0.791[g,h] 0.078[l]	0.206	0.2049[g], 0.2048[y]	0.219	0.2168[g]
Ne^{6+}	0.525	0.522[d], 0.525[e,g,h]	0.095	0.0946[g,y]	0.077	0.0762[g]

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TABLE II. Singlet-singlet transition energies and effective quantum numbers for the Be isoelectronic sequence.

		Excitation energies (a.u.)				Effective quantum number		
Atom or Ion	Transition scheme	Calc.	Expt.[a]	Deviation (%)	Other theoretical values	Calc.	Expt.[a]	Other values
Be	$2\,^1S \to 3\,^1S$	0.2296	0.2491	7.83	0.224 85[b]	2.505	2.312	2.4337[b]
	$\to 4\,^1S$	0.2680	0.2973	9.86	0.266 83[b]	3.481	3.322	3.4323[b]
	$\to 5\,^1S$	0.2842	0.3159	10.03	0.283 82[b]	4.466	4.326	4.4325[b]
	$\to 6\,^1S$	0.2938	0.3250	9.6		5.685	5.327	
	$\to 7\,^1S$	0.2996	0.3301	9.24		7.191	6.319	
	$\to 8\,^1S$	0.3018	0.3333	9.45		8.181	7.324	
	$\to 2\,^1P$	0.1763	0.194	9.12	0.176 34[b], 0.188[c], 0.176 35[d], 0.1764[e,f], 0.194 09[g], 0.222[h], 0.177[i], 0.201[j], 0.1758[k]	1.939	1.834	1.9394[b]
	$\to 3\,^1P$	0.2470	0.2742	9.92	0.247 06[b], 0.266[c], 0.247 07[d], 0.2490[e], 0.2633[f]	2.834	2.703	2.8350[b]
	$\to 4\,^1P$	0.2749	0.3054	9.99	0.274 95[b], 0.292[c], 0.274 96[d], 0.3211[e]	3.814	3.665	3.8176[b]
	$\to 5\,^1P$	0.2879	0.3195	9.89	0.287 67[b], 0.311[c], 0.287 75[d], 0.4881[e]	4.837	4.650	4.8108[b]
	$\to 6\,^1P$	0.2960	0.3269	9.45		6.138	5.64	
	$\to 7\,^1P$	0.3013				7.921		
	$\to 8\,^1P$	0.3036				9.391		
	$\to 3\,^1D$	0.2543	0.2936	13.38	0.254 31[b], 0.254 32[d], 0.2548[e], 0.2560[f]	3.016	3.194	3.0163[b]
	$\to 4\,^1D$	0.2782	0.3134	11.23	0.278 28[b], 0.278 29[d], 0.3003[e], 0.3201[f]	4.012	4.137	4.0168[b]
	$\to 5\,^1D$	0.2894	0.3235	10.54	0.289 40[b], 0.3998[e]	5.016	5.114	5.0162[b]
	$\to 6\,^1D$	0.2954	0.3292	10.27		6.004	6.104	
	$\to 7\,^1D$	0.2996	0.3327	9.95		7.191	7.100	
	$\to 8\,^1D$	0.3017	0.3350	9.94		8.127	8.100	
	$\to 4\,^1F$	0.2780	0.3109	10.58	0.278 04[d], 0.2856[e],	3.999	3.970	
	$\to 5\,^1F$	0.2893	0.3224	10.27	0.289 28[d], 0.3430[e]	5.004	4.973	
	$\to 6\,^1F$	0.2954	0.3285	10.08		6.004	5.950	
	$\to 7\,^1F$	0.2998	0.3323	9.78		7.266	6.960	
	$\to 8\,^1F$	0.3027				8.724		
B^+	$2\,^1S \to 3\,^1S$	0.5823	0.6178	5.75		2.62	2.554	
	$\to 4\,^1S$	0.7206	0.7652	5.83		3.612	3.544	
	$\to 5\,^1S$	0.7798	0.8273	5.74		4.612	4.536	
	$\to 6\,^1S$	0.8103				5.610		
	$\to 7\,^1S$	0.8290				6.676		
	$\to 8\,^1S$	0.8398				7.662		
	$\to 2\,^1P$	0.3063	0.3344	8.40	0.306 33[d], 0.3068[e], 0.3063[f], 0.347[j], 0.3838[l]	1.878	1.840	
	$\to 3\,^1P$	0.6235	0.6566	5.04	0.623 51[d], 0.6228[e], 0.6247[f]	2.826	2.732	
	$\to 4\,^1P$	0.7371	0.7773	5.17		3.824	3.686	
	$\to 5\,^1P$	0.7879	0.8322	5.32		4.824	4.656	
	$\to 6\,^1P$	0.8149				5.824		
	$\to 7\,^1P$	0.8309				6.824		
	$\to 8\,^1P$	0.8428				8.024		
	$\to 3\,^1D$	0.6537	0.7048	7.25	0.6583[e], 0.6537[f]	3.014	3.018	
	$\to 4\,^1D$	0.7494	0.7999	6.31	0.8920[e], 0.7666[f]	4.008	4.006	
	$\to 5\,^1D$	0.7941	0.8444	5.96		5.008	4.998	
	$\to 6\,^1D$	0.8184				6.006		
	$\to 7\,^1D$	0.8334				7.031		
	$\to 8\,^1D$	0.8432				8.077		
	$\to 4\,^1F$	0.7489	0.7970	6.04	0.7489[e]	4.000	3.960	
	$\to 5\,^1F$	0.7939	0.8428	5.80		5.002	4.948	
	$\to 6\,^1F$	0.8183	0.8677	5.69		6.0	5.936	
	$\to 7\,^1F$	0.8342				7.102		
	$\to 8\,^1F$	0.8431				8.064		

