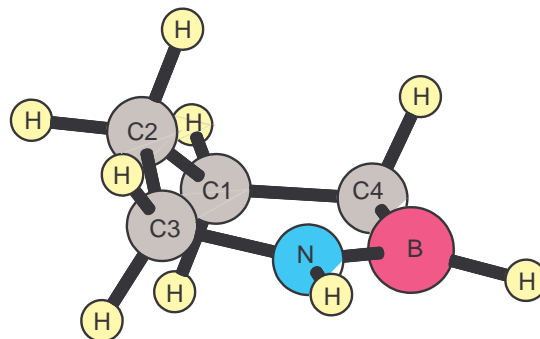


IDENTIFICATION AND CHARACTERIZATION OF 1,2-BN CYCLOHEXENE USING MICROWAVE SPECTROSCOPY^a

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1,2-BN Cyclohexene was produced from 1,2-BN Cyclohexane through the loss of H₂ and characterized and identified using a pulsed-beam Fourier-transform microwave spectrometer. The first microwave spectra for 1,2-¹⁰BN Cyclohexene 1,2-¹¹BN Cyclohexene have been measured in the frequency range of 5.5-12.5 GHz, providing accurate rotational constants and nitrogen and boron quadrupole coupling strengths for two isotopologues. High-level ab initio calculations provided rotational constants and quadrupole coupling strengths for the precursor 1,2-BN Cyclohexane (C₄H₁₂BN) and 1,2-BN Cyclohexene (C₄H₁₀BN). Calculated molecular properties for 1,2-BN Cyclohexene are in very good agreement with measured parameters. Calculated parameters for the starting material, 1,2-BN Cyclohexane do not agree with the experimental data. Rotational constants for 1,2-¹¹BN Cyclohexene are A = 4702.058(2) MHz, B = 4360.334(1) MHz and C = 2494.407(1) MHz. The inertial defect is $\Delta_0 = -20.78 \text{ amu}\cdot\text{\AA}^2$ clearly indicating a nonplanar structure. These microwave experiments show that heating the initial compound, 1,2-BN Cyclohexane, to 60 C in a 1 atm neon stream results in the loss of H₂ and conversion to 1,2-BN Cyclohexene. This appears to be the first characterization of the 1,2-BN Cyclohexene monomer.



^aSupported by the NSF CHE-1057796 and DOE DE-EE-0005658