

Total photoionization cross sections of atomic oxygen from threshold to 44.3 Å

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The relative photoionization cross section of atomic oxygen for the production of singly charged ions has been remeasured in more detail and extended to cover the wavelength range 44.3–910.5 Å by use of synchrotron radiation. In addition, the contribution of multiple ionization to the cross sections has been measured, allowing total photoionization cross sections to be obtained below 250 Å. The results have been made absolute by normalization to our previously measured data. The use of synchrotron radiation has enabled measurements of the continuum cross section to be made between the numerous autoionizing resonances that occur near the ionization thresholds. This in turn has allowed a more critical comparison of the various theoretical estimates of the cross section to be made. The series of autoionizing resonances leading to the 4P state of the oxygen ion have been observed for the first time in an ionization-type experiment, and their positions have been compared with both theory and previous photographic recordings.

I. INTRODUCTION

It has long been realized that the photoionization of atomic oxygen plays an important role in the interpretation of solar-terrestrial effects and in the study of stellar atmospheres. Experimental difficulties associated with its measurement, however, meant that, for many years, a knowledge of the magnitude of the photoionization cross section was limited to theoretical estimates. The first calculation was made by Bates *et al.*¹ in 1939 using a Hartree-Fock approximation, but it was not until 1949 that Bates and Seaton² reported more detailed calculations that took into account the effect of exchange. Since then many authors^{3–17} have reported calculations that incorporate increasing degrees of sophistication and complexity associated with the photon-atom interaction. An interesting review on the progress of our understanding of the photoionization of atomic oxygen since 1939 has been given recently by Seaton.¹⁸

The first absolute measurement of the atomic oxygen photoionization cross section was made in 1965 by Cairns and Samson¹⁹ who used an absorption tube technique to measure its total absorption cross section. It was remeasured by Comes *et al.*²⁰ using a crossed beam method, but the agreement was not good. Subsequent measurements by Kohl *et al.*²¹ were made covering a limited energy range using the dissociation produced in a shock-heated gas. In 1985 Samson and Pareek²² reported absolute measurements made using a mass spectrometric technique; they also showed that for photon energies above ~25 eV the atomic cross section was very close to one-half of the total molecular ionization cross section. Huffman *et al.*²³ used a photographic technique to classify the autoionizing resonances leading to the $^4S^\circ$, $^2D^\circ$, and $^2P^\circ$ thresholds and Dehmer *et al.*²⁴ measured relative photoionization cross sections in the same region. In addition, several measurements have been made of the branching ratios for the production of the $^4S^\circ$, $^2D^\circ$, and $^2P^\circ$ states,^{25–27} and of the angular distributions of the

ejected photoelectrons.^{26,28}

The purpose of the present experiment was to remeasure the relative photoionization cross section of atomic oxygen, including the effects of multiple ionization, over as wide an energy range as possible using the continuum radiation available from a synchrotron storage ring. This would also allow more detailed measurements at the ionization threshold to be made. In addition, a clearer picture of the variation of the continuum cross section between the autoionizing resonances from the $^4S^\circ$ to the $^2P^\circ$ ionization thresholds could be obtained, in order to give an indication of which of the presently available theories describes most closely the ionization process in this region. The continuum radiation would also allow observation of the Rydberg series $2s2p^4(^4P)np$, the presence of which had been indicated at only a few discrete wavelengths in our previous work.²²

II. EXPERIMENTAL APPROACH AND ANALYSIS OF RESULTS

The experiment was performed at the University of Wisconsin synchrotron storage ring, Aladdin, using radiation from both a 4-m normal incidence and a Mark II Grasshopper grazing incidence monochromator. Figure 1 shows a schematic diagram of the apparatus used in the experiment. Molecular oxygen was partially dissociated in a microwave discharge sustained by the air cooled cavity, *C*. The discharge, operated at 2450 MHz and with up to 100 W microwave power, was initiated by a spark from a Tesla coil. The discharge products flowed along the pyrex tube, *T*, which was coated with phosphorus pentoxide to minimize recombination on the walls, and passed, via a 0.5-mm orifice through the center of the collision region, *R*, and then to the turbo-molecular pump, *P*₁. The differential pumping region, *D*, evacuated by the turbomolecular pump, *P*₂, separated the relatively high-pressure collision region (~10⁻⁶ torr) from the ultrahigh vacuum of the monochromator output mirror box

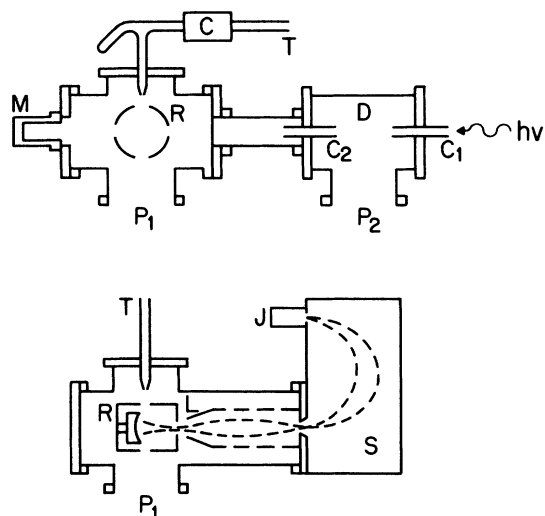


FIG. 1. Schematic diagram of the apparatus showing the side view (upper diagram) and end view (lower diagram) as seen from *M* looking towards *D* (for symbols see text).

