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R-matrix calculations of electron molecule collision data for plasma models

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Models of low-pressure plasma require electron collision cross sections for many processes. For transient molecular species, almost none of these data are available from laboratory measurements so theory has to be the chosen means of providing the necessary information. The R-matrix method is a well-established fully quantal procedure for computing low-energy electron-collision cross sections. The R-matrix calculations using the UK Molecular R-matrix codes (UKRMol)[1], which are run by the Quantemol-N expert system, are being employed to provide a wide range of collision cross sections. These are augmented by use of suitable high-energy approximations, such as BEB for ionisation, and a novel procedure to give branching ratios for the fragmentation pattern following electron impact ionisation and electron impact dissociation. Examples, such as recently generated complete cross section sets for the molecules NF, NFand NF [2], will be given at the meeting. [1] J.M. Carr et al, (2016) Euro J. Phys. D, , 58. [2] J.R. HAMILTON, J. TENNYSON, S.HUANG AND M.J. KUSHNER (2016) IN PREPARATION FOR SUBMISSION TO PLASMA SCI. SOURCES TECH.