

GL-TR-90-0229

**AD-A230 572**

**Ionization and Neutralization Processes**

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**29 April 1990**

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**Scientific Report No. 1**

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## REPORT DOCUMENTATION PAGE

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| 1a. REPORT SECURITY CLASSIFICATION<br>Unclassified                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |       |                                                 | 1b. RESTRICTIVE MARKINGS                                                                                                                                                          |                               |
| 2a. SECURITY CLASSIFICATION AUTHORITY                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |       |                                                 | 3. DISTRIBUTION/AVAILABILITY OF REPORT<br>Approved for public release; distribution unlimited                                                                                     |                               |
| 2b. DECLASSIFICATION/DOWNGRADING SCHEDULE                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |       |                                                 |                                                                                                                                                                                   |                               |
| 4. PERFORMING ORGANIZATION REPORT NUMBER(S)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |       |                                                 | 5. MONITORING ORGANIZATION REPORT NUMBER(S)<br>GL-TR-90-0229                                                                                                                      |                               |
| 6a. NAME OF PERFORMING ORGANIZATION<br>Queen's University of Belfast                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |       | 6b. OFFICE SYMBOL<br>(If applicable)            | 7a. NAME OF MONITORING ORGANIZATION<br>European Office of Aerospace Research and Development                                                                                      |                               |
| 6c. ADDRESS (City, State, and ZIP Code)<br>Department of Applied Mathematics and Theoretical Physics<br>Belfast BT7 INN, Northern Ireland                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |       |                                                 | 7b. ADDRESS (City, State, and ZIP Code)<br>Box 14<br>FPO New York 09510-0200                                                                                                      |                               |
| 8a. NAME OF FUNDING/SPONSORING ORGANIZATION<br>Geophysics Laboratory                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |       | 8b. OFFICE SYMBOL<br>(If applicable)<br>PHK     | 9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER<br>AFOSR-83-0190                                                                                                                  |                               |
| 8c. ADDRESS (City, State, and ZIP Code)<br>Hanscom AFB, MA 01731-5000                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |       |                                                 | 10. SOURCE OF FUNDING NUMBERS                                                                                                                                                     |                               |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |       |                                                 | PROGRAM ELEMENT NO.<br>61102F                                                                                                                                                     | PROJECT NO.<br>2303           |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |       |                                                 | TASK NO.<br>G2                                                                                                                                                                    | WORK UNIT ACCESSION NO.<br>AI |
| 11. TITLE (Include Security Classification)<br>IONIZATION AND NEUTRALIZATION PROCESSES                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |       |                                                 |                                                                                                                                                                                   |                               |
| 12. PERSONAL AUTHOR(S)<br>BATES, Sir David R                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |       |                                                 |                                                                                                                                                                                   |                               |
| 13a. TYPE OF REPORT<br>Scientific #1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |       | 13b. TIME COVERED<br>FROM 1 Apr 89 to 31 Mar 90 | 14. DATE OF REPORT (Year, Month, Day)<br>1990 April 29                                                                                                                            | 15. PAGE COUNT<br>16          |
| 16. SUPPLEMENTARY NOTATION                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |       |                                                 |                                                                                                                                                                                   |                               |
| 17. COSATI CODES                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |       |                                                 | 18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)                                                                                                 |                               |
| FIELD                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | GROUP | SUB-GROUP                                       | Dissociative recombination. Termolecular association. Termolecular ionic recombination. Deactivation. $O_2$ bands. $O(^1S)$ production. F-region. Negative ions. Photoionization. |                               |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |       |                                                 |                                                                                                                                                                                   |                               |
| 19. ABSTRACT (Continue on reverse if necessary and identify by block number)<br>Dissociative recombination in polyatomic ions is discussed. A new process, tidal termolecular ionic recombination has been discovered. Deactivation of $O_2(^5\Pi)$ by $N_2$ is discussed in connection with termolecular association of oxygen. The temperature-dependence of termolecular association has been explained. An experimentally-determined rate of $N(^4D)$ quenching by $O(^1P)$ is shown to be incompatible with forbidden-red-line observations. Transition probabilities for some $O_2$ bands have been computed. The $O(^1S)$ production-mechanisms, relevant to observations on the nocturnal F-region, are discussed. A review on negative ions has been written. Cross sections for photoionization of $O(2p^4 3p, 1D, 1S)$ $O(2p^3 3s 3, 5S^o)$ and $O(2p^3 3p 3, 5P)$ have been calculated by the R-matrix method. A preliminary study of photoionization of $N(2p^3 4S^o)$ has been made. R-matrix calculations of electronic excitation of $N_2$ by electron-impact agree well with experiment for the $X \rightarrow A$ and $X \rightarrow W$ transitions and reveal the importance of resonances, and preliminary studies of excitation of $O_2$ indicate reasonable agreement with experiment. An accurate R-matrix calculation |       |                                                 |                                                                                                                                                                                   |                               |
| 20. DISTRIBUTION/AVAILABILITY OF ABSTRACT<br><input checked="" type="checkbox"/> UNCLASSIFIED/UNLIMITED <input type="checkbox"/> SAME AS RPT. <input type="checkbox"/> DTIC USERS                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |       |                                                 | 21. ABSTRACT SECURITY CLASSIFICATION<br>Unclassified                                                                                                                              |                               |
| 22a. NAME OF RESPONSIBLE INDIVIDUAL<br>DR. ED MURAD                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |       |                                                 | 22b. TELEPHONE (Include Area Code)<br>(617) 377-3176                                                                                                                              | 22c. OFFICE SYMBOL<br>GL/PHK  |

