Electron-impact ionization of O^{5+}: Improved measurements

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New measurements of total cross sections for single ionization of O^{5+} by electron impact are reported in the energy range 120–580 eV. The improved experimental accuracy reveals the structure of the inner-shell excitation-autoionization threshold. Comparison with distorted-wave calculations for direct ionization shows good overall agreement, but up to 9% difference in the shape for direct ionization in the energy region below the onset of $1s$-nl excitation-autoionization. An effort was made to measure structure in the cross section due to resonant-excitation–auto-double-ionization which was suggested by earlier measurements. No clear evidence of these processes is observed, and their contribution to the total single-ionization cross section is determined to be less than 10^{-20} cm^2.

I. INTRODUCTION

One of the atomic processes basic to an understanding of astronomical and laboratory plasmas is electron-impact ionization. Because of the approximations required to perform calculations, accurate experimental data are needed to check theoretical approaches. Measurements of total ionization cross sections can provide valuable information about the various processes involved. Li-like ions are prime candidates for an extensive study by experiment and theory. The experiments benefit from the absence of metastable ions in the beams, so a well-defined collision system can be investigated. The electronic structure is simple enough to make fairly detailed calculations possible, but the presence of inner-shell electrons make possible various indirect processes.

Cross sections for electron-impact ionization of Li-like O^{5+} have already been reported by this group.[1,2] The experimental principle is straightforward. Ions of energy 10 kV$\times q$ (q is the ionic charge) are crossed at right angles by a variable-energy electron beam. The ionized ions are carefully separated from the primary beam and detected. The background level is determined by chopping the electron beam. Recently more accurate results have become possible due to improvements in the experiment.[3] These include major changes in the separation and detection system, which reduced the sensitivity to space-charge modulation of the ion beam (as described in Ref. 2), thereby reducing the systematic uncertainties. Also, the output of the electron-cyclotron-resonance heated (ECR) ion source providing the O^{5+} beam was increased, allowing accumulation of better statistics in a shorter period of time. The current status of the experiment is described elsewhere in detail.[3]

The basic process of direct ionization,

$$O^{5+}+e^- \rightarrow O^{6+}+2e^- , \tag{1}$$

is well understood. The semiempirical Lotz formula[4] provides a very simple way to estimate direct ionization and is usually correct within a factor of two. Distorted-wave calculations frequently give a much more accurate description.[5]

States produced by inner-shell ($1s$ to nl) electron-impact excitation of Li-like ions are very likely to decay via autoionization [excitation-autoionization (EA)], thus contributing to single ionization,

$$O^{5+}(1s^2 2s)+e^- \rightarrow O^{5+}(1s2snl)+e^- \searrow O^{6+}+e^- . \tag{2}$$

For low-Z ions and excitation to low principal quantum levels n the branching ratio to autoionization approaches 100%. By measuring the threshold for EA with sufficient energy resolution to distinguish between the onsets of excitation into different levels it is possible to gain information about the cross section for excitation to these levels.

In an earlier experiment[2] the question was raised about the possible contribution of resonant-excitation–auto-double-ionization (READI) to the total single-ionization cross section. In this process, an electron is captured by the ion followed by auto-double-ionization,

$$O^{5+}+e^- \rightarrow (O^{4+})^{**} \rightarrow O^{6+}+2e^- . \tag{3}$$

Energetically the $(O^{4+})^{**}$ intermediate state can only decay to O^{6+} by ejection of two electrons in a single correlated event. Although the cross section for the first step (resonant excitation) can be large ($\sim 10^{-18}$ cm^2), the branching ratio for decay of the excited intermediate state by auto-double-ionization is predicted[6] to be small. This process can most likely be observed for recombination into the lower states of O^{4+} such as $1s2s^22p\,^3P$ and $1s2s2p^2\,^3D$. Auto-double-ionization is still possible for these states, which are well separated in energy, so the peaks are resolvable within the experimental energy spread. The branching ratio for auto-double-ionization is expected to be near maximum for these transitions due to good overlap of the wave functions of the electrons involved in the process.[6]

II. RESULTS

A. Total cross section

Experimental cross sections for ionization of O^{5+} are listed in Table I and plotted in Fig. 1. One-standard-deviation uncertainties due to counting statistics are indicated and are representative of the relative uncertainty of the measurements. Total absolute systematic uncertainty for a typical measurement near the peak cross section is $\pm 8\%$ at 90% confidence level. These measurements are in quantitative agreement with previously published, but less precise, cross-section data.[2] Table II provides a comparison chart of typical experimental parameters for the three measurements of O^{5+} ionization made in this laboratory.

