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Low-energy elastic scattering of O-atoms by atmospheric species

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LOW ENERGY ELASTIC SCATTERING OF O-ATOMS BY
ATMOSPHERIC SPECIES

by

Gerald J. Smith

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Abstract

Low Energy Elastic Scattering of O-atoms by Atmospheric Species

by

Gerald J. Smith

This thesis reports measurements of absolute differential cross sections for elastic scattering of atomic oxygen at 0.5- and 1.5-keV laboratory energies. Measurements for targets of He, Ne, Ar, Kr, Xe, H₂, N₂, O₂, CO, CO₂, H₂O, CH₄, CF₄, SF₆, SO₂, and NH₃ are performed over a laboratory angular range of 0.2 to 5.0 degrees. Using a partial wave analysis, the cross sections for several targets are inverted and estimates of model interaction potentials are made. These potentials are then used to predict the elastic scattering cross sections at a laboratory energy of 100 eV.
Acknowledgements

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I. Introduction

Measurements of differential scattering cross sections involving fast oxygen atoms have been of continuing interest to both experimentalists and theorists due to their importance in a wide range of environments. In the earth's atmosphere, significant fluxes of precipitating $O^+$ ring current ions have been observed at altitudes of around 200 km to 1000 km during geomagnetic storms$^{1-3}$. With energies ranging from a few hundred to several thousand eV, these fast ions undergo charge-transfer collisions with thermospheric hydrogen and oxygen atoms producing a flux of fast neutral oxygen atoms. As these atoms penetrate the atmosphere and collide with atmospheric atoms and molecules they can undergo elastic scattering, charge-transfer, excitation, and collisional ionization. The energy they deposit through these collisions causes phenomena such as local heating, optical emissions, and loss of some atmospheric constituents$^4$. Similarly, collisions involving oxygen atoms play a significant role in other environments ranging from extraterrestrial planetary atmospheres to fusion plasmas$^5$ and lasers$^6$. A lack of experimentally derived cross section data has forced researchers to rely on simple models and estimates of cross sections, making accurate modelling of these phenomena difficult$^{4,7}$.

Accurate information regarding the differential cross sections (DCS's) for collisions involving oxygen atoms over a range of energies helps to fill this need. To this end, this thesis reports measurements of elastic scattering DCS's for 0.5 keV and 1.5 keV laboratory energy O atoms incident on He, Ne, Ar, Kr, Xe, H$_2$, N$_2$, O$_2$, CO, CO$_2$, CH$_4$, CF$_4$, SF$_6$, H$_2$O, SO$_2$, and NH$_3$ over a laboratory angular range of 0.2 to 5.0 degrees. Since 0.5 keV
represents the minimum practicable energy for which the present apparatus is suited, the interaction potentials for a subset of the targets above have been estimated through inversion of the experimental measurements, allowing calculation of the DCS's at lower energies and thus increasing the utility of the measurements. A detailed description of the calculations performed and resulting DCS's for 0.1 keV O atoms are presented.
II. Experimental Method

Apparatus

A fast beam technique, based on previous work performed by Newman et al.\textsuperscript{8}, is used to measure absolute DCS's. A schematic diagram of the apparatus used is shown in figure 1. Oxygen ions are produced by electron impact on CO$_2$ in a low pressure, magnetically confined plasma ion source. As ions exit the source they are accelerated to the desired beam energy, and focused by a three element electrostatic lens. Ions exiting the lens pass through a pair of 60° sector magnets where the charge to mass ratio of the desired ionic species is selected by tuning of the magnetic field intensities. After passing through the magnets, the beam passes through collimating apertures defining the exit of the charge-transfer cell (CTC) and the entrance of the target cell (TC). For 0.5 keV and 1.5 keV beams, pairs of 50 μm and 30 μm diameter apertures respectively are used. Separated by 19 cm, these aperture pairs give a maximum beam divergence of 0.015° and 0.009° respectively. Further, previous measurements\textsuperscript{9} have shown that similar collimation geometries combined with the bending magnets limit the energy spread in the resulting beam to a few eV's, a negligible percentage of the beam energy, regardless of the energy spread of the ions leaving the ion source. As the beam passes through the CTC, a small fraction of the fast ions are converted to fast neutral O atoms through charge-transfer collisions with N$_2$. A detailed discussion of the neutral beam production is deferred until the next section. After the CTC, a pair of electrostatic deflection plates (DP1) serves to remove remaining ions in the beam, allowing only neutral atoms to enter the TC.
Figure 1. Schematic of the apparatus.
With typical target gas pressures of around 4 mtorr and a TC length of 1.6 mm, only a small percentage (1 - 4%) of the primary beam passing through the TC is scattered by the target gas. This keeps secondary collisions in the TC at an insignificant level, while still providing a target thickness over 700 times greater than that existing between the TC and the detector due to background gas (nominally at $< 1 \times 10^{-7}$ torr). The high degree of beam collimation and the shortness of the TC combine to form a very well defined scattering volume, thus contributing to the high angular resolution of the measurements. Another set of electrostatic deflection plates (DP2) immediately after the TC serves to remove any charged scattering products formed through electron capture or loss.

Scattered atoms and primary beam atoms strike the front surface of the position-sensitive detector (PSD) which is located on the beam axis 10.4 cm from the TC. The PSD has an active area 2.5 cm in diameter and consists of two microchannel plates (MCP's) mounted in front of a specially-shaped resistive anode. A full description of the design and operation of the PSD can be found in Gao et al.\textsuperscript{10}. Briefly, the MCP's act as electron multipliers for energetic particles which strike the surface of the PSD, with a gain of $10^6$ to $10^7$. The charge deposited on the anode by the resulting electron clouds is collected at four corner connections, from which the position of each particle impact is determined. A negative bias voltage applied to the front surface of the detector prevents stray electrons from initiating an electron cascade and being recorded as a real event. The basic design of the PSD is illustrated in figure 2.
Figure 2. Position-sensitive detector (PSD) with biasing network.