18 (subject terms-cont)

Electronic excitation of molecules.    Dielectronic recombination.

19 (Abstract-contd)

of dielectronic recombination in oxygen has given a rate coefficient about one-half of distorted-wave results.

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## SECTION I

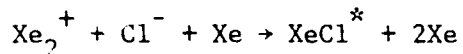
### A. Dissociative recombination of polyatomic ions

The key question in the context of the dissociative recombination of polyatomic ions is: What are the dissociation products? One of the factors which controls this is the occurrence of favourable crossings of potentials. It is not possible to determine theoretically whether or not there is a favourable crossing without doing very lengthy ab initio quantal computations but some relevant elementary considerations have been discovered. There are two main classes of saturated polyatomic ion. A member of the first class has a free valence or contains an ionized atom (for example  $C^+$ ) the number of whose valences increases on neutralization. Breaking a bond yields radicals, and generally there are enough accessible potentials to make a crossing quite likely. A member of the second class contains an ionized atom (for example  $N^+$  or  $O^+$ ) the number of whose valences decreases on neutralization so that one of the products of breaking a bond is a saturated molecule and only a single potential is accessible. In this circumstance there is unlikely to be a favourable crossing. However in many cases a favourable crossing is to be expected for the channel in which two H atoms are shed and a  $H_2$  molecule is formed from them. This is because of the considerable spread in the vibrational energy that may be carried by the  $H_2$  molecule. Branching ratios cannot easily be predicted. Each depends on the product of the favourability of the crossing (as measured by the Frank-Condon factor) and the probability of the transition (D. R. Bates, *Astrophys. J.* 344, 531, 1989).

### B. Tidal termolecular ionic recombination

A new recombination process, tidal termolecular ionic recombination, has been discovered. It arises from calculations

aimed at explaining measurements (S. P. Mezyk, R. Cooper and J. Sherwell, J. Phys. Chem. 93, 8187, 1989) on processes like



which were carried out in connection with rare gas halide lasers. The experiments proved that the recombination coefficient is far higher than expected. Monte Carlo simulation that allowed for the  $\text{Cl}^- - \text{Xe}^+$ ,  $\text{Cl}^- - \text{Xe}$  and  $\text{Xe}^+ - \text{Xe}$  forces showed that the rotational and vibrational modes of  $\text{Xe}_2^+$  tend to be excited by the passage of  $\text{Cl}^-$  through perihelion. Because of this electrostatic tidal action the orbit contracts and the internal energy of  $\text{Xe}_2^+$  increases leading to dissociation. The measured values of the recombination coefficient have been reproduced satisfactorily (D. R. Bates and W. Lowell Morgan (Phys. Rev. Lett. 64, in press 1990).

#### C. Deactivation of $\text{O}_2$ and termolecular association of oxygen

It has been shown that the rate coefficient for the deactivation of  $\text{O}_2(^5\Pi_g)$  by  $\text{N}_2$  is probably low enough to ensure that collisional dissociation  $\text{O}_2(^5\Pi_g) + \text{N}_2 \rightarrow 2\text{O} + \text{N}_2$  prevents the reaction  $\text{O} + \text{O} + \text{N}_2 \rightarrow \text{O}_2(^5\Pi_g) + \text{N}_2$  from contributing appreciably to the measured total termolecular association coefficient (D. R. Bates, Chem. Phys. Lett. 162, 313, 1989).

