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Radiative lifetimes of triply excited states of the Li isoelectronic sequence

Nicos A. Piangos and Cleanthes A. Nicolaides
Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Avenue, Athens 116 35, Greece

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Singly, doubly, and triply excited states of the Li isoelectronic sequence have been represented by small expansions of self-consistent, state-specific wave functions containing important contributions from localized and asymptotic correlation components. These wave functions have been used for the prediction of wavelengths and probabilities of one-, two-, and three-electron radiative transitions along the sequence, up to Ne^{7+}. For Z around 8–10, the radiative lifetimes of the triply excited states are about 10^{-11}–10^{-13} s, a fact which might render them observable in emission.

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I. INTRODUCTION

Absorption from the ground state of one short-wavelength photon, or of many photons, or a variety of collisions at high energy, tend to involve parts of the electronic spectrum containing multiply excited states (MES's).

Although most of these are low-lying doubly excited states (DES's), triply excited states (TES's) are also known to appear in a variety of experiments (e.g., [1–5]). A few types of these (along the nonrelativistic isoelectronic sequence) belong to the discrete spectrum due to symmetry restrictions most often connected to their high spin. Their existence and properties were first predicted theoretically, such as, for example, the $1s2p^3 3s\ ^6S^0$, $1s2p^3 3p\ ^6P$, and $1s2p^3\ ^5S^0$ states of the boron and beryllium sequence [6,7], or the $2p^2 3p\ ^2S$ state of Li [8] or the $2p^3\ ^4S$ state [9,10], which in fact is the lowest member of a special class of TES's with a characteristic energy spectrum and geometric localization [11,12].

On the other hand, the overwhelming number of types of TES's are autoionizing nonrelativistically. Judging from the theoretical results on Li $2s^2 2p\ ^2P^0$ [13] and on He^- $2s2p^2\ ^4P$ [14] as well as from the experimental ones on He^- $2s2p^2\ ^2D$ [1], we estimate that along the isoelec-

TABLE I. Comparison of two sets of results for the absorption oscillator strengths to triply excited states of Li. In spite of the smallness of these numbers, the deviation between the results from small, state-specific wave functions of this work and those from large CI calculations done by Chung [20] is generally small. The accuracy of our results for the ionized members of the sequence is expected to be higher.

Transition	This work		Ref. [20]
	Length	Velocity	Length
$1s^2 2s\ ^2S \rightarrow 2s^2 2p\ ^2P^0$	1.0×10^{-3}	5.0×10^{-4}	1.424×10^{-3}
$2p^3\ ^2P^0$	1.2×10^{-3}	1.1×10^{-3}	7.848×10^{-4}
$1s^2 2p\ ^2P^0 \rightarrow 2s2p\ ^2D$	7.0×10^{-4}	2.4×10^{-4}	4.501×10^{-4}
^2S	3.0×10^{-4}	3.7×10^{-5}	3.254×10^{-4}
^2P	1.1×10^{-3}	3.7×10^{-4}	6.427×10^{-4}
$1s2s^2\ ^2S \rightarrow 2s^2 2p\ ^2P^0$	3.3×10^{-1}	2.3×10^{-1}	2.395×10^{-1}
$2p^3\ ^2P^0$	3.8×10^{-3}	9.6×10^{-3}	1.376×10^{-2}
$1s2s^2\ ^2P \rightarrow 2s^2 2p\ ^2P^0$	1.4×10^{-2}	1.6×10^{-2}	1.452×10^{-2}
$2p^3\ ^2D^0$	2.0×10^{-1}	1.7×10^{-1}	1.731×10^{-1}
$^2P^0$	7.5×10^{-2}	8.5×10^{-2}	7.326×10^{-2}
$1s2p^2\ ^2D \rightarrow 2s^2 2p\ ^2P^0$	2.5×10^{-3}	3.8×10^{-3}	3.568×10^{-3}
$2p^3\ ^2D^0$	1.2×10^{-1}	1.1×10^{-1}	1.195×10^{-1}
$^2P^0$	2.4×10^{-2}	2.3×10^{-2}	2.876×10^{-2}
$[1s(2s2p)^3P^0]^2P^0 \rightarrow 2s2p^2\ ^2D$	2.2×10^{-1}	2.3×10^{-1}	2.292×10^{-1}
^2S	4.4×10^{-2}	4.5×10^{-2}	4.397×10^{-2}
^2P	1.3×10^{-2}	1.3×10^{-2}	1.455×10^{-2}
$[1s(2s2p)^1P^0]^2P^0 \rightarrow 2s2p^2\ ^2D$	1.7×10^{-2}	2.4×10^{-2}	2.345×10^{-2}
^2S	4.5×10^{-2}	4.5×10^{-2}	4.397×10^{-2}
^2P	1.5×10^{-1}	1.5×10^{-1}	1.601×10^{-1}