Electronic State of the Primary Beam

Production of a ground state neutral oxygen atom beam from an $O^+$ beam is obtained through charge-transfer with $N_2$ in the CTC, with about 10% of the fast ions being converted to fast neutrals. In order to obtain predominantly ground state neutrals it is necessary to control the excited electronic state fraction in the parent $O^+$ beam by appropriate choice of the ion source operating conditions. Specifically, for reasons outlined below, production of the $O^+({^2}D)$ state in significant quantities is useful in producing a ground state neutral beam (see electronic energy level diagram, figure 3.). Other investigators have found\(^1\) that this can be achieved through electron impact on $CO_2$, which has been verified with the present ion source using the
\[ \begin{array}{ll}
O^+ & ^2P \quad 18.6 \text{ eV} \\
& ^2D \quad 16.9 \text{ eV} \\
& ^4S \quad 13.6 \text{ eV} \\
O & ^1S \quad 4.2 \text{ eV} \\
& ^1D \quad 2.0 \text{ eV} \\
& ^3P \quad 0.0 \text{ eV} \\
\end{array} \]

**Figure 3.** Electronic states of O and O$^+$.

attenuation method of Turner *et al.*\textsuperscript{12}. This method involves measuring the attenuation of an ion beam as it passes through a gas cell as a function of gas pressure. An appropriate choice of attenuating gas results in different states of the ions suffering different attenuations due to different charge-transfer cross sections. A plot of \( \log(I/I_0) \) vs. gas pressure, where \( I \) is the attenuated ion current and \( I_0 \) is the ion current at zero gas pressure, reveals the presence and relative fractions of multiple states in the ion beam. For single state beams, this plot is a straight line whose slope depends on the charge-transfer cross section, while multiple state beams produce a curve resulting from the
superposition of each individual state's attenuation. Using this method, Guest et al.\textsuperscript{11} have found that the three states of O\textsuperscript{+} seen in figure 3 all have sufficiently different charge-transfer cross sections with N\textsubscript{2} to make this an appropriate choice of attenuation gas. Their attenuation results were found to be consistent when checked against measurements of O\textsuperscript{+} + Xe elastic scattering, where each of the three states of O\textsuperscript{+} introduces a different type of oscillatory structure into the cross section. An attenuation curve for O\textsuperscript{+} in N\textsubscript{2} using the present ion source is shown in figure 4, which can be resolved into contributions from two states identified as O\textsuperscript{+}(4\textit{S}) and O\textsuperscript{+}(2\textit{D}). The O\textsuperscript{+}(2\textit{P}) state is identified as the third absent state based on studies\textsuperscript{5,11} showing that production of this state can be avoided by limiting the electron impact energy in the source, which is done in the present case, and on the unlikelihood of the absence of either the O\textsuperscript{+}(4\textit{S}) or O\textsuperscript{+}(2\textit{D}) state in the presence of the O\textsuperscript{+}(2\textit{P}) state. Using this analysis, O\textsuperscript{+}(2\textit{D}) beam fractions as high as 30\% to 40\% are routinely observed in the present apparatus. The essentially resonant charge transfer reaction

\[
\text{O}^+ (2\text{D}) + \text{N}_2 (X^1\Sigma_g^+) \rightarrow \text{O}(3\text{P}) + \text{N}_2^+ (A^2\Pi_u) \quad (1)
\]

then leads to a predominantly ground state neutral beam, with other reaction channels from the O\textsuperscript{+}(2\textit{D}) state to the O(1\textit{D}) and O(1\textit{S}) states occurring far less frequently due to energy defects of 0.6 eV and greater\textsuperscript{13}. Additionally, at scattering angles below 0.1° the differential cross section for reaction (1) has been shown\textsuperscript{14} to be about two orders of magnitude larger than that for the non-resonant O\textsuperscript{+}(4\textit{S}) + N\textsubscript{2} charge transfer reaction, the products of which
Figure 4. $O^+ + N_2$ attenuation curves for A) $O^+(^4S)$ state-, B) $O^+(^2D)$ state-, and C) multi-state-beam containing both $O^+(^4S)$ and $O^+(^2D)$. 
include neutral oxygen in both the ground and excited states. Thus the collimation of the neutral beam to $\leq 0.015^\circ$ discriminates against these reaction products, further limiting excited state contamination of the beam. Note that the $\text{O}^+({}^2\text{D})$ and $\text{O}^+({}^2\text{P})$ states are metastable (radiative lifetimes of 2.1 hrs. and 6.0 sec. respectively)$^{15}$, as are the $\text{O}({}^1\text{D})$ and $\text{O}({}^1\text{S})$ states (radiative lifetimes of 110 sec. and 0.74 sec. respectively)$^{16}$ due to dipole selection rules. Thus, $\text{O}^+$ excited states formed in the ion source will live long enough to reach the CTC, and any O excited states formed in the CTC will reach the TC and detector.

While this is a reasonable strategy for obtaining a ground state O beam, there is no easy method of directly measuring the neutral beam excited state fraction to verify its composition. However, it is relatively simple to investigate the effects of an unexpectedly significant excited state contamination by deliberately contaminating the beam and looking for sensitivity to this contamination in the measured elastic scattering cross sections. To this end, several source gases were used ($\text{CO}_2$, $\text{CO}$, $\text{O}_2$) with varying electron impact energies (40 - 100 eV) and a different CTC gas (Kr) in a series of DCS measurements involving several different targets. It has been shown$^{11,13}$ that the state composition of an $\text{O}^+$ beam is dependent on the source gas used and the electron impact energy. Further, there are no clearly preferred reaction channels to any one atomic O state given an assortment of $\text{O}^+$ states charge-transferring with Kr. These circumstances guarantee a mixed state O beam for the DCS measurements, as demonstrated in figure 5 where two measurements of the state-sensitive reaction $\text{O} + \text{O}_2 \rightarrow \text{O}^-$ are compared$^{17}$ using $\text{N}_2$ and Kr as charge-transfer gases for production of the neutral O beam. When Kr is used, the presence of excited states in the O
Figure 5. DCS's for 1.5-keV O + O$_2$ → O$^{-}$ using A) Kr and B) N$_2$ as charge-transfer gases for production of the neutral O beam.
beam is evident by the dramatic change in the DCS's at small angles. Comparing the elastic scattering DCS's measured under the same conditions reveals absolutely no discernible differences for any of the targets tested, leading to the conclusion that atomic O elastic scattering cross sections are insensitive to excited states in the beam.

