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Electron-molecule collision cross section calculations

2019 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.

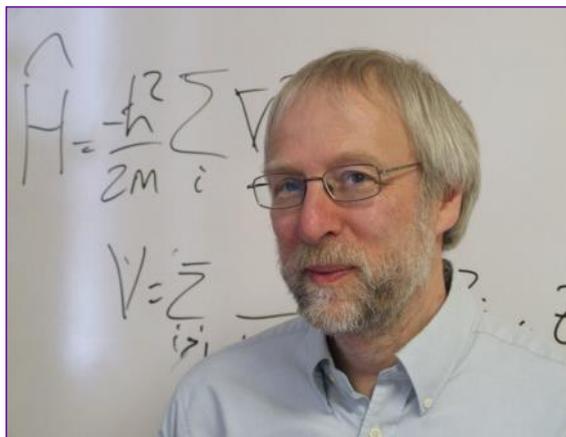
Quantemol-N uses an older version UK R-matrix codes to calculate electron and photon molecule scattering cross sections. It is Quantemol's first product equally appreciated by academia and industry.

Quantemol-EC is a new generation highly automated software to calculate electron-molecule scattering cross sections using a suit of new R-matrix codes alongside Molpro, a quantum chemistry program. **Coming in 2019!**

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

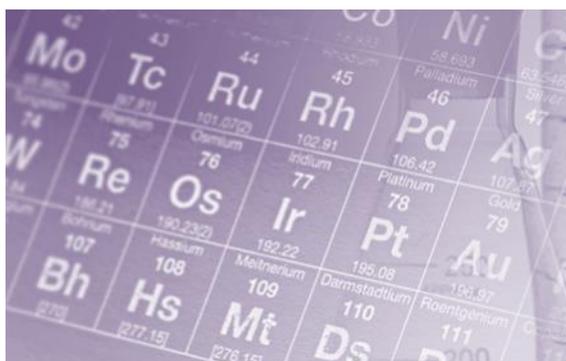
Quantemol-DB (QDB) is a leading sustainable database, representing the chemical and radiative transport properties of a very wide range of plasmas. The database contains chemistry data for plasma chemistry modelling with pre-assembled and validated chemistry sets, and is regularly updated with the most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



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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R-matrix codes have proven to be the leading and most reliable method for electron-molecule scattering calculations.

Quantemol has 15 years of experience in developing software based on R-matrix codes.

Quantemol-N, the Java-based interface, was launched in 2004 and enabled our customers in academia and industry to produce results with practical impact and well-rated publications

Taking the idea of providing user-friendly interfaces to our customers even further, we are happy to introduce the new generation of R-matrix - based software, Quantemol Electron Collisions (QEC). QEC is a new Python interface taking an advantage of world-renown Molpro package for molecular properties calculations.

Quantemol-EC offers additional features to Quantemol-N software:

⇒ V1 (April 2019):

- automatic generation of configurations
- automatic detection of symmetry
- automatic handling of degenerate states
- more accurate ionisation cross-section calculations
- 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

⇒ V2: dissociative recombination estimation and branching ratio estimates. (2020)

⇒ V3: effective core potentials (2020)

⇒ V3: vibrational excitations for ions (2021)

⇒ V4: vibrational excitations for neutrals (2021)

Based on integration with Molpro quantum chemistry package

What does Quantemol-EC 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
- Calculations for isotopes
- Integration with Molpro
-

** features not present in standard R-matrix codes

Quantemol-EC Products:

Quantemol-EC is MPI and openMP parallelisation compatible. QEC includes a large suite of molecular examples (currently ~40) and the user can get started immediately.

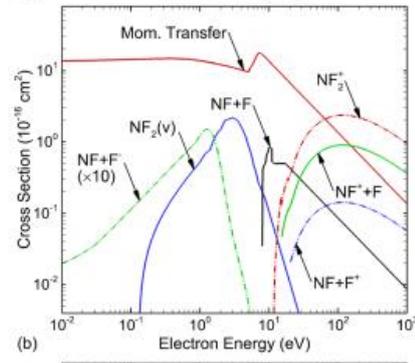
What range of problems can be tackled with Quantemol-EC?

