J. Phys. B: At. Mol. Opt. Phys. 23 (1990) 745-750. Printed in the UK

Total electron scattering cross sections for molecular oxygen at low electron energies

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Received 26 July 1989, in final form 26 October 1989

Abstract. Absolute total electron scattering cross sections for molecular oxygen have been measured at low electron energies using a photoelectron source. The measurements have been carried out at 38 electron energies varying from 0.15-10 eV with an accuracy of ±2.7%. The cross sections obtained in the present experiment have been compared with other measurements and theoretical computations.

Low-energy electron scattering by molecular gases has been studied for many years. Total cross section measurements are of importance in a variety of applications such as the study of planetary atmospheres and interstellar clouds, plasma physics, laser physics, gaseous dielectrics, diffuse-discharge switching etc. As a result interest in the subject has grown enormously in the last decade.

Electron scattering by molecular oxygen has been extensively studied experimentally, but relatively little theoretical work has been reported. A great majority of these measurements include the work carried out by Brüche (1927), Ramsauer and Kollath (1930), Sunshine *et al* (1967), Salop and Nakano (1970), Griffith *et al* (1982), Shyn and Sharp (1982), Zecca *et al* (1986) and Dababneh *et al* (1988). Recent high-resolution studies of electron scattering by molecular oxygen leading to the formation of temporary negative ions (O_2^-) have been reported by Zecca *et al* (1986) and Field *et al* (1988). These measurements below 1.5 eV electron energy have yielded the relative sizes of the oxygen resonances as they appear in the total scattering cross section. Not much theoretical work has been done to compute the electron-scattering cross sections for molecular oxygen at low energies. The theoretical calculation for elastic cross sections by Fisk (1936) is one of the very few reliable results reported so far. There appears to be a large discrepancy both in the shape of the cross section curve and in the cross section values reported by various researchers (mentioned above) in the electron energy range from 0-10 eV. In view of this, more measurements in this direction are needed, possibly using new techniques.

This paper is part of the ongoing research work which aims to measure total electron scattering cross sections for atoms and molecules at low electron energies using a photoelectron source. Previously, absolute electron-scattering cross sections for helium, neon (Kumar *et al* 1987), argon, krypton, xenon (Subramanian and Kumar 1987) and molecular hydrogen (Subramanian and Kumar 1989) have been measured at electron energies from 0-10 eV. In this paper, we present measurements of scattering cross sections for electrons scattered by molecular oxygen with projectile energy varying from 0.15-10 eV.

0953-4075/90/040745+06$03.50

A detailed description of the experimental set-up used for the study, the method for analysis of the data and error analysis has been reported previously (Kumar *et al* 1987, Subramanian and Kumar 1987). In brief, the experiment consists of measuring the intensities of the peaks in the photoelectron spectra of the source gas such as argon, krypton, xenon or molecular oxygen itself. The photoelectrons thus produced by the source gas are scattered by the target gas, the cross section of which is to be determined. Each peak in the photoelectron spectrum of the source gas provides one point in the electron energy scale. Complete scanning of the electron energy is performed by varying the energy of the ionising radiation as well as changing the source gas. Using different combinations of photons of three different wavelengths (HeI, 58.4 nm, NeI, 73.6 and 74.4 nm) and four different source gases and neglecting the energy points where the statistics for the photoelectron intensity were poor, it was possible to measure scattering cross sections at 38 electron energies.

The electron-scattering cross sections for molecular oxygen were measured using the method described previously. When source and target species are different, the electron scattering cross section σ can be evaluated by using the following equation:

$$\ln\left(\frac{I_{e2}}{I_{e1}}\frac{I_{\lambda 01}}{I_{\lambda 02}}\right)=\frac{P_1-P_2}{760}[n_0\sigma x+k(al_1+l_2)]. \tag{1}$$

Here I_{e1} and I_{e2} are the amplitudes of the photoelectron peaks at two different gas pressures P_1 and P_2, $I_{\lambda 01}$ and $I_{\lambda 02}$ are the incident photon intensities monitored during the experiment by the beam monitor at the two pressures, l_1 is the distance from the centre of the beam splitter to the circular aperture covering the ionisation region, l_2 is the distance from the same aperture to the actual ionisation region defined geometrically by different slits in the acceleration region and cylindrical mirror analyser, x is the scattering path length, a is the ratio of the pressures of the target gas outside and inside the ionising region and k is the photoabsorption coefficient of the target gas at a particular photon wavelength. The total photoabsorption cross sections at the three incident photon wavelengths have been taken from Samson *et al* (1977). The ratios of $I_{\lambda 01}$ and $I_{\lambda 02}$ were determined from the beam splitter as described previously (Kumar *et al* 1987).

