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Dissociative Electron Attachment to HCCH, HCN/HNC and HCCCN SLIM CHOUROU, ANN OREL, UC Davis — Previous work on the dissociative electron attachment (DEA) to acetylene, hydrogen cyanide and its isomer and cyano-acetylene shows that the dissociation process for these systems is inherently polyatomic. We present a comparative summary of the study of these species believed to play a role in the chemistry of interstellar media and to present key elements in the prebiotic synthesis in early Earth. Our treatment was carried out in the low energy range (0-6 eV for HCCH and HCN/HNC and 0-12 eV for HCCCN) using a suitable coordinate system that allows taking into account distortions in the symmetry of the polyatomic target molecule. We have performed electron scattering calculations using Complex Kohn Variational method to determine the low-lying shape resonance energies and autoionization width for various geometries of these molecules. The resonance parameters are then used to construct the complex potential energy surfaces relevant to the metastable negative ion formed in each case. The nuclear dynamics is performed using the Multiconfiguration Time-Dependent Hartree (MCTDH) approach and the flux of the propagating wavepacket is used to compute the DEA cross section associated with the dissociation channels addressed for each system. The computation results are then compared to the available experimental results.

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