#### D. Temperature dependence of termolecular association

The dependence of the rate coefficient  $k$  for termolecular association between the diatomic ions  $\text{A}^+$  and diatomic molecules  $\text{B}$  on the temperature  $T$  of the ambient gas has been considered. There is experimental evidence that  $k$  decreases rapidly as  $T$  is increased if the association energy is small. It was shown that the required  $T$  variation could ensue if the reactants in the energized complex  $\text{AB}^{+*}$

repel one another at some relative orientations (D. R. Bates, J. Chem. Phys. 90, 87, 1989).

#### E. $N(^2D)$ quenching and the forbidden red line

Theoretical considerations show that if the rate coefficient for  $N(^2D) + O(^3P) \rightarrow N(^4S) + O$  is indeed  $2.8 \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$  as measured by L. E. Jusinski, G. Black and T. G. Slanger (J. Phys. Chem. 92, 5977, 1988) the product oxygen atoms must be in the  $^1D$  state. This is incompatible with observational data on the forbidden red line emission. It was inferred that the  $N(^2D) + O(^3P)$  quenching measurement must have been vitiated by some factor which did not enter a companion  $N(^2D) + O_2(X)$  quenching measurement (D. R. Bates, Planet Space Sci. 37, 1145, 1989).

#### F. Transition probabilities for $O_2$ bands

Absolute transition probabilities have been computed for the bands of the Herzberg I, Chamberlain, Herzberg II and Herzberg III systems of molecular oxygen (D. R. Bates, Planet. Space Sci. 37, 881, 1989).

#### G. $O(^1S)$ production and the nocturnal F-region

The  $O(^1S)$  quantum yield in  $O_2^+$  dissociative recombination  $f(^1S)$  in the nocturnal F-region and processes  $O^+ + O_2 \rightarrow O + O_2^+$  ( $v \leq 7$ ) and  $O_2^+(v) + O \rightarrow O_2^+(v' < v) + O$  have been discussed. The values of  $f(^1S)$  obtained from the Visible Airglow Experiment (V. J. Abrev, S. C. Solomon, W. E. Sharp and P. B. Hayes J. Geophys. Res. 88, 4140, 1983) do not seem explicable in terms of the ab initio results of Guberman (Nature, 327, 408, 1987) on the  $\alpha(^1S, v)$  direct dissociative recombination coefficients. Arguments have been advanced to show that the discrepancy cannot be attributed to an overlooked  $O(^1S)$  source in the F-region. Doubt has been thrown on the correctness of the results of the Visible Airglow Experiment by a recent determination of the  $f(^1S)/f(^1D)$  ratio by H. Takahashi, B. R.

Clemensha, P. P. Batista, Y. Sahai, M. A. Abdu and P. Muralikrishna (Planet. Space Sci. 38, 547, 1990) from equatorial F-region profile measurements. These are consistent in general with theoretical expectations. However discrepancies appear in detailed facets of the data. If they are real they may conceivably be due to the computed  $\alpha(^1S, v)$  being less accurate than has been supposed. The possibility has been raised that  $\alpha(^1S, 0)$ , in particular, is affected by the neglected indirect dissociative recombination Laboratory measurements on  $f(^1S)$  by J. L. Queffelec, B. R. Rowe, F. Vallee, J. C. Gomet and M. Morlais (J. Chem. Phys. 91, 5335, 1989) have been considered and it has been concluded that they conflict with so much independent evidence that they must be regarded with reserve (Dr. R. Bates, Planet. Space Sci. 38, in press 1990).

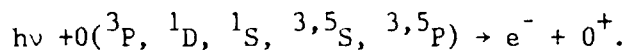
#### H. Negative ions

A long review article "Negative ions: structure and spectra" has been written (D. R. Bates, Adv. Atomic. Molec. and Optical Physics, 27, in press 1990).

