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Microwave Spectrum and Molecular Structure Parameters for the 1,2-Cyclohexanedione (monoenoic) - Formic Acid Dimer

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Highlights

- This paper describes measurements and calculations of a doubly-hydrogen bound dimer.
- Rotational constants and hydrogen-bonding parameters are obtained from the experiments and compared with new theoretical values.
- No proton tunneling effects were observed for this complex.

Abstract:

The microwave spectrum for the 1,2-cyclohexanedione (monoenoic) - formic acid dimer was measured for four isotopologues in the 4.5-9 GHz range using a Flygare-Balle type spectrometer. Rotational and distortion constants ( $A$ ,  $B$ ,  $C$ ,  $D_J$ ,  $D_{JK}$ ) were obtained. Measured rotational constants were used in a least squares fit to determine some of the gas phase structural parameters of the dimer. Rotational constants and distortion constants of the parent isotopologue are  $A=2415.044(18)$  MHz,  $B=543.6907(2)$  MHz,  $C=451.6663(2)$  MHz,  $D_J=0.0220(13)$  kHz, and  $D_{JK}=0.119(31)$  kHz. The experimental hydrogen bond lengths are  $1.97\text{\AA}$ , somewhat longer than the values calculated using Gaussian 09 with MP2/6-311++G\*\*.

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