

$e^-$



# **Electron-molecule collision cross section calculations**

2020 Brochure

## Company Profile

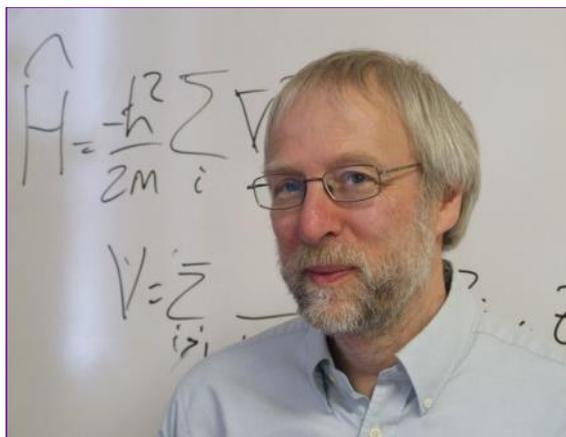
Quantemol was founded by [Prof. Jonathan Tennyson FRS](#) (right) and [Dr. Daniel Brown](#) in 2004. We develop unique software tools that bring accessibility to highly sophisticated research codes.

**Quantemol-N and Quantemol-EC** allow the UK molecular R-matrix code, used to model electron-polyatomic molecule interactions, to be employed quickly with reduced set-up times.

**Quantemol-VT** brings an unsurpassed user experience to the world-renowned plasma simulation codes of Prof. Mark Kushner from the University of Michigan.

**Quantemol-DB (QDB)** is a leading sustainable database, representing the chemical and radiative transport properties of a very wide range of plasmas. The database contains chemistry data for plasma chemistry modelling with pre-assembled and validated chemistry sets, and is regularly updated with the most recent and relevant data.

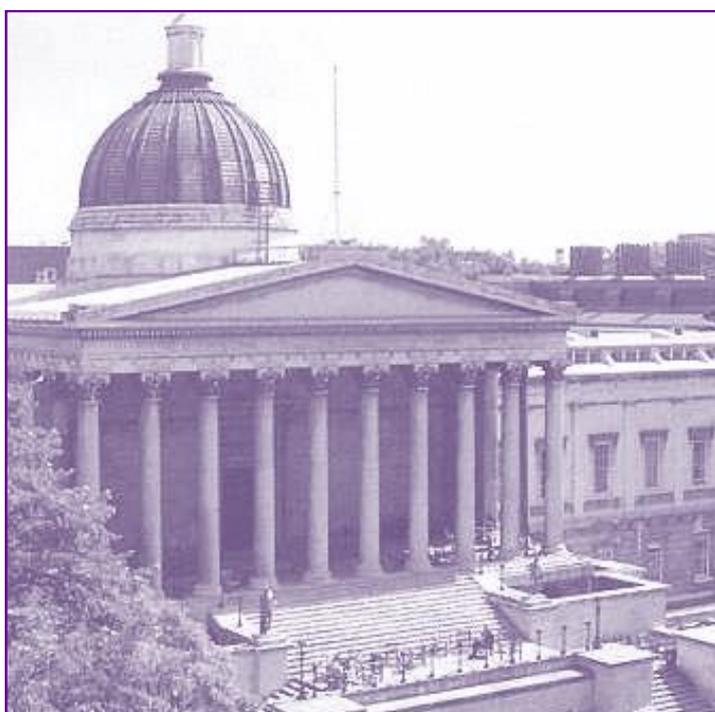
With an expanding research team, Quantemol is able to offer consultancy projects that are carried out by world leading scientists in their respective fields.



Prof. Jonathan Tennyson, FRS, UCL

## Our mission statement

*“To serve our users in industry and academia to simulate complex processes more efficiently, reliably, accurately and cost-effectively and thereby accelerate technological and scientific innovation.”*



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## Background

Collisions of low-energy electrons with molecules affect many aspects of the environment and modern technologies, including:

- Initiating plasma etching processes
- Controlling the action of lasers
- Controlling the ignition of internal combustion engines
- Determining edge effects in fusion plasmas
- Causing radiation damage in biological tissue
- Dictating the behaviour of the earth's ionosphere.

Measurements of such collisions are both expensive and difficult to perform, and their theoretical determination requires sophisticated procedures based on the application of quantum mechanics.

Quantemol-N is an expert interface that simplifies the process of using the sophisticated UK molecular R-Matrix codes.

