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Dissociative Electron Attachment to HCCCN SLIM CHOUROU, ANN OREL, UC Davis — Experiments on dissociative electron attachment (DEA) to HCCCN below 12 eV have led predominantly to formation of $CCCN^-$, CN^-, HCC^- and CC^- negative ions. It has been concluded that these fragments result mainly from the decay of π^*-shape resonant state upon electron attachment that involves distortion of the symmetry of the linear neutral molecule. In order to study the dynamics of dissociation in these channels, we subdivided the molecule into three fragments (H), (CC) and (CN); therefore, four internal coordinates consisting in the distances between the center of masses of (H) and (CC) fragments, (CC) and (CN) fragments, the (H)-(CC) angle and the (CC)-(CN) angle are included in the calculation. We have performed electron scattering calculations using Complex Kohn Variational method to determine the resonance energies and autoionization width for various geometries of the system and construct the complex potential energy surfaces relevant to the metastable $HCCCN^{-*}$ ion. The nuclear dynamics is treated using the Multiconfiguration Time-Dependent Hartree (MCTDH) formalism and the flux of the propagating wavepacket is used to compute the DEA cross section relevant to 4 channels in question. The results are then compared to the available findings.

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