TABLE II. (*Continued*).

Atom or Ion	Transition scheme	Excitation energies (a.u.) Calc.	Expt.[a]	Deviation (%)	Other theoretical values	Effective quantum number Calc.	Expt.[a]	Other values
C^{2+}	$2\,{}^1S\rightarrow 3\,{}^1S$	1.0799	1.1262	4.11		2.706	2.664	
	$\rightarrow 4\,{}^1S$	1.3657	1.4204	3.85		3.702	3.642	
	$\rightarrow 5\,{}^1S$	1.4903	1.5425	3.38		4.698	4.548	
	$\rightarrow 6\,{}^1S$	1.5555				5.7		
	$\rightarrow 7\,{}^1S$	1.5937				6.696		
	$\rightarrow 8\,{}^1S$	1.6194				7.764		
	$\rightarrow 2\,{}^1P$	0.4246	0.4664	8.96	0.424 59[b,d], 0.4246[e], 0.4245[f], 0.470 54[g], 0.520[h,l], 0.428[i], 0.484[j]	1.884	1.866	1.8828[b]
	$\rightarrow 3\,{}^1P$	1.1419	1.1798	3.21	1.141 97[b,d], 1.1420[e], 1.1505[f]	2.856	2.784	2.8550[b]
	$\rightarrow 4\,{}^1P$	1.3912	1.4690	5.3	1.391 30[b], 1.391 23[d]	3.855	3.933	3.8553[b]
	$\rightarrow 5\,{}^1P$	1.5031	1.5641	3.9	1.503 22[b]	4.854	4.794	4.8561[b]
	$\rightarrow 6\,{}^1P$	1.5628	1.6272	3.96		5.856	5.823	
	$\rightarrow 7\,{}^1P$	1.5983	1.6627	3.87		6.855	6.804	
	$\rightarrow 8\,{}^1P$	1.6213	1.6856	3.81		7.866	7.782	
	$\rightarrow 3\,{}^1D$	1.1975	1.2598	4.94	1.1977[e], 1.1974[f]	3.009	3.0	
	$\rightarrow 4\,{}^1D$	1.4133	1.4773	4.33	1.4134[e], 1.4201[f]	4.002	3.990	
	$\rightarrow 5\,{}^1D$	1.5141	1.5796	4.15		5.001	4.995	
	$\rightarrow 6\,{}^1D$	1.5690	1.6346	4.01		6.0	5.991	
	$\rightarrow 7\,{}^1D$	1.6031	1.6678	3.88		7.035	6.99	
	$\rightarrow 8\,{}^1D$	1.6247				8.055		
	$\rightarrow 4\,{}^1F$	1.4130	1.4704	3.90	1.4151[e]	4.002	3.942	
	$\rightarrow 5\,{}^1F$	1.5141	1.5896	4.75		5.001	5.139	
	$\rightarrow 6\,{}^1F$	1.5691	1.6364	4.11		6.000	6.036	
	$\rightarrow 7\,{}^1F$	1.6023				7.002		
	$\rightarrow 8\,{}^1F$	1.6244				8.037		
N^{3+}	$2\,{}^1S\rightarrow 3\,{}^1S$	1.7174	1.7718	3.07		2.760	2.728	
	$\rightarrow 4\,{}^1S$	2.2000	2.2557	2.47		3.756	3.676	
	$\rightarrow 5\,{}^1S$	2.4130	2.4912	3.14		4.756	4.74	
	$\rightarrow 6\,{}^1S$	2.5252	2.6026	2.97		5.756	5.72	
	$\rightarrow 7\,{}^1S$	2.5915	2.6655	2.78		6.756	6.636	
	$\rightarrow 8\,{}^1S$	2.6352	2.7164	2.99		7.80	7.820	
	$\rightarrow 2\,{}^1P$	0.5387	0.5955	9.54	0.652[h,l], 0.544[i], 0.617[j]	1.896	1.884	
	$\rightarrow 3\,{}^1P$	1.8006	1.8432	2.31		2.876	2.824	
	$\rightarrow 4\,{}^1P$	2.2349	2.3103	3.26		3.88	3.860	
	$\rightarrow 5\,{}^1P$	2.4306	2.5071	3.05		4.88	4.848	
	$\rightarrow 6\,{}^1P$	2.5353	2.6096	2.85		5.88	5.804	
	$\rightarrow 7\,{}^1P$	2.5977	2.6791	3.04		6.88	6.900	
	$\rightarrow 8\,{}^1P$	2.6379	2.7169	2.91		7.88	7.836	
	$\rightarrow 3\,{}^1D$	1.8822	1.9555	3.75		3.008	2.996	
	$\rightarrow 4\,{}^1D$	2.2668	2.345	3.33		4.000	3.992	
	$\rightarrow 5\,{}^1D$	2.4464	2.5257	3.14		4.996	4.988	
	$\rightarrow 6\,{}^1D$	2.5442	2.624	3.04		5.996	5.988	
	$\rightarrow 7\,{}^1D$	2.6032	2.6833	2.98		6.996	6.984	
	$\rightarrow 8\,{}^1D$	2.6419	2.7218	2.94		8.004	7.988	
	$\rightarrow 4\,{}^1F$	2.2670	2.3779	4.66		4.000	4.128	
	$\rightarrow 5\,{}^1F$	2.4469	2.5288	3.24		5.000	5.012	
	$\rightarrow 6\,{}^1F$	2.5446	2.6245	3.04		6.000	5.992	
	$\rightarrow 7\,{}^1F$	2.6035				7.000		
	$\rightarrow 8\,{}^1F$	2.6426				8.028		

TABLE II. (*Continued*).

