REINVESTIGATION OF THE ROTATIONAL SPECTRUM AND STRUCTURE OF CYCLOHEXYLAMINE

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Cyclohexylamine was re-investigated by high-resolution Fourier transform microwave spectroscopy. In order to interpret the microwave spectrum, high-level first-principle quantum chemical calculations were carried out at the B3LYP and MP2 methods using the aug-cc-pVTZ basis set. Two potential energy surface scans (one for the axial and another for equatorial conformer) were performed along the H-N-C-C dihedral angle at the B3LYP/6-311++G level of theory. The scan identified four conformers which correlates with previously reported vibrational spectra and theoretical calculations. Eighteen rotational transitions were assigned to the gauche-equatorial conformer and fit to A= 4264.343(57) MHz, B=2222.446 (39) MHz, and C=1604.877(31) MHz. Ring strain and spectral assignment for additional conformers will be discussed.