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TABLE II. Nonrelativistic excitation energies of the $n=2$ intrashell TES's of the Li isoelectronic sequence, in eV above the corresponding ground-state "exact" nonrelativistic energies (Li$=7.478\,025$ a.u. [23], Be$^{+}=-14.323\,50$ a.u. [24], C$^{3+}=-34.775\,509$ a.u. [25], O$^{3+}=-64.228\,540$ a.u. [25], and Ne$^{7+}=-102.682\,229$ a.u. [25]). Our results are obtained according to the state-specific theory (SST) of such states, whose major first step is finding a stationary discrete solution in the continuous spectrum by solving for the important few configurations self-consistently. The numbers in parentheses next to the state label refer to the number of these configurations.

State	Li	Be^{+}	C^{3+}	O^{5+}	Ne^{7+}
$2s^22p\,^2P^0$ (15)					
SST (MCHF)	142.37	268.85	644.62	1183.71	1886.08
Ref. [21]	142.272	268.748			
Ref. [22]	142.598	269.248	645.252	1184.479	1886.943
$2s2p^2\,^2D$ (11)					
SST (MCHF)	145.03	272.88	651.38	1193.17	1898.27
Ref. [21]	144.817	272.653			
Ref. [22]					
$2s2p^{2\,2}S$ (11)					
SST (MCHF)	146.85	275.65	655.92	1199.47	1906.29
Ref. [21]	146.517	275.330			
Ref. [22]	147.443	276.654	657.302	1201.076	1908.002
$2s2p^2\,^2P$ (9)					
SST (MCHF)	147.26	276.12	656.64	1200.48	1907.61
Ref. [22]	146.990	275.842			
Ref. [22]					
$2p^3\,^2D^0$ (8)					
SST (MCHF)	147.14	276.19	657.10	1201.31	1908.80
Ref. [21]	146.960	275.998			
Ref. [22]					
$2p^3\,^2P^0$ (11)					
SST (MCHF)	149.31	279.36	662.24	1208.41	1917.86
Ref. [21]	148.972	278.978			
Ref. [22]	149.251	280.264	663.664	1210.115	1919.748
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Ref. [22]					

TABLE II. (*Continued.*)

State	Li	Be^+	C^{3+}	O^{5+}	Ne^{7+}
$2p^3\,{}^2P^0$ (11)					
SST (MCHF)	149.31	279.36	662.24	1208.41	1917.86
Ref. [21]	148.972	278.978			
Ref. [22]	149.251	280.264	663.664	1210.115	1919.748

tronic sequence the autoionization lifetimes of such $n=2$ intrashell states ought to be of the order of $10^{-13}-10^{-15}$ s, depending on the availability of open channels, on the electronic structure, and on the degree of bound-continuum wave-function overlaps. At the neutral end of the isoelectronic sequence, such lifetimes do not allow any observation of radiative transitions to lower states. Nevertheless, absorption oscillator strengths are still useful since the MES's of the neutral end can in principle be probed during photoabsorption.

As the energy differences increase along the isoelectronic sequence, it is reasonable to expect that radiative transitions to lower states can indeed occur in ions, with rates of the order of $10^{12}-10^{13}$ s^{-1}, so that they could be identified in beam-foil spectra [15], or during gaseous collision processes, or after dielectronic recombination in

TABLE III. Transition wavelengths from the MCHF energies of this work (column a) and from previous configuration-interaction calculations (column b) (Refs. [20,21,23–27]).

