

Abstract Submitted
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Electron induced bond-breaking at low energies in HCOOH and Glycine: The role of very short-lived σ^* anion states¹ ILYA FABRIKANT, PAUL BURROW, GORDON GALLUP, University of Nebraska-Lincoln — Cross sections for dissociative electron attachment (DEA) to formic acid and glycine are calculated by the resonant R-matrix theory. A model with one effective reaction coordinate close to the O-H stretch motion is employed. The choice of the anion R-matrix pole and the surface amplitude as functions of the reaction coordinate for formic acid are based on scattering phase shift calculations using the finite element discrete model. For glycine the input parameters are adjusted to reproduce experimental data. The results show that the mechanism of DEA in these molecules is similar to that for the hydrogen halides and involves electron capture into a $\sigma^*(\text{OH})$ orbital, so that no σ^*/π^* coupling is required. Nonlocal effects play an important role for both molecules. In particular, pronounced steps and cusps are seen at the vibrational excitation thresholds. A sharp threshold peak in glycine is interpreted as a vibrational Feshbach resonance.

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