Partial autoionization rates of O^{4+} $(1s2s^22p)^3P^0$ and $^1P^0$: A crucial test of electron correlation in Be-like systems

R. Bruch,* S. Datz, P. D. Miller, P. L. Pepmiller, H. F. Krause, J. K. Swenson, and N. Stolterfoht†
Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831
(Received 10 October 1986)

For the first time, ratios of partial autoionization widths have been measured for highly ionized oxygen projectiles. In particular we have studied the Auger decay of the Be-like $(1s2s^22p)^3P^0$ and $^1P^0$ states in 0^{4+} decaying to the $1s^22p$ and $1s^22s$ final ionic states. Our experimental intensity ratios for the $^3P^0$ and $^1P^0$ states are 1.7 and 16, respectively. We also present new results on the partial and total autoionization widths of these states from calculations which include electron correlation and interchannel coupling via the application of the many-electron theory of ionic resonances in terms of complex coordinates.

Electron correlation manifests itself distinctly in the level structure and transition probabilities of highly excited few-electron systems. Such many-body effects may be tested by measuring specific autoionization transition energies, line intensities, branching ratios, and line widths. Specifically, singly core-excited states isoelectronic with beryllium generally decay to two adjacent continua, giving rise to a double-line structure associated with each initial state. The intensity ratios of such lines represent a direct measure of ratios of partial Auger widths which are strongly affected by the strength of the mutual Coulomb interaction.

A striking example of the power of projectile Auger spectroscopy[1–3] to elucidate many-body effects[4,5] is found in the recent measurement of the $(1s2s^22p)^3P^0$ and $^1P^0$ Auger decay[6] in O^{4+}, conducted at the Oak Ridge National Laboratory EN Tandem facility using the zero-degree Auger spectroscopy apparatus temporarily transported from the Hahn-Meitner Institut, Berlin. The only previous information on the Auger deexcitation of such core-excited multiply ionized systems comes from the theoretical work of Chen and Crasemann.[7] The Herman-Skillman Hartree-Slater model with $X\alpha$ exchange potential was used in these calculations to generate the wave functions needed for computing the $(1s2s^22p)^3P^0$ and $^1P^0$ matrix elements. In the case of the Ne^{6+} $1s2s^22p$ $^3P^0$ state, both Auger decay channels are intense, whereas in the case of the $^1P^0$ state the $1s^22s$ ^2S channel has very small intensity, corresponding to a theoretical ratio $(1s^22p)^2P^0/(1s^22s)^2S$ of 286.7. A similar large ratio for O^{4+}, namely, 74.1, has been predicted recently by Chen[8] using the multiconfiguration Dirac-Fock (MCDF) model. In order to account for electron correlation and interchannel coupling, Nicolaides and collaborators have applied the complex rotation method.[9–12] Their timely, new application of the state-specific theory of autoionizing states in terms of real or complex coordinates yields an intensity ratio of 14.7, for the $^1P^0$ Auger decay in O^{4+} which is in good agreement with our experimental result of about 16.

The procedure of measuring line-intensity ratios of highly ionized Be-like states and the comparison of measured and predicted ratios of partial Auger widths are discussed in the following. For the details of the solutions of the complex eigenvalue problem the reader is referred to the preceding paper by Nicolaides and Mercouris.[9]

In this work the zero-degree projectile Auger spectroscopy method has been used to study intensity or branching ratios of core-excited multiply charged ions. The potential of this method[2] lies in its (i) high energy resolution and accuracy, (ii) accessibility of multiply ionized few-electron systems, (iii) selectivity of the excitation process, and finally (iv) cascade-free depopulation of specific Auger states. Here we present high-resolution oxygen K Auger spectra associated with the charge state O^{4+}. In particular we have confined ourselves to the $(1s2s^22p)^3P^0$, $^1P^0$, and $(1s2s2p^2)^5P$ states decaying to the O^{5+} $(1s^22p)^2P^0$ and $(1s^22s)^2S$ final ionic states. Such Be-like inner-shell vacancy levels play an important role in understanding few-body quantum systems.