Transition	Li		Be^+		C^{3+}		O^{5+}		Ne^{7+}	
	a	b	a	b	a	b	a	b	a	b
One-electron transitions										
$1s^22s\,{}^2S\rightarrow[1s(2s2p)^3P^0]^2P^0$	210.08	210.45	104.30		41.26		22.02		13.66	13.66
$1s^22p\,{}^2P^0\rightarrow 1s2p^2\,{}^2D$	209.35	209.37	104.63		41.54		22.13		13.72	13.71
^2P	207.40	207.48	104.03	104.05	41.37	41.37	22.06	22.048	13.68	13.67
^2S	201.50		101.46		40.67		21.78		13.55	13.54
$1s2s^2\,{}^2S\rightarrow 2s^2p\,{}^2P^0$	144.60	144.38	80.35		35.15		19.59		12.46	
$[1s(2s2p)^3P^0]^2P^0\rightarrow 2s2p^2\,{}^2D$	144.48	144.34	80.62		35.37		19.68		12.52	
^2P	140.89	140.77	78.98		34.85		19.46		12.40	
^2S	141.51	141.53	79.19		34.91		19.49		12.42	
$1s2p^2\,{}^2D\rightarrow 2p^3\,{}^2D^0$	144.36	144.35	80.78		35.40		19.72		12.54	
$\rightarrow {}^2P^0$	141.00	141.05	79.18		34.90		19.50		12.42	
$^2P\rightarrow {}^2D^0$	145.30	145.28	81.14	81.09	35.52		19.77		12.57	
$\rightarrow {}^2P^0$	141.89	141.94	79.53	79.53	35.01		19.55		12.45	
$^2S\rightarrow {}^2P^0$	144.79		81.10		35.53		19.78		12.57	
Two-electron transitions										
$1s^22s\,{}^2S\rightarrow 2s^22p\,{}^2P^0$	87.22	87.15	46.16	46.13	19.24		10.48		6.57	
$1s^22p\,{}^2P^0\rightarrow 1s2p^2\,{}^2S$	227.14	227.26	112.38		43.74		23.03		14.17	14.16
$\rightarrow 2s2p^2\,{}^2D$	86.70	86.72	46.15	46.13	19.28		10.50		6.59	
$\rightarrow {}^2P$	85.39	85.43	45.61	46.34	19.13		10.44		6.56	
$\rightarrow {}^2S$	85.62	85.70	45.68	45.68	19.15		10.14		6.56	
$1s^23d\,{}^2D\rightarrow[1s(2s2p)^3P^0]^2P^0$	224.58	225.21	116.06		47.61		25.85		16.19	16.20
$1s2p^2\,{}^2D\rightarrow 2s^22p\,{}^2P^0$	152.87	152.68	84.84		36.71		20.29		12.83	
$^2P\rightarrow {}^2P^0$	153.93	153.73	85.24	85.12	36.84		20.35		12.85	
$^2S\rightarrow {}^2P^0$	157.35		87.05		37.42		20.59		12.99	
Three-electron transitions										
$1s^22s\,{}^2S\rightarrow 2p^3\,{}^2P^0$	83.22	83.23	44.43	44.44	18.73		10.26		6.47	
$1s^23d\,{}^2D\rightarrow 2s^22p\,{}^2P^0$	89.62	89.58	48.32	48.31	20.52		11.27		7.11	
$\rightarrow 2p^3\,{}^2P^0$	85.40	85.45	46.43	46.46	19.94		11.02		6.98	
$\rightarrow {}^2D^0$	86.63	86.65	46.98	46.98	20.10		11.09		7.02	
$1s2s^2\,{}^2S\rightarrow 2p^3\,{}^2P^0$	133.93	135.94	75.26		33.48		18.86		12.08	

plasmas. Thus, in order to facilitate future spectroscopic studies and at the same time to contribute to our understanding of the electronic structure and properties of TES's, we undertook a series of computations of the wavelengths (λ in Å) and of the radiative transition probabilities (A in s^{-1}) for one-, two-, and three-electron intershell transitions involving many doublet states of the Li sequence, of which the autoionizing TES's are assigned the configurations $2s^2 2p\ ^2P^0$, $2s2p^2\ ^2D$, ^2S, ^2P, $2p^3\ ^2D^0$, $^2P^0$.

Although the *ab initio* calculations stop at $Z=10$, extrapolation to higher stages of ionization, where the wavelengths as well as the radiative lifetimes will be shorter, can be carried out straightforwardly. However, given the increasing importance of relativistic corrections and the fact that many nonrelativistic wavelengths approach each other already at $Z=10$ (Table III), such an extrapolation should probably aim at estimates for transitions between averaged configurations rather than between nonrelativistic LS states. We note that we also computed the probabilities for the intrashell transitions among the TES's. These turned out to be too small for the radiative decay to be observable. For example, even for $Z=10$ where the wavelengths are in the neighborhood of 600–1200 Å, the corresponding lifetimes are of the order of 10^{-9}–10^{-8} s.

