

Abstract Submitted
for the DAMOP14 Meeting of
The American Physical Society

Ab initio electron collisions with N_2^+ : Application to dissociative recombination¹ DUNCAN LITTLE, JONATHAN TENNYSON, Univ Coll London — Extensive ab initio scattering calculations have been performed using the well established R-matrix method to comprehensively map out the electronic structure of N_2 above and below the ionisation threshold. Advances in computational efficiency meant it was possible to use a fine grid of internuclear separations to characterise the many avoided crossings and complex mixing of valence and Rydberg type states brought about the proximity of the ground and first excited state. It was shown that with this approach, a scattering calculation outperforms a standard multireference configuration interaction with respect to the calculation of Rydberg states. This is the most comprehensive study of the electronic structure of N_2 to date and sets a benchmark for future calculations of Rydberg–valence type states. The R-matrix method provides a self-consistent means to find all of the parameters needed to find a dissociative recombination (DR) cross-section. These parameters have now been used to calculate a cross-section for the DR of N_2^+ using multi-channel quantum defect theory including so called “core-excited” Rydberg states. The calculated cross-section is completely ab initio and agrees well with experiment at low electron energies.

¹Funded by Themisys Ltd. and UCL

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Date submitted: 01 Apr 2014

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