Atom or Ion	Transition scheme	Excitation energies (a.u.) Calc.	Expt.[a]	Deviation (%)	Other theoretical values	Effective quantum number Calc.	Expt.[a]	Other values
O^{4+}	$2\,^1S \to 3\,^1S$	2.4946	2.5575	2.46		2.80	2.770	
	$\to 4\,^1S$	3.2226	3.3339	3.34		3.795	3.830	
	$\to 5\,^1S$	3.5468				4.795		
	$\to 6\,^1S$	3.7184				5.795		
	$\to 7\,^1S$	3.8200				6.795		
	$\to 8\,^1S$	3.8855				7.805		
	$\to 2\,^1P$	0.6507	0.7236	10.07	0.6507[b,d], 0.725 24[g], 0.782[h,l], 0.658[i], 0.749[j]	1.905	1.900	1.9062[b]
	$\to 3\,^1P$	2.5988	2.6465	1.80	2.5988[b,d]	2.895	2.85	2.8946[b]
	$\to 4\,^1P$	3.2670	3.3621	2.83	3.2671[b,d]	3.895	3.895	3.8958[b]
	$\to 5\,^1P$	3.5693	3.6564	2.38	3.5695[b]	4.895	4.860	4.8972[b]
	$\to 6\,^1P$	3.7312	3.8257	2.47		5.895	5.890	
	$\to 7\,^1P$	3.8280	3.9226	2.41		6.90	6.890	
	$\to 8\,^1P$	3.8907	3.9844	2.35		7.905	7.875	
	$\to 3\,^1D$	2.7069	2.7914	3.03		3.005	2.995	
	$\to 4\,^1D$	3.3089	3.4004	2.69		4.0	3.990	
	$\to 5\,^1D$	3.5898	3.6832	2.55		4.995	4.985	
	$\to 6\,^1D$	3.7428	3.837	2.46		5.995	5.985	
	$\to 7\,^1D$	3.8355	3.9296	2.39		7.0	6.985	
	$\to 8\,^1D$	3.8954				8.0		
	$\to 4\,^1F$	3.3099	3.4166	3.12		4.0	4.030	
	$\to 5\,^1F$	3.5910	3.6858	2.57		5.0	4.995	
	$\to 6\,^1F$	3.7436	3.8312	2.29		6.0	5.935	
	$\to 7\,^1F$	3.8357				7.0		
	$\to 8\,^1F$	3.8970				8.030		
F^{5+}	$2\,^1S \to 3\,^1S$	3.4110	3.4828	2.06		2.826	2.802	
	$\to 4\,^1S$	4.4336	4.5448	2.45		3.822	3.822	
	$\to 5\,^1S$	4.8912				4.824		
	$\to 6\,^1S$	5.1343				5.820		
	$\to 7\,^1S$	5.2788				6.822		
	$\to 8\,^1S$	5.3754				7.878		
	$\to 2\,^1P$	0.7615	0.8513	10.55	0.911[h,l], 0.771[i], 0.879[j], 0.8631[m]	1.914	1.914	
	$\to 3\,^1P$	3.5363	3.5897	1.49		2.904	2.868	
	$\to 4\,^1P$	4.4873	4.5922	2.28		3.906	3.90	
	$\to 5\,^1P$	4.9186	5.0094	1.81		4.908	4.848	
	$\to 6\,^1P$	5.1500	5.2601	2.09		5.910	5.910	
	$\to 7\,^1P$	5.2887	5.3970	2.01		6.912	6.894	
	$\to 8\,^1P$	5.3791				7.926		
	$\to 3\,^1D$	3.6709	3.7675	2.56		3.006	2.994	
	$\to 4\,^1D$	4.5390	4.6447	2.28		3.996	3.990	
	$\to 5\,^1D$	4.9439	5.0518	2.14		4.992	4.986	
	$\to 6\,^1D$	5.1643	5.2736	2.07		5.994	5.988	
	$\to 7\,^1D$	5.2974	5.4068	2.02		6.996	6.984	
	$\to 8\,^1D$	5.3845				8.004		
	$\to 4\,^1F$	4.5411	4.6586	2.52		4.002	4.014	
	$\to 5\,^1F$	4.9457				4.998		
	$\to 6\,^1F$	5.1657				6.000		
	$\to 7\,^1F$	5.2983				7.002		
	$\to 8\,^1F$	5.3866				8.034		

TABLE II. (*Continued*).