**Measured Quantities**

Under thin target conditions, the differential cross section can be expressed as

\[
\frac{d\sigma(\theta,\phi)}{d\Omega} \approx \frac{\Delta S(\theta,\phi)}{S_0 \tau \Delta \Omega}
\]

(2)

where \(S_0\) is the primary beam flux, \(\Delta S(\theta,\phi)\) is the flux scattered into the solid angle \(\Delta \Omega = \sin \theta \Delta \theta \Delta \phi\), and \(\tau\) is the target thickness. Each of the quantities on the right hand side of (2) is measured, and the experimental uncertainties relating to each are summarized in table 1.

Very simply, the target thickness \(\tau\) can be expressed as the product \(n \ell\), where \(\ell\) is the TC length and \(n\) is the gas number density. More accurately, integration of the gas density along the TC axis is needed to account for changes in the density near the apertures. However, modelling of the axial and radial target gas density distributions relevant to the type of cell used in this experiment\(^8,18\) indicates that the integrated value is sufficiently represented by the product \(n \ell\). The gas density is obtained by measuring the TC pressure far from the apertures using an MKS Baratron capacitance manometer. The TC length \(\ell\) is found by measuring the displacement of a
Table 1. Experimental Uncertainties

<table>
<thead>
<tr>
<th>Experimental Quantity</th>
<th>Uncertainty</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Cross Section Amplitude Uncertainties:</strong></td>
<td></td>
</tr>
<tr>
<td>Counting statistics</td>
<td>3% - 20%</td>
</tr>
<tr>
<td>PSD operating point</td>
<td>3%</td>
</tr>
<tr>
<td>Primary beam/scattered signal efficiency</td>
<td>3%</td>
</tr>
<tr>
<td>TC length $\ell$</td>
<td>2%</td>
</tr>
<tr>
<td>TC pressure (number density $n$)</td>
<td>2%</td>
</tr>
<tr>
<td>Baratron thermal transpiration</td>
<td>2%</td>
</tr>
<tr>
<td><strong>Cross Section Angular Uncertainties:</strong></td>
<td></td>
</tr>
<tr>
<td>TC to PSD distance</td>
<td>1%</td>
</tr>
<tr>
<td>Beam divergence</td>
<td>0.015°</td>
</tr>
<tr>
<td>Analysis ring width</td>
<td>0.035° - 0.140°</td>
</tr>
<tr>
<td>PSD position encoding error $^{20}$</td>
<td>~ 0.035°</td>
</tr>
<tr>
<td>PSD Linearity</td>
<td>2%</td>
</tr>
</tbody>
</table>

microscope body as the microscope is focused through the cell on the entrance and exit apertures.

Measurements of $S_0$ and $\Delta S(\theta,\phi)$, that is the primary beam and elastically scattered atoms, are determined coincidentally on the PSD. Because they are of the same species and energy, and are collected on the same detector, there is no need to know the absolute detection efficiency of the PSD. However, their detection efficiencies relative to one another are affected by their vastly different flux densities. When a small region of the
PSD is subjected to a high flux of particles, there is a local depletion of electrons in the MCP leading to smaller output pulses. These smaller pulses are discriminated against by the PSD decoding electronics, leading to a lower detection efficiency for the primary beam. By increasing the voltage on the MCP's the gain is increased, and detection efficiency rises. However, the increased gain causes overly large pulses of electrons to result from impacts by scattered particles, where flux density is low and there is no electron depletion. These large pulses are also discriminated against, decreasing the detection efficiency for scattered particles. By measuring the relative detection efficiencies for high and low fluxes versus PSD bias voltage, it is possible to operate the PSD at a point where the two relative detection efficiencies are equal. Such measurements are made before each daily data run, since the PSD characteristics change with time and use.

Primary beam and scattered particle impacts resulting in electron pulses of appropriate size are counted as valid events. Their impact positions are decoded as described earlier with a Surface Sciences decoding electronics unit. For each event, this unit outputs a TTL strobe pulse which is counted by a Bira Model 2101 Scaler/Timer, and two analog x and y position signals, which are digitized with nine bits of resolution and converted to a position in a 360 x 360 computer memory array. For each event, the appropriate array element is incremented by one, with each element corresponding to a 65 x 65 μm² area on the detector face. Over time, a two dimensional histogram of the primary beam and scattered particles is built up, as seen in figure 6. The memory array and scaler/timer total are recorded on an MVME Motorola 131 computer, along with the Baratron pressure measurement.
Since the scattering data is azimuthally symmetric, it is summed into concentric rings about the scattering center. A finite ring width is needed in order for a statistically meaningful number of events to be counted at each incremental value of the scattering angle $\theta$ (where $\theta$ is defined as the average angle subtended by the ring). Thus, $\Delta\Omega$ is determined primarily by the ring width, and its accuracy is limited by uncertainty in the TC-to-PSD distance measurement, the finite size of the primary beam, and the position-finding uncertainty of the PSD. Concurrently, these factors, along with the discrete nature of the analysis rings, determine the angular resolution of the measurement. The relevant uncertainties are listed in table 1.
Detector Diagnostics and Considerations

In order to insure an accurate measure of the DCS's, the detection efficiency uniformity and linearity across the face of the detector must be characterized. The linearity is measured by mounting a 40 lines per inch electroformed mesh immediately in front of the PSD face, and sweeping an ion beam across it. The shadow of the mesh visible in the recorded histogram can then be measured to determine linearity and to calibrate physical area per memory array element. The detector is found to be linear to within 2%. The PSD uniformity is measured by rastering a stable ion beam over an array of localized positions on the PSD face, with the beam spending an equal amount of time at each location. Summing the number of counts at each spot then reveals any irregularities in detection efficiency over the surface of the PSD. The PSD used in these experiments is found to be uniform to within 2%, with the exception of one side where the incident angle of the ions approaches parallel incidence with the channels in the MCP, which are biased at 5°, reducing detection efficiency dramatically. This behavior has been characterized previously\textsuperscript{10} and is corrected with a software mask over the memory array. This mask discounts the non-uniform area (approximately 15% of the PSD's active area) as well as the extreme edges of the PSD, where uniformity and linearity are unreliable.

