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LETTER TO THE EDITOR

Scattering of 4·5 eV electrons by ground ($x\ ^3\Sigma_g^-$) state and metastable ($a\ ^1\Delta_g$) oxygen molecules†

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Abstract. Differential and integral cross sections have been determined for scattering of 4·5 eV electrons by ground ($x\ ^3\Sigma_g^-$) state and metastable ($a\ ^1\Delta_g$) oxygen molecules. The cross section for the excitation of the $b\ ^1\Sigma_g^+$ state from the $a\ ^1\Delta_g$ state is more than an order of magnitude larger than from the ground ($x\ ^3\Sigma_g^-$) state. The principle of detailed balancing was found to be applicable to the rotationally unresolved ($x \rightarrow a$) vibrational bands of the electronic transition.

Very little experimental work has been reported so far on electron scattering from metastable species (Burrow 1967, Burrow and Davidovits 1968, Hertel and Stoll 1974, Dixon *et al* 1973) in spite of their importance in plasma and laser systems. Measurements of this type are also needed to test theoretical methods and will yield some insight into the similarities and differences between electron scattering from ground and excited state species. A natural choice for study is metastable ($a\ ^1\Delta_g$) O_2 which has a long life with respect to radiation and collisional deactivation, is easily generated by microwave discharge, and plays an important role in aurora (Noxon 1970) and airglow (Noxon 1968) phenomena.

We report here differential and integral cross sections for scattering of 4·5 eV electrons by ground-state ($x\ ^3\Sigma_g^-$) and metastable ($a\ ^1\Delta_g$) oxygen molecules in the $-2{\cdot}0$ eV to $+2{\cdot}0$ eV energy-loss range. The cross section for the ($a\ ^1\Delta_g \rightarrow b\ ^1\Sigma_g^+$) transition was found to be more than an order of magnitude larger than that of the excitation of the b state from the ground state. It was found that the principle of detailed balance can be applied to the rotationally unresolved inelastic and superelastic electronic transitions ($x\ ^3\Sigma_g^- \rightleftarrows a\ ^1\Delta_g$), indicating that for this transition one may neglect the very different rotational level structure of the two states in estimating superelastic cross sections from inelastic data to an accuracy of about 15%.

The electron impact spectrometer was described earlier (Hall *et al* 1973). It consists of a molecular-beam target, cylindrical electrostatic energy analysers, aperture lenses and an electron-multiplier detector. An energy-selected electron beam about 50 meV full-width-at-half-maximum of energy E_0 is scattered from an O_2 molecular-beam target which contains about 7% O_2 ($a\ ^1\Delta_g$) species when a microwave discharge is

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applied to the O_2 sample gas. The scattered-electron intensity is measured at fixed scattering angles (θ) ranging from 20° to 135° as a function of energy loss ΔE using pulse-counting and multichannel-scaling techniques. The memory of the 1024 channel scaler was divided into two 512 channel parts and the energy-loss spectra with the microwave discharge on and off were collected alternately into each half of the memory under otherwise identical conditions. A typical set of spectra is shown in figure 1.

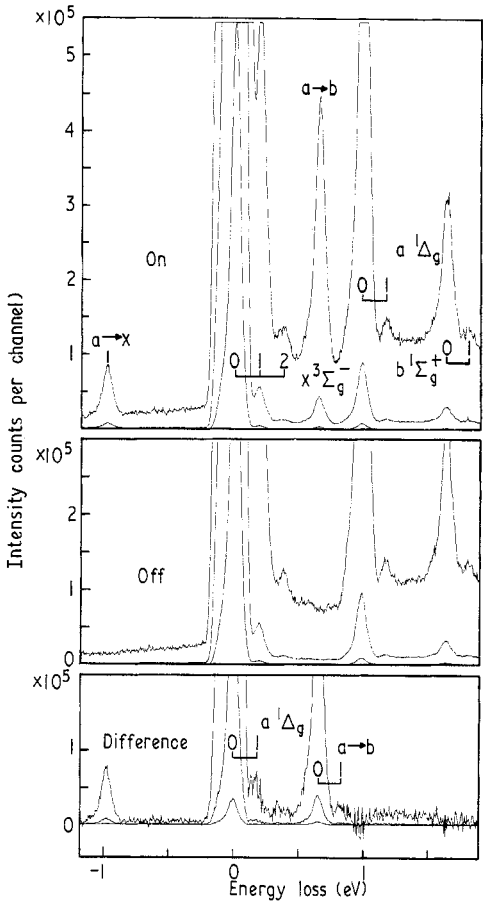

Figure 1. Energy-loss spectra for 4·5 eV electrons in O_2 at 110° scattering angle. Top and centre with and without microwave excitation, respectively, and bottom the difference of the two spectra. Each spectrum is shown with a sensitivity of 1, 10 and 100.