The curve shown in Fig. 1 represents the results of various calculations.[6–8] At energies below the excitation-autoionization threshold the theories for direct ionization agree within 1.5%. Overall, experiment and theory are in good agreement. However, the experimental cross section rises slightly less steeply from the threshold than all the calculations and is essentially constant from 300 eV to the

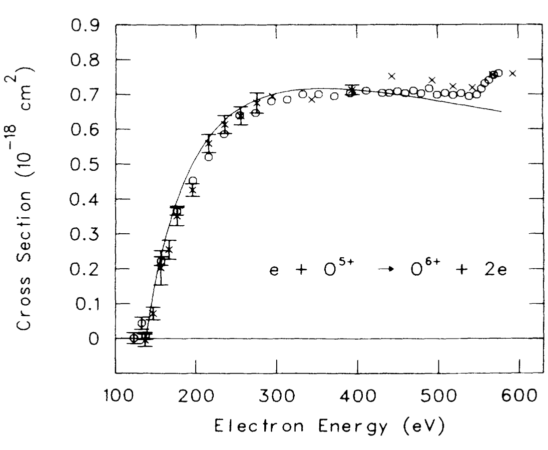

FIG. 1. Cross section vs interaction energy for electron-impact ionization of O^{6+}. The circles are present results, with one-standard-deviation relative uncertainties. The crosses are previous experimental results (Ref. 2). Where no error bars are plotted the relative uncertainty was smaller than the symbol. The calculations (Refs. 6–8) are represented by one curve since on the scale of this figure the theoretical results are indistinguishable.

TABLE I. Experimental electron-impact ionization cross sections for O^{5+}. Uncertainties listed here are one-standard-deviation relative only.

Energy (eV)	Cross section (10^{-18} cm^2)
122.9	0.0008±0.0158
132.7	0.0440±0.0176
137.5	0.0073±0.0100
157.1	0.2224±0.0124
176.7	0.3650±0.0105
196.3	0.4529±0.0064
215.8	0.5194±0.0064
235.4	0.5861±0.0080
254.9	0.6405±0.0072
274.5	0.6468±0.0070
293.9	0.6806±0.0051
313.5	0.6856±0.0052
332.8	0.7004±0.0071
352.4	0.7004±0.0075
372.0	0.6946±0.0066
391.5	0.7035±0.0039
411.2	0.7106±0.0037
431.1	0.7036±0.0033
439.8	0.7039±0.0044
450.0	0.7086±0.0031
459.5	0.7029±0.0042
469.8	0.7107±0.0032
479.3	0.7025±0.0040
489.4	0.7168±0.0029
499.1	0.6992±0.0038
508.9	0.7037±0.0033
518.8	0.6981±0.0037
528.7	0.7032±0.0031
538.6	0.6942±0.0036
541.1	0.7009±0.0031
542.3	0.6994±0.0031
543.5	0.6963±0.0031
544.7	0.6999±0.0031
545.8	0.6996±0.0031
547.0	0.6958±0.0030
548.2	0.7020±0.0030
548.4	0.6985±0.0035
549.4	0.6967±0.0030
550.6	0.6998±0.0030
551.8	0.7025±0.0030
553.0	0.7057±0.0030
554.2	0.7158±0.0030
555.3	0.7200±0.0030
556.5	0.7258±0.0030
557.7	0.7359±0.0030
558.4	0.7314±0.0035
558.9	0.7411±0.0030
560.1	0.7398±0.0030
561.3	0.7460±0.0030
562.5	0.7412±0.0030
563.7	0.7404±0.0030
564.9	0.7401±0.0030
566.0	0.7458±0.0030
567.2	0.7510±0.0030
568.4	0.7522±0.0030
569.6	0.7554±0.0030
570.8	0.7571±0.0030

TABLE I. (*Continued*).

Energy (eV)	Cross section (10^{-18} cm^2)
572.0	0.7588±0.0030
573.1	0.7625±0.0030
574.4	0.7592±0.0030
575.5	0.7603±0.0030

onset of excitation-autoionization at 550 eV, whereas the theories predict a maximum around 350 eV. The measurements yield zero cross section below threshold for ionization of ground-state O^{5+} (138 eV). This confirms the absence of any metastable O^{5+} ions in the primary beam as well as the absence of modulated background due to the space charge of the electron beam. (For discussion of these and related potential problems in crossed-charged-particle-beams experiments see, e.g., Ref. 9.)

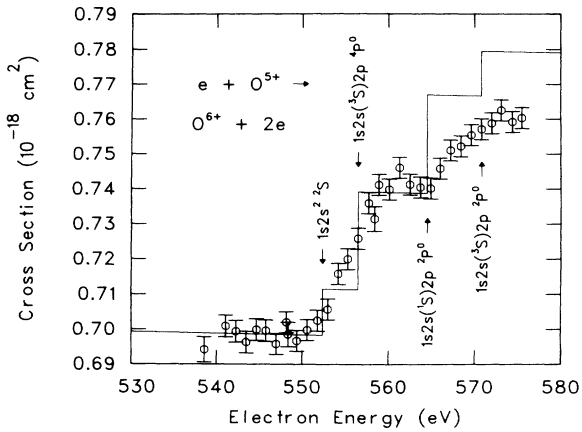

FIG. 2. Energy range from 530–580 eV in more detail. The onsets of the levels leading to excitation autoionization are marked. The straight line is based on the calculations by Henry (Ref. 10) as explained in the text.

