Electron-impact ionization of B^{2+} and O^{5+}: Excitation-autoionization in Li-like ions

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(Received 19 August 1985; revised manuscript received 28 April 1986)

New measurements for the total, single ionization of B^{2+} and O^{5+} by electron impact are reported with particular attention directed to the indirect contribution of excitation-autoionization. For B^{2+} these are the first measurements to our knowledge while for O^{5+} the present data improve on previous measurements. In both cases the direct total ionization cross sections are in good agreement with recent distorted-wave predictions of Younger, and the excitation-autoionization contribution is consistent with measurements for other Li-like ions. For O^{5+} an additional small increase in the cross section is observed at an energy well below the excitation-autoionization threshold; this feature may be attributable to resonance recombination followed by auto-double-ionization. For the Li-like ions Be^{+}, B^{2+}, C^{3+}, N^{4+}, and O^{5+}, the ionization theory of Younger is used as a basis to subtract the direct ionization component from the total measured ionization cross sections in order to extract the $1s^22s \rightarrow \sum_l 1s2s2l$ excitation cross section. The deduced inner-electron excitation cross sections are quantitatively compared with excitation theory including new close-coupling calculations for Be^{+} and B^{2+} presented here. For all cases except Be^{+}, the close-coupling theory is in agreement with the deduced experimental excitation cross sections. These new results and analysis improve confidence in excitation theory for highly charged ions.

I. INTRODUCTION

Measurements of electron-impact ionization of ions are of general interest because of the uncertain state of basic collision theory as applied to ionization and because of the important role of ionization in laboratory and astrophysical plasmas. In the past few years we have endeavored to provide accurate experimental data from crossed-beam experiments along isoelectronic sequences in order to test theoretical approaches in a consistent manner, and to provide tests for cases with initial ionic charge greater than +1.

The present data for B^{2+} and O^{5+} complete a series of experiments on ionization of Li-like ions for the first five ions of the isoelectronic sequence. Because of the absence of metastable ions in the beams, simple electronic structure, and prominence of emission lines from plasmas, the lithium isoelectronic sequence is a prime candidate for extensive study by experiment and theory. It is desirable to extend these measurements to more highly charged ions of this series; the required apparatus is being developed for these formidable experiments. However, the present results provide improved understanding of electron-ion collisions for Li-like ions.

The first measurements on ionization of Li-like ions[1,2] of C^{3+}, N^{4+}, and O^{5+} provided a mild surprise in that inner-shell excitation followed by autoionization produced a measurable contribution to the ionization cross section. Subsequent calculations[3] showed that, for these ions, such excitation should decay totally (99% or higher) by autoionization and that the calculated inner-shell excitation cross sections, $1s^22s \rightarrow \sum_l 1s2s2l$ were roughly appropriate for the observed structure in the ionization cross sections. However, trends in the experimental data indicated that the relative importance of the excitation-autoionization increased more rapidly with ionic charge along the isoelectronic sequence than any of the theoretical predictions. In addition to the basic questions about collision physics, this discrepancy implied significant uncertainty for even the most refined predictions of ionization and excitation rates for other, more highly charged ions, such as Li-like Fe^{23+} which is important in analyzing high-temperature plasmas of fusion and astrophysical interest.

Since the first measurements, the theoretical community has responded with improved excitation calculations,[3,4] ionization calculations,[5,6] and attempts to include quantum interference between these processes;[7] these changes did not qualitatively improve the agreement between theory and experiment. A goal for our experiments is to extend the range of comparison, but as yet we have been unable to pursue measurements at higher charge states for Li-like ions. The current B^{2+} and O^{5+} results and recent Be^{+} results[8] are new experimental information on this problem.

Assuming that sophisticated ionization calculations[6] (slightly renormalized in some cases) provide the best direct ionization cross sections, we have attempted to extract the excitation cross sections by subtracting the direct ionization from the measured total ionization cross sections. The resultant $1s^2 2s \rightarrow \sum_l 1s\,2s\,2l$ excitation cross sections for each case are compared with theory. The new measurements and current analysis for O^{5+} remove the discrepancy between theory and experiment for the excitation component but introduce a possible new feature contributing to ionization through recombination resonances.

For the Be^{+} case the present six-state close-coupling excitation calculations are more than a factor of 2 lower than the experimentally deduced excitation cross section. For the Be^{+} case, there appears to be a true discrepancy between the experiment and the "best" predicted values. In all other cases (B^{2+} through O^{5+}) the agreement in deduced experimental excitation cross sections and best predicted values is excellent.

II. B^{2+} RESULTS

The present measured electron-impact ionization cross sections were obtained using crossed beams of electrons and ions. The technique[9] and the specific apparatus used in this experiment[10] have been thoroughly described. The B^{2+} experiments used the Oak Ridge National Laboratory Penning ion gauge (ORNL-PIG) ion source while the O^{5+} experiments used the new electron-cyclotron-resonance heated (ECR) ion source.[11] A primary intent of the present measurements has been to examine the excitation-autoionization structure. Thus, the measurements were pursued with the highest level of precision in the energy region where the excitation thresholds occur.

Table I presents the measured cross section values for B^{2+}. Two different forms of relative uncertainty are given in the table. The values designated by ± are obtained by the quadrature sum of 1 standard deviation (s.d.) counting statistics, relative variations (reproducibility) of measured beams overlap factors, and estimated relative variation of detector sensitivities. These are total relative uncertainties at 67% confidence level. Within the energy range indicated as "structure scans" the point-to-point variations of form factors is considered to be negligible. In addition, the relative variations in detector sensitivity and any variations due to ion-beam focusing, transmissions, or other factors which can vary slightly with time are eliminated by cyclical repetitions of measurements at each energy. (These cycled scans have no apparent time correlation in any event.) The measured value at each energy is the variance weighted mean of the repeated measurements. Within this range marked structure scans all relative variations are estimated to be negligible except for counting statistics which are given, within the parentheses, at 1 s.d. level. Finally, the total absolute uncertainty is influenced by absolute uncertainties in detector efficiencies, current measurements, form factors (beams overlap), ion transmission through analyzers, and ion-beam velocity. The estimated absolute uncertainties in these quantities are the same as for other recent measurements with this apparatus.[10,12] By deliberate varia-

TABLE I. Measured cross sections for electron-impact ionization of B^{2+}. The relative uncertainties are given at standard confidence level of 67% by combining (in quadrature) counting statistics with relative variations in form factor and detection sensitivity except within the 150—235-eV range. Within this range marked structure scans the counting statistics are assumed to be the only significant relative variation as described in the text. The total absolute uncertainty at good-confidence level of 90% is ±8.1% for the 144-eV cross-section value.