The Be-like K vacancy states of the type $1s2s^22p$ and $1s2s2p^2$ have been predominantly excited in 10-MeV $O^{3+}+He$ collisions. The experimental apparatus used in these measurements has been described in detail previously.[6] In brief electrons were measured at an observation angle of zero degrees with respect to the beam direction by a spectrometer of two consecutive parallel-plate analyzers connected in a tandemlike arrangement. High resolution of the order of $\Delta E/E \sim 10^{-3}$ was achieved by deceleration of the electrons between two grids in front of the second analyzer.

In Fig. 1 a segment of the high-resolution 10-MeV $O^{3+}+He$ spectrum is shown. Background has been subtracted and electron energies have been transformed to the projectile rest frame. The most prominent Auger peaks were fitted by a Lorentzian curve folded by a Gaussian-type spectrometer response function. The most intense peak, at 423.9 eV, corresponds to the $(1s2s^22p)^3P^0 \rightarrow (1s^22p\epsilon l)^3P^0$ decay channels[13] with $l=0$ and 2. We note that in a pure single-particle model the $l=2$ (ϵd) channel would be forbidden. The line identification is based on previous studies by Bruch *et al.*[14] Another pronounced peak observed at 435.9 eV results from the competing $(1s2s^22p)^3P^0 \rightarrow (1s^22s\epsilon p)^3P^0$

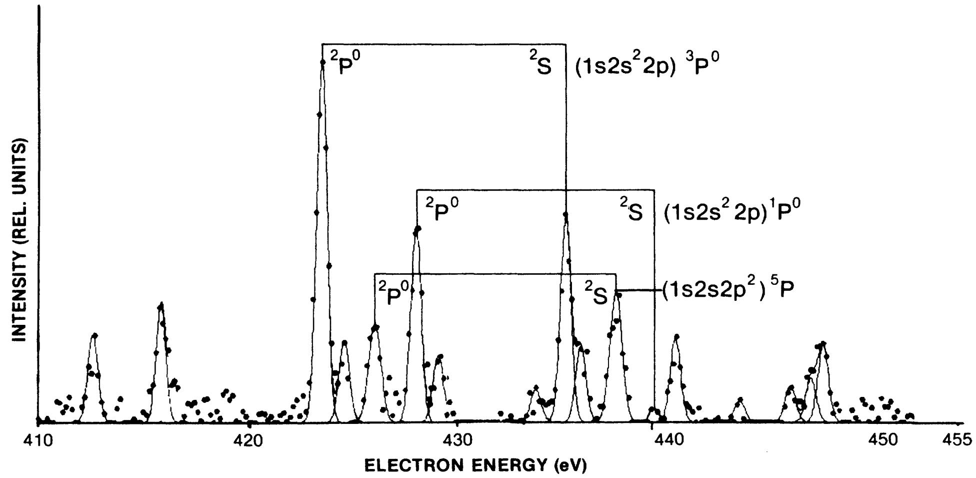

FIG. 1. High-resolution Auger-electron spectrum for 10-MeV O^{3+} on He gas. The electron emission was measured at an observation angle of zero degrees. Background has been subtracted and electron energies have been transformed to the projectile rest frame.

decay channel.

In Table I we have listed our experimentally determined intensity ratios for the $^3P^0$ state in comparison with theoretical data of Chen[8] and Nicolaides and Mercouris.[9] We note that for the $^3P^0$ state the predicted ratios of Chen and Nicolaides and Mercouris are very close to the experimental value of 1.7. We further note that the intensity ratio associated with the $^3P^0$ and $^1P^0$ initial states leading to the $(1s^22p)^2P^0$ and $(1s^22s)^2S$ final states are a direct measure of squares of Auger matrix elements. In particular the ratio for $(1s2s^22p)^1P^0$ should be very sensitive to the fine details of the wave functions in four-electron systems and therefore can be used to discriminate among different many-body theoretical descriptions of autoionization.