Atom or Ion	Transition scheme	Excitation energies (a.u.) Calc.	Expt.[a]	Deviation (%)	Other theoretical values	Effective quantum number Calc.	Expt.[a]	Other values
Ne^{6+}	$2\,{}^1S \rightarrow 3\,{}^1S$	4.4664	4.5485	1.80		2.849	2.828	
	$\rightarrow 4\,{}^1S$	5.8322	5.9558	2.08		3.843	3.836	
	$\rightarrow 5\,{}^1S$	6.4460				4.844		
	$\rightarrow 6\,{}^1S$	6.7729				5.845		
	$\rightarrow 7\,{}^1S$	6.9681				6.846		
	$\rightarrow 8\,{}^1S$	7.0958				7.875		
	$\rightarrow 2\,{}^1P$	0.8716			1.04[h,l], 0.885[i], 1.01[j],0.9889[m]	1.925		
	$\rightarrow 3\,{}^1P$	4.6129				2.919		
	$\rightarrow 4\,{}^1P$	5.8954				3.92		
	$\rightarrow 5\,{}^1P$	6.4783				4.921		
	$\rightarrow 6\,{}^1P$	6.7915				5.922		
	$\rightarrow 7\,{}^1P$	6.9794				6.923		
	$\rightarrow 8\,{}^1P$	7.1027				7.945		
	$\rightarrow 3\,{}^1D$	4.7742				3.003		
	$\rightarrow 4\,{}^1D$	5.9570				3.997		
	$\rightarrow 5\,{}^1D$	6.5084				4.991		
	$\rightarrow 6\,{}^1D$	6.8086				5.992		
	$\rightarrow 7\,{}^1D$	6.9903				7.0		
	$\rightarrow 8\,{}^1D$	7.1079				8.001		
	$\rightarrow 4\,{}^1F$	5.9603				4.004		
	$\rightarrow 5\,{}^1F$	6.5112				4.998		
	$\rightarrow 6\,{}^1F$	6.8104				5.999		
	$\rightarrow 7\,{}^1F$	6.9908				7.0		
	$\rightarrow 8\,{}^1F$	7.1116				8.036		

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TABLE III. Dipole and quadrupole oscillator strengths as obtained from frequency-dependent calculations. In the last column, powers of 10 have been inserted in square brackets, i.e., $m\,[\pm n] \equiv m \times 10^{\pm n}$.

Atom or ion	Transition scheme	Dipole Oscillator Strength (a.u.) Calc.	Expt.	Other theoretical values	Transition scheme	Quadrupole oscillator strength (a.u.) Calc.
Be	$2{}^1S \rightarrow 2\,{}^1P$	1.381	1.34±0.05[α],	1.71[a], 1.82[b], 1.378[c,d],	$2\,{}^1S \rightarrow 3\,{}^1D$	2.72[−6]
			1.08±0.05[β],	1.25[e], 1.814[f], 1.372[g],	$\rightarrow 4\,{}^1D$	1.14[−6]
			1.21±0.03[γ]	1.344[h], 1.774[i], 1.424[i],	$\rightarrow 5\,{}^1D$	5.76[−7]
				1.813[j], 1.410[j], 1.371[k],	$\rightarrow 6\,{}^1D$	3.26[−7]
				1.386[l], 1.36[m], 1.356[n],	$\rightarrow 7\,{}^1D$	1.73[−7]
				1.254[o], 2.029[p], 1.38[q],	$\rightarrow 8\,{}^1D$	7.27[−8]
				1.28[r], 1.38[s], 1.42[t]		
	$\rightarrow 3\,{}^1P$	0.0206		0.003[a], 0.0227[c,d], 0.208[f], 0.0225[g], 0.016[o], 0.0106[q], 0.0251[s]		
	$\rightarrow 4\,{}^1P$	0.000 76		0.0007[a], 0.001 02[c,d], 0.0002[g], 0.010[n], 0.001 35[s]		
	$\rightarrow 5\,{}^1P$	0.000 005		0.0012[a], 0.000 053[c], 0.000 08[g], 0.013[n]		

TABLE III. (*Continued*).

