

A THEORETICAL CHARACTERIZATION OF ELECTRONIC STATES OF CH₂IOO AND CH₂OO RADICALS RELEVANT TO THE NEAR IR REGION

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Criegee intermediates (R₁R₂COO or CIs) arise from ozonolysis of biogenic and anthropogenic alkenes, which is an important process in the atmosphere. Recent breakthroughs in producing them in the gas phase have resulted in a flurry of experimental and theoretical studies. Producing the simplest CI (CH₂OO) in the lab via photolysis of CH₂I₂ in the presence of O₂ yields both CH₂OO and CH₂IOO with pressure dependent branching.

As discussed in the preceding talk, both species might be expected to have electronic transitions in the near IR (NIR). Here we discuss electronic structure calculations used to characterize the electronic states of both systems in the relevant energy range. Using explicitly-correlated multireference configuration interaction (MRCI-F12) and coupled-cluster (UCCSD(T)-F12b) calculations we were first able to exclude CH₂OO as the carrier of the observed NIR spectrum. Next, by computing frequencies and relaxed full torsional scans for the \tilde{A} and \tilde{X} states, we were able to aid in analysis and assignment of the NIR spectrum attributed to CH₂IOO.