	Energy (eV)	Cross section (10^{-18} cm^2)
	25.8	−0.37±0.33
	30.8	+0.02±0.30
	35.7	+0.03±0.29
	40.6	1.70±0.29
	45.5	3.08±0.30
	50.4	4.07±0.29
	55.3	5.22±0.29
	60.2	5.38±0.29
	65.2	5.94±0.29
	70.1	6.62±0.29
	80.0	6.89±0.28
	86.8	7.49±0.35
	95.0	7.42±0.26
	104.6	7.40±0.32
	114.5	7.87±0.33
	124.3	7.47±0.30
	134.2	7.25±0.29
	144.0	7.37±0.22
Structure Scans	153.6	7.33 (0.14)
	163.4	7.22 (0.13)
	168.6	7.22 (0.15)
	173.2	7.05 (0.09)
	178.1	7.10 (0.11)
	183.0	7.08 (0.11)
	187.9	7.01 (0.10)
	193.2	6.91 (0.06)
	195.0	6.96 (0.08)
	196.7	7.19 (0.08)
	198.5	7.23 (0.06)
	201.0	7.09 (0.08)
	203.0	7.16 (0.06)
	204.8	7.08 (0.08)
	212.9	6.90 (0.10)
	222.7	6.79 (0.09)
	232.5	6.83 (0.09)
	251	6.54±0.25
	291	6.35±0.22
	388	5.56±0.18
	488	5.05±0.16

tion and direct measurements, we estimate the absolute uncertainties at "good confidence" intended to be equivalent to 90% confidence level on counting statistics. The quadrature sum of these estimated absolute uncertainties with the counting statistics at 90% confidence level provides an overall good-confidence absolute uncertainty—typically ±8% of the peak cross-section value for these B^{2+} data.

The relative energy spread in the experimental measurements is about 1 eV [full width at half maximum (FWHM)] in the energy range where excitation structures occur. This estimate is founded on previous measurements[13] and analysis, and the energy spread is attributed to combined energy spread in cathode emitted electrons, space charge within the magnetically confined electron beams, and variation of externally applied electric fields over the finite extent of the electron beam. The energy spreads in the other measurements on Li-like ions were not all the same. For C^{3+}, N^{4+}, and O^{5+} in Ref. 2 the energy spread is estimated at 2 eV (FWHM) and for the Be^{+} data of Ref. 8 the energy spread is estimated to be 0.5 eV.

The B^{2+} measurements are presented in Fig. 1 along with predicted values. The general agreement with the distorted-wave theory of Younger[6] for direct ionization is satisfactory, while results based upon the Lotz semiempirical formula[14] are significantly larger than the measured cross section. The Younger results are calculated using the parameters and formula given[6] to represent ionization along the Li isoelectronic sequence. The reader should be aware that Younger has found a simple but significant error in the published parameters for this sequence as explained in Ref. 6.

Within the energy region where inner-shell excitation should enhance the total ionization via excitation-autoionization, Fig. 1 is expanded in the inset to show detailed comparison with the predicted inner-electron excitation cross sections. The excitation thresholds[15] for $1s^22s \rightarrow 1s2s2l$, $1s2s3l$, and $1s2s4l$ are indicated by the arrows which are labeled by orbital of the excited electron. The three fine-structure energy levels with $2p$ orbitals (^4P, $^2P_{1/2}$, $^2P_{3/2}$) are reasonably separated and indicated by separate arrows while for $4l$ orbitals all of the excited states occur between the two arrows labeled $4l$. The label "I_{1s}" indicates the threshold for direct ionization of an inner-shell electron. The onset of excitation-autoionization is clearly apparent at 195 eV. Also in the Fig. 1 inset, the upper solid line represents direct ioniza-