Atom or ion	Transition scheme	Dipole Oscillator Strength (a.u.) Calc.	Expt.	Other theoretical values	Transition scheme	Quadrupole oscillator strength (a.u.) Calc.
B^+	$2\,^1S \rightarrow 2\,^1P$	1.004	0.83±0.09$^{\delta}$, 0.73±0.07$^{\varepsilon}$, 0.9±0.2$^{\zeta}$	1.004^{d}, 1.00^{e}, 1.495^{f}, 1.01^{g}, 1.048^{i}, 1.021^{k}, 1.013^{l}, 1.1^{m}, 0.816^{n}, 1.003^{q}, 1.05^{t}, 1.069^{u}	$2\,^1S \rightarrow 3\,^1D$ $\rightarrow 4\,^1D$ $\rightarrow 5\,^1D$ $\rightarrow 6\,^1D$	1.60[−5] 4.99[−6] 2.24[−6] 1.20[−6]
	$\rightarrow 3\,^1P$	0.091		0.0908^{d}, 0.0256^{f}, 0.0957^{g}, 0.165^{n}, 0.092^{q}	$\rightarrow 7\,^1D$ $\rightarrow 8\,^1D$	7.68[−7] 5.61[−7]
	$\rightarrow 4\,^1P$	0.039		0.039^{d}, 0.0529^{g}, 0.078^{n}		
	$\rightarrow 5\,^1P$	0.02		0.042^{n}		
	$\rightarrow 6\,^1P$	0.011				
	$\rightarrow 7\,^1P$	0.006				
	$\rightarrow 8\,^1P$	0.0026				
C^{2+}	$2\,^1S \rightarrow 2\,^1P$	0.749	0.65±0.03$^{\eta}$	0.749^{c,d}, 0.76^{e}, 1.113^{f}, 0.764^{g,l}, 0.7654^{h}, 1.0746^{i}, 0.793^{i}, 1.112^{j}, 0.770^{j}, 0.776^{k}, 0.81^{m}, 0.674^{n}, 0.75^{q}, 0.794^{r}, 0.753^{s}, 0.797^{t}, 0.791^{u}	$2\,^1S \rightarrow 3\,^1D$ $\rightarrow 4\,^1D$ $\rightarrow 5\,^1D$ $\rightarrow 6\,^1D$ $\rightarrow 7\,^1D$ $\rightarrow 8\,^1D$	3.80[−5] 9.92[−6] 4.07[−6] 2.07[−6] 1.37[−6] 1.18[−6]
	$\rightarrow 3\,^1P$	0.223		0.223^{c,d}, 0.166^{f}, 0.236^{g}, 0.26^{m}, 0.302^{n}, 0.24^{q}, 0.216^{s}		
	$\rightarrow 4\,^1P$	0.078		0.0779^{c}, 0.0775^{d}, 0.054^{g}, 0.016^{m}, 0.022^{n}, 0.0783^{s}		
	$\rightarrow 5\,^1P$	0.036		0.0367^{c}, 0.085^{n}		
	$\rightarrow 6\,^1P$	0.02				
	$\rightarrow 7\,^1P$	0.012				
	$\rightarrow 8\,^1P$	0.009				