($\sim 5 \times 10^{-10}$ torr). Radiation passed via the low conductance canals, C_1 and C_2 , through the middle of the collision region, *R*, and was then incident on the photon detector, *M*. This was either a sodium salicylate-photomultiplier combination or an aluminum photodiode, the current from either of which was recorded by a picoammeter. Ions produced in the collision region were extracted and focused by the electrostatic lens system, *L*, onto the entrance of the 180° electromagnetic mass spectrometer, *S*, where the ions of interest were separated and directed to the first dynode of the Johnston type MM1 particle multiplier, *J*, the signal from which was recorded using particle-counting techniques. The signals from the photon detector and the ion rate meter were simultaneously recorded on a strip chart recorder.

The experimental investigation was conducted as follows. Previous investigations in our laboratory have shown that the dissociation fraction produced by the microwave discharge requires a considerable period in which to stabilize but that once it has done so the atomic production remains essentially constant. Consequently, pure O_2 was admitted to the discharge tube via a needle valve and the microwave discharge struck. This was then left to stabilize for up to 4 h. The electromagnet was tuned to select O^+ ions and the monochromator scanned over the wavelength range of interest. A similar scan was made of the parent molecular ion, the whole process being repeated with the microwave discharge extinguished. Repeat measurements were made at several discharge gas pressures between 200 and 700 μm and, in the case of the 4-m monochromator, with both the photomultiplier and photodiode as photon detector.

The number, N^+ , of ions produced when a flux I_0 of photons passes through a gas whose number density-path length product is nl is given by the equation

$$N^+ = I_0 n l \sigma, \quad (1)$$

provided $n l \sigma \ll 1$, where σ is the photoionization cross

section. If the ion extraction, analysis, and detection system has an overall efficiency F and if the efficiency of the photon detector is G , then Eq. (1) becomes

$$N_D^+ / F = (I_D / G) n l \sigma, \quad (2)$$

where N_D^+ and I_D are the ion count rates and photon signals, respectively, actually recorded. It may be seen that for constant n , l , and F we obtain the expression

$$\sigma \propto (N_D^+ / I_D) G. \quad (3)$$

Relative values for the efficiency G of the photodiode used in the experiment could be obtained by running a noble gas (neon or argon) through the collision region in place of the oxygen and recording the ion count rate and photodiode signal simultaneously. Since the noble-gas absorption cross sections $\sigma(\text{Ar, Ne})$ are known,^{29,30} Eq. (3) shows that

$$G \propto (I_D / N_D^+) \sigma(\text{Ar, Ne}). \quad (4)$$

For the salicylate-screen-photomultiplier combination the efficiency is known to be constant up to photon energies of ~ 60 eV;³¹ this detector was never used for wavelengths shorter than ~ 400 Å. Thus, using either photon detector, Eq. (3) may be used to determine the relative variation of the photoionization cross section for the gases under study.

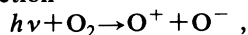
Data were recorded on the 4-m monochromator from well before the ionization threshold to approximately 400 Å. Between the atomic ionization threshold (910.4 Å) and 662 Å the ion signal arose purely from the ionization of the atom; at wavelengths shorter than this a component caused by dissociative ionization was also present. At these wavelengths the relative atomic ionization cross section is given by the expression

$$\sigma \propto G [(N_D^+ / I_D) - \alpha (N_D^+ / I_D)_{\text{off}}], \quad (5)$$

where the second bracket represents the ion to photon ratio with the microwave discharge turned off and α is the fraction of molecular oxygen left undissociated. It should be noted, however, as observed by Samson and Pareek,²² that Eq. (5) is strictly true only in the absence of excited states of the oxygen molecule. Several groups^{19,25,32} have shown that the production of atomic oxygen in a microwave discharge leads to the formation of molecular oxygen in its $a(^1\Delta)$ excited state. Thus, the presence of this species must be considered. However, it can be shown²² that this has a negligible effect on the atomic cross section provided that the continuum photoionization cross section of O_2 in its ground $X(^2\Sigma_u)$ state is comparable to O_2 in the $a(^1\Delta)$ state. From the theoretical calculations of Roche *et al.*³³ It appears that this is a reasonable assumption.