II. THEORETICAL APPROACH

Autoionizing states are embedded in the continuous spectrum while in most cases their wave functions are strongly correlated. Therefore, for the *ab initio* computation of a large number of data involving such states, it is necessary for the theoretical approach not only to be properly justified but also to combine physically meaningful accuracy with economy. The computations herein are based on the state-specific approach ([16,17], and references therein), which starts with a multiconfigurational Hartree-Fock (MCHF) wave function consisting of properly selected few configurations and continues, if necessary by the requirements of the problem, with the inclusion of the remaining localized and asymptotic multichannel correlation. In this way it is possible to obtain efficiently properties of a variety of polyelectronic highly excited states and not of just specialized cases of two- or three-electron systems.

In this work, we computed two types of correlated wave functions for the TES's. The first was obtained by the numerical MCHF method [18]. The justification of such computations for states embedded in the continuum is discussed in [16,17]. These MCHF wave functions contained only a few symmetry-adapted configurations (SAC's) consisting of $n=2$ and 3 orbitals. According to the arguments given in [17] and in earlier papers, strongly mixing open-channel-like (OCL) configurations representing continuum contributions were included. It is noteworthy that in one or two cases where inclusion of OCL configurations prevented convergence of the MCHF calculation for the negative ion of the sequence, He$^-$, for the neutral and the positive ions this did not happen. For example, for the $2s2p^2\ ^2S$ TES, the inclusion of the OCL $2s^2 3s$ does not allow convergence in He$^-$, but it causes no

TABLE IV. Absolute values of the coefficients of the major configurations constituting the localized part of the autoionizing $n=2$ intrashell triply excited states of the Li isoelectronic sequence (not normalized to unity). The criterion used for their choice is that they are larger than 0.05 in Li. The number in parentheses below each label represents the total number of MCHF configurations used in the computation.

State	Z	3	4	6	8	10	State	Z	3	4	6	8	10
$^2P^0$	$2s^2 2p$	0.908	0.919	0.928	0.932	0.934	^2D	$2s2p^2$	0.969	0.983	0.993	0.996	0.997
(15)	$(2s2p)^1P^0 3d$	0.113	0.089	0.062	0.047	0.038	(11)	$2s^2 3d$	0.147	0.106	0.067	0.049	0.039
	$(2s2p)^3P^0 3d$	0.117	0.092	0.064	0.049	0.039		$2s3p^2$	0.070	0.047	0.028	0.020	0.016
	$2p^3$	0.378	0.369	0.359	0.354	0.351		$2s3d^2$	0.057	0.044	0.030	0.023	0.018
								$3d(2p^2)^3P$	0.161	0.126	0.087	0.066	0.053
								$(3s2p)^3P^0 3p$	0.058	0.040	0.025	0.018	0.014
^2S	$2s2p^2$	0.961	0.987	0.995	0.997	0.998	^2P	$2s2p^2$	0.956	0.973	0.986	0.991	0.993
(11)	$2s^2 3s$	0.184	0.081	0.041	0.028	0.021	(9)	$3s3p^2$	0.052	0.035	0.021	0.015	0.011
	$2s3p^2$	0.108	0.071	0.042	0.029	0.023		$3d(2p^2)^3P$	0.157	0.120	0.080	0.060	0.048
	$2s4d^2$	0.116	0.091	0.061	0.045	0.036		$3d(2p^2)^1D$	0.218	0.171	0.117	0.088	0.071
	$(3s2p)^3P^0 3p$	0.074	0.047	0.027	0.019	0.015		$(3s2p)^1P^0 3p$	0.057	0.040	0.025	0.018	0.014
	$2s3s^2$	0.054	0.030	0.017	0.012	0.009		$(3s2p)^2P^0 3p$	0.055	0.036	0.021	0.015	0.012
	$3s2p^2$	0.092	0.054	0.045	0.042	0.004		$3s2p^2$	0.063	0.067	0.071	0.073	0.074
$^2D^0$	$2p^3$	0.955	0.977	0.991	0.995	0.997	$^2P^0$	$2p^3$	0.886	0.909	0.924	0.930	0.933
(8)	$(2s2p)^1P^0 3d$	0.093	0.075	0.052	0.040	0.032	(11)	$2s^2 2p$	0.384	0.371	0.362	0.357	0.353
	$(2s2p)^3P^0 3d$	0.248	0.175	0.108	0.077	0.060		$(2s2p)^1P^0 3d$	0.142	0.107	0.069	0.050	0.040
	$2p(3s^2)^3P$	0.065	0.051	0.035	0.027	0.021		$(2s2p)^3P^0 3d$	0.095	0.075	0.049	0.036	0.029
	$2p(3d^2)^1D$	0.055	0.048	0.034	0.026	0.021		$2p(3d^2)^1S$	0.119	0.091	0.060	0.045	0.035
	$2p(3p^2)^3P$	0.059	0.041	0.025	0.018	0.014		$2p(3p^2)^1S$	0.086	0.058	0.035	0.025	0.019
	$2p(3p^2)^1D$	0.080	0.055	0.034	0.025	0.019		$2p(3p^2)^3P$	0.057	0.039	0.024	0.017	0.013
								$2p(3p^2)^1D$	0.060	0.041	0.024	0.017	0.014
								$2p3s^2$	0.083	0.043	0.023	0.016	0.012