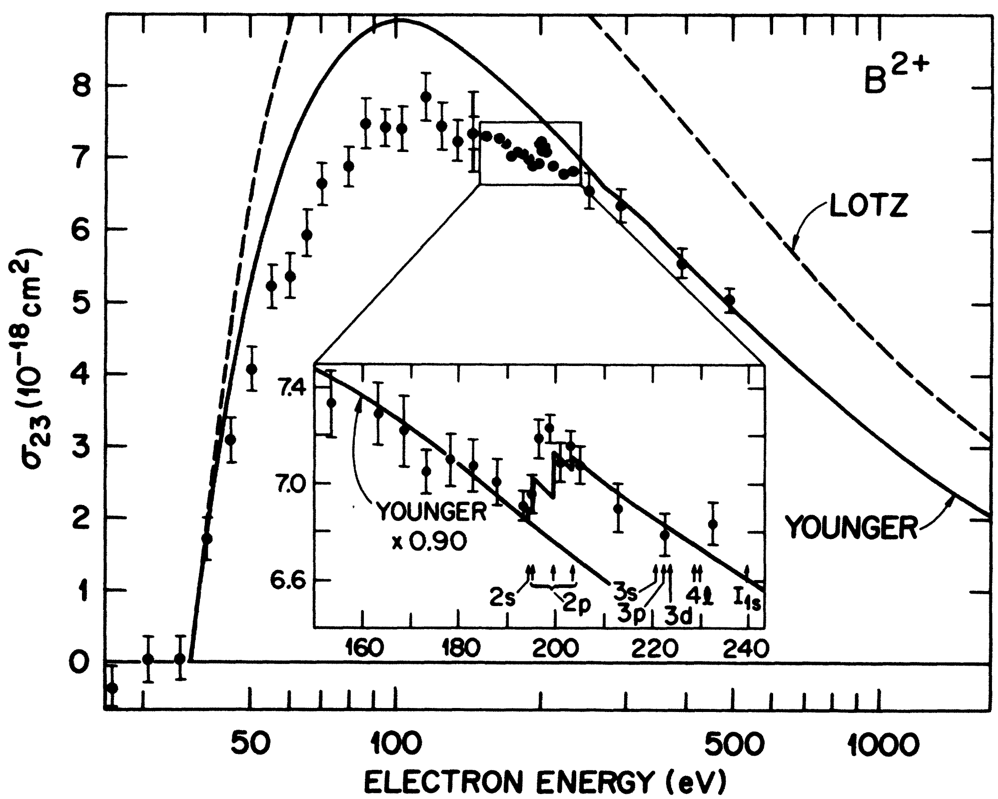

FIG. 1. Electron-impact ionization of B^{2+}. Points are present measurements with relative uncertainties at 1 s.d. except outer bar at 144 eV is total absolute uncertainty at 90% confidence level. The Lotz prediction (Ref. 14, dashed curve) and the distorted-wave prediction of Younger (Ref. 6, solid curve) are shown for comparison. The inset shows the energy region where excitation-autoionization should contribute. Within the inset, the Younger theory of direct ionization has been multiplied by 0.90 and the arrows indicate the energies for inner-shell excitation of a $1s$ electron to the nl orbital indicated (energies from Ref. 15). The upper curve in the inset adds the present six-state close-coupling calculations of excitation of $2l$ substates (from Table II) to the direct ionization.

TABLE II. Threshold energies in eV for excitation-autoionization levels, calculated as in Ref. 15.

State	Be^+	B^{2+}	C^{3+}	N^{4+}	O^{5+}
$1s\,2s^2\,{}^2S$	115.2	194.1	293.6	412.8	552.4
$1s\,2s\,({}^3S)2p\,{}^4P^\circ$	116.1	194.9	296.9	416.4	556.5
$1s\,2s\,({}^1S)2p\,{}^2P^\circ$	119.3	199.7	301.8	423.0	564.5
$1s\,2s\,({}^3S)2p\,{}^2P^\circ$	122.6	203.7	306.8	428.6	550.8
$1s\,2s\,3s$[a]	129.4	220.6	336.1	475.8	639.8
$1s\,2s\,3p$[a]	130.5	222.2	338.2	478.5	643.0
$1s\,2s\,3d$[a]	131.3	223.5	339.9	480.6	645.6
$1s\,2s\,4s$[a]	133.3	228.6	349.4	495.8	667.8
$1s\,2s\,4p$[a]	133.7	220.2	350.2	496.9	669.1
$1s\,2s\,4d$[a]	134.0	229.7	350.9	497.7	670.1
$1s\,2s\,4f$[a]	134.1	229.9	351.2	498.1	670.6

[a]Center-of-gravity energies.

tion plus excitation-autoionization which proceeds through $2l$ states. For reference, the excitation-autoionization thresholds for all of the cases discussed here are given in Table II (Ref. 15).

Contributions from inner-shell excitation have been calculated in a six-state close-coupling approximation and have been added to the renormalized (factor of 0.90) predictions of direct ionization obtained from Younger's parameters. The present six-state close-coupling calculations are performed in a manner similar to that described by Henry.[3] Cross sections for excitation of various inner-shell states are given in Table III for B^{2+} and Be^+ at the three energies: 1.1, 1.2, and 1.3 times the first inner-shell threshold energy.

The excitation-autoionization features associated with $3l$, $4l$, and higher excited states ($\Delta n \geq 2$ excitations) should be smaller than those for $2l$ excited states ($\Delta n = 1$ excitations). Hence features associated with $\Delta n \geq 2$ transitions are not expected to be visible within resolution of the B^{2+} experiment.

Present measurements of the total ionization cross section are 35% lower at the peak than those recommended by Bell et al.[16] for B^{2+}. This difference is similar to the C^{3+} case where they chose to recommend values 25% higher than the measured cross sections. Scaled cross sections for all Li-like species for which measurements have been made are shown in Fig. 2 which emphasizes similarity of the C^{3+} and B^{2+} measurements.

Because of the agreement between the B^{2+} experiment and Younger's predictions for the shape of the direct ionization cross section found here, as well as for Na-like ions,[12] the Younger results are taken as a base for subtracting direct ionization, leaving only the excitation component. In general, this procedure requires slight renormalization of Younger's predictions. For the B^{2+} data an excellent fit to the present results, just below the excitation thresholds, is given by decreasing Younger's results by 10% as shown in the inset on Fig. 1. Since the excited states will decay totally by ionization, this subtraction of the direct ionization gives the total inner-shell excitation cross section. In the region 205–212 eV only the sum of the cross sections for the excitation to the $1s\,2s\,2l$ states contribute, totaling $(4.0\pm1.0)\times10^{-19}$ at 208 eV. The assigned uncertainty is a standard confidence-level (67%) estimate based on the uncertainty in renormalizing Younger's results and the relative uncertainties in measurements near 208 eV. The inner-shell excitation-autoionization cross section as calculated in a six-state close-coupling approximation is 4.1×10^{-19} cm^2 at 208 eV. We note that this is smaller than the 4.5×10^{-19} cm^2 value extrapolated from an isoelectronic fit to C^{3+}, N^{4+}, and O^{5+} calculations.[3] The excellent agreement between the experiment and the excitation calculation for B^{2+} is apparent in Fig. 1.