N^{3+}	$2\,^1S \rightarrow 2\,^1P$	0.596		0.596^{d}, 0.605^{e}, 0.614^{g}, 0.629^{i}, 0.619^{k}, 0.613^{l}, 0.64^{m,v}, 0.560^{n} 0.634^{r}, 0.641^{t}, 0.654^{w}, 0.631^{u}	$2\,^1S \rightarrow 3\,^1D$ $\rightarrow 4\,^1D$ $\rightarrow 5\,^1D$	1.63[−5] 5.77[−6] 2.53[−6]
	$\rightarrow 3\,^1P$	0.323		0.323^{d}, 0.336^{g}, 0.55^{m}, 0.390^{n}	$\rightarrow 6\,^1D$ $\rightarrow 7\,^1D$	1.33[−6] 7.80[−7]
	$\rightarrow 4\,^1P$	0.104		0.104^{d}, 0.107^{g}, 0.116^{n}	$\rightarrow 8\,^1D$	4.48[−7]
	$\rightarrow 5\,^1P$	0.047		0.046^{n}		
	$\rightarrow 6\,^1P$	0.025				
	$\rightarrow 7\,^1P$	0.015				
	$\rightarrow 8\,^1P$	0.010				
O^{4+}	$2\,^1S \rightarrow 2\,^1P$	0.495	0.42±0.05$^{\theta}$	0.495^{c,d}, 0.513^{e,g}, 0.742^{f}, 0.5146^{h}, 0.7055^{i}, 0.525^{i}, 0.741^{j}, 0.517^{j}, 0.518^{k}, 0.512^{l}, 0.53^{m}, 0.529^{r}, 0.499^{s}, 0.536^{t}, 0.550^{w}, 0.527^{u}	$2\,^1S \rightarrow 3\,^1D$ $\rightarrow 4\,^1D$ $\rightarrow 5\,^1D$ $\rightarrow 6\,^1D$ $\rightarrow 7\,^1D$	1.05[−4] 2.08[−5] 7.38[−6] 3.50[−6] 1.99[−6]
	$\rightarrow 3\,^1P$	0.4		0.400^{c,d}, 0.371^{f}, 0.406^{g}, 0.59^{m}, 0.394^{s}, 0.46^{x}	$\rightarrow 8\,^1D$	1.20[−6]
	$\rightarrow 4\,^1P$	0.121		0.121^{c,d,s}, 0.089^{g}		
	$\rightarrow 5\,^1P$	0.054				
	$\rightarrow 6\,^1P$	0.029				
	$\rightarrow 7\,^1P$	0.017				
	$\rightarrow 8\,^1P$	0.011				
F^{5+}	$2\,^1S \rightarrow 2\,^1P$	0.424		0.424^{d}, 0.435^{e}, 0.449^{i}, 0.440^{l}, 0.62^{m}, 0.454^{r}, 0.460^{t}, 0.475^{w}, 0.452^{u}	$2\,^1S \rightarrow 3\,^1D$ $\rightarrow 4\,^1D$ $\rightarrow 5\,^1D$ $\rightarrow 6\,^1D$	1.50[−4] 2.64[−5] 8.87[−6] 4.04[−6]
	$\rightarrow 3\,^1P$	0.458		0.458^{d}, 0.48^{m}, 0.51^{x}	$\rightarrow 7\,^1D$	2.25[−6]
	$\rightarrow 4\,^1P$	0.133		0.133^{d}	$\rightarrow 8\,^1D$	1.22[−6]
	$\rightarrow 5\,^1P$	0.058				
	$\rightarrow 6\,^1P$	0.031				
	$\rightarrow 7\,^1P$	0.018				
	$\rightarrow 8\,^1P$	0.011				

