Quantemol

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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.

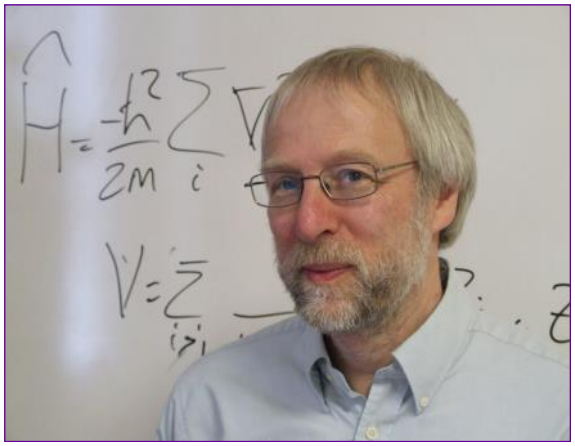
Quantemol-N uses an older version UK R-matrix codes to calculate electron and photon molecule scattering cross sections. It is Quantemol's first product equally appreciated by academia and industry.

Quantemol-EC is a new generation highly automated software to calculate electron-molecule scattering cross sections using a suit of new R-matrix codes. **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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QEC
electron collisions

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-known Molpro package for molecular properties calculations.

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

⇒ V1 (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 estimations and branching ratio estimations. (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.

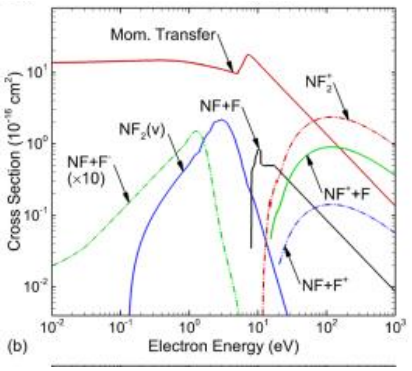
What range of problems can be tackled with Quantemol-EC?

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

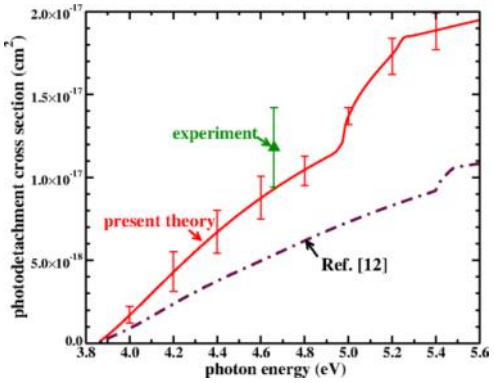
R-Matrix codes validation

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 (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 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 NF_3, NF_2 and 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 ofCN^-,C_3N^-, andC_5N^-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 O_2 and 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

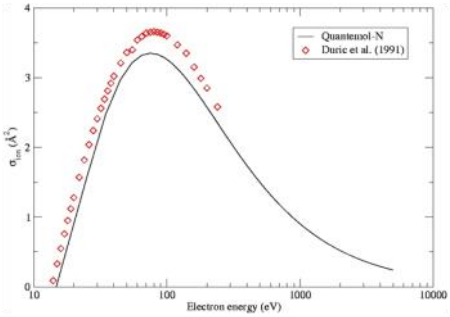
Comparison with experimental data



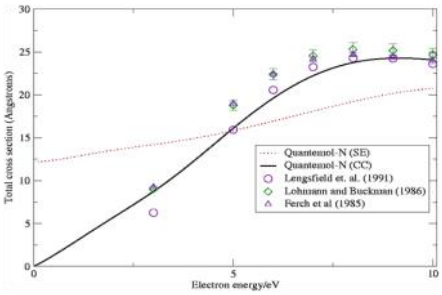
Cross sections for electron impact reactions of NF_2 using the *ab initio* molecular R-matrix method. Huang et al, 2017.



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



BEB ionisation cross-section of CH_4. Here the Quantemol-N data is compared with experimental data (Duric et.al., red diamonds).