TABLE III. Calculated $1s^2 2s \rightarrow \sum_l 1s\,2s\,2l$ excitation cross sections in $10^{-3}\pi a_0^2$, with x in threshold energy units for $1s^2 2s \rightarrow 1s\,2s^2$.

x	$1s\,2s^2\,{}^2S$	$1s\,2s\,2p\,{}^4P^\circ$	$1s\,2s\,({}^1S)2p\,{}^2P^\circ$	$1s\,2s\,({}^3S)2p\,{}^2P^\circ$
		Be^+		
1.1	1.54	2.80	3.79	0.90
1.2	1.28	2.15	3.69	0.84
1.3	1.13	1.69	3.93	0.80
		B^{2+}		
1.1	0.64	1.40	1.83	0.52
1.2	0.56	1.11	2.01	0.50
1.3	0.50	0.88	2.13	0.45

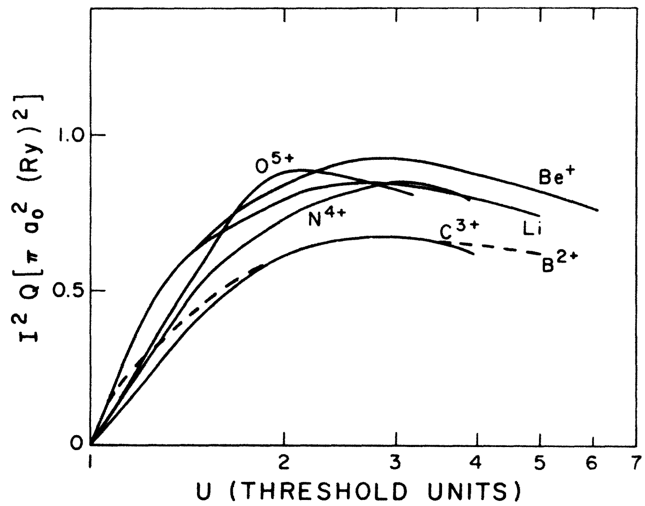

FIG. 2. Measured electron-impact ionization cross sections for Li-like ions scaled by the square of the outer-electron ionization potential vs energy in units of this ionization potential. A similar figure (without the B^{2+} results) was given in Ref. 8.

III. O^{5+} RESULTS FOR EXCITATION-AUTOIONIZATION

The new measurements of total ionization of O^{5+} were obtained with the apparatus previously described[2,10,12] except that the ion beam was obtained from the new ECR source[11] rather than from the ORNL-PIG source used for B^{2+} and in the earlier measurements. The new source provided stable and reproducible ion beams of O^{5+}, typically at 50 keV and 300 nA intensity within the collision region, compared with less-stable beams of 50 keV and 10—40 nA from the ORNL-PIG source used in the previous O^{5+} measurements.[2] The new ion source allowed a substantial improvement in the O^{5+} ionization experiment.

Improvement of the parallel-plate analyzer used to separate O^{6+} signal ions from incident O^{5+} beam ions was attempted for the present measurement. A baffle plate was added within the parallel-plate analyzer. The baffle plate was removed for final cross-section measurements because of a spurious signal which was four times smaller after the baffle plate was removed.

The spurious signal appeared as a positive apparent cross section below threshold for O^{5+} ionization. Systematic checks revealed that this same effect occurred with other ion beams, for example He^{2+}, provided the analyzer parameters were maintained as required for separation of 6 + signal ions from 5 + incident ions. The same effect could be produced with the electron beam off but voltage modulation applied to steering plates in the collision region. We conclude that the spurious signal is due to modification of the trajectory of the primary ion beam by electron-beam space charge. This type of systematic problem has been recognized for some time[17] as a difficulty in crossed-charged-beam experiments and also occurred in the original O^{5+} ionization cross-section measurements.[1] In the present case, a small component of the primary beam striking the baffle plate within the analyzer or the analyzer exit aperture could result in background counts at the O^{6+} detector. The amplitude of the background is modulated due to space-charge focusing of the ion beam, as the electron beam (or other source of space potential) is turned on and off, giving a spurious signal. The fraction of the incident beam striking the baffle plate could not be detected as loss of transmitted O^{5+} ion current in this case but was still sufficient to give measurable false signal in the O^{6+} channel. The spurious signal was observed to be proportional to the applied space potential or to the density of electrons in the electron beams. Specifically this electron density and the spurious signal changed with the electron energy as $E_e^{-1/2}$. This scaling of the spurious signal, together with measurement of the apparent below-threshold cross section for ionization of O^{5+}, have been used to correct the O^{5+} ionization cross sections both with and without the baffle present. The two sets of corrected data are completely indistinguishable except for precision, but only data acquired without the baffle plate are presented here because the correction is substantially less and these data are also more precise. In particular, data given in Table IV are corrected for the

TABLE IV. Corrected experimental cross sections for electron-impact ionization of O^{5+}. The relative uncertainties (given in parentheses) are one standard deviation counting statistics only. Corrections applied to obtain these data and additional uncertainties contributing to total absolute uncertainty are given in the text. Total absolute uncertainty is ±11% at good confidence corresponding to 90% confidence level.

Energy (eV)	Cross section (10^{-18} cm^2)	
97	0.005	(0.018)
137	−0.005	(0.018)
147	0.072	(0.018)
157	0.203	(0.049)
167	0.255	(0.027)
177	0.352	(0.028)
196	0.426	(0.018)
216	0.559	(0.026)
236	0.614	(0.026)
256	0.639	(0.026)
276	0.676	(0.029)
295	0.695	(0.012)
344	0.685	(0.013)
394	0.713	(0.014)
443	0.752	(0.012)
493	0.741	(0.008)
519	0.723	(0.009)
543	0.719	(0.009)
568	0.756	(0.008)
593	0.759	(0.008)
618	0.764	(0.009)
693	0.717	(0.016)
793	0.707	(0.016)
892	0.642	(0.017)
995	0.634	(0.011)

spurious signal according to

$$\sigma=\sigma_m-(1.35\times10^{-18})(E_e)^{-1/2},$$

where σ is a corrected cross section, while σ_m is a measured apparent cross section in cm^2 and E_e is the electron energy in eV. For data presented here, the magnitude of the correction is about 7% near the excitation-autoionization threshold energy.

Figure 3 and Table IV present the corrected new measurements of the total, single ionization of O^{5+} by electron impact. These measured cross sections are consistent with previous measurements[2] except that they are somewhat lower above the excitation-autoionization threshold. These O^{5+} data were acquired with the specific interest of investigating the excitation-autoionization occurring near 560 eV. All of the data were acquired in a manner similar to that of the structure scans portion of the B^{2+} data described in Sec. II of this paper.

