Abstract Submitted
for the DAMOP10 Meeting of
The American Physical Society

Dissociative Electron Attachment to Polyatomics[1] 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 may exhibit intrinsically polyatomic effects. 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. The Complex Kohn Variational Method was used to determine the resonance energies and the autoionization widths; thus allowing the construction of the multidimensional complex potential energy surfaces of the temporary polyatomic anion. The dissociation dynamics calculation is then performed using the Multi-Configuration Time-Dependent Hartree approach to compute the DEA cross sections.

[1]NSF Grant PHY-05-55401

Slim Chourou
UC Davis

Date submitted: 21 Jan 2010 Electronic form version 1.4