Detection efficiency at the spot where the primary beam impacts the front MCP can also be affected by ageing of the surface with use. Atomic oxygen is particularly damaging to the MCP surface, and areas subjected to a high flux density quickly develop an efficiency "hole", leading to a decrease in the measured primary beam signal. To counteract this problem, the PSD
is mounted on a moveable slide (perpendicular to the beam axis) so that no one spot on its surface is exposed to the primary beam for an extended length of time. By frequently testing the detection efficiency around the beam impact point with a rastered ion beam and moving the PSD after every few data runs, efficiency holes are prevented from forming.

**Data Analysis**

When gas is in the TC, the signal measured on the PSD is comprised of scattering from the target gas, primary beam counts, and noise. The sources of noise are scattering from the edges of apertures, scattering from background gas, and dark counts. A second data set collected with an empty TC (gas-out) contains only primary beam counts and noise, and is subtracted from the gas-in data to find the signal due to scattering from the target gas alone. This requires matching of the primary beam intensity and time of accumulation between the two data sets, which is easily achieved due to the good stability of the beam. The gas-out data is then used as a measure of the primary beam, since by comparison the noise is insignificant. The location of the scattering center in the 360 x 360 gas-in array is found through a "center-of-mass" calculation performed on the distribution of counts in a small area around the primary beam peak. Concentric rings are then defined about this center, and the number of counts in each ring is totaled. The width of the rings increases with increasing radius from the center, trading high angular resolution for better statistics at the larger scattering angles. The same is done with the gas-out file, and the corresponding ring sums are subtracted, as mentioned above, to give the scattered flux $\Delta S(\theta)$. The DCS's are then calculated directly from equation (2).
III. Theoretical Calculations

In an ideal scattering experiment, a perfect source of incident particles produces a completely monoenergetic beam which is perfectly collimated. The incident particles collide with a target, and a perfect detector collects 100% of the scattered incident particles and nothing else. Operated in a constant, steady-state manner, the scattering can be considered time-independent. For elastic scattering events, one can consider two spinless, structureless particles interacting through a single, spherically symmetric interaction potential. This requires that the initial and final quantum states of the system are identical, and no interactions with other states occur. For such a system, the method of partial waves can be applied, and has been described in detail\textsuperscript{19-21}, where a wave function $\Psi(r)$ describing the motion of a particle with mass $\mu$ under the influence of a real, central potential $V(r)$ satisfies the time-independent Schrödinger equation

$$\left[ -\frac{\hbar^2}{2\mu} \nabla^2 + V(r) \right] \Psi(r) = E\Psi(r) \quad (3)$$

where $\nabla^2$ is the Laplacian operator, and $E$ is the kinetic energy of the particle (center-of-mass frame) far from the scattering center where the potential is equal to zero. Working in spherical coordinates, the solution to eqn. (3) is the function

$$\Psi_{lm}(r) = \frac{1}{r} u_l(r) \ Y_{lm}(\theta,\phi) \quad (4)$$
where the spherical harmonics $Y_{lm}(\theta, \phi)$ are the solutions to the angular part of (3), and $u_l(r)$ is a solution to the radial equation

$$\frac{d^2 u_l(r)}{dr^2} + \left[ k^2 - U(r) - \frac{1(l+1)}{r^2} \right] u_l(r) = 0$$

(5)

where $k^2 = (2\mu/h^2)E$ and $U(r) = (2\mu/h^2)V(r)$.

Taking advantage of the azimuthal symmetry of the physical situation, a solution to (3) which is independent of $\phi$ can be written as the linear combination

$$\Psi(r) = \frac{1}{kr} \sum_{l=0}^{\infty} u_l(r)Y_{l0}(\theta)$$

(6)

where $u_l(r)$ satisfies the radial equation. With the imposed boundary conditions that the potential $V(r)$ vanishes at large $r$ values, and that $u_l(r)$ vanish at $r=0$ (from the requirement that $\Psi(r)$ and its gradient be finite everywhere), the asymptotic solution of the radial equation (5), beyond the range of the potential, may be written as a linear combination of the asymptotic forms of the spherical Bessel and spherical Neumann functions

$$u_l(r) \xrightarrow{r \to \infty} A \sin(kr - \frac{1}{2}l\pi) + B \cos(kr - \frac{1}{2}l\pi)$$

(7)

or, alternately

$$u_l(r) \xrightarrow{r \to \infty} N_l \sin(kr - \frac{1}{2}l\pi + \delta_l)$$

(8)
where \( N_1 = (A^2 + B^2)^{1/2} \) is a normalization constant, and the phase shift \( \delta_1 = \arctan(B/A) \) is introduced. The phase shift is interpreted as the difference in phase between the free particle solution and the solution in the presence of the potential.

The normalization of \( u_i(r) \) is determined by the requirement that \( \Psi(r) \) in the asymptotic region be represented by an incident plane wave and an outgoing scattered wave

\[
\Psi(r)_{r \to \infty} \rightarrow e^{ikz} + \frac{1}{r} e^{ikr} f(\theta)
\] (9)

where \( k \) is taken to be along the \( z \) axis and \( f(\theta) \) is the complex scattering amplitude. By using expression (8) in the series (6), and comparing the result to the asymptotic expression (9) for \( \Psi(r) \) above, the normalization constant is determined to be

\[
N_1 = i^l e^{idl} [4\pi(2l + 1)]^{1/2}
\] (10)

and, using the same comparison along with the expression

\[
Y_{l0}(\theta) = \left[ \frac{(2l + 1)}{4\pi} \right]^{1/2} P_l(\cos \theta)
\] (11)

the scattering amplitude can be expressed as
\[
f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) (e^{i\delta_l} - 1) P_l(\cos \theta)
\]

where \(\theta\) is the scattering angle in the center-of-mass frame and \(P_l(\cos \theta)\) is the \(l\)th Legendre polynomial. The scattering amplitude is used to calculate the differential cross section with the familiar relation

\[
\frac{d\sigma(\theta)}{d\Omega} = \left| f(\theta) \right|^2.
\]