The fraction α was determined from the molecular ion to photon ratio obtained from runs with the microwave generator turned on and off. It was found to be of the order 0.83–0.93 depending on the pressure in the discharge tube and the condition of the phosphorous pentoxide coating. Values for the ion count rate and photon signal were measured from the chart recorder traces at appropriate wavelengths, chosen to be at positions not

influenced by the many autoionizing resonances observed. The relative cross sections were determined using either Eq. (3) or (5), depending on whether the wavelength was above or below the dissociative ionization threshold. A further correction to the O^+ production cross section was necessary between 700 and 725 Å because of the production of O^+ from the pair production reaction



which was previously reported by Dehmer and Chupka³⁴ and which was clearly visible in the O^+ signal trace recorded with the microwave switched off. No new information could be gained from the width of the autoionizing resonances over that already obtained by Dehmer *et al.*²⁴ because the 4-m monochromator, although having a designed resolution of 0.07 Å for a 100- μ m exit aperture, was found to have an actual resolution of 0.6 Å that was largely independent of the monochromator slit width. For this reason, and because of the number of peaks involved, values for the photoionization cross section have not been calculated over the autoionizing peaks.

Data on the grazing incidence monochromator were recorded from its long-wavelength limit of 310 to 44.3 Å at which point considerable photon loss was apparent because of increasing absorption at the carbon *K* edge caused by carbon deposited on the mirrors and grating. All the oxygen ion signals, except O^{3+} , taken on this monochromator had dissociative ionization components associated with them. Thus Eq (5) was used exclusively to determine the relative photoionization cross section. Equation (5) also applies in determining multiple-ionization cross sections provided N_D^{n+} is substituted for N_D^+ , where *n* is the degree of ionization. The relative cross section can then be placed on an absolute basis by determining the constant of proportionality for Eq. (5). This constant is the same for single or multiple ionization. More details on the multiple ionization of atomic oxygen are given in a separate paper.³⁵

A major difficulty associated with the use of a continuum as opposed to a discrete line source is the separation of true signal from that arising from second- and higher-order spectra and scattered radiation. Subsidiary experiments were carried out on both monochromators to try to determine the extent of the contamination by unwanted radiation. On the 4-m normal incidence monochromator using the photomultiplier detector the following technique was used.

At any particular wavelength it was assumed that the radiation consisted of components of both the first and second orders I'_0 and I''_0 . These in turn would produce ion signals N' and N'' with cross sections σ' and σ'' , according to Eq. (2). In the experiment the measured ratio of ions per photon was given by

$$\mathcal{R} = \frac{(N'_D + N''_D)}{(I'_D + I''_D)} .$$

Thus,

$$\mathcal{R} = \frac{F/G(I'_D n l \sigma' + I''_D n l \sigma'')}{(I'_D + I''_D)} .$$

Because *F*, *G*, and the number-density–path-length product *nl* are assumed to be constant, this may be reduced to

$$\mathcal{R} = \frac{C[\sigma' + (I''_D/I'_D)\sigma'']}{[1 + (I''_D/I'_D)]} ,$$

where *C* is a constant. The ratio above could be determined at wavelengths just above and below the onset of ionization for a particular gas target yielding two equations for the two unknowns *C* and (I''_D/I'_D) , where it is assumed that this ratio is constant over a restricted wavelength range. This process was carried out at the argon and neon ionization thresholds, (787 and 575 Å, respectively) and at the threshold for O_2^+ production (1026 Å). (I''_D/I'_D) was found never to exceed 4%. Higher-order corrections to data gathered on the 4-m monochromator thus had only a small effect on the final result.

For the grazing incidence monochromator a different approach was necessary. Because the lowest energy available from the machine was 40 eV, no threshold for single ionization was available. The thresholds for the production of doubly, triply, and, in some cases, quadruply charged ions were accessible, however, and, by tuning the magnetic mass spectrometer to the appropriate position, the variation of the production of the multiply charged ion with respect to the photon energy could be obtained. It was assumed that any signal at energies below the threshold was primarily caused by second-order radiation. By comparing this signal with the signal obtained at the appropriate second-order wavelengths, an estimate of the higher-order fraction present was derived. Using this estimate, corrections to the ion production rate and the photon signals for both noble gas and molecular oxygen targets were made. The photodiode efficiency was calculated from the noble-gas data, and, using this, the relative singly charged molecular oxygen production cross section was determined. A second estimate of the higher-order percentage was then made that forced these molecular oxygen cross sections to agree, when normalized, with the previously measured absolute values of Samson *et al.*³⁶ This second estimate of the contamination component was then used to recorrect the ion production rates and diode signals. The photodiode efficiency was recalculated and the new value used to redetermine the molecular oxygen cross section. This procedure was repeated until no further change in the higher-order component was necessary. As a check on this higher-order subtraction, molecular nitrogen was introduced into the collision region and the cross section for the production of molecular nitrogen ions was calculated using the correction factors as determined above. Figure 2 shows both the variation of the molecular oxygen and nitrogen cross sections as a function of wavelength, compared to previously measured data.^{36,37} Although the agreement between the present data and the previously measured molecular oxygen cross sections is to be expected, the good agreement between the two measurements of the molecular nitrogen cross section acts as a confirmation that the second-order subtraction applied to the data is approximately correct.