## Quantemol-N Products:

Quantemol-N is available in standard (SE) and parallel (PE) editions. PE includes all the features of the SE with the addition of a batch job feature, and a parallel version of SCATCI (which significantly reduces calculation times on multicore machines). Both versions also include a large suite of molecular examples (currently ~40) so the user can get started immediately.

## What range of problems can be tackled with Quantemol-N?

- Closed shell molecules
- Open shell molecules, radicals
- Neutral and positively charged species
- Molecules with up to 17 atoms tested

## What does Quantemol-N v 6.1 do?

Calculates a variety of observables for electron molecule collisions including:

- Zero – high electron energy extension for all cross sections \*\*
- Elastic cross-sections
- Electronic excitation cross-sections
- Super-elastic cross-sections
- Quenching cross-sections
- Electron impact dissociation
- Scattering reaction rate
- Arrhenius parameters for reaction rates
- Resonance parameters
- Estimate dissociative electron attachment\*\*
- Differential cross-sections
- Momentum transfer cross-sections
- Electron impact ionisation at all energies\*\*
- Cross-sections for oriented molecules
- Rotational excitation cross-sections
- Inelastic photoionization cross-sections
- Oriented molecule photoionization cross-sections
- Calculations for isotopes
- Integration with Molpro

\*\* features not present in standard R-matrix code

## The key advantages of Quantemol-N?

- Based on the world leading UK molecular R-matrix code
- Easy to use graphical interface: set up a calculation in 9 steps
- Results presented in a flexible, user-friendly form
- Can run on a desktop machine or laptop
- Now also with the Q-N Express feature, speeding up the set-up time of well known molecules\*
- Help with referencing publications
- Compatibility with quantum chemistry software packages

\* - the molecular geometry is imported from the NIST open access database and symmetries are automatically completed by the program

## Photoionization

The response of atomic systems to ionising radiation is a dominant process in the universe. It involves neutral atoms, molecules and clusters as well as their ions (positive or negative) and takes place in many physical systems including a variety of astrophysical objects, the upper atmosphere, fission and fusion plasmas as well as laser-produced plasma.

In many cases the role of the photoionization process is central for determining the overall properties of a system and in addition optical transitions are often used as a diagnostic tool.

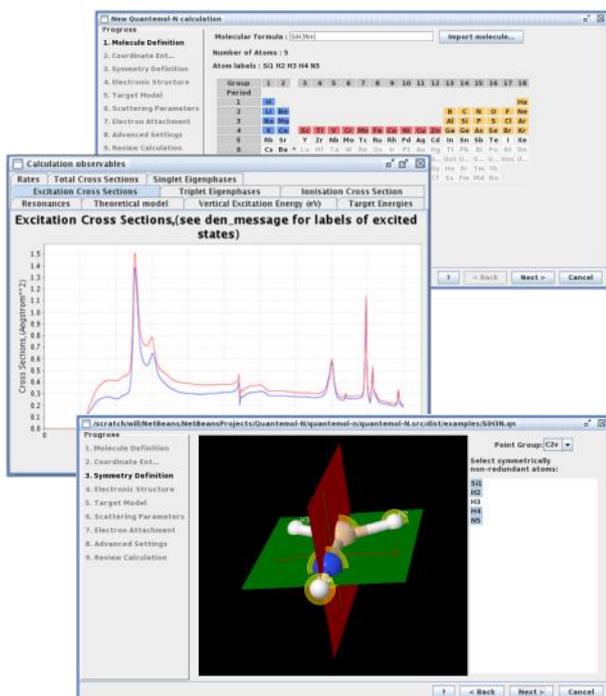
Photoionization cross-sections are now included within the Quantemol-N suite.

## Underlying model

A recent development in the R-matrix method and Quantemol-N is an adaptation allowing for calculations of photoionization cross-sections.

1. Harvey AJ, D. Brambila, F. Morales and O. Smirnova "CDENPROP: Transition matrix elements involving continuum states" arXiv: 1401.0229 [physics.chem-ph] 2013
2. Harvey AJ, D. Brambila, F. Morales and O. Smirnova "Photoelectron angular distributions from aligned molecules using the R-matrix method" arXiv: 1402.3853 [physics.chem-ph]

Extensive experimental comparisons have been performed in order to validate the code.



