DETERMINATION OF SUBSTITUTION EFFECTS ON THE STRUCTURES OF 2-, 3-, AND 4-PICOLYLAMINE USING FOURIER TRANSFORM MICROWAVE SPECTROSCOPY

RYAN G BIRD, CALEB B SHIERY, KAYLEE X SHOOK, *Chemistry, University of Pittsburgh Johnstown, Johnstown, PA, USA*.

This is a continued discussion regarding the substitution effectcts on the three-dimensional shape and electron distribution of three methylamine substituted pyridines, 2-, 3-, and 4-picolylamine. The microwave spectra of all three molecules were collected over the frequency range of 4-18 GHz. In addition, the ^{13}C and ^{15}N isotopologues, along with the deuterated amine groups, were collected for each molecule in natural abundance. From these spectra, exact structures were determined which allowed for accurate rotation of the quadruple constants from the molecular frame into an internal axis. Next, an extended Townes and Dailey analysis was used to determine the lone pair density around each nitrogen and then compared to those of benzylamine and pyridine. Results of this analysis and how it explains the configuration of the methylamine group in each of the picolylamines will be discussed.