Oxygen data, taken on both the 4-m and grazing in-

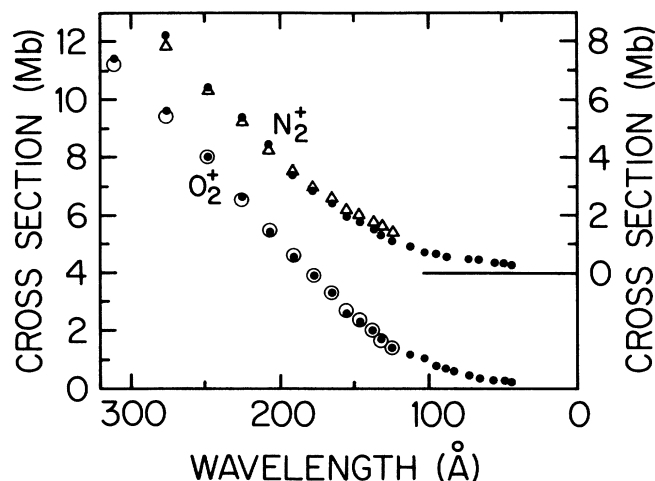


FIG. 2. Photoionization cross section for production of O_2^+ from O_2 (left ordinate) and N_2^+ from N_2 (right ordinate). ●, present data; ○, (O_2^+), Samson *et al.* (Ref. 36); △, (N_2^+), Samson *et al.* (Ref. 37).

vidence monochromator, were normalized to the absolute measurements of Samson and Pareek.²² For the 4-m data this was done at 584 Å since Samson and Pareek had taken considerable care in the laboratory to ensure the accuracy of the cross-section measurement at this wavelength. In addition, although the ion signals (taken both with the microwave on and off) revealed considerable structure in the long-wavelength region, caused by molecular transitions, the region of 584 Å was almost entirely free from them. For the grazing incidence measurements a factor was determined that gave a good fit between the two sets of data over the wavelength range of overlap.

III. RESULTS AND DISCUSSION

The absolute values of the photoionization cross section obtained in the present work are tabulated in Table I for wavelengths between 911 and 260 Å. Because multiple ionization cannot occur in this wavelength range, the tabulated values represent the total photoionization cross sections. The actual wavelengths used between 911 and 677.5 Å, a region of structure, are tabulated in the first portion of Table I. Towards shorter wavelengths the data have been averaged with the previous results and smoothed to give a best fit to the data. Table II lists the specific cross sections for single, double, and triple photoionization between 254.4 and 44.3 Å. The final column of Table II gives the total photoionization cross section.

The present results (not smoothed) are shown in Fig. 3 along with previous experimental results. The present measurements are shown as closed circles, while the previous data of Samson and Pareek²² are shown as open circles. Also shown are the experimental results of Kohl *et al.*²¹ (inverted triangles) and those of Comes *et al.*²⁰ (triangles). The data at the oxygen *K* edge, shown at twice the normal scale, were taken from the compilation of Henke *et al.*³⁸

The two points measured by Samson and Pareek at 700.3 and 684.6 Å appear to be lower than would be expected. However, examination of the recorder traces re-

veals that at precisely these wavelengths the ion production rate passes through a minimum because of the influence of the autoionizing resonances leading to the $^2P^o$ threshold [see Fig. (5)].

The partial cross sections for producing O^+ in the $^4S^o$ ground state and $^2D^o, ^2P^o$ excited states are also shown in Fig. 3. These results were obtained from the product of

TABLE I. Absolute photoionization cross sections of atomic oxygen between 911 and 260 Å. Units in Mb ($1 \text{ Mb} = 10^{-18} \text{ cm}^2$).

λ (Å)	Cross section	λ (Å)	Cross section
911.00	0.15	690.6	9.47
910.50	0.70	690.0	9.80
910.00	1.15	683.9	9.25
909.80	2.45	683.0	9.65
907.50	2.75	682.8	9.69
905.00	2.75	677.5	10.0
900.00	2.85	665.3	12.0
895.00	2.75	660	12.6
890.00	2.70	650	13.0
885.00	2.85	640	13.3
870.00	3.10	630	13.4
865.00	3.10	620	13.4
860.00	3.10	610	13.4
855.00	3.10	600	13.3
850.00	3.20	590	13.2
845.00	3.25	580	13.0
840.00	3.30	570	12.9
835.00	3.30	560	12.7
830.00	3.30	550	12.5
825.00	3.30	540	12.3
785.00	3.70	530	12.1
780.00	3.70	520	12.0
765.00	4.00	510	11.9
760.22	4.06	500	11.9
760.0	3.90	490	12.0
752.3	4.15		structure
732.2	8.03	430	11.5
730.6	8.40	420	11.3
729.0	9.17	410	11.0
727.5	8.90	400	11.8
722.5	9.02	390	10.5
720.9	8.91	380	10.2
720.0	9.00	370	9.90
719.2	9.00	360	9.57
717.6	8.79	350	9.25
715.7	9.24	340	8.92
714.1	9.18	330	8.60
712.5	9.26	320	8.25
710.8	9.30	310	7.90
710.0	9.15	303.8	7.70 ^a
709.2	9.71	300	7.55
707.6	9.88	290	7.40
705.9	9.71	280	6.85
705.0	9.60	270	6.50
695.3	9.06	260	6.15
693.8	9.00		
692.5	9.60		
692.2	9.51		

