Production of excited $Be^+ 1s^2 2p$ ions from decay of $1s2s^2 2p$

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Based on a photoabsorption experiment on Be I, Caldwell *et al.* [Phys. Rev. A **41**, 542 (1990)] have shown that the $1s2s^2 2p\ ^1P^\circ$ state decays mainly through the $(1s^2 2p,e)$ Auger channel. It is also remarked that this can be regarded as a common feature for the Be-like series. We present accurate energies of $^1P^\circ$ on Be I, B II, C III, and O V that lead to identifications in high-resolution Auger experimental measurements from ion-atom and ion-molecule collisions. We show that, while the $1s2s^2 2p\ ^1P^\circ \rightarrow (1s^2 2p,e)$ decay channels are clearly seen in the reported spectra, the $1s2s^2 2p\ ^1P^\circ \rightarrow (1s^2 2s,e)$ channels are either extremely weak or not reported at all. This gives unambiguous support to the conclusion of Caldwell *et al.* The calculated $1s2s^2 2p\ ^1P^\circ$ energy in this work is 115.52 eV above the $1s^2 2s^2$ level of Be I. This agrees well with the 115.5 eV found in the experiment.

In a recent Rapid Communication, Caldwell *et al.*[1] reported a photoabsorption experiment on Be I. They found that the $1s$-$2p$ resonance absorption occurred at 115.5 eV. By studying the decay of this $1s2s^2 2p\ ^1P^\circ$ resonance, they found further that the $(1s^2 2p,e)$ channel is 95% of the entire decay of this resonance state. This is a surprise in that the ground-state Be II $(1s^2 2s,e)$ decay channel is almost invisible. The experiment of Caldwell *et al.* is particularly valuable because the photoabsorption experiment is strongly symmetry selective. As a consequence, the resulting spectrum is much easier to analyze. Furthermore, in most cases, the photon energies can be measured to a high degree of accuracy, thus giving a smaller error bar for the energy of a resonance state. By comparing with the B II calculation of Petrini,[2] Caldwell *et al.* speculate that this $(1s^2 2p,e)$ decay channel dominance can be regarded as a common feature for the Be-like series.[1]

In 1979, high-resolution Auger spectra on beryllium, boron, and carbon were reported by Rødbro, Bruch, and Bisgaard.[3] The experiment was carried out using ion-atom and ion-molecule collision systems. The boron and carbon spectra from this experiment were subsequently recalibrated.[4,5] Mann also reported a high-resolution Auger spectrum for carbon ions using a multiple-electron-capture technique.[6] High-resolution *KLL* Auger spectra of oxygen ions on helium were reported by Bruch *et al.*[7] A special feature of these experiments is the breakdown of selection rules. As a result, resonances of assorted symmetry show up in the measured spectra. However, for four-electron resonances, due to the lack of accurate theoretical data, most of these spectral lines have not been unambiguously identified. Although the interesting phenomena reported by Caldwell *et al.*[1] [i.e., the weak or nonobservance of $(1s^2 2s,e)$ from $1s2s^2 2p\ ^1P^\circ$] should be true in each of these Auger spectra mentioned above, only the decays of $1s2s^2 2p\ ^1P^\circ$ of oxygen were studied by Bruch and co-workers.[8]

The lithiumlike Auger lines in the spectra of Refs. 3–7 were unambiguously identified by theoretical data from the saddle-point method.[9] In the past, the applications of this method have been limited to two- or three-electron systems. Recently, we have constructed the computer code necessary for the calculation of four- or more electron atomic resonances. Extensive calculations have been carried out for over 60 $(1s2l2l'2l'')$ resonances for the Be I, B II, C III, and O V systems. These results give very interesting and consistent identification to the four-electron lines in the observed spectra. Among these results are the $1s2s^2 2p\ ^1P^\circ$ resonances of Be I, B II, C III, and O V. In this work, the calculated results of this resonance will be used to compare with observed experiments. One can show that the conclusion of Caldwell *et al.* is actually supported by all these existing collision experiments.

To calculate the $1s2s^2 2p\ ^1P^\circ$ resonance a multiconfiguration wave function is used. The method and procedure is very similar to our earlier work.[10] The angular partial waves of this singlet P resonance are represented by

$$Y^L = [(l_1,l_2)l_{12},l_3]l_{123},l_4 \ . \tag{1}$$

This implies that the angular momenta of electrons 1 and 2 couple into l_{12} which in turn couples with l_3 into l_{123}. The final P state is obtained by coupling l_{123} with l_4. Similarly, the two singlet spinor functions are given by

$$\chi_1 = [(s_1,s_2)1,s_3]_{\frac{1}{2}},s_4 \tag{2}$$

and

$$\chi_2 = [(s_1,s_2)0,s_3]_{\frac{1}{2}},s_4 \ . \tag{3}$$

The basis set for the radial functions are given by Slater-type orbitals

$$\varphi(1,2,3,4) = r_1^i r_2^j r_3^m r_4^n \exp[-(\alpha_1 r_1 + \alpha_2 r_2 + \alpha_3 r_3 + \alpha_4 r_4)] \ . \tag{4}$$