Calculation of the cross sections using the above analysis is performed using various forms for the interaction potentials, which will be discussed in detail in the Results section of this thesis. The phase shifts are calculated from these potentials using the semi-classical JWKB approximation in the form\(^{22}\)

\[
\delta_l^{\text{JWKB}} = kb \left( \frac{\pi}{2} - \frac{r_0}{b} + I_1 \right)
\]

where \(b = (1 + 1/2)/k\) is the classical impact parameter, \(r_0\) is the associated turning point, and \(I_1\) is the integral

\[
I_1 = \frac{1}{b} \int_{r_0}^{\infty} \left[ \left( 1 - \frac{V(r)}{E} - \frac{b^2}{r^2} \right)^{1/2} - 1 \right] dr
\]
In the limit of large \( l \) the phase shifts become small and can be obtained using the Jeffreys-Born (JB) approximation

\[
\delta l^{\text{JB}} = \frac{-k}{2E} \int_b^\infty \frac{V(r)}{(1 - b^2 r^2)^{1/2}} \, dr = \frac{-k}{2E} I_2
\]  

(16)

where

\[
I_2 = b \int_0^1 \frac{V(b/z)}{z^2 (1 - z^2)^{1/2}} \, dz
\]  

(17)

with \( z = (b/r) \). Further details concerning the numerical techniques and checks used in the determination of the phase shifts have previously been described at length\(^{22}\).
IV. Results and Discussion

**Elastic Scattering Measurements**

Experimental absolute differential cross sections have been obtained for elastic scattering of atomic oxygen at laboratory-frame collision energies of 0.5 and 1.5 keV as a function of laboratory scattering angle. The results are plotted in figures 7 through 14, and in most cases display a featureless, monotonic behavior. The vertical error bars in the DCS results are due strictly to counting statistics, while the horizontal error bars reflect the measured size of the beam on the detector, which takes into account the beam divergence and the PSD position encoding error. Comparison of the present results with those of Schafer et al.\textsuperscript{23} for He, N\textsubscript{2}, and O\textsubscript{2} targets shows agreement within the stated error bars at collision energies of 1.5 keV. However, the agreement at 0.5 keV is poor, and is attributed to secondary collision effects in the Schafer measurements due to an unacceptably thick target. To confirm this, the Schafer results were accurately duplicated in the present experiment through use of a similarly thick target. As a further test of the validity of the present experimental method, well-known benchmark measurements were made of He + He and He + N\textsubscript{2} elastic scattering and were found to be in excellent agreement with previous measurements\textsuperscript{8} for both 0.5 and 1.5 keV projectiles.

While most of the cross sections measured are featureless, some structure is seen at the higher energy for the lighter rare gas targets. In these cases it is likely that potential energy curve crossings corresponding to target excitation give rise to the structure. Other typical sources of structure fail to fit the circumstances, such as rainbow and glory scattering which are
Figure 7. DCS's for elastic scattering of 0.5 keV atomic O from He, N$_2$, O$_2$, and H$_2$. The cross sections have been multiplied by the factors indicated.
Figure 8. DCS's for elastic scattering of 1.5 keV atomic O from He, N₂, O₂, and H₂. The cross sections have been multiplied by the factors indicated.
Figure 9. DCS's for elastic scattering of 0.5 keV atomic O from Xe, Kr, Ar, and Ne. The cross sections have been multiplied by the factors indicated.
Figure 10. DCS's for elastic scattering of 1.5 keV atomic O from Xe, Kr, Ar, and Ne. The cross sections have been multiplied by the factors indicated.
Figure 11. DCS's for elastic scattering of 0.5 keV atomic O from CF$_4$, CH$_4$, CO$_2$, and CO. The cross sections have been multiplied by the factors indicated.
Figure 12. DCS's for elastic scattering of 1.5 keV atomic O from CF₄, CH₄, CO₂, and CO. The cross sections have been multiplied by the factors indicated.
Figure 13. DCS's for elastic scattering of 0.5 keV atomic O from SF$_6$, H$_2$O, SO$_2$, and NH$_3$. The cross sections have been multiplied by the factors indicated.
Figure 14. DCS's for elastic scattering of 1.5 keV atomic O from SF₆, H₂O, SO₂, and NH₃. The cross sections have been multiplied by the factors indicated.
associated with attractive potentials, Demkov scattering which occurs under conditional circumstances in some charge-transfer collisions, and the so-called forward diffraction peak which occurs at very small angles.

One notable observation regarding the cross sections is their similarity to one another in both amplitude and functional form. This similarity remains consistent for a wide variety of dissimilar targets, from small atoms to large complex molecules. Comparing the DCS's in the center-of-mass reference frame accentuates this phenomenon, as seen in figures 15 and 16. With few exceptions, all of the cross sections lie within approximately ± 50% of a central average cross section throughout the entire angular range studied. Analogous similarities in elastic scattering DCS's are also observed for other projectiles. Figures 17 and 18 show this behavior for hydrogen and helium projectiles at lab energies of 0.5-, 1.5-, and 5.0-keV scattering from a limited number of targets.

Interaction Potentials

Calculations of DCS's for 100 eV O atoms scattering from N₂, CO, CO₂, and H₂O have been made using the higher energy scattering data and the partial wave analysis described earlier. All of the quantities in equations (12) through (17) are either known through measurement or can be directly calculated from measurements with the sole exception of the interaction potential V(r). To deal with this some analytic form and initial value of the potential is chosen, and the resulting calculated DCS is compared with the measured DCS. Using a nonlinear least-squares fitting routine for the comparison, the fit to the measured results is improved through iterative adjustments to the potential. Since the interaction potential is independent of
Figure 15. DCS's for elastic scattering of 0.5 keV (lab energy) atomic O from each of the targets studied, plotted in the center-of-mass reference frame.
Figure 16. DCS's for elastic scattering of 1.5 keV (lab energy) atomic O from each of the targets studied, plotted in the center-of-mass reference frame.
Figure 17. DCS's for elastic scattering of H from H$_2$, N$_2$, O$_2$, He and Ar at lab energies of A) 0.5-, B) 1.5-, and C) 5.0-keV, plotted in the center-of-mass reference frame. The cross sections have been multiplied by the factors indicated.
Figure 18. DCS's for elastic scattering of He from H₂, N₂, O₂, and Ar at lab energies of A) 0.5-, B) 1.5-, and C) 5.0-keV, plotted in the center-of-mass reference frame. The cross sections have been multiplied by the factors indicated.
the collision energy (assuming the absence of inelastic processes), an empirical potential which accurately predicts the DCS at one energy can be used to calculate the DCS at another energy, in this case 100 eV. While it is possible to avoid this computationally-intensive procedure and obtain a potential through integration of an empirical reduced deflection function using classical scattering theory, as was done by Lane and Everhart\textsuperscript{24}, Smith \textit{et al.}\textsuperscript{25} point out that scatter in experimental data can make this method ambiguous, making it more profitable to assume an analytic potential form and fit the data as described above.

