STRUCTURE FOR THE PROPIOLIC ACID - FORMIC ACID COMPLEX FROM MICROWAVE SPECTRA FOR MULTIPLE ISOTOPOLOGUES [a]

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New microwave spectra were measured to obtain rotational constants and centrifugal distortion constants for the DCCCOOH—HOOCH and HCCCOOD—DOOCH isotopologues. Transitions were measured in the 4.9-15.4 GHz range, providing accurate rotational constants which, combined with previous rotational constants allowed an improved structural fit for the propiolic acid - formic acid complex. The new structural fit yields orientations for both the propiolic and formic acid monomers in the complex and more accurate structural parameters describing the hydrogen bonding. The structure is planar, with a positive inertial defect of Δ = 1.33 amu Å^2.The experimental structure exhibits a greater asymmetry for the two hydrogen bond lengths than was obtained from the ab initio mp2 calculations.The average of the two hydrogen bond lengths is R(exp) = 1.76 Å, in good agreement with R(theory) = 1.72 Å.

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