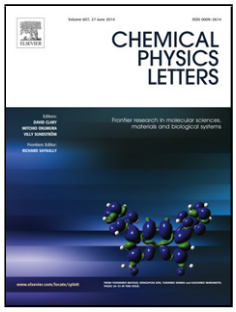

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Microwave Spectrum and Molecular Structure Parameters for the 1,2-Cyclohexanedione (monoenolic) - Formic Acid Dimer

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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 1,2cyclohexanedione (monoenolic) - 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 1.97Å, somewhat longer than the values calculated using Gaussian 09 with MP2/6-311++G**.