Using spherically symmetric potentials as called for in the partial wave analysis keeps the problem simple enough to be workable. In reality, however, none of the targets studied here has such physical symmetry. Whether or not this is an oversimplification becomes apparent in the success or failure of applying these potentials to the measurements. One form used for the potentials is comprised of a screened coulomb term plus an exponential term:

\[ V_1(r) = A_1 \frac{e^{-\alpha_1 r}}{r} + A_2 e^{-\alpha_2 r} \quad (18) \]

and has been used with a high degree of success in modelling elastic scattering of H atoms from rare gases\textsuperscript{26}. While this form works well for some targets, it is inadequate for others where the DCS's exhibit some minor structure. In these cases, a slight variation of a potential form proposed by Ceperley and Partridge\textsuperscript{27} for the interaction of two helium ions at small distances is found to be effective:
\[ V_2(r) = \sum_{n=-1}^{2} B_n e^{-\beta_n r} r^n. \] (19)

These potential forms are but two among many physically plausible forms which have been used by investigators to model collision processes. In particular, the interactions of He and He\(^+\) with He and other rare gases have been studied extensively and have spawned many empirical formulas for the interaction potentials\(^{25-33}\). For reasons why the forms shown above are used over other likely candidates, one need look no further than that they serve very well in providing fits to the experimental results. It would be pointless to over-analyze the forms chosen in relation to the real physical interaction potential, since the empirical potential providing the best fit must necessarily be some "average" over many target orientations and many contributing molecular states.

**Calculated Cross Sections**

The parameters providing the best fit to the experimental results are summarized in table 2. For N\(_2\), CO, and H\(_2\)O targets, the potential form \( V_1(r) \) provides an excellent fit at both 0.5 and 1.5 keV, as seen in figures 19 through 21. Figure 22, however, shows a poor fit to CO\(_2\) using this form. The greater flexibility of the potential form \( V_2(r) \) provides a much better fit for CO\(_2\) as seen in figure 23, and is also able to provide as good a fit to CO (figure 24) as that using \( V_1(r) \). In each of the figures shown, a single potential is used to fit the DCS data at both energies (except for fig. 22, where only one energy is used). That this is possible suggests that the measurements
Table 2. Interaction Potential Parameters

**Screened Coulomb plus Exponential Form:**

\[
V_1(r) = A_1 \frac{e^{-\alpha_1 r}}{r} + A_2 e^{-\alpha_2 r}
\]

<table>
<thead>
<tr>
<th>Parameters:</th>
<th>O + N₂</th>
<th>O + CO</th>
<th>O + CO₂</th>
<th>O + H₂O</th>
</tr>
</thead>
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<tr>
<td>(A_1) (eV Å)</td>
<td>1.43 E7</td>
<td>7.56 E7</td>
<td>3.09 E8*</td>
<td>5.04 E12</td>
</tr>
<tr>
<td>(\alpha_1) (Å⁻¹)</td>
<td>10.69</td>
<td>13.52</td>
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</tr>
<tr>
<td>(A_2) (eV)</td>
<td>256</td>
<td>403</td>
<td>620*</td>
<td>1.68 E4</td>
</tr>
<tr>
<td>(\alpha_2) (Å⁻¹)</td>
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<td>2.728</td>
<td>2.610*</td>
<td>4.169</td>
</tr>
<tr>
<td>Active Range:</td>
<td>1.19 – 2.38</td>
<td>1.08 – 2.24</td>
<td>1.27 – 2.58</td>
<td>1.56 – 2.42</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>*Fit to 500eV data only</td>
</tr>
</tbody>
</table>

**Modified Ceperley and Partridge Form:**

\[
V_2(r) = \sum_{n = -1}^{2} B_n e^{-\beta_n r} r^n.
\]

<table>
<thead>
<tr>
<th>Parameters:</th>
<th>O + N₂</th>
<th>O + CO</th>
<th>O + CO₂</th>
<th>O + H₂O</th>
</tr>
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<tr>
<td>(B_{-1}) (eV Å)</td>
<td>—</td>
<td>1.12 E8</td>
<td>8.21 E5</td>
<td>—</td>
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<tr>
<td>(\beta_{-1}) (Å⁻¹)</td>
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<td>(B_0) (eV)</td>
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<td>-1.35 E4</td>
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<td>(\beta_0) (Å⁻¹)</td>
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<td>4.335</td>
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<td>(B_1) (eV Å⁻¹)</td>
<td>—</td>
<td>-103</td>
<td>4.95 E3</td>
<td>—</td>
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<tr>
<td>(\beta_{1,2}) (Å⁻¹)</td>
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<td>3.939</td>
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<tr>
<td>(B_2) (eV Å⁻²)</td>
<td>—</td>
<td>549</td>
<td>1.46 E3</td>
<td>—</td>
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<tr>
<td>Active Range:</td>
<td>—</td>
<td>1.24 – 2.32</td>
<td>1.19 – 2.58</td>
<td>—</td>
</tr>
</tbody>
</table>
Figure 19. DCS's for O + N₂ elastic scattering from measurement (+) and calculation using the $V_1(r)$ potential form (———). The cross sections have been multiplied by the factors indicated.
Figure 20. DCS's for O + CO elastic scattering from measurement (+) and calculation using the $V_1(r)$ potential form (——). The cross sections have been multiplied by the factors indicated.
Figure 21. DCS's for O + H₂O elastic scattering from measurement (+) and calculation using the V₁(r) potential form (———). The cross sections have been multiplied by the factors indicated.
Figure 22. DCS's for 0.5-keV O + CO$_2$ elastic scattering from measurement (+) and calculation using the $V_1(r)$ potential form (———).
Figure 23. DCS's for O + CO$_2$ elastic scattering from measurement (+) and calculation using the V$_2$(r) potential form (——). The cross sections have been multiplied by the factors indicated.
Figure 24. DCS's for O + CO elastic scattering from measurement (+) and calculation using the $V_2(r)$ potential form (——). The cross sections have been multiplied by the factors indicated.
are relatively free from inelastic processes, which become more significant at higher projectile energies and smaller impact parameters. Difficulties in fitting multiple-energy DCS's with a single potential due to target excitation have in fact been observed\textsuperscript{26} for the cases of H + Kr and H + Xe direct scattering.

