USING HYPERFINE STRUCTURE TO QUANTIFY THE EFFECTS OF SUBSTITUTION IN 2-, 3-, AND 4-PICOLYLAMINE

LINDSEY M McDIVITT, TIMOTHY J McMAHON, JOSIAH R BAILEY, CALEB B SHIERY, RYAN G BIRD, Chemistry, University of Pittsburgh Johnstown, Johnstown, PA, USA.

Last year we presented preliminary results on three methylamine substituted pyridines, 2-, 3-, and 4-picolylamine. After helpful feedback, the microwave spectra of all three molecules were recollected over the frequency range of 7-18 GHz using by zero-fitting the free induction decay. Each molecule showed a distinctive quadrupole splitting, which is representative of the local electronic environment around the two different ¹⁴N nuclei, with the pyridine nitrogen being particularly sensitive to the pi-electron distribution within the ring. An extended Townes and Dailey analysis was used to determine the lone pair density around each nitrogen and compared to that of benzylamine and pyridine. Results of this analysis and how it explains the configuration of the methylamine group with respect to the pyridine ring in each of the picolylamines will be discussed.