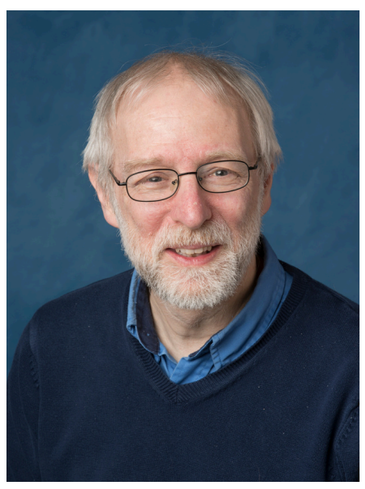
Quantemol Database (QDB)

'Your Trusted Plasma Chemistry Data'

Company Profile

Quantemol was founded in 2004 as a spin-out from the University College London (UCL) Physics and Astronomy department by Prof. Jonathan Tennyson FRS and Dr Daniel Brown. Quantemol is a leader in the plasma chemistry market, specialising in calculating and estimating essential data for electron-molecule scattering. This unique capability is fundamental to understanding and predicting plasma behaviour.

Dr. D. Brown



Prof. J. Tennyson

Products

QDB database

Access a comprehensive database of plasma chemistry data.

QEC electron collisions

Simulate electron-molecule scattering to obtain cross sections.

QVT virtual tool

Model low temperature plasmas in two dimensions.

QCS consultancy services

Access our in-house expertise and modelling tools to gain new insights in your research.

Free Trial

Contact Us:
Info@quantemol.com
www.quantemoldb.com

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QDB database

QDB is a **leading sustainable database** for plasma chemistry. Offering pre-assembled chemistry sets, regularly updated data, and integration with plasma modelling software.

Why Choose QDB?

All of Your Data in One Place

QDB supports streamlined comparisons of multiple data sets, such as: electron scattering, heavy particle collisions and surface chemistry.

Use Your Data with Confidence

QDB uses trustworthy, validated data and chemistry sets that are monitored regularly, so you can be confident in your results.

Save Precious Time

QDB's easy-to-use tools will help you to assemble the chemistry set you need in minutes. It intuitively exports data in flexible formats & avoids human error.

Connect with Our Team

We offer ongoing data updates and support - so you don't have to struggle alone!

Advantages:

- Estimations of branching ratios for dissociative ionisation
- Order and calculate your own custom cross sections
- Machine Learning estimations for heavy particle collisions
- Delivery to your plasma modelling software via an API

Read our most recent publication here

Details a major QDB update, describes its expanded plasma modelling data, structure, web interface, API, and use cases that demonstrate data validation through application.

Reference: Jonathan Tennyson et al 2022 Plasma Sources Sci. Technol. 31 095020

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Quantemol Global Model

Included with your Gold or Platinum QDB membership, the Quantemol Global Model (QGM) is a powerful tool that calculates reactor-averaged particle densities and electron temperature. To perform these calculations, it uses your defined plasma process conditions, such as pressure, power, gas flow rates, and reactor size. The QGM is effective for quick assessments and trend analysis in plasma behaviour. You can test the online free version on pre assembled chemistry sets, contact the Quantemol team to find out more!

Key Features:

- Zero-dimensional plasma model
- Calculates volume-averaged species densities and electron temperature
- Based on user-defined process conditions
- Features error checking for the input
- Includes a reduction mechanism and species ranking
- Fast simulations due to solving Ordinary Differential Equations (ODEs) instead of Partial Differential Equations (PDEs)
- Does not require detailed reactor geometry or spatially-resolved boundary conditions

‘Trusted by Scientists’

Read our Publications here

Membership Options

Free Standard Membership

- Search for reactions/species
- Graphs for cross-section data
- Access to global models and Boltzmann solver
- Download up to 20 datasets/month

Gold Membership

- Access to Quantemol-DB GM app/software
- Flexible downloads compatible with COMSOL, STAR CCM+, CHEMKIN, HPEM, VizGlow
- Unlimited download of individual reactions and up to 20 preassembled chemistry sets
- Dedicated support from our team of Scientists

Platinum Membership

- All Gold benefits
- Cross-section calculations for up to 6 molecules/ions annually with detailed reports
- Dedicated support from our team of Scientists

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Machine Learning

Quantemol applies machine learning to enhance its QDB platform by providing tools to estimate missing data (reaction rates, fragmentation patterns) and to aid in the construction of comprehensive plasma chemistry sets, thereby accelerating research and modelling efforts in plasma science.

On over 1,000 test reactions, 87% of predicted rate coefficient values had an error of less than one order of magnitude

Features:

Estimator for Rate Coefficients:

Quickly fill in missing data for your plasma simulations. This tool rapidly estimates reaction rate coefficients for heavy particle collisions, helping you build more complete chemistry sets for your research. This feature is available to all members.

Estimator for Mass Spectra & Partial Cross Sections:

Gain deeper insights into electron impact ionisation processes. This method predicts mass spectra to help estimate previously unavailable partial ionisation cross sections, enriching your datasets for more accurate plasma modelling.

Diffusion Coefficient Estimators:

Obtain crucial transport data more efficiently with machine learning-based estimations for binary diffusion coefficients. Allowing faster parameterisation of your plasma models, particularly when experimental data for diffusion coefficients are scarce or difficult to obtain.

“The money we saved pays for the subscription to QDB about 100 times over. We are quite satisfied!”

-Industrial user

“We are fully satisfied with your software and support. We are convinced it is absolutely beneficial to our business.”

-Another Industrial User

Free Trial »

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