The fits achieved in the present analysis improve upon those of Foreman \textit{et al.}\textsuperscript{29}, who determined interaction potentials using a two-parameter exponential form (sometimes referred to as the Born-Mayer potential). The relative inflexibility of this form results in calculated DCS's that fit the measurements to within a factor of two, but fail to do better than meet the general slope and amplitude of the data. Similarly general agreement is attained using the Universal potential of Biersack and Ziegler\textsuperscript{34}. However, this latter case is most noteworthy in that the Universal potential, which was derived exclusively for atomic targets and projectiles, is an analytical form depending only on the atomic numbers of the reactants and has no other adjustable parameters. Yet despite the absence of fitting to individual measurements and being misapplied to molecular targets, a respectable agreement is attained for all four targets studied.

Whatever potentials are used, they are in theory independent of energy and thus can be used to extrapolate the DCS's to any energy desired. There are, however, practical limitations to their use. In the present analysis, the primary limitation comes from the semiclassical JWKB approximation, which deteriorates at low energies, such that at energies on the order of 10 eV the calculated phase shifts are no longer accurate\textsuperscript{35}. 
Additional Interaction Potential Considerations

For each energy, the range of the potential considered significant to the fitting (referred to here as the active range) lies between the two classical turning points corresponding to the largest and smallest angles of the experimental data. These angles, $\theta_{\text{max}}$ and $\theta_{\text{min}}$, are used to find the impact parameters $b_{\text{min}}$ and $b_{\text{max}}$ through use of the classical deflection function $\theta = \theta(b)$, derived through a knowledge of the phase shifts and the expressions

$$\theta(l) = 2 \frac{d\delta}{dl}$$  \hspace{1cm} (20)

$$b = (l + \frac{1}{2}) k.$$  \hspace{1cm} (21)

The impact parameters $b_{\text{min}}$ and $b_{\text{max}}$ then lead directly to the turning points. On average, these typically lie at approximately 1.3 Å and 2.4 Å internuclear separation for the targets and energies studied (actual values are given in table 2). At these points, the radial motion of the nuclei is at a minimum and thus the time available for the potential forces to act is longest. Although the wave packet extends some small distance (roughly 0.01 to 0.02 Å) past the smallest turning point, the potential at smaller internuclear separations goes essentially unseen, and the accuracy of the potential in this region is unknown. In fact it has been found that at small enough internuclear separation ($r$), the screened coulomb treatment used is inappropriate, as the interaction becomes a pure nuclear coulombic repulsion\textsuperscript{25}. Thus, extrapolation of the measurements to larger scattering angles, though tempting, is avoided. At large $r$ the potential is viewed by every incoming
wave packet, and the importance of its accuracy in this region must be assessed. Cross section calculations performed using identical potentials in the active range with well behaved but very different potentials at large $r$ produced identical results, confirming the exclusive importance of the potential in the active range. Probing the accuracy of the upper and lower limits of the active range as defined by the classical turning points is performed with a more sensitive method, where a small artificial bump is added to the potential and the resulting perturbation in the calculated DCS is observed\textsuperscript{17}. Figures 25 and 26 illustrate this method for the sample case of O(500eV) + N$_2$. Moving the bump on the potential to smaller $r$ values shifts the perturbation in the DCS to larger scattering angles as expected. The lower limit (smaller $r$ value) of the active range then corresponds to the point at which the perturbation begins to appear at the largest angle in the experimental data. In the sample case studied this limit was found to be at $r = 1.725$ Å. Comparing this with the $r = 1.740$ Å limit calculated from the classical turning point, the width of the wave packet is estimated to be, very roughly, 0.03 Å. Further, this result indicates that the classical turning points provide an excellent estimate of the region of the potential important to the scattering calculations.

Fitting potentials to the DCS measurements yields the interesting result of non-uniqueness of the potentials for a given reactant pair. While it is observed that a slight change in slope or shift in magnitude by itself can cause significant changes in the calculated DCS, changing the parameters in concert can result in two or more significantly different potentials which all yield excellent fits to the data. To illustrate this point quantitatively, a study of the O + N$_2$ collision reveals that a 1.0% change in individual potential
Figure 25. Artificial bump superimposed on the $V_1(r)$ potential form for the $O+N_2$ elastic scattering calculation.
Figure 26. DCS's for 0.5-keV O + N₂ elastic scattering calculated using the $V_1(r)$ potential form with a bump added at 1.8 Å (— — —) and with no bump added (— - - -).
parameters (using the $V_1(r)$ form) can elicit a change in the measure of the fit (chi squared) as small as 0.02% or as large as 9.8%. Nonetheless, two very different potentials, seen in figure 27, produce nearly identical cross sections at all of the energies studied (figure 28). Keep in mind that the active range of the potentials lies somewhere between 1 and 3 Å, where the divergence of the potentials is pronounced. Efforts to find a large family of such potentials, either continuous or discrete, failed, with the refining process always converging the potentials into one of the two seen in the figure. This suggests that two distinct local minima in the 4-fold "parameter space" are responsible for the observed effects, with the possible existence of additional undiscovered minima left open. Similar results are seen for O + CO (two potentials found) and O + H$_2$O (three potentials found), with the results for the latter case shown in figures 29 and 30. No attempt was made to find multiple potentials for O + CO$_2$ due to the substantial time required to fit the $V_2(r)$ form.

