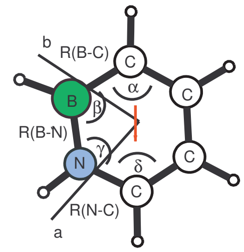
MICROWAVE SPECTRUM, STRUCTURAL PARAMETERS AND QUADRUPOLE COUPLING FOR AZABORINE AND 1-ETHYL-AZABORINE [a]

ADAM DALY, STEPHEN G. KUKOLICH, *Department of Chemistry and Biochemistry, The University of Arizona, Tucson, Arizona 85721.*; CHAKREE TANJAROON, *Department of Chemistry and Physics, Arkansas State University, Jonesboro, AR 72467*; ADAM J. V. MARWITZ and SHIH-YUAN LIU, *Department of Chemistry, University of Oregon, Eugene, OR 97403*.



The first microwave spectra for the unusual and elusive aromatic molecules, 1,2-dihydro-1,2-azaborine (azaborine) and 1-ethyl-azaborine have been measured, in the 7-18 GHz range, providing accurate rotational constants, nitrogen and boron quadrupole coupling strengths, important bond lengths and other structural parameters. Azaborine (BNC_4H_6)is an aromatic, B-N substituted analog of benzene, the quintessential aromatic molecule. The experimental bond lengths determined for azaborine are: R(B-N) = 1.45(3) Å, R(B-C) = 1.51(1) Å, and R(N-C) = 1.37(3) Å. Accurate measurements of ^{14}N, ^{11}B, and ^{10}B nuclear quadrupole coupling were obtained. The inertial defect Δ = 0.02 amu Å^2 indicating a planar structure. A Townes-Dailey population analysis of the B and N quadrupole coupling constants provided the valence p-electron occupancy

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