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Quantemol-N calculation of electron molecule cross sections and related parameters WILL BRIGG, ADAM WILLIAMS, DEREK MONAHAN, JONATHAN TENNYSON, University College London — Quantemol-N was originally developed as a wrapper for the UK Molecular R-Matrix codes, significantly accelarating data production rates for electron molecule collision calculations. Since its conception Quantemol-N has continuously been developed in the direction of the plasma industry, with many features being added to produce extended cross sections sets and related parameters. Recent additions include the calculation of differential cross sections, which provide momentum transfer and rotational excitation cross sections. These are used in turn to provide transport coefficients for verification of swarm calculations. Electron collisions with water have been used as a test bed. The code has also been generalised to calculate cross sections for aligned molecules, for example ones trapped on surfaces.

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