The relative uncertainties ascribed to these O^{5+} data are taken to be only due to counting statistics which are given in parentheses in Table III and shown on Fig. 3 at the 1-s.d. (67% confidence) level. The uncertainty in the correction for spurious signal and all other systematic uncertainties are considered to contribute to the total absolute uncertainty, but not to the relative uncertainty. To obtain a total absolute uncertainty the counting statistics for each individual data point and for the scaled "spurious-signal" correction are taken at 90% confidence level (about 1.7 times the standard deviation) and summed in quadrature with similar good-confidence estimates of all other systematic uncertainties. This absolute uncertainty is about ±11% for most of the present O^{5+} data compared to ±8% for the B^{2+} data and other measurements with this apparatus. The increase in absolute uncertainty for these O^{5+} data relative to the other cases is due to the uncertainty in subtraction of the spurious background signal.

The inner-shell electron excitation cross section is deduced from the present O^{5+} total ionization cross section measurements by subtracting values from Younger's calculation of the direct ionization cross sections. In this

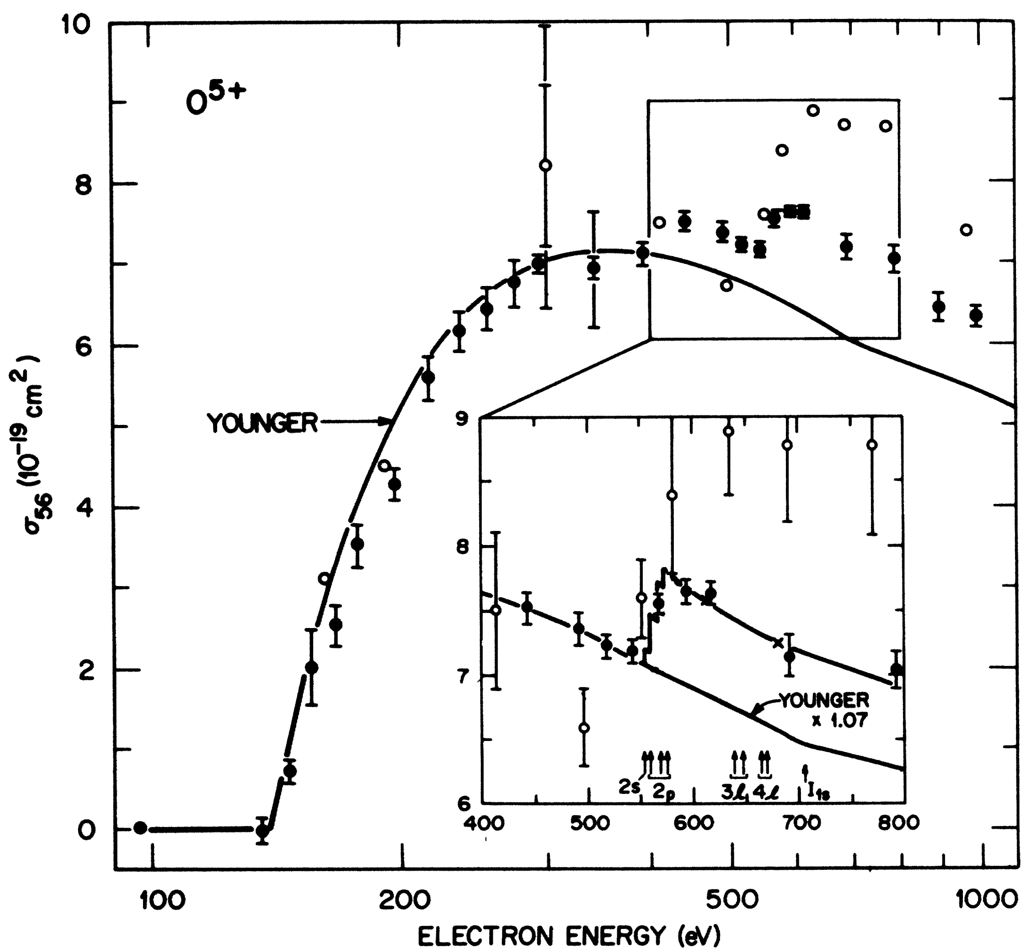

FIG. 3. Electron-impact ionization of O^{5+}. Solid points are present experiment (Table III) with relative uncertainties at 1 s.d. except outer bars on point at 344 eV which are absolute uncertainty at 90% confidence level. Open circles are experiment from Ref. 2 with 1 s.d. relative uncertainties. Solid curve is direct-ionization calculation of Younger (Ref. 6). The inset shows the excitation-autoionization region in greater detail with Younger's direct ionization multiplied by 1.07 to obtain the best fit to data between 400 and 550 eV. The inset includes Henry's calculation (Ref. 3) for excitation $1s^22s\rightarrow\sum_l 1s2s2l$ as a solid line added to the renormalized Younger calculations. Henry provides cross sections only at energies indicated by $\times$ on the figure.

case we have multiplied Younger's results by 1.07 for the best fit in the excitation-autoionization region. The resultant experimental, inner-shell excitation cross section at 612 eV is $(0.8\pm0.3)\times10^{-19}$ cm^2 and can be compared with Henry's calculation[3] of the inner-shell excitation to the $2l$ substates which are the only states that can contribute by excitation-autoionization in the energy range 580—630 eV. That comparison is shown in the inset of Fig. 3 and given in Table V.

The inner-shell excitation cross section deduced from the present O^{5+} measurements is in good agreement with several theoretical calculations[3,5,7] in striking contrast to previous analysis[18] of the earlier less-precise measurements.[2] The present estimate of the inner-shell excitation-autoionization resulting from these experiments is considerably more reliable because of the improved theoretical basis of the direct ionization and the improved statistical precision of the measured total ionization cross sections.

The Coulomb-Born with exchange (CBX) calculations of Jakubowicz and Moores[7] for ionization of O^{5+} include the excitation-autoionization component by using close-coupling wave functions including the inner-shell excited states in a Coulomb-Born calculation of the ionization cross section. This procedure allows for interference between the atomic states included in the calculation, but no significant interference effect is found for the total ionization cross sections. The experimentally deduced excitation step is about 70% of this CBX prediction (see Table V).

Other experiments on electron impact ionization of O^{5+} have been carried out by Defrance *et al.*[19] Those experimental results will provide independent information on this important test case.

