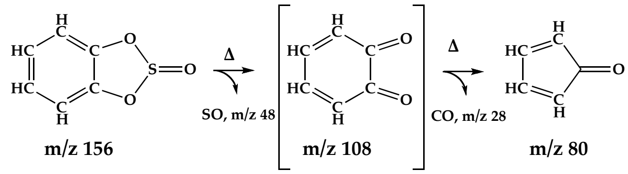
POLARIZED MATRIX INFRARED SPECTRA OF CYCLOPENTADIENONE

THOMAS K. ORMOND, ADAM M. SCHEER, G. BARNEY ELLISON, *Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO 80309-0215*; MARK R. NIMLOS, *Center for Renewable Chemical, Technologies & Materials, NREL, 1617 Cole Blvd., Golden, CO 80401*; JOHN W. DAILY, *Department of Mechanical Engineering, University of Colorado, Boulder, CO 80309-0427*; JOHN F. STANTON, *Institute for Theoretical Chemistry, Department of Chemistry, University of Texas, Austin, TX 78712*.

We are developing a resistively-heated SiC μtubular reactor with a 100 μsec residence time to study the thermal cracking of biomass monomers. The decomposition products are identified by two independent techniques: 118.2 nm VUV photoionization mass spectrometry (PIMS) and matrix infrared spectroscopy. Many lignins thermally crack[a] to produce cyclopentadienone (m/z 80) and its derivatives. Subsequent decomposition of these cyclopentadienones results in formation of substituted acetylenes which are known precursors to polycyclic aromatic hydrocarbons and soot. Due to its anitaromatic character, cyclopentadienone is highly reactive and presents an interesting spectroscopic system. Pyrolysis of *o*-phenylene sulfite (m/z 156) is a convenient precursor for cyclopentadienone. In this work we report the polarized matrix infrared absorption spectra of cyclopentadienone and d_4-cyclopentadienone. The PIMS results corroborate the thermal decomposition steps of phenylene sulfite. *Ab initio* coupled-cluster anharmonic force field calculations are used to guide the vibrational assignments.



[a] A. M. Scheer, C. Murkarakate, D. J. Robichaud, M. R. Nimlos, and G. B. Ellison *J. Phys. Chem. A* **115**, 13381 (2011)