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Low energy electron scattering from \textit{N}_2\textit{H} molecules

BRENDAN M. MCLAUGHLIN, School of Mathematics and Physics, QUB, ROBERT C. FORREY, Department of Physics, Pennsylvania State University at Berks — Electron collisions with the \textit{N}_2\textit{H} radical are an important constituent of understanding electron detachment in low energy \textit{H}^− + \textit{N}_2 collisions. Potential energy curves for both the neutral \textit{N}_2\textit{H} and anion \textit{N}_2\textit{H}^− molecules are calculated in \textit{C}_s symmetry for perpendicular, colinear and bent geometry using valence-CI and CASSCF approximations. Low energy electron scattering from the \textit{N}_2\textit{H} molecule are carried out using the R-matrix approach to determine the elastic scattering cross-section as a function of the colliding electron energy. Resonance energies and the autoionization linewidth (Γ) found in the elastic scattering cross sections are determined as a function of the stretching of the \textit{N}_2 - \textit{H} bond length, where the \textit{N}_2 molecule is fixed at its equilibrium geometry. A complex potential is then constructed from the resonance parameters and used in the heavy particle dynamical calculations to determine the low energy electron detachment cross sections and rates. Results for isotopic replacement of \textit{H}^− by \textit{D}^− have also been obtained for this cold molecular complex. Further details will be presented at the meeting.

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