problem in Li (where its coefficient is 0.193) up to Ne^{7+} (where its coefficient is reduced to 0.021) (Table IV). In addition, in certain cases the final choice of the MCHF function was made after careful analysis of the effect of singly excited configurations in the presence of doubly excited ones, to which they may be connected by orbital rotation (e.g., $2s2p^2$, $2s2p3p$, $2s3p^2$ or $1s2s^2$, $1s2s3s$, $1s3s^2$).

Compact MCHF wave functions with selected configurations representing the most important electron correlations were also computed for the lower-lying states to which the TES's decay radiatively. The corresponding total energies were used for the determination of the energy differences. On the other hand, following the arguments on the interplay between atomic structure and the dynamics of photoabsorption ([19], and references therein) we also computed a second type of correlated TES wave functions for the transition probabilities, where *all* possible SAC's were included that can be constructed from $n=2$ and 3 orbitals. However, for reasons of economy and/or of convergence, the additional configurations were not subjected to self-consistent optimization. In other words, these wave functions were obtained by a single diagonalization using the orbitals of the small MCHF computation.

III. RESULTS

Our results are presented in Tables I–VI. In order to have an indication of their level of accuracy, we have compared when possible, directly or indirectly, with results of other computations which used much larger correlated wave functions obtained by configuration-interaction (CI) methods [20–27] (Tables I–III).

Table I presents nonrelativistic excitation energies. The state-specific MCHF wave functions were obtained with orthogonality constraints to the 1*s* orbital of the corresponding hydrogenic ion. Only 15 symmetry-adapted configurations were used for the $2s^22p\,^2P^0$ state, 11 for the $2p^3\,^2P^0$, 11 for the $2s2p^2\,^2D$, 11 for the $2s2p^2\,^2S$, 9 for the $2s2p^2\,^2P$, and 8 for the $2p^3\,^2D^0$. We also list the re-

TABLE V. Transition probabilities in s^{-1}, for one-, two-, and three-electron jumps, involving triply, doubly, and singly excited states of the Li isoelectronic sequence. The number in brackets stands for the power of ten.