IV. RESONANCE RECOMBINATION WITH AUTO-DOUBLE-IONIZATION IN O^{5+}

Close examination of Fig. 3 discloses that the excitation-autoionization feature at 560 eV is about the same size as another feature occurring at 440 eV. In fact, renormalizing the Younger ionization calculation by 1.07, as in the inset, only gives a best fit to the four data points between 443 and 543 eV just below the excitation-autoionization under investigation. However, a significantly better fit to all of the experimental data below 440 eV is obtained without any renormalization of the Younger theoretical results.

Figure 4 shows the present experimental data near the cross-section peak compared to the Younger results without any renormalization. The data acquired in this energy range were spaced to concentrate on the excitation-autoionization threshold, but the increase in the cross section near 440 eV is just as apparent as the excitation-autoionization. This feature was not anticipated and has led us to examine the data and experimental procedures for possible systematic errors. We have repeated some measurements in this energy range; they are no more definitive than the data presented here, but show the same feature. We find no reason to doubt that the feature in the data near 440 eV is real, and we suggest that it may be due to formation of resonance-recombination levels that decay via auto-double-ionization (also known as double Auger decay).

For every excited state of these Li-like ions there is a Rydberg series of resonance-recombination levels of the Be-like ions extending to lower energies. These levels require addition of another electron to the initial ion and consequently can be formed in the present collisions through dielectronic capture.

In all of the cases under discussion here these resonance-recombination levels are in electron configuration with one inner-shell vacancy and three electrons in excited levels relative to this vacancy. Such resonances are likely to be formed in the present collisions, but their decay by emission of two electrons while the third electron fills the inner-shell vacancy was not anticipated. The process is

$$e+1s^22s\rightarrow 1s\,2sln'l'\rightarrow 1s^2+2e\ .$$

TABLE V. $1s^22s\rightarrow\sum_l 1s\,2s\,2l$ excitation cross sections in 10^{-19} cm^2.

Ion	Energy (eV)	Previously deduced expt.[a]	Scaled Coulomb-Born[b]	Jakubowicz and Moores, CBX[c]	Six-state close coupling[d]	Presently deduced expt.	Ratio of expt. to six-state CC theory
Be^+	125	17	23 (10.1)		9.3	$20\ \pm8$[e]	2.1
B^{2+}	208		6.7 (3.5)		4.1	4.0 ± 1.0	1.0
C^{3+}	325	3.2	3.7 (2.2)	3.0	2.24	2.3 ± 0.7	1.0
N^{4+}	460	1.8	2.0 (1.3)	2.0	1.27	1.6 ± 0.4	1.3
O^{5+}	612	2.8	1.1 (0.8)	1.2	0.74	0.8 ± 0.3[f]	1.1

[a]From Ref. 18.

[b]From Sampson and Golden, Ref. 5, which cautions that these results are not appropriate to low ionic charge cases such as Be^+ and B^{2+}. Values in parentheses have been rescaled as described in the text and Ref. 5.

[c]Extracted from the CBX calculations of Jakubowicz and Moores (Ref. 7) which obtain total ionization including the $2l$ excitation-autoionization.

[d]From Henry (Ref. 3) for C^{3+}, N^{4+}, and O^{5+} and present paper for Be^+ and B^{2+}.

[e]Uncertainties are standard confidence level (67%) values estimated by combining the uncertainty in the renormalization of the Younger direct-ionization component and the relative uncertainties in the measured total-ionization cross sections near the energy of interest.

[f]Based on the new O^{5+} data in the present paper.

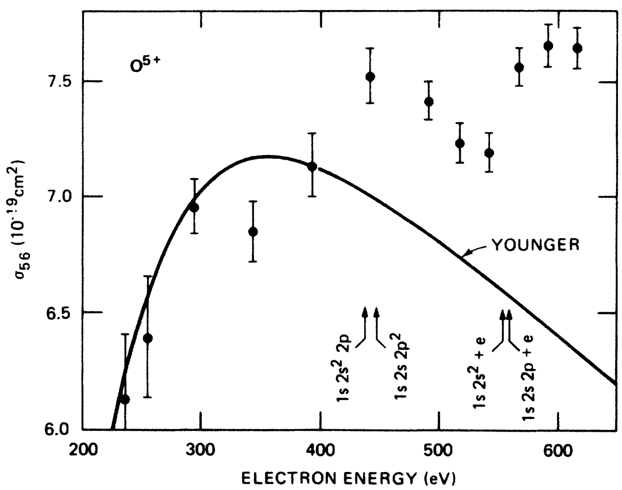

FIG. 4. Electron-impact ionization of O^{5+} in the region of peak cross section. Solid points are present data with relative uncertainties at 1 s.d. Solid curve is direct ionization calculation of Younger (Ref. 6). Arrows indicate center-of-gravity energies (Ref. 15) for formation of the lowest-energy recombination resonances and for inner-shell excitation.

The final step has alternate decay routes that do not contribute to ionization. Specifically, decay of $1s2sln'l'$ to $1s^2nl+e$ by single autoionization is expected to dominate and gives rise to resonances in excitation processes in electron-ion collisions. The resonance states can also decay by emission of photons, which results finally in dielectronic recombination. This mode should dominate the decay branches for sufficiently high ionic charges (about + 20 for these states).

Intermediate states with an inner-shell vacancy and three or more excited electrons can be formed in many ways, including inner-shell ionization, electron transfer in ion-atom collisions, and photoionization. Decay of such states by simultaneous emission of two electrons has been previously identified following photoionization of Ne and Kr.[20] The decay process was named "double Auger" in those photoionization studies, but we have adopted the terminology auto-double-ionization.[21] These terminologies refer only to decay in which at least three electrons make simultaneous transitions as opposed to decay by one- or two-electron transitions which in some cases can proceed sequentially to similar final states.