The α's are the nonlinear parameters determined in the optimization process. In order to account for the correlation of the system a large basis set is chosen. In the case of Be I, a 29 partial-wave 496-term wave function is

used. A smaller wave function is selected by eliminating some terms with small energy contributions. The final wave function contains 286 terms, giving a nonrelativistic energy of $-10.420\,905$ a.u. The convergence of this calculation is shown in Table I. It is apparent from this table that various angular couplings contribute strongly to the correlation of this four-electron $1s$ core-excited state, making a precision calculation very challenging.

The relativistic effects contribute significantly to the energies of systems in this work. The relativistic corrections included are corrections to the kinetic energy, Darwin term, electron-electron Fermi contact term, and orbit-orbit interaction.[11] The nonrelativistic mass polarization correction is also included. The explicit expression of these operators was given in an earlier work.[12] The corrections to the energy are computed using first-order perturbation theory. The corrected total energy becomes $-14.422\,946$ a.u. for this $^1P^\circ$ resonance. Compared with the relativistic corrected energies $-14.325\,852$ a.u. for $1s^22s$ and $-14.180\,132$ a.u. for $1s^22p$, it implies that the energy of the Auger electron in the $(1s^22p,e)$ channel is 102.24 eV and that of the $(1s^22s,e)$ channel is 106.20 eV. The conversion factor 1 a.u. = 27.211 66 eV is used in this work. It should be noted that the nonrelativistic $1s^22s$ energies used in this work are slightly higher than the very precise results of King[13] but our total energies are much lower. They are more reliable due to the relativistic corrections included in our energies.

To compare with the 115.5-eV photon energy given by Caldwell *et al.*, we need an accurate $1s^22s^2$ energy. The most accurate experimental energy of a ground state is usually given by its ionization potential. We used the experimental Be I ionization energy of 9.322 eV from Bashkin and Stoner.[14] Adding the electron energy of 106.20 eV in the $(1s^22s,e)$ channel, the result implies that the calculated $1s2s^22p\ ^1P^\circ$ energy is 115.52 eV above the experimental $1s^22s^2$ energy. This agrees well with the experiment. Our energy agrees with that of Safronova and Kharitonova[15] but is lower than that of the result of Mercouris and Nicolaides by about 0.81 eV.[16]

Similar calculations have been done on this $^1P^\circ$ resonance of B II, C III, and O V. These results and their comparison with Auger experiments are given in Table II. Notice that the difference in the $1s^22s$-$1s^22p$ energies in this table agree well with that of Bashkin and Stoner.[14] Here we have 3.965, 6.010, 8.017, and 12.011 eV for Be, B, C, and O, respectively. In Bashkin and Stoner, they are 3.960, 5.999, 8.005, and 11.999 eV, respectively.

For Be I, the calculated $^1P^\circ \rightarrow (1s^22p,e)$ electron energy

TABLE I. Convergence of Be I $1s2s^22p\ ^1P^\circ$ energy. ($q = 3.36$ in the vacancy orbital, ΔE is the binding energy contributed by adding the partial wave, and for notation see text and Ref. 10.)