^aAbsolute value used for normalization (from Ref. 22).

TABLE II. Absolute photoionization cross section for single, double, and triple photoionization from 44 to 254 Å.

$h\nu$ (eV)	λ (Å)	O ⁺ (Mb)	O ²⁺ (10 ⁻² Mb)	O ³⁺ (10 ⁻³ Mb)	σ_{tot} (Mb)
48.736	254.402	6.00	0.0		6.00
50	248.0	5.75	2.0		5.77
60	206.6	4.25	18.7		4.44
70	177.1	3.20	22.5		3.43
80	155.0	2.37	23.0		2.60
90	137.8	1.84	22.1		2.06
100	124.0	1.44	20.5		1.65
110	112.7	1.20	18.5	0.28	1.39
120	103.3	1.01	16.4	1.01	1.17
130	95.4	0.86	14.2	1.65	1.00
140	88.6	0.72	12.1	2.02	0.84
150	82.7	0.62	10.3	2.20	0.73
160	77.5	0.52	8.4	2.12	0.61
170	72.9	0.45	6.9	1.95	0.52
180	68.9	0.39	5.8	1.75	0.45
190	65.3	0.33	4.8	1.51	0.38
200	62.0	0.286	3.9	1.28	0.33
210	59.0	0.250	3.2	1.07	0.28
220	56.4	0.220	2.55	0.87	0.25
230	53.9	0.197	2.05	0.69	0.22
240	51.7	0.180	1.75	0.54	0.20
250	49.6	0.168	1.50	0.44	0.18
260	47.7	0.161	1.30	0.37	0.17
270	45.9	0.154	1.20	0.32	0.17
280	44.3	0.150	1.05	0.27	0.16

the total atomic cross section and the branching ratios for producing these states. The branching ratios have been measured by the technique of photoelectron spectroscopy at 584 Å by Samon and Petrosky,²⁵ at 304 Å by

Dehmer and Dehmer,²⁶ and between 725 and 580 Å by Hussein *et al.*²⁷ The dashed lines show a reasonable extrapolation of the present data through the partial cross section points at 584 and 304 Å. The solid line represents

