Abstract Submitted
for the DAMOP11 Meeting of
The American Physical Society

Threshold photodetachment of $HOCO^-$: a theoretical study[1] S. MIYABE, D.J. HAXTON, K.V. LAWLER, A.E. LAWLER, C.W. MCCURDY, T.N. RESCIGNO — The HOCO radical is an important intermediate in combustion. Information about its electronic structure has been obtained from studies of the photodetachment of $HOCO^-$. We present the results of a theoretical study of $HOCO^-$ photodetachment, with a view toward understanding the origin of two peaks observed in the photoelectron kinetic energy spectrum very close to threshold. Fixed-nuclei variational electron-HOCO scattering calculations are used to compute photodetachment cross sections and laboratory-frame photoelectron angular distributions. We show that the observed peaks cannot, as previously assumed, be narrow shape resonances and argue that they can be attributed to vibrational Feshbach resonances of dipole-bound trans-$HOCO^-$.

[1]LBNL, UC Davis. Work performed under auspices of US DOE and supported by OBES, Division of Chemical Sciences.

Thomas Rescigno

Date submitted: 03 Feb 2011 Electronic form version 1.4