	Li		Be^+		C^{3+}		O^{5+}		Ne^{7+}	
Transition	*L*	*V*	*L*	*V*	*L*	*V*	*L*	*V*	*L*	*V*
					One-electron transitions					
$1s^22s\,^2S \rightarrow [1s(2s2p)^3P^0]^2P^0$	1.6[10]	1.3[10]	9.1[10]	8.1[10]	7.9[11]	7.9[11]	2.8[12]	2.7[12]	7.7[12]	7.4[12]
$1s^22p\,^2P^0 \rightarrow 1s2p^2\,^2D$	8.2[9]	7.0[9]	5.2[10]	4.7[10]	4.2[11]	3.9[11]	1.6[12]	1.5[12]	4.4[12]	4.2[12]
$\rightarrow {}^2P$	2.1[10]	2.1[10]	1.3[11]	1.3[11]	1.1[12]	1.1[12]	4.5[12]	4.4[12]	1.2[13]	1.2[13]
$\rightarrow {}^2S$	9.1[9]	7.6[9]	5.4[10]	4.2[10]	4.24[11]	3.5[11]	1.6[12]	1.4[12]	4.2[12]	3.7[12]
$1s2s^2\,^2S \rightarrow 2s^22p\,^2P^0$	3.5[10]	2.5[10]	1.2[11]	9.6[10]	6.4[11]	5.8[11]	2.1[12]	2.0[12]	5.3[12]	5.1[12]
$[1s(2s2p)^3P^0]^2P^0 \rightarrow 2s2p^2\,^2D$	4.1[10]	4.4[10]	1.7[11]	1.8[11]	1.0[12]	1.0[12]	3.6[12]	3.7[12]	9.4[12]	9.6[12]
$\rightarrow {}^2P$	4.3[9]	4.2[9]	1.7[10]	1.6[10]	1.6[11]	1.5[11]	3.7[11]	3.5[11]	9.5[11]	9.1[11]
$\rightarrow {}^2S$	4.4[10]	4.5[10]	1.8[11]	1.8[11]	1.1[12]	1.0[12]	3.7[12]	3.7[12]	9.6[12]	9.6[12]
$1s2p^2\,^2D \rightarrow 2p^3\,^2D^0$	3.9[10]	3.4[10]	1.6[11]	1.4[11]	9.4[11]	8.9[11]	3.2[12]	3.1[12]	8.1[12]	7.8[12]
$\rightarrow {}^2P^0$	1.3[10]	1.3[10]	6.8[10]	6.1[10]	4.6[11]	4.1[11]	1.6[12]	1.5[12]	4.1[12]	3.8[12]
${}^2P \rightarrow {}^2D^0$	3.7[10]	3.2[10]	1.5[11]	1.3[11]	9.1[11]	8.6[11]	3.1[12]	3.0[12]	8.0[12]	7.8[12]
$\rightarrow {}^2P^0$	2.5[10]	2.8[10]	1.1[11]	1.2[11]	7.3[11]	7.4[11]	2.6[12]	2.6[12]	6.7[12]	6.7[12]
${}^2S \rightarrow {}^2P^0$	1.5[10]	1.6[10]	6.4[10]	6.8[10]	4.0[11]	4.1[11]	1.4[12]	1.4[12]	3.6[12]	3.6[12]
					Two-electron transitions					
$1s^22s\,^2S \rightarrow 2p^22p\,^2P^0$	3.0[8]	1.5[8]	9.7[8]	4.2[7]	3.9[9]	1.5[9]	8.8[9]	3.1[9]	1.6[10]	5.2[9]
$1s^22p \rightarrow 1s2s^2\,^2S$	2.6[9]	1.4[8]	9.2[9]	1.7[9]	4.8[10]	2.2[10]	1.6[11]	9.8[10]	4.2[11]	2.9[11]
$\rightarrow 2s2p^2\,^2D$	3.7[8]	1.3[8]	1.4[9]	4.8[8]	4.6[9]	1.7[9]	9.1[9]	3.8[9]	1.4[10]	6.5[9]
$\rightarrow {}^2P$	9.7[8]	3.4[8]	3.8[9]	1.3[8]	1.3[10]	5.0[9]	2.6[10]	1.1[10]	4.1[10]	1.9[10]
$\rightarrow {}^2S$	8.2[8]	1.0[8]	1.7[9]	4.5[8]	5.5[9]	1.7[9]	1.2[10]	3.4[9]	2.3[10]	6.4[9]
$1s^23d\,^2D \rightarrow [1s(2s2p)^3P^0]^2P^0$	1.6[8]	5.2[6]	5.5[8]	1.3[7]	2.0[9]	7.3[7]	3.6[9]	4.7[7]	6.1[9]	7.8[7]
$1s2p^2\,^2D \rightarrow 2s^22p\,^2P^0$	1.2[9]	1.8[9]	5.8[9]	9.0[9]	4.3[10]	6.2[10]	1.5[11]	2.1[11]	4.1[11]	5.3[11]
${}^2P \rightarrow {}^2P^0$	4.0[9]	4.5[9]	1.6[10]	1.8[10]	9.7[10]	1.1[11]	3.3[11]	3.7[11]	8.6[11]	9.4[11]
${}^2S \rightarrow {}^2P^0$	6.4[6]	1.1[8]	1.2[6]	2.8[8]	4.7[7]	1.5[9]	2.6[8]	4.2[9]	1.0[9]	9.6[9]
					Three-electron transitions					
$1s^22s\,^2S \rightarrow 2p^3\,^2P^0$	2.6[8]	1.8[7]	6.2[8]	3.1[7]	2.1[9]	8.5[7]	4.4[9]	1.7[8]	7.7[9]	2.9[8]
$1s^23d\,^2D \rightarrow 2s^22p\,^2P^0$	1.7[7]	3.1[3]	5.0[7]	8.3[3]	4.6[7]	1.7[6]	6.8[7]	2.6[6]	9.1[7]	3.4[6]
$\rightarrow 2p^3\,^2P^0$	4.6[7]	7.4[5]	2.3[8]	4.4[6]	1.1[9]	1.7[7]	2.8[9]	3.5[7]	5.1[9]	5.9[7]
$\rightarrow {}^2D^0$	7.2[4]	2.1[3]	3.7[6]	4.3[5]	5.3[7]	1.1[7]	1.9[8]	4.6[7]	4.2[8]	1.1[8]
$1s2s^2\,^2S \rightarrow 2p^3\,^2P^0$	4.1[8]	1.2[9]	7.5[8]	2.4[9]	3.3[9]	9.1[9]	1.1[10]	2.5[10]	2.8[10]	5.6[10]

