Quantemol

Electron-molecule collision cross section calculations

2022 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.

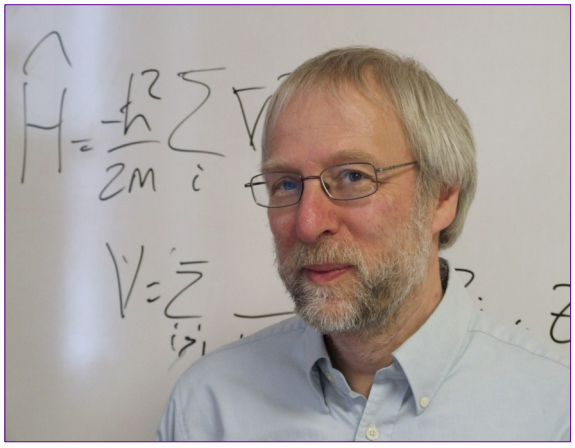
Quantemol-N uses older version UK R-matrix codes to calculate electron and photon molecule scattering cross sections. Quantemol's first product is equally appreciated by academia and industry.

Quantemol-EC is a new generation highly-automated software. It calculates electron-molecule scattering cross sections using a suit of new R-matrix codes alongside Molpro, a quantum chemistry program.

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 properties of a very wide range of plasmas. The database contains chemistry data for plasma chemistry modelling with pre-assembled and validated chemistry sets, Global Model and Boltzmann Solver 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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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.
We are now happy to introduce Quantemol Electron Collisions (QEC), our new generation of R-matrix based software. Even more user-friendly, QEC features a new Python interface and takes advantage of the world-renowned Molpro package for molecular properties calculations.

*"**The speed with which you provided me a trial of QEC is greatly appreciated. I am very impressed with the software and plan to purchase it very soon**."*

Dr Paul Adamson, Naval Research Laboratory, USA

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

V1.2 (February 2021):
- 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
- vibrational excitations for neutrals
- dissociative recombination for ions
- effective core potentials for ionisation cross sections

Request a free trial today:
http://www.quantemol.com/quantemol-ec/

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/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
- Vibrational excitation (non resonant)*
- Effective Core potentials for ionisation
- Approximation of electron scattering from* condensed state: turning off long range moments in the outer region of the calculation

* features not present in standard R-matrix codes

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)

What do I need to run Quantemol-EC?

- Molpro Quantum Chemistry software package installed (version 2012 or more recent).
- Linux operating system, preferably Ubuntu 18/ equivalent or a more recent.
- 16 or 32 GB of RAM, especially if you plan to work with large molecules.

QEC publications

Why SF_6 eats electrons: identifying high electrical strength molecules from their electron collision properties. Wang et al, J. Phys. B, 54, 025202 (2021)

The efficient calculation of electron impact ionization cross sections with effective core potentials V. Graves et al, J Chem Phys, 154,114104 (2021)

Theoretical study of the alkali hydride anions XH^-(X=Li, Na, and K) Zeid et al, Chem Phys, 538, 110825 (2020)

R-Matrix codes validation

Electron and positron scattering cross sections for propene. Singh et al,
J. Appl. Phys., 124, 034901 (2018)

Study of electron impact inelastic scattering of chlorine molecule (Cl_2)Yadav et al,
J. Phys. B: At. Mol. Opt., 51, 045201 (2018)

An R-matrix study of electron-induced processes in BF_3 plasma. Gupta et al,
Phys. Plasmas, 24, 123511 (2017)

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, 065010 (2017)

Global model of an iodine gridded plasma thruster. P. Grondein et Al, Phys. Plasmas, 23, 033514 (2016)

Formation of CN^-,C_3N^-, and C_5N^- Molecules by Radiative Electron Attachment and their Destruction, Khamesian et al, Phys. Rev. Lett., 117, 123001 (2016)

Electron induced chemistry of thiophene. M. Vinodkumar et al, RSC Advances, 5, 24564 (2015)

Total cross sections for O_2 and S_2 by electron impact.
R. Naghma et al, Radiat. Phys. Chem., 97, 6 (2014)

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)

Read about more about the software in *Quantemol Electron Collisions (QEC): An Enhanced Expert System for Performing Electron Molecule Collision Calculations Using the R-matrix Method*
Cooper, B.; Tudorovskaya, M.; Mohr, S.; O'Hare, A.; Hanicinec, M.; Dzarasova, A.; Gorfinkiel, J.; Benda, J.; Masin, Z.; Al-Refaie, A.; Knowles, P.; Tennyson, J.