## Quantemol-EC

New Quantemol software **Quantemol-EC** is offering additional features to Quantemol-N software:

- ⇒ V1.1 (April 2020):
- automatic generation of configurations
  - automatic generation of symmetry
  - automatically handling of degenerate states
  - more accurate ionisation cross-section calculations
  - an automatically generated summary with the results and the level of theory used to generate the results in order to help your understanding and publication
  - access to the most recent version of R-Matrix code
  - Feature to cut off long range interactions

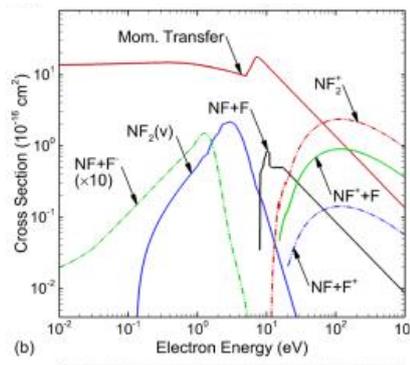
- ⇒ V2: dissociative recombination estimations for ions(2020)
- ⇒ V3: effective core potentials (2020)
- ⇒ V4: vibrational excitations for neutrals (2021)

Based on integration with Molpro quantum chemistry package

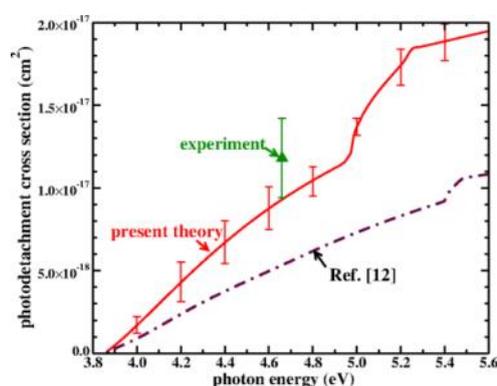
## Recent Citations

1. [Electron and positron scattering cross sections for propene](#), Singh et al, Journal of Applied Physics **124**, 034901 (2018)
2. [Study of electron impact inelastic scattering of chlorine molecule \( \$\text{Cl}\_2\$ \)](#), Yadav et al, Journal of Physics B: Atomic, Molecular and Optical Physics, Volume **51**, Number 4 (2018)
3. [An R-matrix study of electron-induced processes in  \$\text{BF}\_3\$  plasma](#), Gupta et al, Physics of Plasmas **24**, 123511 (2017);
4. [QDB: a new database of plasma chemistries and reactions](#), Tennyson et al, PSST, GEC special issue, (2017)
5. [Calculated cross sections for electron collisions with  \$\text{NF}\_3\$ ,  \$\text{NF}\_2\$  and  \$\text{NF}\$  with applications to remote plasma sources](#), Hamilton et al, Plasma Sources Sci. Technol. **26** (2017) 065010
6. [Global model of an iodine gridded plasma thruster](#) P. Grondein, T. Lafleur, P. Chabert and A. Aanesland, Phys. Plasmas **23**, (2016)
7. [Formation of  \$\text{CN}^-\$ ,  \$\text{C}\_3\text{N}^-\$ , and  \$\text{C}\_5\text{N}^-\$  Molecules by Radiative Electron Attachment and their Destruction](#), Khamesian et al, Physical Review Letters, 117(12 (2016))
8. [Electron induced chemistry of thiophene](#) Vinodkumar, M: Desai, H and Vinodkumar, PC, RSC ADVANCES, V5, Issue: **31** (2015)
9. [Total cross sections for  \$\text{O}\_2\$  and  \$\text{S}\_2\$  by electron impact](#), R Naghma et al, Radiation Physics and Chemistry, **97** (2014) 6-11
10. [Total Scattering Cross Sections for Ethylene by Electron Impact for Incident Electron Energies from 1 to 2000 eV](#) . Naghma, R and Antony, B., International Journal of Quantum Chemistry, v 114, issue 4 (2014)
11. [Electron induced chemistry of disilane](#). D Gupta et al, RSC Advances vol. 4 Issue: 18 (2014) 9197-9204