	Angular partial wave	Spin	No. of terms	Nonlinear parameters α_1	α_2	α_3	α_4	ΔE (a.u.)
1	[(0,0)0,0]0,1	χ_2	32	4.00	1.311	1.386	1.170	10.342 510 2
2	[(0,0)0,0]0,1	χ_1	33	4.00	1.707	1.248	1.391	0.008 656 6
3	[(0,1)1,1]0,1	χ_1	37	3.711	1.436	1.651	1.253	0.039 095 5
4	[(0,0)0,1]1,2	χ_2	27	4.00	1.037	1.771	1.697	0.019 179 5
5	[(0,1)1,1]0,1	χ_1	7	1.239	4.013	3.416	1.125	0.001 473 4
6	[(0,0)0,1]1,2	χ_1	6	4.00	0.942	1.936	1.943	0.002 080 8
7	[(0,0)0,1]1,2	χ_2	7	0.642	0.884	4.356	3.933	0.001 151 7
8	[(0,0)0,2]2,3	χ_2	11	4.00	0.777	2.080	2.363	0.000 858 6
9	[(0,0)0,2]2,3	χ_1	6	4.00	0.896	1.843	2.073	0.000 357 2
10	[(2,2)0,0]0,1	χ_2	7	1.940	1.935	3.780	1.157	0.001 571 4
11	[(3,3)0,0]0,1	χ_2	5	2.286	2.286	3.780	1.129	0.000 252 1
12	[(0,1)1,2]1,2	χ_1	3	4.00	1.270	1.925	1.513	0.001 036 9
13	[(0,1)1,2]1,2	χ_2	5	4.00	1.329	1.915	1.513	0.000 571 6
14	[(0,0)0,2]2,3	χ_2	6	1.068	1.398	4.177	5.382	0.000 166 4
15	[(0,1)1,1]0,1	χ_2	9	0.841	4.515	2.992	1.132	0.000 266 9
16	[(0,0)0,1]1,0	χ_2	12	1.718	0.795	1.960	3.043	0.000 096 1
17	[(0,0)0,1]1,0	χ_1	11	1.369	2.482	1.083	4.00	0.000 209 9
18	[(0,1)1,1]0,1	χ_2	4	3.720	1.231	1.846	1.257	0.000 125 2
19	[(0,1)1,1]2,3	χ_2	4	4.00	1.219	1.520	1.791	0.000 421 3
20	[(1,1)0,1]1,2	χ_2	7	1.014	2.220	2.964	3.940	0.000 102 6
21	[(0,0)0,1]1,2	χ_1	6	4.00	0.957	2.421	2.052	0.000 172 9
22	[(0,1)1,3]2,3	χ_2	2	4.00	1.135	2.398	2.897	0.000 018 5
23	[(0,1)1,3]2,3	χ_1	2	4.00	1.261	2.502	2.031	0.000 036 0
24	[(0,0)0,3]3,4	χ_2	9	4.00	0.782	2.752	3.150	0.000 218 4
25	[(0,0)0,3]3,4	χ_2	8	0.588	1.088	6.608	7.328	0.000 049 0
26	[(0,0)0,3]3,4	χ_1	5	4.00	0.964	1.830	2.587	0.000 046 0
27	[(0,0)0,4]4,5	χ_2	5	4.00	0.862	3.163	3.479	0.000 074 7
28	[(4,4)0,0]0,1	χ_2	4	2.950	2.924	3.780	1.327	0.000 074 9
29	[(5,5)0,0]0,1	χ_2	3	3.540	3.219	4.00	1.328	0.000 031 2
	Subtotal		286					10.420 905 0

TABLE II. Energies of the $1s2s^22p\ ^1P^\circ$ states of Be-like ions and comparison with experimental energies in the $(1s^22s\ ^2S,e)$ and $(1s^22p\ ^2P,e)$ channels. (1 a.u.=27.211 66 eV.)

	$-E$ (a.u.)				Auger energy (eV)		
Z	E (nonrel.)	Relativistic corrections	E_{total}	Decay channel energy	This work	Expt.	Remark
4	10.420 905	0.002 051	10.422 956	^2S 14.325 852	106.20	106.0±0.2[a]	Very weak
				^2P 14.180 132	102.24	102.12±0.1[a]	Weak
5	17.200 680	0.005 307	17.205 987	^2S 23.429 444	169.35	Not reported	
				^2P 23.208 600	163.34	163.38±0.2[b]	
6	25.836 574	0.011 497	25.743 027	^2S 34.787 883	246.13	Not reported	
				^2P 34.493 275	238.11	238.21±0.2[c]	
						238.0±0.2[d]	
8	48.044 268	0.038 595	48.082 863	^2S 64.274 607	440.60	440.5±0.2[e]	Very weak
				^2P 63.833 216	428.59	428.5±0.2[e]	

[a]Reference 3; the experimental lines are also identified as coming from $1s2s2p2p\ ^5P\rightarrow(1s^22p,e)$ predicted at 102.20 eV and $1s2s2p2p\ ^5\rightarrow(1s^22s,e)$ at 106.16 eV.
[b]Reference 4.
[c]Reference 5.
[d]Reference 6.
[e]Reference 7.

is 102.24 eV, slightly outside the experimental result 102.12±0.1 eV.[3] However, due to the good agreement of our result with Caldwell *et al.*, it is likely that the correct energy of the Auger electron probably lies in the upper half of the quoted uncertainty. An extremely weak line at 106.0±0.2 eV is also reported in the experiment which does agree with our 106.20 eV. Both lines are very weak in the spectra. It is important to point out that the $1s2s2p2p\ ^5P\rightarrow(1s^22p,e)$ energy is predicted at 102.20 eV and the $1s2s2s2p\ ^5P\rightarrow(1s^22s,e)$ energy is at 106.16 eV. If the experimental result of Caldwell *et al.* is accurate, then the observed 106.0±0.2 eV line observed in Rødbro, Bruch, and Bisgaard[3] is probably mostly coming from this ^5P state.

