

## MILLIMETER-WAVE AND HIGH-RESOLUTION INFRARED SPECTROSCOPY OF CYCLOBUTANONE

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The gas-phase rotational spectrum from 85 to 750 GHz and the high-resolution infrared spectrum of cyclobutanone ( $C_4H_6O$ , Cs) have been analyzed for the ground and low-energy vibrationally excited states of the ring-puckering vibration ( $\nu_{20}$ ). The extension of the ground-state rotational spectrum provides the foundation for astronomical searches across most of the frequency range covered by modern radiotelescopes. Observation of the rotational spectrum in frequency range above 350 GHz, reveals transition frequencies perturbed by b-axis Coriolis-coupling interactions between the ground vibrational state and the ring-puckering vibration ( $\nu_{20}$ ). As a result, meaningful analysis of the rotational spectrum of the ground vibrational state of cyclobutanone cannot be accomplished via a single-state, distorted-rotor Hamiltonian. Thus, a combined global fit of the rotational and infrared data has been obtained using a sextic, centrifugally distorted rotor Hamiltonian with Coriolis coupling between appropriate states. Prior to the acquisition of the high-resolution infrared spectrum from the Canadian Light Source (CLS), initial analysis of the ground state and several quanta of the  $\nu_{20}$  series provided accurate and precise band origins of  $\nu_{20}$  at  $35.730957(40) \text{ cm}^{-1}$  and  $2\nu_{20}$  at  $92.031027(47) \text{ cm}^{-1}$ , due to the observation of many nominally interstate transitions and resonant transitions. Experimental spectroscopic constants and vibrational energies are compared to their computed values.