R-matrix calculations of electron-molecule collisions at low and intermediate energies

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The R-matrix method is now well-established as a reliable and flexible procedure for treating electron collision problems. In particular the UK molecular R-matrix codes have been applied to an increasing variety of electron molecule collision problems. Recent calculations on low-energy electron collisions with water have found outstandingly good agreement with published measurements of differential and momentum transfer cross sections. However the calculated elastic cross sections differ significantly from those inferred from experiment, suggesting that the published data still does not correctly measure the strong forward peak for this process. New calculations have been performed on the 13-atom organic ring molecule tetrahydrofuran with special attention paid to the low-lying resonances in this system: these are found to be numerous, narrow and Feshback in contrast to the standard interpretation of experiment in terms of a few, rather broad, (high energy) shape resonances. No evidence for such shape resonances has been found. A new molecular R-matrix with pseudo-states (MRMPS) procedure has been developed which allows the correct ab initio treatment of electron collision processes, including ionisation, above the molecular ionisation threshold. Initial studies on benchmark systems suggest that this method works well.