THEORETICAL AND MICROWAVE SPECTROSCOPIC CHARACTERIZATION OF CYCLOBUTENONE

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Cyclobutenone has been characterized by high-resolution Fourier transform microwave spectroscopy for the first time. High level first-principles quantum chemical calculations at the B3LYP, MP2, and CCSD levels of theory were employed to better understand the molecular structure and obtain model rotational and centrifugal distortion constants to aid spectral assignment. Results from the different levels of theory are compared. Nine rotational transitions were measured and fit to a Watson A-reduced Hamiltonian (3 kHz error) and S-reduced Hamiltonian (4.2 kHz error). Cyclobutane and its derivatives are known to undergo ring-puckering inversion and were observed to have tunneling splittings of their rotational transitions. No tunneling splittings were observed for cyclobutenone indicating no significant ring-puckering tunneling in this four-membered ring system.