TABLE VI. Absorption oscillator strengths (length form) from the ground and the $1s^22p\ ^2P^0$ and $1s^23d\ ^2D$ excited states of Li and Ne^{7+} to triply excited states, from state-specific Hartree-Fock (HF) and correlated wave functions. The results show again (see Refs. [19,28]) that the occurrence of multielectron transitions does not always have electron correlation as the exclusive cause. They are also allowed by the nonorthonormality between the self-consistent orbitals of initial and final states. In fact, the HF and the correlated results are often quite similar—given the very small order of magnitude of such transitions—suggesting that, depending on zeroth-order electronic structure, the dynamics of multielectron photoabsorption can be understood semiquantitatively without invoking electron correlation.

Transition	Li		Ne^{7+}	
	HF	Correlated	HF	Correlated
$1s^22s\ ^2S \rightarrow 2s^22p\ ^2P^0$	1.0×10^{-3}	1.0×10^{-3}	4.1×10^{-4}	3.0×10^{-4}
$1s^22p\ ^2P^0 \rightarrow 2s2p^2\ ^2D$	1.6×10^{-3}	7.0×10^{-4}	3.3×10^{-4}	1.6×10^{-4}
^2P	2.7×10^{-3}	1.1×10^{-3}	6.5×10^{-4}	2.7×10^{-4}
^2S	3.4×10^{-4}	3.0×10^{-4}	6.9×10^{-5}	5.0×10^{-5}
$1s^23d\ ^2D \rightarrow 2s^22p\ ^2P^0$	6.0×10^{-6}	1.2×10^{-5}	2.0×10^{-7}	4.2×10^{-7}

sults of earlier calculations [21,22]. Those of Ahmed and Lipsky [22] were obtained from large CI calculations with hydrogenic basis sets where the three-electron product functions exclude the $1s$ orbital. Considering the difference in the size of the computations of the two methods, it is clear that the major part of the interelectronic interactions in TES's is described by a few configurations, if they are computed self-consistently. On the other hand, in the extensive calculations of Chung and Davis on Li and Be^+ [21] large Slater-type orbital (STO) bases have been used with variationally optimized nonlinear parameters, and we expect them to be reliable to at least the first decimal digit. Thus they constitute good reference points. Comparison with the present state-specific results suggests that the inaccuracy which is to be expected for the remaining ions of the sequence is in the neighborhood of 0.2–0.3 eV. Of course, improvement of our results by inclusion of additional localized correlation is straightforward (e.g., [17]). Nevertheless, it was considered unnecessary for the practical purposes of the present work which aimed at economically producing a large number of *energy differences* and of transition probabilities for wave functions computed at approximately the same level of accuracy involving hitherto unexplored states in ions.

Table IV presents MCHF configurations whose mixing coefficients are larger than 0.05, from which the basic electronic structure features of these TES's can be understood. As Z increases, the single configurational or the hydrogenic degeneracy description dominates, while contributions from localized or asymptotic correlation components are reduced drastically.

Tables III and V give the computed wavelengths and transition probabilities [length (L) and velocity (V) forms] for a large number of transitions. These have been classified into categories of one-electron, two-electron, and three-electron intershell transitions. It is probable that many of these transitions are identifiable experimentally. The present MCHF wave functions contain the most important nonrelativistic correlation effects and we expect that what is left out does not alter the result significantly when energy differences are computed. This proposition is corroborated by the favorable comparison with wavelengths deduced from a combination of published accurate total energies (Refs. [20,21,23–27]) (column b of Table III). The good agreement for the cases where comparison can be made suggests that the remainder of our predicted wavelengths ought to offer useful guidance to spectroscopic research on the MES's of this isoelectronic sequence. For one- and two-electron transitions, the reliability of these probabilities is in general high. The results for the simultaneous transition of three electrons are not expected to have the same level of accuracy because the oscillator strengths are very small (order of 10^{-3}–10^{-7}). Nevertheless, they are also useful since not much information exists for such transitions. The numbers for C^{3+}, O^{5+}, and Ne^{7+} show that the radiative lifetimes of these TES's are about 10^{-12}–10^{-13} s. Also of interest is the fact that the inner hole states $1s2s^2$, $1s2s2p$, and $1s2p^2$ acquire relatively short lifetimes, 10^{-12}–10^{-13} s, after C^{3+}.

