

# Electron Impact Dissociation of Ground and Metastable States of O<sub>2</sub> Molecule

J. Tennyson<sup>1,2</sup>, A. Dzarasova<sup>1,2</sup>, J. R. Hamilton<sup>1,2</sup>, J. P. Booth<sup>3</sup>, T. Gans<sup>4</sup>, A. Gibson<sup>3,4</sup>

1. Department of Physics & Astronomy, University College London, London, WC1E 6BT, UK
2. Quantemol Ltd., University College London, London, WC1E6BT, United Kingdom
3. LPP, Ecole Polytechnique-CNRS-Univ Paris-Sud-UPMC, 91128 Palaiseau, France
4. York Plasma Institute, Department of Physics, University of York, Heslington, York, YO10 5DD, UK

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plasma chemistry

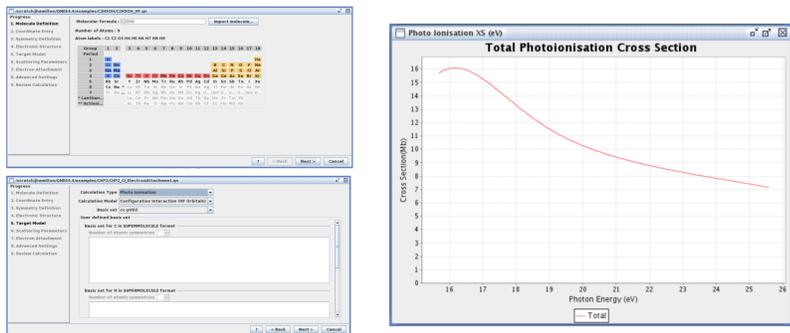
## Quantemol Ltd

Quantemol is based at University College London and was founded by Prof. Jonathan Tennyson FRS and Dr Daniel Brown in 2004. The company develops unique software tools that bring accessibility to highly sophisticated research codes



The *ab initio* UK polyatomic R-matrix method is a sophisticated method to study the scattering interactions of electrons and photons with molecules<sup>2</sup>. The R-Matrix methods are very highly regarded however they are also notoriously hard to use both in terms of understanding the physics behind the method and using the codes computationally.

Quantemol-N<sup>1</sup> is a java interface that allows users to run the R-Matrix codes with minimum scientific knowledge of scattering physics and minimum computational difficulty efficiently providing very good quality data to its users.



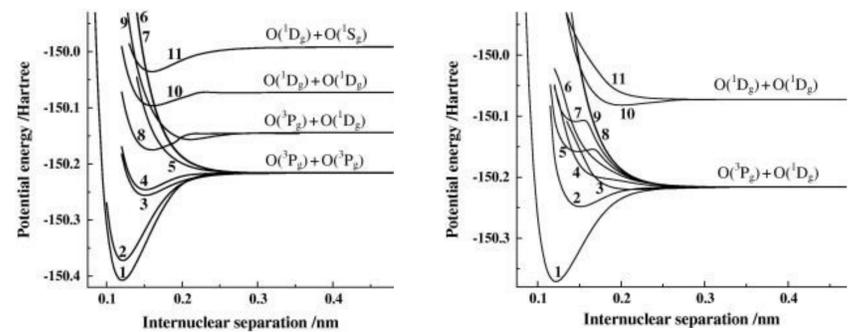
Quantemol-N can be used to perform electron-molecule scattering calculations producing elastic, electronic excitation, super-elastic excitation, impact dissociation, ionization, dissociative attachment, momentum transfer, rotational excitation cross sections and rate coefficients as well as resonance parameters and photoionization cross sections and rate coefficients as a function of energy.

## Quantum Chemistry Method

In this work we have carried out Close Coupling Complete Active Space Configuration Interaction (CAS-Cl) R-Matrix calculations<sup>3</sup> within Quantemol-N to model the excitation cross sections from the ground of the Oxygen molecule O<sub>2</sub>(X<sup>3</sup>Σ<sub>g</sub><sup>-</sup>) and its two metastable states O<sub>2</sub>(a<sup>1</sup>Δ<sub>g</sub>) and O<sub>2</sub>(b<sup>1</sup>Σ<sub>g</sub><sup>+</sup>) to its excited bound and repulsive states.

The ground state of O<sub>2</sub> was found to be (3σ<sub>g</sub><sup>+</sup>, 1π<sub>u</sub>, 2σ<sub>u</sub><sup>+</sup>)<sup>14</sup>(1π<sub>g</sub>)<sup>2</sup>. Orbitals were calculated using the augmented Dunning aug-cc-pVTZ basis set. A CAS-Cl calculation freezing the lowest 5 orbitals and leaving active the degenerate π orbitals open and an additional 5 valence orbitals: (1-3 σ<sub>g</sub><sup>+</sup>, 1-2 σ<sub>u</sub><sup>+</sup>)<sup>10</sup>(4-5 σ<sub>g</sub><sup>+</sup>, 1-2 π<sub>u</sub>, 3 σ<sub>u</sub><sup>+</sup>, 1-2 π<sub>g</sub>)<sup>6</sup> was carried out.

We have then used the potential energy curves (PECs) of Liu *et al.*<sup>4</sup> to match these excited states to dissociation channels thus deriving the electron impact dissociation cross sections.