The B spectrum of Rødbro, Bruch, and Bisgaard[3] was recalibrated by Chung and Bruch.[4] In Ref. 4, line 6 (Fig. 15 in Ref. 3) is reported at 163.88±0.2 eV. This agrees well with the calculated 163.34 eV in this work. Line 6 is clearly visible. We identify this to be the $1s2s^22p\ ^1P^\circ\rightarrow(1s^22p,e)$ transition. However, the corresponding $(1s^22s,e)$ Auger line at 169.35 eV is missing. Line 11 at 169.04±0.2 eV is also a very weak line which comes mostly from $(1s2s2p2p)^5P$. This shows clearly that the decay to the $(1s^22s,e)$ channel is either extremely weak or unobserved.

In the recalibrated carbon spectrum of Bruch *et al.*,[5] line 5 at 238.21±0.2 eV was identified to be the $1s2s^22p\ ^1P^\circ\rightarrow(1s^22p,e)$ transition. It is based on the prediction of Safronova and Kharitanova at 238.5 eV.[15] The corresponding transition to the $1s^22s$ channel was not reported. Mann reported a line (8) in his spectra at 238.0±0.2 eV. He identified it as coming from the $1s2s^23s$ and $1s2s2p3p$ states based on the code from Grant *et al.*[17] The $1s2s^22p\ ^1P^\circ$ is completely absent from his spectra. Our calculated result for the $1s2s^22p\ ^1P^\circ\rightarrow(1s^22p,e)$ is 238.11 eV, within the quoted experimental uncertainties of both experiments. It appears that we have reconfirmed the identification of Bruch *et al.*[5] The corresponding line for the $(1s^22s,e)$ channel at 246.13 eV was completely missing in both experiments, again confirming the conclusion of Caldwell *et al.* We noticed that all the spectral lines observed by Mann[6] between 235 and 260 eV can be identified as coming from $1s2l2l'2l''$ resonances (except the four well-known lithiumlike lines). These identifications are consistent with those for Be I, B II, O V, and the C III spectra from Bruch and co-workers.[3,5,7]

For oxygen, the branching ratio of the two decay channels has been studied.[8] These results also agreed with the conclusion of Ref. 1. Energies for the Auger electrons calculated here again reconfirm the identifications of Bruch *et al.*[7]

In conclusion, we find that what was seen in Be I in Ref. 1 also appeared in the high-resolution spectra of B II, C III, and O V and that the near 100% production of the $(1s^22p,e)$ decay channel of $1s2s^22p\ ^1P^\circ$ is a common feature of the Be-like series.

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[1]C. D. Caldwell, M. Flemming, M. O. Krause, P. van der Meulen, C. Pan, and A. F. Starace, Phys. Rev. A **41**, 542 (1990).
[2]D. Petrini, J. Phys. B **14**, 3839 (1981).
[3]M. Rødbro, R. Bruch, and P. Bisgaard, J. Phys. B **12**, 2413 (1979).
[4]K. T. Chung and R. Bruch, Phys. Rev. A **28**, 1418 (1983).
[5]R. Bruch, K. T. Chung, W. L. Luken, and J. C. Culberson, Phys. Rev. A **31**, 310 (1985).
[6]R. Mann, Phys. Rev. A **35**, 4988 (1987).

[7]R. Bruch, N. Stolterfoht, S. Datz, P. D. Miller, P. L. Pepmiller, Y. Yamazaki, H. F. Krause, J. K. Swenson, K. T. Chung, and B. F. Davis, Phys. Rev. A **35**, 4114 (1987).

[8]R. Bruch, S. Datz, P. D. Miller, P. L. Pepmiller, H. F. Krause, J. K. Swenson, and N. Stolterfoht, Phys. Rev. A **36**, 394 (1987).

[9]See, for example, K. T. Chung and B. F. Davis, in *Autoionization—Recent Developments and Applications,* edited by A. Temkin (Plenum, New York, 1985), Chap. 3.

[10]K. T. Chung, Phys. Rev. A **23**, 2957 (1981); B. F. Davis and K. T. Chung, J. Phys. B **15**, 3113 (1982).

[11]H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Springer-Verlag, Berlin, 1957), p. 193.

[12]K. T. Chung, Phys. Rev. A **40**, 4203 (1989).

[13]F. W. King, Phys. Rev. A **40**, 1735 (1989); **38**, 6017 (1988).

[14]S. Bashkin and J. O. Stoner, Jr., *Atomic Energy Level and Grotrian Diagrams* (North-Holland, New York, 1975).

[15]U. I. Safronova and V. N. Kharitonova, Opt. Spektrosk. **27**, 550 (1969) [Opt. Spectrosc. (U.S.S.R.) **27**, 300 (1969)].

[16]T. Mercouris and C. A. Nicolaides, Z. Phys. D **5**, 1 (1987).

[17]J. P. Grant, B. J. Mckenzie, P. H. Norrington, D. F. Mayers, and N. C. Pyper, Comput. Phys. Commun. **21**, 207 (1980).