- Closed shell molecules
- Open shell molecules, radicals
- Neutral and positively charged species
- Large molecules (up to 25 atoms, preferably lighter than Ar)

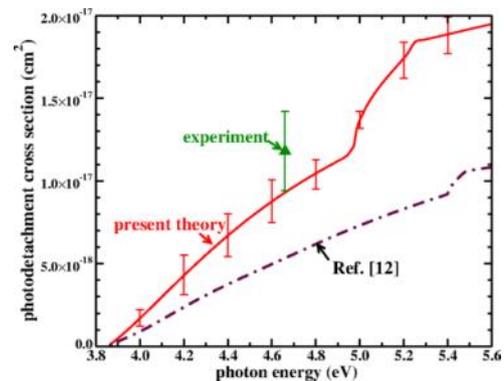
Comparison with experimental data

R-Matrix codes validation

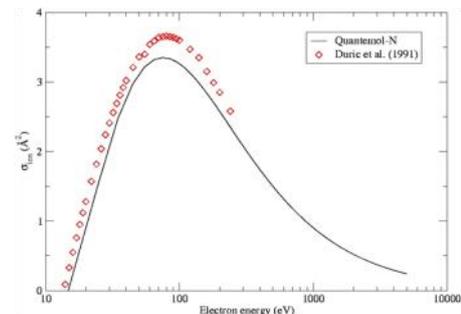
1. [Electron and positron scattering cross sections for propene](#), Singh et al, J. Appl. Phys., **124**, 034901 (2018)
2. [Study of electron impact inelastic scattering of chlorine molecule \(Cl₂\)](#), Yadav et al, J. Phys. B: At. Mol. Opt., **51**, 045201 (2018)
3. [An R-matrix study of electron-induced processes in BF₃ plasma](#), Gupta et al, Phys. Plasmas, **24**, 123511 (2017)
4. [QDB: a new database of plasma chemistries and reactions](#), Tennyson et al, Plasma Sources Sci. Technol., **26**, 055014 (2017)
5. [Calculated cross sections for electron collisions with NF₃, NF₂ and NF with applications to remote plasma sources](#), Hamilton et al, Plasma Sources Sci. Technol., **26**, 065010 (2017)
6. [Global model of an iodine gridded plasma thruster](#) P. Grondein, T. Lafleur, P. Chabert and A. Aanesland, Phys. Plasmas, **23**, 033514 (2016)
7. [Formation of CN⁻, C₃N⁻, and C₅N⁻ Molecules by Radiative Electron Attachment and their Destruction](#), Khamesian et al, Phys. Rev. Lett., **117**, 123001 (2016)
8. [Electron induced chemistry of thiophene](#) M. Vinodkumar, H. Desai, and P.C. Vinodkumar, RSC Advances, **5**, 24564 (2015)
9. [Total cross sections for O₂ and S₂ by electron impact](#), R. Naghma et al, Radiat. Phys. Chem., **97**, 6 (2014)
10. [Total Scattering Cross Sections for Ethylene by Electron Impact for Incident Electron Energies from 1 to 2000 eV](#) . R. Naghma and B. Antony, Int. J. Quantum Chem., **114**, 127 (2014)
11. [Electron induced chemistry of disilane](#). D. Gupta et al, RSC Advances, **4**, 9197 (2014)



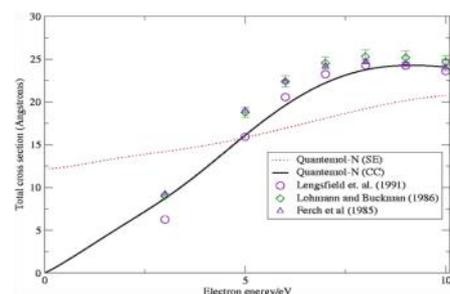
Cross sections for electron impact reactions of NF₂ using the *ab initio* molecular R-matrix method. Huang et al, 2017.