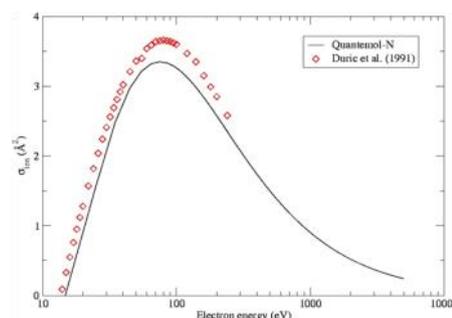
## Comparison with experimental data



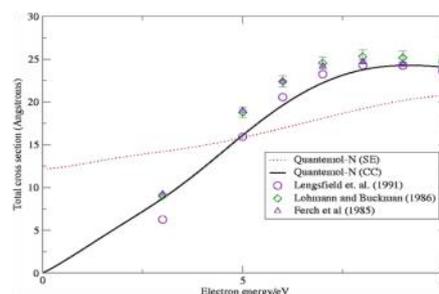
Cross sections for electron impact reactions of  $\text{NF}_2$  using the *ab initio* molecular R-matrix method. Huang et al, 2017.



Here the Quantemol interface has been used to compare experimental and theoretical photodetachment cross sections. The R-matrix code was used for the  $\text{CN}$  and  $\text{CN}^-$  molecules by Khamesian et al, 2016 .



BEB ionisation cross-section of  $\text{CH}_4$ . Here the Quantemol-N data is compared with experimental data (Duric et al., red diamonds).



Total cross-sections of  $\text{CH}_4$ . Here the Quantemol-N results (black & red lines) are shown with theory (Lengsfeld et al., circles) and experiment (Lohmann & Buckham, diamonds, Ferch et al., triangles).

## Price list \*

Use Case	Type of Licence	Version	Licence term		
			1 year	3 years	Annual Support
Non-commercial research	Single Workstation	SE	£4,730	£11,000	£2,310
		PE	£5,500	£12,320	£2,750
	Research group	SE	£5,610	£13,750	£3,300
		PE	£6,160	£16,500	£3,630
	Institution	SE	£7,480	£20,570	£4,180
		PE	£8,910	£24,750	£4,950
Commercial research	Single Workstation	SE	£19,250	£38,500	£4,730
		PE	£22,000	£44,000	£5,500
	Site	PE	£30,250	£60,500	£7,480

## General terms

**Commercial research** - research by commercial organisations or for commercial organisations with results not disclosed to public access.

**Non-commercial research** - research by not-for-profit organisations producing publishable results.

All licences are floating type licences and can be moved from one PC to another.

**SE** - Standard Edition

**PE** - Parallel Edition

**Single workstation licence** - to be used on a single workstation with a possibility of access by multiple users.

**Research group licence** - includes up to five workstations used by researchers in one group, can be installed on the cluster but the number of users should be limited to five within one group only.

**Institution licence** - covers an unlimited number of users across different groups within an institution.

**Site licence** - covers an unlimited number of users within a company.

### Min spec:

Quantemol-N software Linux x86, 64 bit operating system, 4 GB RAM (large calculations will require more RAM), 10 GB free disk space.

## FAQ

**Standard Edition** on single workstation can use any number of cores to be run.

**Parallel Edition** includes a feature enabling the SCATCI part of the code to be run in parallel, with Q-N which significantly speeds up calculations of large molecules. This edition includes a command line interface. To gain access to use the photoionization module you will need a parallel edition licence.

**Annual support** includes initial training, e-mail and telephone support, and bug fixes throughout the year.

**Add on modules** should be purchased separately and we can advise which ones you might need.

**Set up molecule examples** supplied with Q-N free of charge:

AlCl <sub>3</sub>	C <sub>3</sub>	CF	CO	H <sub>2</sub> O	I <sub>2</sub>	SiF <sub>2</sub>	C <sub>4</sub>
BF <sub>3</sub>	C <sub>3</sub> H <sub>4</sub>	CF <sub>2</sub>	CO <sub>2</sub>	H <sub>2</sub> S	N <sub>2</sub>	SiH <sub>4</sub>	C <sub>2</sub>
C <sub>2</sub>	C <sub>3</sub> N	CF <sub>4</sub>	CO <sub>2</sub> <sup>+</sup>	HBr	NH <sub>3</sub>	SiO	CF <sub>3</sub>
C <sub>2</sub> H <sub>2</sub>	C <sub>3</sub> F <sub>8</sub>	CFCs	COS	HCHO	NO <sub>2</sub>	SO <sub>2</sub>	CF <sub>4</sub>
C <sub>2</sub> H <sub>2</sub> <sup>+</sup>	C <sub>3</sub> HF <sub>7</sub>	CH	CS	HCN	O <sub>2</sub>	C <sub>2</sub> F <sub>2</sub>	CF
C <sub>2</sub> H <sub>4</sub>	C <sub>6</sub> H <sub>6</sub>	CH <sup>+</sup>	F <sub>2</sub> O	HCONH <sub>2</sub>	O <sub>3</sub>	C <sub>2</sub> F <sub>6</sub>	F <sub>2</sub>
C <sub>2</sub> H <sub>5</sub> OH	CaF	CH <sub>4</sub>	H <sub>2</sub>	HCP	PH <sub>3</sub>	C <sub>3</sub> F <sub>8</sub>	Benzene
	CaF <sup>+</sup>	CN	H <sub>2</sub> <sup>+</sup>	HNC	SF <sub>6</sub>	C <sub>3</sub>	