## PHOTOIONIZATION OF OXYGEN AND NITROGEN

### A. Oxygen

In the work performed, studies have been made for the photoionisation of the  $2p^4\ ^3P$ ,  $^1D$ ,  $^1S$ ;  $3s\ ^{3,5}S^o$  and  $3p\ ^{3,5}P$  states of atomic oxygen



Whilst photoionisation of the  $2p^4\ ^3P$  ground state has been investigated theoretically for the last fifty years, limited research has been carried out on the photoionisation of excited states. Indeed for all of the above excited states the theoretical work has been limited to the extent that none of it has included autoionising resonances. An important feature of the present work is therefore the inclusion of such resonances. Despite all of the work on the ground state, there are still several discrepancies between theory and experiment, particularly above the  $^4S^o$  threshold and the  $^2P^o$  threshold. Part of this work therefore has been to improve on the calculations of Pradhan (J. Phys. B: At. Molec. Phys. 11, L729, 1978) and Taylor and Burke (J. Phys. B: At. Mol. Phys. 9, L353, 1976). These authors employed R-matrix approach and includes some  $O^+$  target states arising from the  $2s^2 2p^3$  and  $2s 2p^4$  configurations.

In all of the calculations performed in this study, we employed the R-matrix method and included eleven target states of  $O^+$ :  $2s^2 2p^3\ ^4S^o$ ,  $^2D^o$ ,  $^2P^o$ ;  $2s 2p^4\ ^4P$ ,  $^2D$ ,  $^2S$ ,  $^2P$ ;  $2s^2 2p 3s\ ^4P$ ,  $^2P$ ,  $^2D$ ,  $^2S$ . Each of these states was represented by configuration-interaction type wave functions and the energies and energy separation between levels agreed closely with experiment and represented a significant improvement on all previous calculations.

### 1. $^3P$ state

Figure 1 displays the present results. The most significant conclusion is that the theoretical data has converged and thus the discrepancies, above the  $^4S^0$  and  $^2P^0$  threshold, with experiment still remain but must almost certainly lie with the experimental procedures. We shall see below that the photoionisation cross sections for the  $^1D$  and  $^1S$  states are dominated by a broad resonance, the position of which lies in the region above the  $^2P^0$  threshold. A possible explanation therefore of the discrepancy above the  $^2P^0$  threshold is that there may exist excited states of atomic oxygen in the experimental beam. However, we note that this is not applicable to experiment of Hussein et al (J. Phys. B: At. Mol. Phys. 18, 2827, 1985).

### 2. $^1D$ , $^1S$ states

Figures 2 and 3 display the present results. The wide divergence among previous results is clearly apparent. The significant discovery of the present study is the occurrence of a broad  $2s2p^5\ ^1P^0$  Coster-Kronig resonance in both the  $^1D$  and  $^1S$  state photoionisation cross sections.

### 3. $3s\ ^{3,5}S^0$ and $3p\ ^{3,5}P$ states

The only theoretical work available for these states is that of Saxon et al (Phys. Rev. A39, 1156, 1989) for the  $3p\ ^3P$  state. Their work did reveal the interesting feature of a Cooper minimum in the  $O^+(^4S^0)ed\ ^3D^0$  final channel, but did not include allowance for autoionising resonances. Thus, the present work is not only the sole data available for the  $3s\ ^{3,5}S^0$  and  $3p\ ^5P$  states (very limited experimental data exists) but is the most sophisticated for all states. Cooper minima was found for both the  $3p\ ^3P$  and  $3p\ ^5P$  states and careful analysis using oscillator strengths for neutral oxygen was performed to confirm both the accuracy of the present calculation

and hence the position of the Cooper minima. For the  $2p^3 3s^3, 5S^0$  states it was found that the photoionisation cross sections are dominated at high energies by the contributions arising from ejection of a 2p electron (the 3s behaving like a 'spectator' electron).

Two papers have occurred from the above work:

Photoionisation of the  $2p^4\ ^3P, ^1D, ^1S$  states of atomic oxygen,

K. L. Bell, P. G. Burke, A. Hibbert and A. E. Kingston,

J. Phys. B: At. Mol. Opt. Phys. 22, 3197, 1989.

Photoionisation of the  $2p^3 3s^3, 5S^0, 2p^3 3p^3, 5P$  states of atomic oxygen,

K. L. Bell, K. A. Berrington, P. G. Burke, A. Hibbert and A. E. Kingston.

J. Phys. B: At. Mol. Opt. Phys. (in press, 1990).

#### B. Nitrogen

A preliminary study of the photoionisation of the ground  $4S^0$  state of atomic nitrogen has been carried out. The R-matrix method was used and nine target states of  $N^+$  have been included in the calculation:  $2s^2 2p^2\ ^3P; 2s2p^3\ ^5S^0, ^3D^0, ^3P^0, ^3S^0; 2s^2 2p3s\ ^3P^0; 2s^2 2p3p\ ^3D, ^3S, ^3P$ . The results are found to differ little from the less sophisticated work of Le Dournuef et al (J. Phys. B: At. Mol. Phys. 12, 2449, 1979). The study however is being continued by attempting to obtain better representation of the above target states. The continuation is important since recent experimental data (Samson and Angel, private communication) differs significantly from the theoretical results.