Finally, Table VI contains the f values for transitions to TES's obtained from state-specific HF (single configuration) and correlated wave functions. The purpose of this table is to support earlier arguments [19,28] that multielectron electric dipole transitions not only are allowed in the single configuration approximation but that their occurrence can be interpreted semiquantitatively as being caused mainly by the coupling of *all* the electrons (and not just the one seemingly making the dipole transition) in the two different self-consistent fields of initial and final states.

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[1] G. J. Schultz, Rev. Mod. Phys. **45**, 378 (1973); P. J. Hicks, C. Cvejanovic, J. Comer, F. H. Read, and J. M. Sharp, Vacuum **24**, 573 (1974).

[2] R. Bruch, G. Paul, J. Andrä, and L. Lipsky, Phys. Rev. A **12**, 1808 (1975); M. Rodbro, R. Bruch, and P. Bisgaard, J. Phys. B **12**, 2413 (1979).

[3] A. Müller, G. Hofmann, B. Weissbecker, M. Stenke, K. Tinschert, M. Wagner, and E. Salzborn, Phys. Rev. Lett.

63, 758 (1989).

[4] E. Träbert, P. H. Heckmann, J. Doerfert, and J. Granzow, J. Phys. B **25**, L353 (1992).

[5] E. Knystautas, J. Phys. B **25**, L395 (1992); Phys. Rev. Lett. **69**, 2635 (1992).

[6] D. R. Beck and C. A. Nicolaides, Phys. Lett. **61A**, 227 (1977).

[7] C. F. Bunge, Phys. Rev. Lett. **44**, 1450 (1980).

[8] D. R. Beck, Int. J. Quantum Chem. **S16**, 345 (1982).

[9] D. R. Beck and C. A. Nicolaides, Chem. Phys. Lett. **59**, 525 (1978).

[10] C. A. Nicolaides and Y. Komninos, Chem. Phys. Lett. **80**, 463 (1981); C. A. Nicolaides, Y. Komninos, and D. R. Beck, Phys. Rev. A **24**, 1103 (1981).

[11] Y. Komninos, M. Crysos, and C. A. Nicolaides, Phys. Rev. A **38**, 3182 (1988).

[12] C. A. Nicolaides, M. Crysos, and Y. Komninos, Phys. Rev. A **41**, 5244 (1990)

[13] R. L. Simons and H. P. Kelly, Phys. Rev. A **22**, 625 (1980).

[14] C. A. Nicolaides, Phys. Rev. A **46**, 690 (1992).

[15] S. Mannervik, Phys. Scr. **40**, 28 (1989).

[16] C. A. Nicolaides, in *Applied Many-Body Methods in Spectroscopy and Electronic Structure,* edited by D. Mukherjee (Plenum, New York, 1992), p. 233.

[17] C. A. Nicolaides, N. A. Piangos, and Y. Komninos, Phys. Rev. A (to be published).

[18] C. Froese-Fischer, Comput. Phys. Commun. **14**, 145 (1978).

[19] C. A. Nicolaides, in *Giant Resonances in Atoms, Molecules, and Solids,* edited by J. P. Connerade, J. M. Esteva, and R. C. Karnatak (Plenum, New York, 1987), p. 213.

[20] K. T. Chung, Phys. Rev. A **24**, 1350 (1981); **25**, 1596 (1982).

[21] K. T. Chung and B. F. Davis, in *Autoionization,* edited by A. Temkin (Plenum, New York, 1985), p. 73.

[22] M. Ahmed and L. Lipsky, Phys. Rev. A **12**, 1176 (1975).

[23] S. Larsson, Phys. Rev. **169**, 49 (1968).

[24] A. W. Weiss, Phys. Rev. **122**, 1826 (1961).

[25] F. W. King, Phys. Rev. A **40**, 1735 (1989).

[26] B. F. Davis and K. T. Chung, Phys. Rev. A **39**, 3942 (1989).

[27] R. Bruch, D. Schneider, M. H. Chen, K. T. Chung, and B. F. Davis, Phys. Rev. A **44**, 5659 (1991).

[28] C. A. Nicolaides, Chem. Phys. Lett. **101**, 435 (1983); J. Phys. B **26**, L291 (1993).