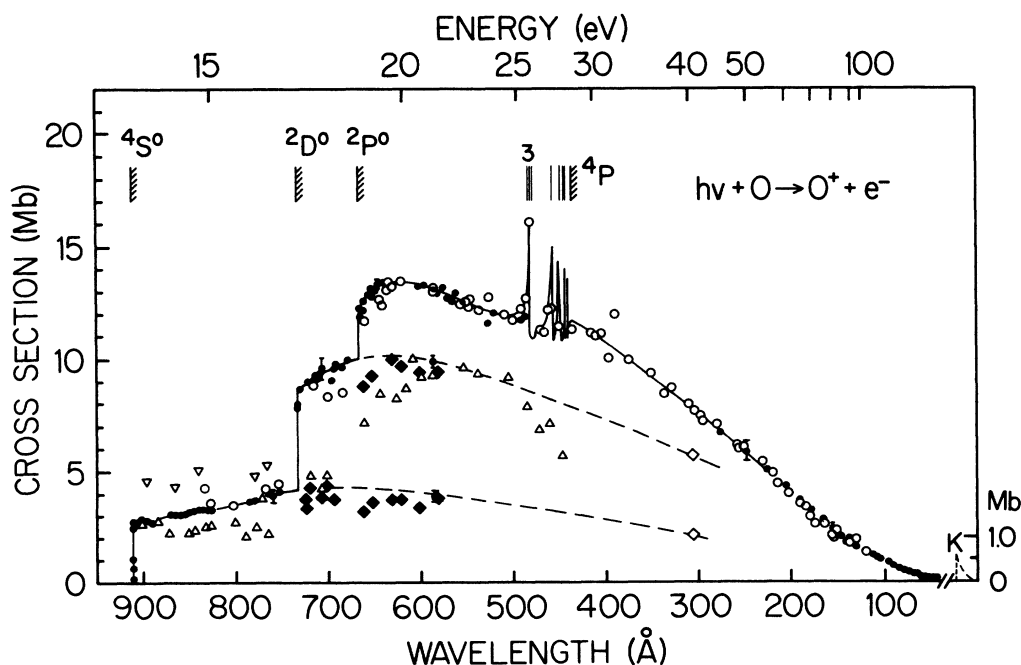


FIG. 3. Photoionization cross section of atomic oxygen for the production of singly charged ions as a function of wavelength. ●, present data; ○, previous data, Samson and Parek (Ref. 22); ▽, Kohl *et al.* (Ref. 21); △, Comes *et al.* (Ref. 20). Partial cross sections; ◆, Hussein *et al.* (Ref. 27); ◇, Dehmer and Dehmer (Ref. 26); ▽ at 584 Å, Samson and Petrosky (Ref. 25).

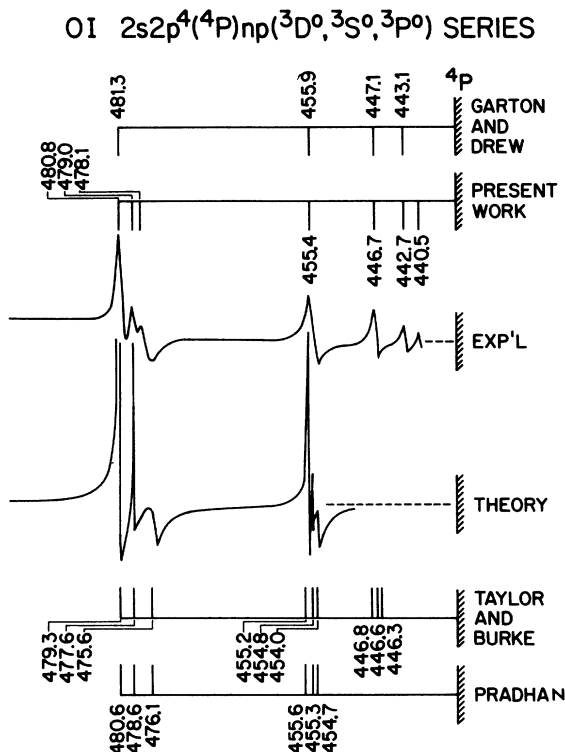


FIG. 4. Autoionizing resonances leading to the 4P threshold; upper curve, the rate meter signal from the present experiment; lower curve, the theoretical predictions of Pradhan (Ref. 10). The upper wavelength assignments are those derived from the present work and the photographic measurements of Garton and Drew (Ref. 40), the lower are those reported by Pradhan (Ref. 10), and Taylor and Burke (Ref. 8).

a best fit to the present data, excluding the resonance structure leading to the 4P threshold. Representative error bars are shown at several points; these were determined from the uncertainty introduced on extracting data from the chart recordings. The overall accuracy of the results depends upon the absolute value of our previous data. An estimated error of $\pm 9\%$ was quoted at that time. However, confidence in the relative and absolute value of the cross sections can be obtained by considering the value of the total oscillator strength for the absorption process. According to the Thomas-Reiche-Kuhn (TRK)-sum rule³⁹ the oscillator strength must add up to a value of 8, the total number of electrons in the atom. Thus, we have evaluated the continuum oscillator strength from the ionization threshold down to 44.3 \AA using the present total photoionization cross sections and from 44.3 to 0 \AA using the cross sections from the compilation by Henke *et al.*³⁸ A value of 7.29 was obtained. Adding this value to our previously quoted line oscillator strength of 0.71 gives a total oscillator strength of 8.00. Obtaining the precise value of the total oscillator strength is, of course, fortuitous because the maximum error in the value of the line oscillator strength ($\pm 50\%$) introduces an error of about $\pm 4.4\%$ in the total oscillator strength. However, this implies that our value of the continuum oscillator strength should be accurate to within $\pm 4.4\%$, which is certainly in keeping with our es-

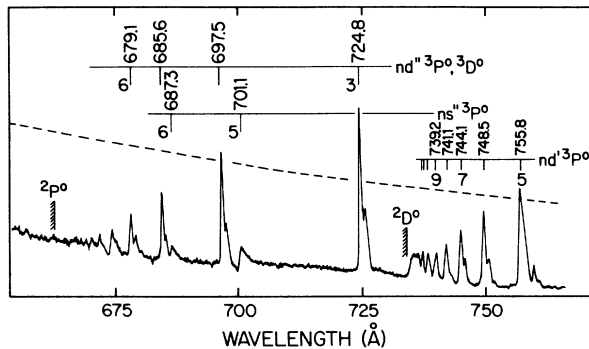


FIG. 5. Rate meter signal in the present experiment showing the autoionizing resonances leading to the $^2D^{\circ}$ and $^2P^{\circ}$ ion thresholds. The wavelength assignments are derived from the present work. The dashed line represents the decrease in the stored ring current over the period that the scan was made and is thus proportional to the photon flux.

timated value of $\pm 9\%$. It should be noted that in our previous work²² we did not take into account the effect of multiple ionization below 250 \AA .