TABLE III. (*Continued*).

Atom or ion	Transition scheme	Dipole Oscillator Strength (a.u.) Calc.	Expt.	Other theoretical values	Transition scheme	Quadrupole oscillator strength (a.u.) Calc.
Ne^{6+}	$2\,^1S \rightarrow 2\,^1P$	0.370	0.336±0.025[ι],	0.370[d], 0.384[e], 0.393[i], 0.386[l],	$2\,^1S \rightarrow 3\,^1D$	2.01[−4]
			0.60[κ]	0.57[m], 0.399[r], 0.378[s], 0.404[t],	$\rightarrow 4\,^1D$	3.22[−5]
				0.418[w], 0.397[u]	$\rightarrow 5\,^1D$	1.03[−5]
	$\rightarrow 3\,^1P$	0.504		0.504[d], 0.493[s], 0.54[x]	$\rightarrow 6\,^1D$	4.63[−6]
					$\rightarrow 7\,^1D$	2.55[−6]
	$\rightarrow 4\,^1P$	0.142		0.143[d,s]	$\rightarrow 8\,^1D$	1.47[−6]
	$\rightarrow 5\,^1P$	0.062				
	$\rightarrow 6\,^1P$	0.033				
	$\rightarrow 7\,^1P$	0.019				
	$\rightarrow 8\,^1P$	0.012				

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transitions with large n, involving higher members of the isoelectronic series, no other data are available for comparison. Our results may serve as a reference for such cases. The number of linear variation parameters is confined to 12 for all the cases for computational simplicity. Results for the higher transitions for all the ions may be more accurately determined by choosing more diffuse basis sets with a larger number of parameters.

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