In fact the structure of 428.5 and 440.5 eV are associated with the $(1s2s^22p)^1P^0$ Auger transitions. It is evident from Fig. 1 that the $(1s2s^22p)^1P^0 \rightarrow (1s^22s\epsilon p)^1P^0$ channel intensity is very weak in accordance with theoretical predictions.[7–9] From the experimental line intensities a ratio of the order 16 has been derived. As can be seen in Table I this value is in close agreement with the theoretical prediction of Nicolaides and Mercouris. On the other hand, the ratios obtained from the Dirac-Fock calculation and the complex rotation method differ by a factor of the or-

TABLE I. $(1s^22p)^2P^0/(1s^22s)^2S$ intensity ratios resulting from Auger decay of the O^{4+} $(1s2s^22p)^3P^0$, $^1P^0$, and $(1s2s2p^2)^5P$ states.

Initial state	Final state	Experiment Transition energy (eV)	Theory Transition energy (eV)	Experiment $(1s^22p)^2P^0/(1s^22s)^2S$ Intensity ratio	Theory $(1s^22p)^2P^0/(1s^22s)^2S$ Intensity ratio	Theory Total autoionization rate (in 10^{13} sec^{-1})
$(1s2s^22p)^3P^0$	$1s^22p$	423.9±0.2[a]	424.2[b]			
			424.54[c]			
				1.7±0.1[a]	1.8[d]	9.0[d]
$(1s2s^22p)^3P^0$	$1s^22s$	435.9±0.2[a]	436.2[b]		1.9[c]	13.0[c]
			436.33[c]			16.3[e]
$1s2s^22p)^1P^0$	$1s^22p$	428.5±0.2[a]	428.5[b]			
			429.07[c]			
				16±10[a]	14.7[d]	5.0[d]
					74.1[c]	8.8[c]
$(1s2s^22p)^1P^0$	$1s^22s$	440.5±0.2[a]	440.5[b]			10.8[e]
			441.16[c]			
$(1s2s2p^2)^5P$	$1s^22p$	426.5±0.2[a]	426.7[b]			
			426.22[c]			
				0.8±0.2[a]		
$(1s2s2p^2)^5P$	$1s^22s$	438.55±0.2[a]	437.7[b]			
			438.33[c]			

[a]This work.
[b]Bruch *et al.* (Ref. 14).
[c]Chen (Ref. 8).
[d]Nicolaides and Mercouris (Ref. 9).
[e]Safronova and Lisina (Ref. 13).

der 5. In Table I we have also tabulated the total autoionization rates of the O^{4+} $(1s2s^2 2p)^3P^0$ and $^1P^0$ states, as predicted by theory. It is clearly seen that these data deviate considerably from each other. When comparing the rates obtained by Safronova and Lisina using $1/Z$ expansion,[13] with those based on the complex solutions of the Schrödinger equation, we find that the autoionization rates differ by a factor of about 2.

The additional structures in Fig. 1 at 426.5 and 438.55 eV correspond to the metastable autoionizing $(1s2s2p^2)^5P$ state. From our experimental data we have deduced an intensity ratio of 0.8. Due to the differential metastability[15] of quintet states, each J fine-structure level (e.g., $^5P_3$, $^5P_2$, and $^5P_1$) is characterized by two partial Auger transition probabilities. Total Auger transition rates for oxygen $^5P_3$, $^5P_2$, and $^5P_1$ levels were calculated by Chen[8] using the MCDF method; however, no partial rates are given. From the work of Chen and Crasemann[7] we were able to estimate a ratio of 0.17 for the Ne^{6+} $(1s2s2p^2)^5P$ state, assuming statistical population of the $J=1$, 2, and 3 fine-structure levels. This theoretical ratio for neon deviates considerably from the experimental value given in Table I for oxygen.