The structure shown in Fig. 3 has not been seen before in photoionization experiments and represents the Rydberg triplet series $2s2p^4(^4P)np(^3D^{\circ}, ^3S^{\circ}, ^3P^{\circ})$. Figure 4 is a trace of the rate meter signal showing the series in detail compared with the theoretical predictions of Pradhan.¹⁰ Also shown are the peak wavelength predictions of Taylor and Burke,⁸ which agree to within 1 \AA with those of Pradhan, and the wavelength assignment of Garton and Drew⁴⁰ who have observed the series photographically in an absorption experiment and obtained an identification for the $np(^3D^{\circ})$ series. As can be seen, the agreement between experiment and theory is good, although the shape and position of the first theoretical triplet differs from that measured experimentally: no attempt has been made to allow for peak shifting or broadening of the measured lines caused by the finite resolution of the monochromator.

Figure 5 illustrates the rate meter signal obtained between 760 and 655 \AA showing the autoionizing resonances leading to the $^2D^{\circ}$ and $^2P^{\circ}$ states of the oxygen

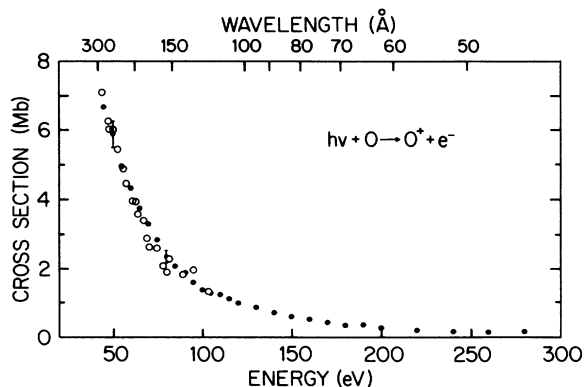


FIG. 6. High-energy region of the photoionization cross section of atomic oxygen leading to the production of singly charged ions. ●, present data; ○, previous data of Samson and Pareek (Ref. 22).

ion. The wavelengths marked agree to within 0.6 Å of the assignments given by Huffmann *et al.*²³ By comparing the height of the autoionizing peaks with the adjacent continuum a lower limit to the peak cross sections may be determined. For example, the peak to background ra-

tio at 724.8 Å is 7.1:1; the adjacent continuum cross section is 8.6 Mb from Fig. 3. Thus, the peak cross section is at least 61 Mb.

Figure 6 shows the high-energy measurements of the atomic oxygen photoionization cross section (closed circles) compared with those of Samson and Pareek²² (open circles) to which they have been normalized. Representative error bars are shown and a further 12% caused by systematic error is estimated. The good agreement of the two sets of data in terms of the variation of the cross section with energy also tends to confirm that the higher-order subtraction previously detailed is correct.

Figures 7(a)–7(c) compare most of the presently available theoretical results with our present data plus those of Samson and Pareek (closed circle data points). The line previously drawn through the experimental points has been omitted as have the $4P$ resonances. The individual theoretical data are identified in the figures by the initials of the authors as given in parentheses in the following description.

In Fig. 7(a) Bates and Seaton² (BS) used Hartree-Fock wave functions to calculate the cross section at the spectral head and then deduced the energy dependence from an approximation given by Bates.¹ Dalgarno *et al.*³ (DL, DV) also used Hartree-Fock wave functions for both the bound and continuum orbitals in their calculations of transitions from the ground state to specific states of the ion. Their data are shown in both the length (L) and velocity (V) approximations. Henry (HL, HV) then investigated the coupling between final-state channels, including as many channels as was technically feasible at the time of computation. McGuire⁴¹ (M) used a development of his semiempirical central potential method to calculate the photoionization cross section of all the elements from helium to xenon, including that of oxygen, whereas, Ganas¹³ (G) used an independent particle model.

In Fig. 7(b) Taylor and Burke⁸ (TB) and Pradhan¹⁰ (P) both introduced close-coupling expansions for the initial and final states, but they used different numerical techniques for the solutions, Taylor and Burke employing the *R*-matrix method while Pradhan used the method of reduction to linear equations; they obtained similar results. Thomas and Helliwell¹⁵ (TH) developed an approximate central potential model for the calculation of the cross section. Koppel¹² (KO) used the scaled Thomas-Fermi method of Stewart and Rotenberg.⁴²

In Fig. 7(c) we show the results of Vesnicheva *et al.*¹⁷ (VL, VV) who used a generalized random-phase approximation with exchange (RPAE) suitable for atoms with a single unfilled shell. Normally, the photoionization cross sections in the RPAE calculations are identical in the length (L) and velocity (V) approximations; however, an approximation used in the calculations resulted in a small difference between the L and V results. Also shown in Fig. 7(c) are the results of Kahler¹¹ (KA) and Saxon *et al.*¹⁶ (SA). Kahler used the scaled Thomas-Fermi method of Stewart and Rotenberg,⁴² as did Koppel (KO) in Fig. 7(b). For photon energies above the $2P^o$ state the two results are almost identical. However, towards lower energies the differences are quite large. Saxon *et al.* used the *R*-matrix technique to calculate the photoionization