\* - all prices are quoted excluding VAT

# CONSULTANCY

As well as providing advanced modelling software, Quantemol delivers a unique consultancy service. With our suite of software and a team of highly-skilled engineers, we provide extensive and in-depth analysis tailored to specific customer requirements. Consultancy projects range from small quick calculations work to comprehensive plasma chemistry development. Typical types of consultancy work provided are:

- Calculations of specific electron-molecule cross sections including:
  - ⇒ Electron impact dissociation cross-sections producing specific products
  - ⇒ Electron impact ionisation dissociation producing specific products
- Heavy particle collision cross-section calculations for neutrals colliding
- Vibrational excitation cross-section calculation for diatomic molecules and ions
- Industrial plasma tool simulations
- Plasma process parameter optimisations
- Plasma chemistry designs
- Plasma etching and deposition calculations
- General multiphysics problems (CFD, etc..)



## Holistic Approach to Consultancy

Quantemol offers two levels of precision for cross section data calculation.

**Academic level** of precision: Convergence is established by running multiple calculations with varied parameters for a parent molecule and fragments.

Example: [“Calculated cross sections for electron collisions with  \$\text{NF}\_3\$ ,  \$\text{NF}\_2\$ , and  \$\text{NF}\$  with applications to remote plasma sources” James R Hamilton, Jonathan Tennyson, Shuo Huang and Mark J Kushner](#)



**Commercial level** of precision: Convergence is established by running multiple calculations with varied parameters for a parent molecule, while the fragments are calculated using the model from the parent molecule. This approach is suitable for plasma modelling input data. Derivative molecules/radicals/ions play a significant role in the plasma, but the cross section data is not readily available in literature.

- ⇒ Pros: essential for plasma modelling; is obtained faster; is consistent
- ⇒ Cons: some additional uncertainty is introduced in fragments; the calculation will be less precise for radicals and excited species

Quantemol has successfully undertaken several large consulting projects for industrial customers. A distinctive feature of our service is that we work with non-standard requests, using computational methods and literature research in order to achieve the results within deadlines. We always strive to deliver results of value to our customers and prioritise research tasks according to our client's development needs.

A formal completion report is delivered at the end of all work to provide our client with results such as raw data, graphs and videos ready for use and in the client's exclusive ownership. We work on the basis of complete confidentiality and understand the importance of protecting intellectual property.

**Appendix**  
**Quantemol N energy ranges and applied models**



Reaction type	formula	0-20 eV	20-50 eV	50-10000
Elastic cross-sections	$AB + e \rightarrow AB + e$	CC	SE	SCOP
Electronic excitation cross-sections	$AB + e \rightarrow AB^* + e$	CC	BEf	BEf
Super-Elastic cross-sections between excited states	$AB^* + e \rightarrow AB + e$	CC	0	0
Metastable Dissociation	$AB^* + e \rightarrow A + B + e$	CC	0	0
Electron impact dissociation	$AB + e \rightarrow A + B + e$	CC	0	0
Estimate dissociative electron attachment	$AB + e \rightarrow A(-) + B$	SE	0	0
Differential cross-sections		CC	SE	SCOP
Momentum transfer cross-sections		CC	SE	SCOP
Electron impact ionisation at all energies	$AB + e \rightarrow AB(+) + e + e$	BEB	BEB	BEB
Rotational excitation cross-sections	$AB(N'') + e \rightarrow AB(N') + e$	CC	0	0

CC (Close Coupling configuration interaction calculation)

SE (Static Exchange model)

SCOP (spherical complex optical potential)

BEB (Binary Encounter Born)

BEf scaling method

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