When source and target gas species are the same, the electron-scattering cross sections could be evaluated by the equation given below:

$$\ln\left(\frac{I_{e2}}{I_{e1}}\frac{I_{\lambda 01}}{I_{\lambda 02}}\frac{P_1}{P_2}\right)=\frac{P_1-P_2}{760}[n_0\sigma x+k(al_1+l_2)]. \tag{2}$$

All errors in the measurement of electron-scattering cross sections have been discussed in detail previously (Kumar *et al* 1987). In the present experiment the probable error was estimated to be ±2.7%.

The electron-scattering cross sections for molecular oxygen were measured using equations (1) and (2) respectively in the two cases described above. In both these equations, all parameters I_{e1}, I_{e2}, $I_{\lambda 01}$, $I_{\lambda 02}$, P_1 and P_2 could be determined experimentally and cross sections could be calculated.

The total electron-scattering cross sections for molecular oxygen as measured in the present experiment are shown in figure 1 for electron energies ranging from 0.15–10 eV along with error bars at three energies only. Also shown in the figure are the measured cross sections reported by Salop and Nakano (1970), Griffith *et al* (1982), Zecca *et al* (1986) and Dababneh *et al* (1988) and theoretically computed elastic cross

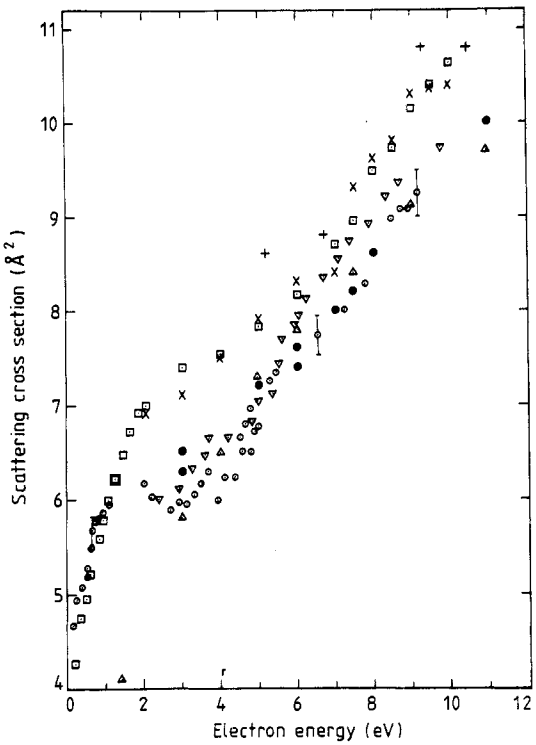

Figure 1. Total electron scattering cross section for molecular oxygen as a function of incident electron energy from 0.15–10 eV obtained by various researchers. The symbols denote: +, Dababneh *et al* (1988); ⊡, Zecca *et al* (1986) Trento; ×, Zecca *et al* (1986) Gdańsk; ●, Salop and Nakano (1970); △, Fisk (1936); ▽, Griffith *et al* (1982); ⊙, present work.

sections by Fisk (1936). The measurements by Zecca *et al* (1986) were carried out independently at the University of Trento (Italy) and the Technical University of Gdańsk (Poland) in the low-energy region (0-100 eV). The Gdańsk experiment was basically a transmission-type system equipped with a cylindrical 127° electrostatic electron monochromator giving an overall random error of less than 2%. The Trento experiment, also a transmission-type system, was equipped with an aperture monochromator (Calicchio *et al* 1982). The random error reported in this case was less than 4% for energies above 1 eV rising to 10% at 0.2 eV. The total cross sections by Dababneh *et al* (1988) were measured using a beam transmission technique in the energy region from 5-500 eV with an estimated error of 5% while measurements by Griffith *et al* (1982) were measured using a similar system and with almost similar errors at electron energies from 2-50 eV. A modified Ramsauer technique has been used by Salop and Nakano (1970) over an energy range from 2.35-21 eV with an estimated error of ±5% associated with the cross section measurement. There is a paucity of theoretical calculations for molecular oxygen. Elastic scattering cross sections have been calculated by Fisk (1936) from about 0.2-25 eV using a semiempirical method (two-centre potential). Measurements for the total cross sections have also been reported by Brüche (1927) from 1-50 eV using an attenuation method, Ramsauer and Kollath (1930) using a Ramsauer-type transmission technique, Sunshine *et al*

(1967) from 0.5–11.3 eV using a recoil method and for total elastic cross sections by Shyn and Sharp (1982) from 2–200 eV using a crossed beam method. These measurements have not been included in figure 1 for reasons of clarity but will be discussed in detail subsequently.