A subtraction of the off spectrum from the on spectrum (properly normalized for the loss of ground-state species due to generation of the metastable species) yielded the difference spectrum which represents electron scattering from the excited species. Transitions originating from other than the a $^1\Delta_g$ excited state, although carefully searched for, were not detected and were, therefore, assumed to be negligible. The concentration of the metastable O_2 (and the correction factor for the on spectrum) was determined on the basis of the decrease of the (X → a) transition intensity which is proportional to the concentration of the ground-state molecules.

Normalization of the experimental measurements to the absolute scale was achieved in two main steps: (i) The absolute elastic cross sections for O_2 were determined by using the known He elastic cross sections (Andrick and Bitsch 1975) as standards; (ii) from the measured inelastic to elastic scattering intensity ratios and from the normalized elastic cross sections, the inelastic cross sections were obtained both for ground-state and metastable O_2. The intensity ratios were corrected for the relative populations (assuming identical cross sections for elastic scattering from x $^3\Sigma_g^-$ and a $^1\Delta_g$ species—see below) and for the variation of the detector-system efficiency with the residual energy of the electrons. The latter correction was carried out by using the known He elastic cross sections (Andrick and Bitsch 1975) as a function of impact (or residual) energy.

The differential cross sections are shown in figure 2 and the integral cross sections (obtained after extrapolations to 0° and 180°) are listed in table 1. The errors in the cross sections for ground-state and a $^1\Delta_g$ molecules are estimated to be about $\pm 25\%$

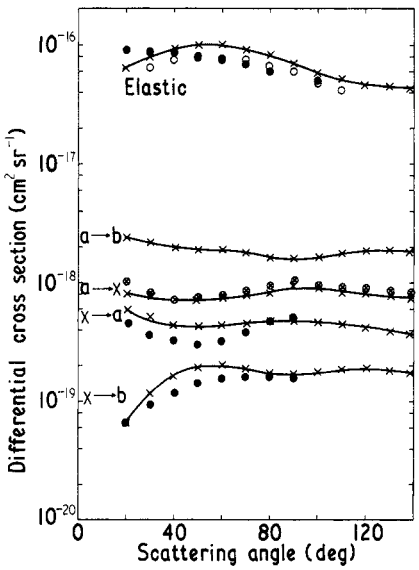

Figure 2. Differential cross sections for 4·5 eV electrons in O_2. Present work: × ; calculated from detailed balance: ⊗; Linder and Schmidt (1971) at 4 eV: ○; and Trajmar *et al* (1971) at 4 eV: ●.

and $\pm 35\%$, respectively. The ground-state elastic scattering and the (x → a) and (x → b) excitation differential cross sections are in good agreement with the previous measurements of Linder and Schmidt (1971) and Trajmar *et al* (1971) obtained by completely different normalization procedures. The (a → b) cross sections are about an order of magnitude larger than the (x → b) cross sections over the whole angular range. This may be attributed to the fact that for the former the initial state is an excited state which may have a more radially-diffused electronic wavefunction; and/or to different symmetries (nodal properties) of the electronic-state wavefunctions involved. The measured and calculated (a → x) cross sections at 4·5 eV agree within the limits of experimental errors. The calculated values were obtained from the (x → a) cross sections measured at 5·5 eV by applying the detailed balance principle to the rotationally unresolved transitions with a statistical weighting factor ratio $gX/ga = 1{\cdot}5$. From the

Table 1. Integral cross sections and comparison with other measurements. Cross sections are in units of 10^{-18} cm^2.

Energy (eV) \ Transition	Elastic	x → a	x → b	a → x	a → b
4·5[a]	850	5·6	2·1	10	23
5·5[a]		6·0			
4·5[b]	700				
4·5[c]	820				
4·5[d]		6·7	1·7		
4·5[e]		5·8	1·9		

[a] This work.
[b] Total cross section, Salop and Nakano (1970).
[c] Total cross section, Sunshine *et al* (1967).
[d] Trajmar *et al* (1971).
[e] Linder and Schmidt (1971).

difference spectra, cross sections for elastic scattering and pure vibrational excitation of the a $^1\Delta_g$ state, as well as for the (a $^1\Delta_g$ ($v = 0$) → b $^1\Sigma_g^+$ ($v = 1$)) transition, could be obtained. The uncertainty in determining these cross sections is quite large for quantitative evaluation. It can be concluded, however, that the magnitude of these excited-state cross sections is similar to those for scattering from the x $^3\Sigma_g^-$ state.

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