Abstract Submitted
for the DAMOP06 Meeting of
The American Physical Society

Electron Collisions with Formic Acid[1] THOMAS RESCIGNO, LBNL, CYNTHIA TREVISAN, ANN OREL, UC Davis — Low-energy electrons (<2 eV) can vibrationally excite as well as fragment gas phase formic acid (HCOOH) molecules through resonant collision processes. Recent experiments have shown that the principal reaction products of dissociative electron attachment are formate ions ($HCOO^-$) and hydrogen atoms. Using first-principles electron scattering calculations, we have identified the responsible negative ion state as a transient π^* anion. Symmetry considerations dictate that the associated dissociation dynamics are intrinsically polyatomic: the anion must first deform to non-planer geometries before dissociating on a second anion surface that can be reached through a conical intersection. The calculations we have performed that support these conclusions will be described. We will also present differential and integrated elastic scattering cross sections and compare our results with recent experiment.

[1]Work performed under auspices of USDOE by LBNL and supported by DOE OBES Division of Chemical Sciences.

Thomas Rescigno
LBNL

Date submitted: 25 Jan 2006 Electronic form version 1.4