

## CONFORMATIONAL ANALYSIS OF CYCLOBUTANECARBOXYLIC ACID

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There has been continued interest in the structure of substituted cyclobutanes. In this work, we measured the rotational spectrum of cyclobutanecarboxylic acid (CBCA) for the first time using a chirp-pulse and a cavity-based Fourier transform microwave spectrometers. To aid in our analysis of the spectrum, we performed potential energy surface scans at B3LYP/aug-cc-pVTZ level in the ring-COOH dihedral angle of both equatorially- and axially-substituted CBCA. These scans revealed a unique local minimum and a shallow, symmetrical double-well at the global minimum, implying the existence of four distinct stable (yet facily interconvertible) conformers. We re-optimized these conformers using both density functional theory and second-order Møller-Plesset perturbation theory with the aug-cc-pVTZ basis set and computed their relative energies, dipole moments, and rotational constants. We will present and discuss the corresponding assignments of features in the rotational spectrum.