The electron-scattering cross sections as measured in the present experiment appear to increase steadily from 0.15–1.09 eV. It was not possible to make measurements in the energy region from 1.09–2 eV as there were no energy points available because of constraints on the photon beam wavelength and the type of source gases used. The cross sections decreased from about 2–2.6 eV before increasing steadily up to 9.14 eV. The shape of the curve below 2.6 eV electron energy suggested the existence of a hump with cross sections possibly peaking somewhere around 1.6 eV. The cross sections reported by Zecca *et al* (1986) using the Trento set-up were in excellent agreement with those reported in the present work in the energy region from 0–1.1 eV. At higher energies, the cross sections given by Zecca *et al* seemed to increase almost linearly up to about 2 eV energy and showed a partially resolved broad hump around 3 eV. The measurements by Sunshine *et al* (1967) from 0.5–1 eV energy were higher by 13 to 7% than the cross sections reported by us. A weak hump was also observed by Sunshine *et al* between 2 and 3 eV. At energies from 0.5–1 eV, the cross sections reported by Ramsauer and Kollath (1930) are approximately 8% higher than the values given in the present work, but at energies smaller than 0.5 eV, the cross section values were in fair agreement with each other.

The hump in the cross section curve observed by the authors and also by Zecca *et al* (1986), although at different energies, could not be explained in terms of present day theories. There was definitely a temptation to explain this hump as being due to the formation of the temporary negative ion state, $X\,^2\Pi_g(O_2^-)$. It is known that the vibrational states corresponding to $v'=0$ to $v'=3$ of $O_2^-(X\,^2\Pi_g)$ lie below the $v=0$ state of $O_2(X\,^3\Sigma_g^-)$ and cannot autodetach. These states are, therefore, stable and are not accessible by direct two-body electron attachment, whereas such electron attachment could be possible in case of higher vibrational states of $O_2^-(X\,^2\Pi_g)$, giving rise to resonances as they appear in the total scattering cross sections of O_2. Field *et al* (1988) observed such resonances corresponding to $v'\geq 4$ states of the temporary negative ion in the electron energy region from 0.1–1.3 eV. Observations in a similar electron energy region were made by Zecca *et al* (1986) in the total scattering cross section measurements of O_2, and resonances corresponding to $v'=4$–13 could be nicely resolved. The resonances appearing at energies less than 1.3 eV could not be observed by us as the number of energy points accessible in this region was not sufficient. It is quite clear that the hump appearing in the present work at around 1.6 eV energy could not be attributed to the formation of the temporary negative ion state $X\,^2\Pi_g(O_2^-)$. The authors find it difficult to explain this hump in terms of present day knowledge.

The scattering cross sections measured in the present work in the electron energy region from 2.6–9.14 eV are in fairly good agreement with those reported by Salop and Nakano (1970). Our results from 2.6–5.5 eV energy are also in good agreement with those given by Griffith *et al* (1982) in the same energy region, but at energies higher than 5.5 eV, the values reported by Griffith *et al* are larger by 3–6.5% at different energies. Again, the cross sections computed theoretically by Fisk (1936) at energies between 3 and 9 eV agree fairly well with our results but at electron energies less than 3 eV, the cross section values by Fisk are comparatively smaller. Dababneh *et al* (1988) have measured cross sections at only four electron energies from 5.2–10.5 eV. The cross sections reported by them are higher by about 12% at 6.7 eV, 19% at 5.2 eV and

about 16% at 9.3 eV. The measurements by Zecca *et al* (1986), both at Trento and Gdańsk, reported much higher cross sections than those given in the present experiment at energies larger than 3 eV. The Trento results are higher by about 23% at 3 eV, 9% at 7 eV and by about 10% at 9 eV. A similar discrepancy seems to exist between our cross sections and those measured by Zecca *et al* at Gdańsk. The total cross sections reported by Sunshine *et al* (1967) and the elastic cross sections by Shyn and Sharp (1982) are even larger than the values given by Zecca *et al* at energies between 3 and 10 eV.

Table 1. Total electron-scattering cross sections for molecular oxygen at various electron energies. Also given are the photon wavelength and the source gas and the photoion state for the corresponding electron energy.