In conclusion, we have determined experimental intensity ratios associated with the Auger decay of the $(1s2s^2 2p)^3P^0$ and $^1P^0$ terms. We have also shown that strong cancellation effects in the transition matrix elements for the O^{4+} $(1s2s2p^2)^1P^0$ Auger decay must occur leading to a very weak $(1s2s^2 2p)^1P^0 \rightarrow (1s^2 2s\epsilon p)^1P^0$ peak intensity. Furthermore, the comparison of theoretical calculations of Nicolaides and Mercouris with experiment suggests that electron correlation is very crucial for the theory of autoionization and therefore cannot be neglected for light atomic systems, such as oxygen. Despite this obvious progress in understanding the Auger decay of Be-like systems, more experimental and theoretical work on branching or intensity ratios of multiply ionized Be four-electron states is necessary, to unravel these interesting many-body effects in more detail.

Reinhard Bruch is indebted to Professor Phil Altick for helpful comments and to Dr. M. H. Chen from the Lawrence Livermore National Laboratory for the communication of unpublished data. This research was sponsored by the U.S. Department of Energy, Division of Chemical Sciences, under Contract No. DE-AC05-84OR21400 with Martin Marietta Energy Systems, Inc.

*Department of Physics, University of Nevada Reno, Reno, NV 89557.
†Hahn-Meitner Institut für Kernforschung Berlin GmbH, D-100 Berlin 39, West Germany.

[1] A. Itoh, T. Schneider, G. Schiwietz, Z. Roller, H. Platten, G. Nolte, D. Schneider, and N. Stolterfoht, J. Phys. B **16**, 3965 (1983).
[2] N. Stolterfoht, A. Itoh, D. Schneider, T. Schneider, G. Schiwietz, H. Platten, G. Nolte, R. Glodde, U. Stettner, W. Zeitz, and T. Zouras (unpublished).
[3] A. Itoh, D. Schneider, T. Schneider, T. J. M. Zouras, G. Nolte, G. Schiwietz, W. Zeitz, and N. Stolterfoht, Phys. Rev. A **31**, 684 (1985).
[4] R. L. Simons, H. P. Kelly, and R. Bruch, Phys. Rev. A **19**, 682 (1979).
[5] A. Temkin, *Autoionization Recent Developments and Applications* (Plenum, New York, 1985), and references given therein.
[6] R. Bruch, N. Stolterfoht, S. Datz, P. D. Miller, P. L. Pepmiller, I. Yamazaki, H. F. Krause, J. K. Swenson, K. T. Chung, and B. F. Davis, Phys. Rev. A **35**, 4114 (1987).
[7] M. H. Chen and B. Crasemann, Phys. Rev. A **12**, 959 (1975).
[8] M. H. Chen, Phys. Rev. A **31**, 1449 (1985); (private communication).
[9] C. A. Nicolaides and Th. Mercouris (private communication); preceding paper, Phys. Rev. A **36**, 390 (1987).
[10] C. A. Nicolaides and Th. Mercouris, Phys. Rev. A **32**, 3247 (1985).
[11] C. A. Nicolaides and D. R. Beck, Int. J. Quantum. Chem. **14**, 457 (1978); Phys. Lett. **65A**, 11 (1978).
[12] C. A. Nicolaides, Th. Mercouris, and Y. Komninos, Int. J. Quantum Chem. Symp. **15**, 355 (1981).
[13] U. I. Safronova and T. G. Lisina, At. Data Nucl. Data Tables **24**, 49 (1979).
[14] R. Bruch, D. Schneider, W. H. E. Schwarz, M. Meinhart, B. M. Johnson, and K. Taulbjerg, Phys. Rev. A **19**, 587 (1979), and references given therein.
[15] R. Bruch, M. Rødbro, P. Bisgaard, and P. Dahl, Phys. Rev. Lett. **30**, 801 (1977), and references given therein.