ROTATIONAL SPECTROSCOPY OF PYRIDYL RADICALS

KELLY S. MEYER, SOMMER L. JOHANSEN, J. H. WESTERFIELD, *Department of Chemistry, The University of California, Davis, CA, USA*; ANAHUT SANDHU, *Department of Chemistry, University of California, Davis, Davis, CA, United States*; JASMINE KEANE, KYLE N. CRABTREE, *Department of Chemistry, The University of California, Davis, CA, USA*.

Radical chemistry is thought to play a role in the formation of complex molecules in space, including nitrogen heterocycles and prebiotic species. Radical derivatives of pyridine, one of the simplest nitrogen heterocycles, have been suggested as key intermediates in barrierless pathways to the formation of nitrogen-containing polycyclic molecules. We have calculated the equilibrium geometries of the *ortho*-, *meta*-, and *para*-pyridyl radicals at the CCSD(T)/cc-pwCVTZ level of theory, along with nitrogen quadrupole and hyperfine interaction terms. Spin-rotation terms were calculated at CCSD(T)/cc-pwCVDZ. Vibrational corrections to the rotational constants have also been evaluated at the CCSD(T)/cc-pwCVDZ level using second-order vibrational perturbation theory. We will discuss the results of these calculations as well as efforts to obtain the rotational spectra of these radicals using Fourier transform microwave spectroscopy.