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



BEB ionisation cross-section of CH₄. Here the Quantemol-N data is compared with experimental data (Duric et al., red diamonds).



Total cross-sections of CH₄. 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 re- search	Single Workstation	PE	£6,000	£13,440	£3,000
	Research group	PE	£6,720	£18,000	£3,960
	Institution	PE	£9,720	£27,000	£5,400
Commercial research	Single Workstation	PE	£24,000	£48,000	£6,000
	Site	PE	£33,000	£66,000	£8,160

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.

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 5 workstations used by researchers in one group, can be installed on the cluster but the number of users should be limited to 5 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-EC software Linux x86, 64 bit operating system, 4 GB RAM (large calculations will require more RAM), 10 GB free disk space

* - all prices are quoted excluding VAT

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.

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-EC free of charge. Molecules tested:

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

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
 - ⇒ Branching ratios.
 - ⇒ Vibrational excitation cross-section calculation for diatomic molecules and ions
 - ⇒ Calculations for molecules with up to 50 atoms
- 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.

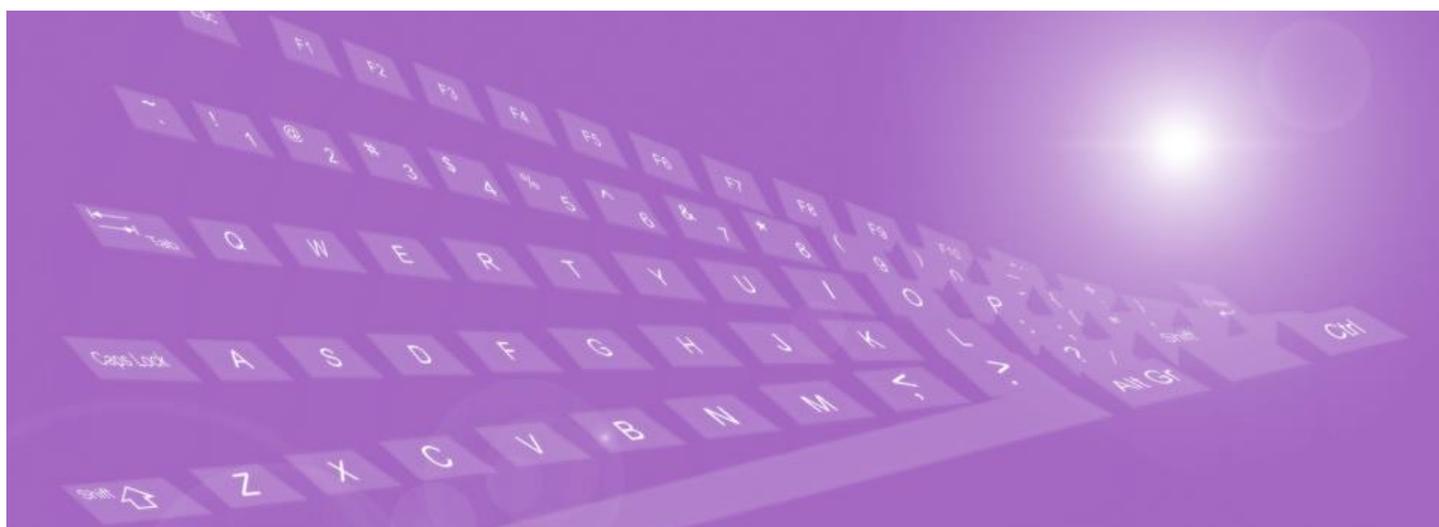
Academic level of precision: Convergence is established by running multiple calculations with varied parameters for a parent molecule and fragments.

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





Tailored and confidential projects

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 providing with the results (raw data, graphs, videos etc...) ready for use and your exclusive ownership. We work on the basis of complete confidentiality and understand the importance of protecting intellectual property.



Appendix
Quantemol EC energy ranges and applied models

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

CC (Close Coupling configuration interaction calculation)

SE (Static Exchange model)

SEP (Static Exchange plus Polarisation model)

SCOP (spherical complex optical potential)

BEB (Binary Encounter Born)

BEf scaling method

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