

ROTATIONAL SPECTROSCOPY OF THE PYRROLYL RADICAL FROM 5 TO 40 GHz

SOMMER L. JOHANSEN, KELLY S. MEYER, J. H. WESTERFIELD, ANNA C WANNENMACHER,
ERIC NGUYEN, KYLE N. CRABTREE, *Department of Chemistry, The University of California, Davis,*
CA, USA.

A wide variety of nitrogen-containing heterocycles have been detected on meteorites with non-terrestrial isotopic abundances, indicative of an interstellar origin. However, no N-heterocycles have been detected in space and their formation pathways are unclear. Experimental work has shown that N-heterocycles can likely form through barrierless radical-neutral gas-phase reactions, which are feasible in the low temperature environments of cold molecular clouds and the outer regions of protoplanetary disks. Astronomical searches for potential precursors and depletion products are critical to determining if such mechanisms play a role in N-heterocycle formation. Here, calculated CCSD(T)/pwCVTZ equilibrium geometries and progress towards measuring and assigning the 5 – 40 GHz rotational spectra of three pyrrolyl isomers (C_4H_4N) will be discussed. Pyrrolyl is both a photodissociation product of the N-heterocycle pyrrole (C_4H_5N) and a potential precursor to larger N-heterocycles. This work will enable astronomical searches, spectroscopy in higher frequency bands, and kinetics and dynamics studies.