Abstract Submitted
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Dissociative Electron Attachment to Polyatomic Systems[1] S.T. CHOUROU, A.E. OREL, UC Davis — We have performed a multi-dimensional computational treatment of the dissociative electron attachment (DEA) dynamics of 3 polyatomic systems; HCCH, HCN/HNC and HCCCCN to investigate predicted inherent polyatomic effects. We have considered the following reaction channels: C_2H_2 ($X^1\Sigma_g^+$, ν)+ $e^-(E) \rightarrow (C_2H_2)^{-*}$ ($^2\Pi_g$) $\rightarrow C_2H^-(^1\Sigma^+,\nu') + H(^2S)$, HCN/HNC $(X^1\Sigma^+,\nu) + e^-(E) \rightarrow (HCN/HNC)^{-*}$ ($^2\Pi_g$) $\rightarrow CN^-(^1\Sigma,\nu') + H$ (^2S) and HCCCN

$$(X^1\Sigma^+,\ \nu)+\ e^-(E)\ \rightarrow\ HCCCN^{-*}\ \rightarrow \begin{cases} CCCN^-(^2\Sigma^+,\nu_I'^-)+H(^2S)\text{: (I)};\\ CN^-(^1\Sigma^+,\nu_{II}'^-)+HCC(^2\Sigma^+,\nu_{II}')\text{: (II)};\\ HCC^-(^1\Sigma^+,\nu_{III}'^-)+CN(^2\Sigma^+,\nu_{III}')\text{: (III)};\\ CC^-(^2\Sigma^+,\nu_{IV}'^-)+HCN(^1\Sigma^+,\nu_{IV}')\text{: (IV)}; \end{cases}.$$

We carried out electron scattering calculations using the Complex Kohn Variational Method with respect to a suitable internal coordinate system to obtain the complex resonant energy surfaces. We use this as input to a dynamics calculation using the Multiconfiguration Time-Dependant Hartree approach. We then compare our DEA cross sections and branching ratios to available experimental results.

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