Intuitively this is a disturbing result, since uniqueness of the interaction potential seems inherent by definition for single channel elastic scattering. However, a rigorous mathematical treatment by Newton$^{36}$ demonstrates both the existence and non-uniqueness of a spherically symmetric potential deduced from a knowledge of all phase shifts at a given energy, provided only that the phase shifts tend to zero sufficiently rapidly with increasing l value. Such a mathematical proof is certainly invaluable, however a plausible physical explanation why this is so is a bit more satisfying. For this one must recall that the empirical potentials generated represent the combined contributions from many different molecular states and target orientations. The empirical rather than physical nature of the
Figure 27. \( V_1(r) \) potentials which yield essentially identical calculated DCS's for \( O + N_2 \) elastic scattering over the angular range studied.
Figure 28. DCS's for O + N₂ elastic scattering calculated using the upper (———) and lower (-----) V₁(r) potentials shown in figure 27. The cross sections have been multiplied by the factors indicated.
Figure 29. $V_1(r)$ potentials which yield essentially identical calculated DCS's for O + H$_2$O elastic scattering over the angular range studied.
Figure 30. DCS's for O + H$_2$O elastic scattering calculated using the upper (———), middle (———), and lower (— —) $V_1(r)$ potentials shown in figure 29. The cross sections have been multiplied by the factors indicated.
Figure 31. $V_2(r)$ potential used to calculate O + CO$_2$ elastic scattering DCS's.
estimated potentials is graphically illustrated by the O + CO\textsubscript{2} potential
generated using the V\textsubscript{2}(r) form (see figure 31). The convex curve does not
conform to expectations of a physical potential, yet the DCS's calculated with
it fit the experimental results well (figure 23).

Extrapolation to Low Energy

As already discussed, the potential at large r (beyond the active range)
is not significant to the DCS calculations, and at small r is unreliable.
Therefore for each reactant pair the cross section at 100 eV is calculated
using the potential only over the union of the active ranges for the two
energies fit, with the results shown in figure 32. The validity of the
extrapolation to lower energy is scrutinized through comparisons between
experimental and calculated DCS's when viewed in reduced coordinates. The
use of reduced coordinates is based on classical expansions of reduced
variables which have been carried out by Smith et al.\textsuperscript{37} and which, to a first
approximation, are dependent only on the impact parameter b. Specifically,
the reduced scattering angle $\tau = E\theta$ and the reduced cross section
$\rho = \theta \sin\theta \frac{d\sigma}{d\Omega}$ (working in the center-of-mass reference frame) can
both be expressed as power series in $1/E$ where the coefficient of each term is
a function of b only:

$$\tau (E,b) = E\theta = \tau_0(b) + E^{-1}\tau_1(b) + ...$$  \hspace{1cm} (22)

$$\rho (\tau,E) = \theta \sin\theta \frac{d\sigma(\theta,E)}{d\Omega} = \rho_0(\tau) + E^{-1}\rho_1(\tau) + ...$$  \hspace{1cm} (23)
Figure 32. Calculated DCS's for 0.1-keV O elastic scattering from CO$_2$, CO, N$_2$, and H$_2$O. The cross sections have been multiplied by the factors indicated.
Figure 33. DCS's for O elastic scattering calculated at 0.1-keV (———), and measured at 0.5-keV (— — —) and 1.5-keV (— — — —) plotted in center-of-mass reduced coordinates. The cross sections have been multiplied by the factors indicated.
The coefficients $\rho_1(\tau), \rho_2(\tau), \ldots$, are functions that decline rapidly as $\tau \rightarrow 0$, unlike $\rho_0(\tau)$. Thus for small angle forward scattering, $\rho(\tau, E) = \rho_0(\tau)$, and a plot of $\rho$ vs. $\tau$ for several values of $E$ yields a set of curves that all follow $\rho_0(\tau)$ at small $\tau$ and then peel away from it at successively higher $\tau$ values as $E$ increases. This method is viewed as a good indicator of the precision of the cross sections, and the present results show excellent agreement when analyzed in this manner (see figure 33). At large angles, the expected divergence seen in the 100 eV data corresponds to laboratory scattering angles as large as $20^\circ \sim 28^\circ$.

In brief summary, previous experience has shown that difficulties encountered in the fitting of measured DCS's at more than one energy with a single potential can arise from inelastic contributions in the measurements due to target excitation. The excellent fits attained in the present work suggest then that inelastic contributions are negligible at the energies and angles studied, and thus the empirical potentials are accurate representations of the physical interactions for elastic scattering. Restricting the range of the potentials used for extrapolation to that for which there is directly corresponding experimental data, and extrapolating to a lower energy where inelastic processes are even less likely to influence the DCS's leaves little room for the introduction of inaccuracies in the 100 eV cross sections. This confidence in the extrapolated DCS's is borne out in the agreement between cross sections at different energies in the reduced coordinate analysis.
V. Conclusion

Absolute differential cross sections for the elastic scattering of oxygen atoms from a wide variety of targets have been presented for projectile energies of 0.5 and 1.5 keV. For several of the targets, single-channel potential scattering calculations have been used to predict the cross sections for projectile energies of 100 eV. Some notable features of the analysis include an illustration of the close similarity among cross sections for different targets when viewed in the center-of-mass frame, derivation of multiple potential curves which all provide excellent fits to measurements for a single pair of reactants, and excellent agreement between calculated low energy cross sections and higher energy experimental results when compared in reduced coordinates.

Measurements of other processes involving atomic oxygen are of great interest to aeronomers and planetary physicists, such as electron loss and capture by fast neutral oxygen, and reactions involving excited states of oxygen. Some preliminary measurements of these processes have been made with interesting results\textsuperscript{17}, such as differential cross sections which increase monotonically with scattering angle and cross sections which show a high degree of sensitivity to the electronic state of the projectile. Measurements of cross sections to larger scattering angles are also of great interest as they reveal information about the interaction potentials at smaller internuclear distances and allow for accurate estimates of total collisional cross sections. Detailed and precise measurements of these processes are realistically achievable with the present research program and basic apparatus. Concurrent measurements with oxygen being carried out in independent
experiments in this research group include electron impact ionization and dissociative ionization of O₂, and differential cross section measurements for H and O projectiles incident on a thermal atomic oxygen target. Together these measurements will provide a reasonably comprehensive picture of the chemistry and scattering of oxygen, and will allow for more accurate modelling of environments where such processes play a significant role.
References