In the O^{5+} case, the lowest-energy, inner-shell, resonance-recombination states of O^{4+} are of configurations $1s2s^22p$ and $1s2s2p^2$, which occur at energies between 437.2 and 461.4 eV relative to the ground state of O^{5+} (with dominant cross sections favoring formation of the lowest energy states).[15] These O^{4+} states cannot decay to the detected state of O^{6+} plus two free electrons by any sequential one- or two-electron transitions. The cross sections for formation of the O^{4+} resonance states, averaged over the experimental energy resolution, are expected to be of order 10^{-19}–10^{-18} cm², and rates[15,22] for single autoionization of these states are as fast as 10^{14} sec^{-1}. The magnitude of the feature at 440 eV is about 3×10^{-20} cm², indicating that, if the calculated cross sections are correct, roughly 10% of the decay of the intermediate O^{4+} resonances must be by auto-double-ionization. In the photoionization[20] of Ne and Kr the auto-double-ionization fractions were deduced to be 10% and 30% of the decays, respectively. Thus, the conjecture that resonance recombination is measurably contributing to ionization of O^{5+} seems reasonable. However, such resonances should not occur at all of the energies between 440 and 560 eV. The resonances of configuration $1s2s2l3l'$ occur between 504 and 530 eV.[15] For example, in the present data, the single point at 493 eV should not be enhanced by resonances.

We have fitted the Younger predictions to the four data points between 440 and 550 eV. We believe that this procedure provides a reasonable estimate of the excitation-autoionization contribution. However, the possible contribution of recombination resonances to the O^{5+} ionization complicates the deduction of the inner-shell excitation cross section presented in Sec. III of this papaer. Such resonances can complicate the deduction of inner-shell excitation in all of the Li-like ionization cases but there are no measurable resonance contributions observed in the other cases so that this problem is not considered serious.

V. EXCITATION-AUTOIONIZATION IN OTHER Li-LIKE IONS

Using the previous total ionization measurements for Be^+, C^{3+}, and N^{4+} and subtracting the direct ionization component, the experimental inner-shell excitation for three additional cases is obtained. A previous similar analysis[18] relied only on the experimental data with extrapolation of the few data points closest to, but distinctly below, the excitation thresholds to establish the magnitude and slope of the direct ionization. Because the predictions of Younger have been used for the present analysis of the B^{2+} and O^{5+} data and in other isoelectronic sequences,[12] we have reanalyzed these other Li-like cases as well.

Figures 5–7 illustrate the results of this analysis for Be^+, C^{3+}, and N^{4+}, respectively. In the Be^+ and C^{3+} cases the predictions based on Younger's Li-like parameters have been renormalized as indicated on the figures, but for N^{4+} renormalization was not required. In all cases the error bars shown are 1 s.d. counting statistics taken to represent relative uncertainties. The threshold energies for excitation of $1s$ electrons are indicated on each of the figures and are all given in Table II from a common source.[15]

In Figs. 5–7, six-state close-coupling calculations (from Table III for Be^+ and from Ref. 3 for C^{3+} and N^{4+}) have been added to the renormalized predictions of direct ionization obtained from the Younger parameters. Recombination resonances may be contributing to the cross sections below excitation thresholds, but might be difficult to discern from statistical variations and, based on the data, the resonance contributions must be small in Figs. 5–7 in any event. The upper solid lines on the figures thus represent direct ionization plus excitation-autoionization proceeding through the $2l$ states. The inner-shell excitation calculations were actually carried out at only a few energies, indicated on the figures by $\times$'s. Nevertheless, the relative contribution of each of the $2l$ substates is

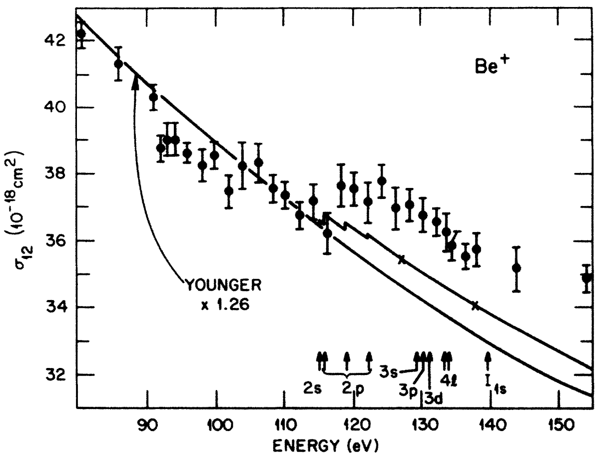

FIG. 5. Electron-impact ionization of Be^{+} (data points from Ref. 8) in the energy region where excitation-autoionization should contribute. The direct ionization theory of Younger (Ref. 6) has been multiplied by 1.26 to obtain best fit to the experimental values between 80 and 115 eV. Other notation is the same as for the inset in Figs. 1 and 3.

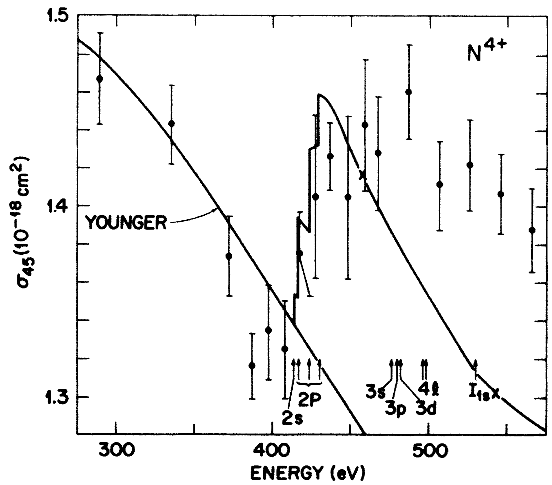

FIG. 7. Electron-impact ionization of N^{4+} (data points from Ref. 2) in the energy region where excitation-autoionization should contribute. The solid curve is Younger's direct ionization theory (Ref. 6) with Henry's inner-shell excitation (Ref. 3) for $1s^22s \rightarrow \sum_l 1s2s2l$ (given at the energies indicated by the $\times$'s) added to Younger's predictions to obtain the upper solid curve. Arrows and error bars are the same as for inset of Figs. 1 and 3.

given by Henry and is approximately represented by the amplitude of the threshold steps shown on the figures.