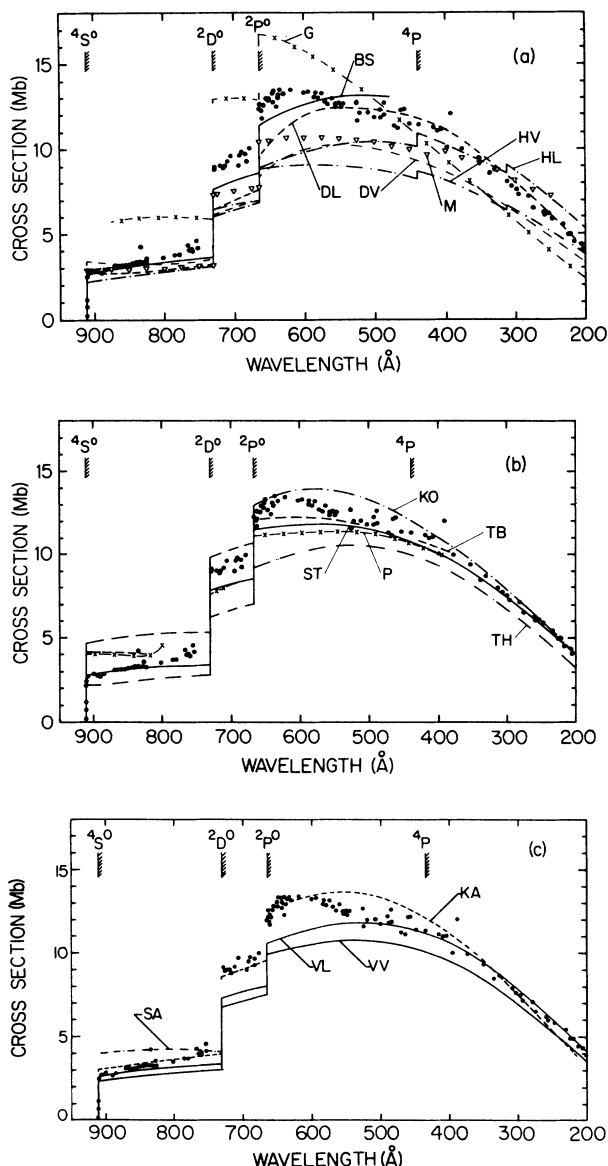


FIG. 7. Comparison of the experimental and theoretical photoionization cross sections of atomic oxygen. The solid circles represent the combined data of the present experiment and the previous measurements of Samson and Pareek (Ref. 22). Theoretical estimates: (a) BS, —, Bates and Seaton, Ref. 2; DL, DV — — — —, Dalgarno *et al.* (length and velocity formulations, respectively), Ref. 3; HL, HV, — · — · —, Henry (length and velocity formulations, respectively), Refs. 5 and 6; M, ▽▽▽, McGuire, Ref. 41; G, -X-X-X-, Ganas, Ref. 13. (b) TB, — — — —, Taylor and Burke (length formulation), Ref. 8; P, -X-X-X-, Pradhan, Ref. 10; TH, — · — · —, Thomas and Helliwell, Ref. 15; KO, — · — · —, Koppel, Ref. 12; ST, — — — —, Starace *et al.*, Ref. 14. (c) VL, VV, — — — —, Vesnicheva *et al.* (length and velocity formulations, respectively), Ref. 17; KA, — — — —, Kahler, Ref. 11; SA, — · — · —, Saxon *et al.*, Ref. 16.

cross section of ground-state atoms leading to the $4S^\circ$ ionic state only as a preliminary to calculating the cross sections for excited oxygen atoms. Their results agree closely with the work of both Taylor and Burke, and Pradhan.

Most of the theoretical data lie within $\pm 40\%$ of the experimental data. However, it is interesting to note that at the $4S^\circ$ ionization threshold the more sophisticated close-coupling and *R*-matrix calculations show a larger disagreement with experiment than many of the other calculations. The theory that most closely describes the variation of the atomic oxygen ionization cross section is that due to Kahler¹¹ [see Fig. 7(c)]. Many of the others accurately predict the variation of the cross section between ionization onset and the $2P^\circ$ threshold though agreement is generally poor between the $2D^\circ$ and $2P^\circ$ onsets. None of the theories accurately predict the shape of the cross section between the $2P^\circ$ and $4P$ thresholds where

the experimental results show a more pronounced peak in the cross section. At higher energies all the theoretical calculations tend to coverage towards the experimental results.

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