Underlying Codes

UKRmol+ is developed by a group of academic researchers who are members of the UK-AMOR consortium and available for download here:

- Inner region codes including GTOLib
- Outer region codes

Read more about the code in the recent publication:

UKRmol+: A suite for modelling of electronic processes in molecules interacting with electrons, positrons and photons using the R-matrix method. Z. Masin, J. Benda, J. Gorfinkiel, A. Harvey, J. Tennyson, Computer Phys. Com. 249, 107092 (2019)

Vibrational Excitation/Dissociative recombination

The method implemented in QEC was developed by Prof. Kokoouline and his co-workers and described in the publications below:

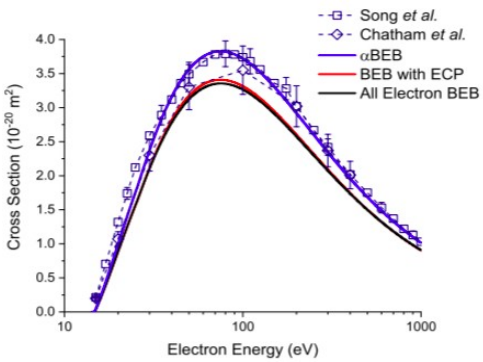
Dissociative Recombination of Highly Symmetric Polyatomic Ions. N. Douguet, A.Orel, C Greene, and V. Kokoouline, Phys. Rev. Lett. 108, 023202 (2012)

Theoretical study of dissociative recombination and vibrational excitation of the BF_2^+ ion by an electron impact. V. Kokoouline, M. Ayouz, J. Z. Mezei, K. Hassouni and I. Schneider,
Plasma Sources Science and Technology, V.27, 11 (2018)

Dissociative recombination of $CH_2NH_2^+$: a crucial link with interstellar methanimine and Titan ammonia. C H Yuen, M A Ayouz, N Balucani, C Ceccarelli, I F Schneider, V Kokoouline, RAS, V. 484, 1, (2019)

Dissociative electron recombination of NH_2CHOH+ and implications for interstellar formamide abundance. M A Ayouz, C H Yuen, N Balucani, C Ceccarelli, I F Schneider, V Kokoouline, RAS, V. 490, 1, (2019)

Comparison with experimental data



Total cross-sections of CH_4. Here the Quantemol-EC results (black & red lines) are shown with experiment (Chatham et al, diamonds, Song et al., squares). Read more in V. Graves et al, J Chem Phys, 154 (2021)

Price list *

Use Case	Type of Licence	Licence Term		
		1 year	3 years	Annual support
Non-commercial research	Single Workstation	£6,300	£14,000	£3,100
	Research group	£7,000	£18,800	£4,100
	Institution	£10,200	£28,200	£5,600
Commercial research	Single Workstation	£25,100	£50,200	£6,300
	Site	£34,500	£69,000	£8,500

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 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-EC software Linux x86 (Ubuntu 18/equiv or more recent), 64 bit operating system, 16 GB RAM (large calculations will require more RAM), 10 GB free disk space.

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

* - all prices are quoted excluding VAT

Molpro

Please be aware that QEC requires Molpro software package. You can order it directly from Molpro web-site or via Quantemol, who is an official reseller of the Molpro Quantum Chemistry package.

The prices range from 250 Euros to a couple of thousand Euros for a licence and depend on the type of licence. Prices for academic institutions can be found here.

You can request a trail licence for Molpro. In order to do that you need to create an account on the Molpro website:

- Register your name, address, and email address. Then submit a request for a trial licence on the account page (or directly) and wait.
- You will be informed where to download the code from, and on first access you will be required to sign a licence agreement and to give details of the machine on which you wish to run the software.
- You will then be provided with the licence token to enable the software for your machine.

Molpro is a comprehensive system of ab initio programs for advanced molecular electronic structure calculations, designed and maintained by H.J. Werner and P.J. Knowles, and containing contributions from many other authors. It comprises efficient and well parallelized programs for standard computational chemistry applications, such as DFT with a large choice of functionals, as well as state-of-the art high-level coupled-cluster and multi-reference wave function methods.

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..)

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.

Training

Quantemol team offers bespoke training courses for individuals or research groups. Our experts will prepare material to suit your needs and knowledge level. We can deliver it online, or with on site visit or if you come to our offices.

Training costs The prices quoted are estimates based on generic materials and an online format. The cost will increase if you require a very specific material to be developed. An in person training format will incur an additional fee to cover our expert's travel costs.

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 H uang 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

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.

Group Size	Duration		
	1 day	2 days	3 days
1 to 1 tutorial	£420	£780	£1000
Small group (up to 5 ppl)	£460	£860	£1100
Large group (up to 15 ppl)	£500	£940	£1300

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 → AB + e	CC/SEP	SE	SCOP
Electronic excitation cross-sections	AB + e → AB* + e	CC/SEP	BEf	BEf
Super-Elastic cross-sections between excited states	AB* + e → AB + e	CC	-	-
Metastable Dissociation	AB* + e → A + B + e	CC	-	-
Electron impact dissociation	AB + e → A + B + e	CC	-	-
Estimate dissociative electron attachment	AB + e → 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 → AB(+) + e + e	BEB	BEB	BEB
Rotational excitation cross-sections	AB(N") + e → 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) – currently not available

BEB (Binary Encounter Born)

BEf scaling method

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