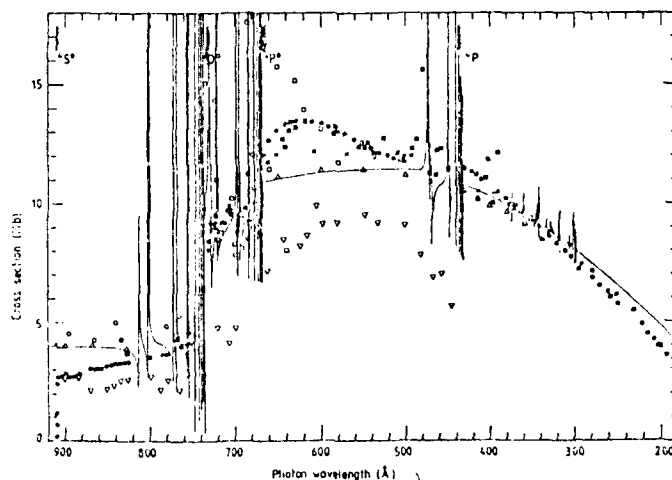


Figure 1. Photoionisation cross section of the  $3P$  state of atomic oxygen. Theory: —, present results;  $\Delta$ , Pradhan (1978);  $\times$ , Taylor and Burke (1976). Experiment:  $\nabla$ , Comes *et al.* (1968);  $\circ$ , Kuhl *et al.* (1978);  $\square$ , Hussein *et al.* (1985);  $\blacksquare$ , Samson and Pareek (1985);  $\bullet$ , Angel and Samson (1988). (Thresholds correspond to experimental values.)

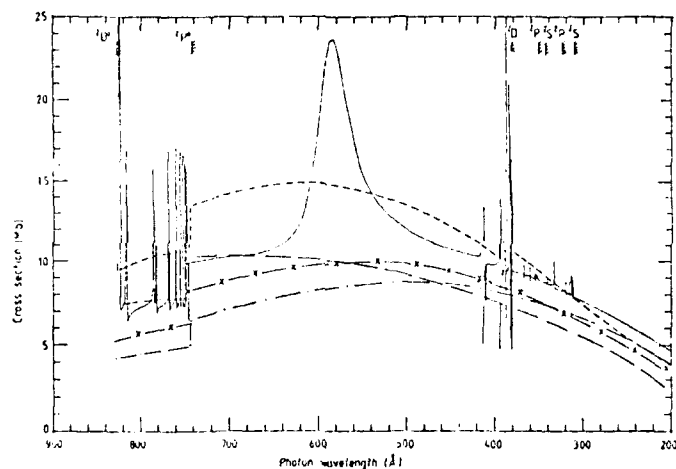


Figure 2. Photoionisation cross section of the  $1D$  state of atomic oxygen. —, present results; --- (length), --- (velocity), Henry (1967);  $\times$ , Thomas and Hellwéll (1970); ---, Koppell (1971). (Thresholds correspond to experimental values.)

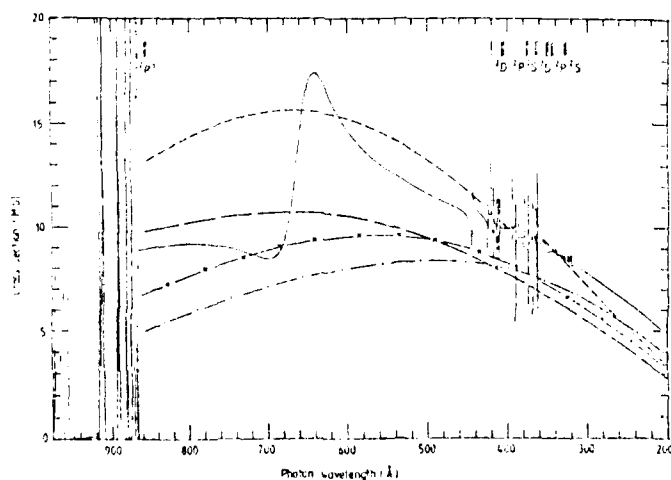


Figure 3. Photoionisation cross section of the  $1S$  state of atomic oxygen. —, present results; --- (length), --- (velocity), Henry (1967);  $\times$ , Thomas and Hellwéll (1970); ---, Koppell (1971). (Thresholds correspond to experimental values.)