The contributions to total ionization by excitation-autoionization through excited states with $n > 2$ have not been included in any of the calculations. A crude estimate of the excitation cross sections for these higher n states can be obtained using the usual n^{-3} scaling rule for formation of highly excited states.[23] This scaling suggests that all n levels above $n = 2$ would contribute an increase of about 60% to the excitation-autoionization component. Such a 60% increase in the indirect component is consistent with the data shown in the figures. Note particularly in Figs. 6 and 7 for C^{3+} and N^{4+} that the measured cross sections do appear to be enhanced by higher n level excitations, roughly as expected.

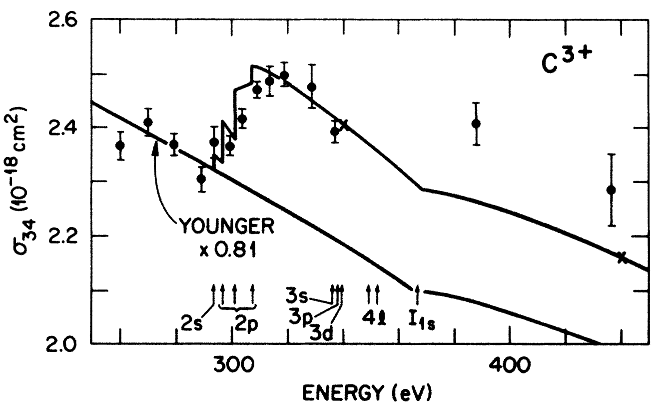

FIG. 6. Electron-impact ionization of C^{3+} (data points from Ref. 2) in the energy region where excitation-autoionization should contribute. The direct-ionization theory of Younger (Ref. 6) has been multiplied by 0.81 for best fit to the four experimental values between 255 and 290 eV. The upper solid curve is simple addition of Henry's coupled-state excitation calculations (Ref. 3) to the Younger theory. The summed excitation calculations for $1s^22s \rightarrow \sum_l 1s2s2l$ are given by Henry only at the energies indicated by the $\times$'s. Arrows and error bars are the same as for inset of Figs. 1 and 3.

For the C^{3+} and N^{4+} cases the CBX ionization calculations of Jakubowicz and Moores[7] which include excitation of $n = 2$ levels are available. These calculations are not shown on Figs. 6 and 7, but the agreement with experiment is quite similar to that obtained by adding Henry's excitation calculation to renormalized Younger direct ionization (see Table V).

Table V shows the comparisons of the $1s \rightarrow 2l$ inner-shell excitation cross sections. Because of statistical precision in the measurements, the B^{2+}, C^{3+}, and N^{4+} measurements provide the most definitive comparisons with excitation theory. The six-state close-coupling calculations by Henry are believed to be the most reliable and are in agreement with experiment except for the Be^{+} case.

The original, scaled-hydrogenic, Coulomb-Born calculations of Sampson and Golden[5] (and Gaunt factor predictions[8]) give best agreement with the Be^{+} case. This agreement with Sampson and Golden may be accidental since these calculations claim no validity for the lower charge states and are not expected to be as accurate as the other calculations for any of the individual cases. Recently Sampson *et al.*[5] have modified their $Z_{\rm eff}$ scaling parameters in order to obtain better agreement with previous experiments and more sophisticated calculations such as those of Henry. Table V gives both the original and rescaled Coulomb-Born results. Agreement with experiment for the Be^{+} case is lost in the rescaling.

For the Be^{+} case, the discrepancy between the deduced experimental cross section and the coupled-state calculations may be indicative of relatively stronger coupling between states in this lowest charge case. The situation is reminiscent of the $2s$-$2p$ outer-electron excitation in Be^{+} compared to C^{3+} and N^{4+}. For the $2s$-$2p$ excitation, the C^{3+} and N^{4+} experimental data agree completely with Coulomb-Born, distorted-wave, or few-state, close-coupling calculations.[24] However, for Be^{+} none of the available calculations agree with experiment, but coupled-state calculations with the greatest number of coupled states (8) are closest.[25] For the present inner-shell excitation calculation, for Be^{+}, the off-diagonal terms in the reactance matrix are rather large (of order 0.1 compared to 10^{-4} in the other Li-like cases). The occurrence of these large off-diagonal terms may be indicating a need to include more coupled states, which is a formidable task.

VI. CONCLUSIONS

We have presented new results comparing experiment and theory for ionization and excitation cross sections. The comparison of excitation is important because there are very few experiments with multicharged ions which can test the validity of theoretical predictions. The ionization comparison is also of fundamental interest and the role of excitation-autoionization becomes more important with increasing ionic charge. The Li isoelectronic sequence is the simplest in which the inner-shell excitation-autoionization can occur. Even in this case some ambiguity may arise due to possible contributions by recombination resonances such as discussed here for O^{5+}.

Previous experiments[2] and analysis[18] raised questions about excitation theory and the relative role of excitation-autoionization as the initial ionic charge of the collision system increased. The present results reduce concern that unexpected discrepancies might occur in excitation predictions for highly charged ions. However, the resonance recombination with auto-double-ionization, discussed here to explain the observed O^{5+} ionization cross section, suggests new challenges in reliably predicting cross sections for inelastic electron-ion collisions.

Resonance interference between the direct ionization and indirect excitation-autoionization channels had been considered as a possible source of discrepancy between experiment and the theory, which simply added excitation-autoionization to direct ionization. In their theory, Jakubowicz and Moores[7] attempted to allow for interference by including states for both channels in the target wave functions. They found no appreciable interference modification of the total cross sections. Within the resolution of the present experiments we find no evidence for interference affecting the total ionization cross sections. Interference effects may still be present and could appear dramatically in differential measurements which observe energy or angle of product electrons.

The best theories[6,7] for direct ionization are found to be in progressively better agreement with experiment for higher charge states along the Li-isoelectronic sequence. The only remaining discrepancy between theory and experiment for excitation is found for the lowest charge-state ion of the sequence. Additional comparisons with improved data for the present cases and for higher ionic charges are desirable.

ACKNOWLEDGMENTS

This work was sponsored by the Office of Fusion Energy of the U.S. Department of Energy. One of us (A.M.H.) acknowledges support by the Department of Energy through the Oak Ridge Associated Universities. Oak Ridge National Laboratory is operated by Martin Marietta Energy Systems, Inc., under Contract No. DE-AC05-840-R21400 with the U.S. Department of Energy.

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