Wavelength λ (Å)	Source gas	Photoion state	Electron energy (eV)	Cross sections (Å^2)
736	Oxygen	$a\,^4\Pi_u$, $v'=5$	0.15	4.69
736	Oxygen	$a\,^4\Pi_u$, $v'=4$	0.26	4.94
736	Oxygen	$a\,^4\Pi_u$, $v'=3$	0.38	5.07
736	Oxygen	$a\,^4\Pi_u$, $v'=2$	0.50	5.27
584	Oxygen	$B\,^2\Sigma_g^-$, $v'=3$	0.53	5.19
736	Oxygen	$a\,^4\Pi_u$, $v'=1$	0.62	5.49
584	Oxygen	$B\,^2\Sigma_g^-$, $v'=2$	0.65	5.67
736	Oxygen	$a\,^4\Pi_u$, $v'=0$	0.75	5.77
584	Oxygen	$B\,^2\Sigma_g^-$, $v'=1$	0.78	5.80
584	Oxygen	$B\,^2\Sigma_g^-$, $v'=0$	0.92	5.85
736	Argon	$^2P_{3/2}$	1.09	5.90
744	Krypton	$^2P_{1/2}$	2.00	6.16
736	Krypton	$^2P_{1/2}$	2.18	6.02
736	Oxygen	$X\,^2\Pi_g$, $v'=10$	2.67	5.88
736	Oxygen	$X\,^2\Pi_g$, $v'=9$	2.87	5.96
736	Oxygen	$X\,^2\Pi_g$, $v'=8$	3.07	5.94
736	Oxygen	$X\,^2\Pi_g$, $v'=7$	3.27	6.04
736	Oxygen	$X\,^2\Pi_g$, $v'=6$	3.47	6.17
736	Oxygen	$X\,^2\Pi_g$, $v'=5$	3.68	6.29
736	Oxygen	$X\,^2\Pi_g$, $v'=4$	3.89	5.98
736	Oxygen	$X\,^2\Pi_g$, $v'=3$	4.11	6.23
736	Oxygen	$X\,^2\Pi_g$, $v'=2$	4.33	6.23
584	Oxygen	$a\,^4\Pi_u$, $v'=5$	4.51	6.65
736	Oxygen	$X\,^2\Pi_g$, $v'=1$	4.55	6.51
584	Oxygen	$a\,^4\Pi_u$, $v'=4$	4.62	6.79
584	Oxygen	$a\,^4\Pi_u$, $v'=3$	4.74	6.96
736	Oxygen	$X\,^2\Pi_g$, $v'=0$	4.78	6.49
584	Oxygen	$a\,^4\Pi_u$, $v'=2$	4.86	6.72
584	Oxygen	$a\,^4\Pi_u$, $v'=1$	4.98	6.77
584	Argon	$^2P_{1/2}$	5.28	7.26
584	Argon	$^2P_{3/2}$	5.46	7.34
584	Krypton	$^2P_{1/2}$	6.55	7.73
584	Krypton	$^2P_{3/2}$	7.22	8.00
584	Xenon	$^2P_{1/2}$	7.78	8.28
584	Oxygen	$X\,^2\Pi_g$, $v'=3$	8.47	8.98
584	Oxygen	$X\,^2\Pi_g$, $v'=2$	8.69	9.07
584	Oxygen	$X\,^2\Pi_g$, $v'=1$	8.91	9.07
584	Oxygen	$X\,^2\Pi_g$, $v'=0$	9.14	9.25

The present experiment and the two experiments of Zecca *et al* (1986) are similar, the main difference being the nature of electron source. The discrepancies in the data obtained in the above three experiments in the electron energy region 2.6-9.14 eV may have two reasons. In the Trento apparatus of Zecca *et al*, the retarding analyser and the entrance of the Faraday cup are very close to the exit aperture of the scattering chamber. The pressure inside those electrodes can therefore be substantially higher than the background pressure in the apparatus. Such a geometry as suggested by the Gdańsk group can influence the effective length, thus increasing the measured values of the total cross section. The systematic error introduced by this effect could be at least 5%. Another reason for the discrepancy could be the angular resolution error which may be different at different electron energies. However, both these reasons can only partly account for the large discrepancy in the data.

In the light of the above discussion, it is clear that some more measurements are needed to obtain electron-scattering cross sections in the energy region from 1-2 eV. This would help in studying the shape and position of the broad hump around 1.6 eV.

The values of cross sections for molecular oxygen as measured in the present experiment are given in table 1 along with the photon wavelength, source gas and photoion state for the corresponding electron energy.

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