PECs of the 11 states of O<sub>2</sub> molecule  
1 X<sup>3</sup>Σ<sub>g</sub><sup>-</sup>; 2 b<sup>1</sup>Σ<sub>g</sub><sup>+</sup>  
; 3 c<sup>1</sup>Σ<sub>u</sub><sup>-</sup>; 4 A<sup>3</sup>Σ<sub>u</sub><sup>+</sup>; 5 1<sup>5</sup>Σ<sub>u</sub><sup>-</sup>  
; 6 1<sup>5</sup>Σ<sub>g</sub><sup>+</sup>; 7 2<sup>5</sup>Σ<sub>g</sub><sup>+</sup>; 8 B<sup>3</sup>Σ<sub>u</sub><sup>-</sup>  
; 9 2<sup>3</sup>Σ<sub>g</sub><sup>-</sup>; 10 2<sup>1</sup>Σ<sub>u</sub><sup>-</sup>; 11 f<sup>1</sup>Σ<sub>u</sub><sup>+</sup>

PECs of the 11 states of O<sub>2</sub> molecule  
1 a<sup>1</sup>Δ<sub>g</sub>; 2 A<sup>3</sup>Δ<sub>u</sub>  
; 3 1<sup>5</sup>Π<sub>g</sub>; 4 1<sup>3</sup>Π<sub>u</sub>; 5 C<sup>3</sup>Π<sub>g</sub>  
; 6 1<sup>1</sup>Π<sub>u</sub>; 7 d<sup>1</sup>Π<sub>g</sub>; 8 1<sup>5</sup>Π<sub>u</sub>  
; 9 1<sup>5</sup>Δ<sub>g</sub>; 10 2<sup>1</sup>Δ<sub>g</sub>; 11 2<sup>1</sup>Π<sub>u</sub>

## Results

Figures 1,3 and 3 show the impact dissociation of the ground, first and second metastable states of O<sub>2</sub> respectively. As noted by Itikawa<sup>5</sup> production of O(<sup>1</sup>S) oxygen atoms is negligible. Our investigation and results agreed with this conclusion and consequently cross sections for this channel are assumed to be zero. There are some noisy areas in the cross sections at medium energies. This is because vibrational excitations which would have been taken into account in these calculations. The large resonances which die off very quickly in the cross sections are triplet resonances and this behaviour is typical of this type of resonance.

Figure 64 shows the electron impact excitation cross section of the ground and metastable states of O<sub>2</sub> exciting these states into bound states. As expected the magnitudes from the metastable states are larger than from the ground state. The low energy behaviour of the O<sub>2</sub>(a<sup>1</sup>Δ<sub>g</sub>) cross section is explained by the situation of the <sup>1</sup>Δ<sub>g</sub> resonance close to the threshold.

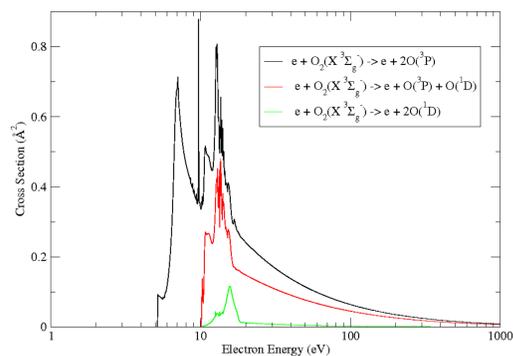


Figure 1: Electron O<sub>2</sub>(X<sup>3</sup>Σ<sub>g</sub><sup>-</sup>) dissociation cross sections to the three non negligible combinations of states of the oxygen atoms.

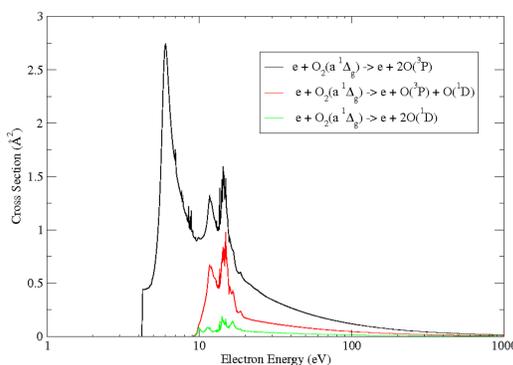


Figure 2: Electron O<sub>2</sub>(a<sup>1</sup>Δ<sub>g</sub>) dissociation cross sections to the three non negligible combinations of states of the oxygen atoms

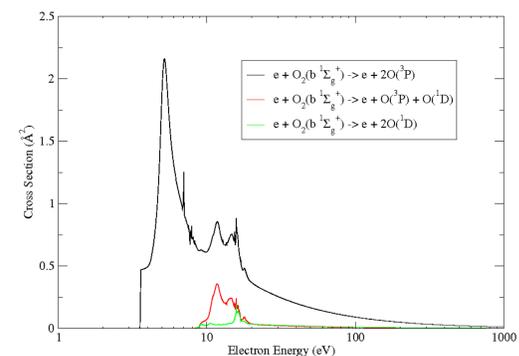


Figure 3: Electron O<sub>2</sub>(b<sup>1</sup>Σ<sub>g</sub><sup>+</sup>) dissociation cross sections to the three non negligible combinations of states of the oxygen atoms

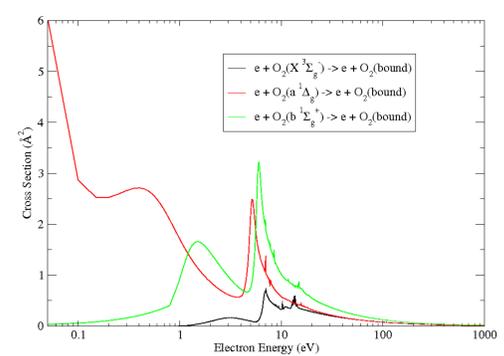


Figure 4: Excitation of ground and metastable states of O<sub>2</sub> to bound states

## References

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PowerBase

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