# ELECTRON MOLECULE COLLISIONS

In the past decade many calculations have been reported on low-energy collisions of electrons with diatomic molecules allowing for rotational and vibrational excitation in the electronic ground state. It is now possible to obtain accurate cross sections for these processes and at Queen's University of Belfast work has been carried out on a number of molecules including  $N_2$ , HF and HCl using the R-matrix method.

By comparison, little work has been carried out on the process of electronic excitation of the target, although such processes, particularly in the cases of  $N_2$  and  $O_2$ , are urgently required in many applications. The only exception to this is work on electronic excitation of  $H_2$ , where calculations for exciting the  ${}^3\Sigma_u^+$  state carried out using the R-matrix method were in good agreement with calculations using the linear algebraic equations method and the Schwinger variational method.

However in the last year a detailed program of work has been initiated at Queen's University Belfast to calculate accurate electronic excitation cross sections for  $N_2$  and  $O_2$  using the R-matrix method. In the case of  $N_2$ , attention has initially been focussed on transitions from the  $X\ {}^1\Sigma_g^+$  ground state to the first three low lying valence excited states of the molecule  $A\ {}^3\Sigma_u^+$ ,  $B\ {}^3\Pi_g$  and  $W\ {}^3\Delta_u$ . Also, for the first time in electron molecule collisions, CI wave functions were used to represent the target states which is important in order to obtain accurate energy spacings and transition moments. The results show that these cross sections are dominated by resonances over the first 10 eV. Good agreement is obtained with experiment for the  $X \rightarrow A$  and  $X \rightarrow W$  transitions but further work needs to be carried out to include more target states and to include the nuclear motion which has been neglected in these preliminary

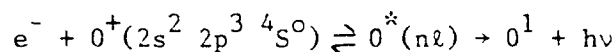
calculations. This work is described in the paper: C. J. Gillan, C. J. Noble and P. G. Burke: Electronic excitation in low energy electron scattering by  $N_2$  molecules. J. Phys. B: At. Mol. Opt. Phys. to be published.

Work on  $O_2$  is also well underway involving a collaboration between Queen's University Belfast and the Daresbury Laboratory. In this case, nine target states arising from the configurations  $1\pi_u^4$   $1f_g^2$  and  $1\pi_u^3 1\pi_g^3$  are being included in the calculation and interest is focussed on transitions from the  $X^3\Sigma_g^-$  ground state to the first two electronically excited states  $1\Delta_g$  and  $b^1\Sigma_g^+$ . Preliminary results indicating reasonable agreement with experiment have been obtained. This work will be submitted for publication in the near future.

It is intended to continue the program of work on electronic excitation of  $N_2$  and  $O_2$ . The nuclear motion will be included in the calculations and transitions involving both electronic and vibrational excitation will be studied.

### DIELECTRONIC RECOMBINATION

Recent accurate calculations on the photoionization of atomic oxygen carried out at Queen's University Belfast by Bell et al (1989, referred to above) raised the prospect of obtaining, for the first time, accurate dielectronic recombination rates given by



where  $O^{*}$  is a resonance state and  $O^1$  an excited bound state of the oxygen atom. Over the last six months, therefore, these earlier R-matrix photoionisation calculations have been extended in this way by Terao et al. It has been found that the rate coefficients are about one half of those obtained by Badwell and Pindzola (1989) using a less accurate distorted wave method, with a maximum value of  $3 \times 10^{-12} \text{ cm}^3 \text{ sec}^{-1}$  at an electron temperature of about 10 eV. This work is described in the forthcoming paper: M. Terao, K. L. Bell, P. G. Burke and A. Hibbert: Theoretical study of dielectronic recombination of  $O^{+}$ . J. Phys. B: At. Mol. Opt. Phys. submitted