Total cross-sections of CH_4. Here the Quantemol-N results (black & red lines) are shown with theory (Lengsfield 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	PE	¥ 930,000	¥ 2,083,200	¥ 465,000
	Research group	PE	¥ 1,041,600	¥ 2,790,000	¥ 613,800
	Institution	PE	¥ 1,506,600	¥ 4,185,000	¥ 837,000
Commercial research	Single Workstation	PE	¥ 3,720,000	¥ 7,440,000	¥ 930,000
	Site	PE	¥ 5,115,000	¥ 10,230,000	¥ 10,230,000

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:

$AlCl_3$	C_3	CF	CO	H_2O	I_2	SiF_2	C_4
BF_3	C_3H_4	CF_2	CO_2	H_2S	N_2	SiH_4	C_2
C_2	C_3N	CF_4	CO_2^+	HBr	NH_3	SiO	CF_3
C_2H_2	C_5F_8	CFCs	COS	HCHO	NO_2	SO_2	CF_4
$C_2H_2^+$	C_5HF_7	CH	CS	HCN	O_2	C_2F_2	CF
C_2H_4	C_6H_6	CH^+	F_2O	$HCONH_2$	O_3	C_2F_6	F_2
C_2H_5OH	CaF	CH_4	H_2	HCP	PH_3	C_3F_8	Benzene
	CaF^+	CN	H_2^+	HNC	SF_6	C_3	

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

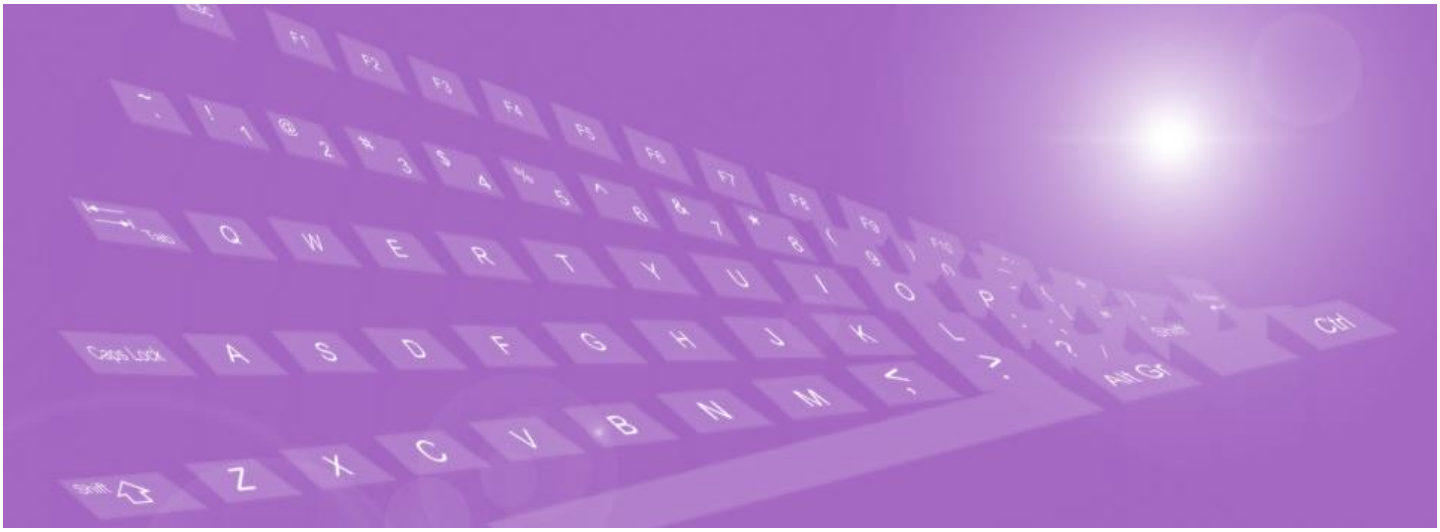
Quantemol offers two levels of precision for cross section data calculation.

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 NF_3, NF_2, and 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



QEC
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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
Elastic cross-sections	AB + e -> AB + e	CC	SE	SCOP
Electronic excitation cross-sections	AB + e -> AB* + e	CC	BEf	BEf
Super-Elastic cross-sections between excited states	AB* + e -> AB + e	CC	0	0
Metastable Dissociation	AB* + e -> A + B + e	CC	0	0
Electron impact dissociation	AB + e -> A + B + e	CC	0	0
Estimate dissociative electron attachment	AB + e -> 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 -> AB(+) + e + e	BEB	BEB	BEB
Rotational excitation cross-sections	AB(N") + e -> 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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