INVESTIGATING THREE CYCLIC DIKETONE MOLECULES USING ROTATIONAL SPECTROSCOPY

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Diketones are a family of compounds extensively investigated in chemistry, mainly due to their keto-enol tautomerism. Rotational spectroscopy is a uniquely powerful tool to probe tautomerization processes owing to its direct sensitivity to molecular structure. The broadband microwave spectra of three cyclic diketone molecules, 4-cyclopentene-1,3-dione, 1,3-cyclopentanedione, and 2-methyl-1,3-cyclopentanedione, have been investigated in the 26-40 GHz frequency range region using a chirped pulse Fourier transform microwave spectrometer coupled to a supersonic expansion. The spectroscopic data were analyzed with the aid of ab-initio calculations to yield complete sets of molecular parameters, including rotational constants and centrifugal distortion constants for all the observed molecules. Details on the molecular structure and the equilibrium between keto- and enol- forms will be discussed.