B. Excitation-autoionization threshold

Figure 2 shows the expanded energy region near the excitation-autoionization threshold. Included are theoretical results for electron-impact excitation as calculated in a six-state close-coupling approximation by Henry,[10] which are added to an extrapolated straight-line fit to the experimental direct-ionization cross section just below the EA threshold. The agreement is excellent for the first two levels [$1s2s^2\,^2S$ and $1s2s(^3S)2p\,^4P^o$], suggesting a close to 100% branching ratio for decay of the excited states by autoionization. Significant discrepancies exist for the higher two levels taken into account in the calculations [$1s2s(^1S)2p\,^2P^o$ and $1s2s(^3S)2p\,^2P^o$], indicating possible inaccuracies in the calculated energy levels or excitation cross sections, or a less-than-unity branching ratio for autoionization.

The accuracy of the experimental energy scale is limited by our knowledge of the space charge of the electron beam (beam current typically 4.7 mA at 550 eV). The space-charge correction to the cathode voltage is essentially proportional to the electron energy and is typically 10.7 eV at 550 eV. Also, the energy spread within the electron beam is determined primarily by the space charge and is estimated to be 2.4 eV. Both the space-charge correction and the electron-beam energy spread are extrapolated from measurements of excitation at low energies.[11] Part of the space charge may be neutralized by ions created from background gas; the amount of neutralization (typical residual gas pressure 2×10^{-9} torr) is not known exactly and may differ from measurements made at low energies. However, the agreement with theory for the first two excitation-autoionization-level onsets confirms the energy correction to be accurate within about 2.5 eV, giving confidence in the estimate of the energy spread.

C. Resonant-excitation–auto-double-ionization

Figure 3 shows a very careful scan made over the energy region where READI would be expected to contribute to the ionization cross section. For recombination into

TABLE II. Typical experimental parameters at 500 eV electron energy. The effects of improvements in the apparatus are reflected in higher ion-beam currents and lower background count rates. The integration time required for a standard deviation of the mean of 1% is provided for comparison; other factors limited the reproducibility obtainable in a single measurement to 7% in 1979, 2% in 1986, and 1% in the present work.

	Electron current (mA)	Ion current (nA)	Background count rate (sec^{-1})	Signal count rate (sec^{-1})	Counting time for 1% standard deviation (min)
1979 (Ref. 1)	4.6	15	30	8	325
1986 (Ref. 2)	2.9	350	1440	180	36
Present work	3.6	800	1080	400	5.5

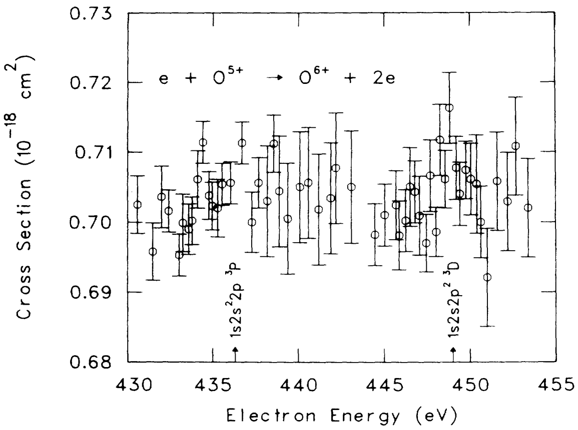

FIG. 3. Energy range from 430–455 eV. For reasons of clarity these results have been omitted from Fig. 1. Plotted uncertainties are one standard deviation relative only. The energies for two levels which could lead to READI in this range are indicated.

the $1s2s\,^22p\,^3P$ state the energy has been calculated[12] to be 436.3 eV and for the $1s2s2p^2\,^3D$ state, 449.0 eV. The error bars in Fig. 3 indicate one-standard-deviation statistical uncertainty only (typically $\pm 0.75\%$). At that level small day-to-day changes (less than 5%) in the absolute experimental calibration became significant, so the average of all points measured in one data run (always more than ten) was normalized to lie on a straight line over this narrow energy range. Since systematic errors are expected to be constant over a short time period, the measurements in one data run were cycled repeatedly with only four seconds integrating time at each energy in each cycle. Although there is some suggestion, no structure in the data can be clearly established, giving an upper limit of the cross section for READI of 10^{-20} cm^2 for an estimated experimental energy spread of 2.4 eV. Also READI into higher (Rydberg) levels does not appear to contribute significantly. These levels are spaced very closely in energy and the READI cross sections should "pile up" within our experimental energy spread below the excitation-autoionization thresholds. Figure 2 does not show clear evidence of this process.

III. SUMMARY

In summary, we have presented improved measurements of the cross section for electron-impact ionization of O^{5+}. For direct ionization, a difference of up to 9% with the shape of the cross section predicted by distorted-wave theory is found. The structure of some of the individual $1s$-nl excitation-autoionization contributions has also been resolved. Evidence for contributions due to resonant-excitation–auto-double-ionization, suggested by an earlier experiment, is not substantiated in the improved measurements. For our 2.4-eV energy resolution an upper limit for the contribution due to this process is determined to be 10^{-20} cm^2.

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