MICROWAVE SPECTRUM OF ACETIC DIFLUOROACETIC ANHYDRIDE

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The rotational spectrum of acetic difluoroacetic anhydride, ($CH_3COOCOCHF_2$) was recorded by microwave spectroscopy and the A and E internal rotor states of the methyl group were analyzed. The A state was easily assigned using the assignment/fitting program DAPPERS, and a combined fit for the A and E state transitions was performed using XIAM. The fitted internal rotation barrier of the methyl group was determined to be 252.646(19) cm^{-1}. Using the M06-2X/6-311++G(d,p) level of theory, one non-planar cis conformer and two non-planar trans conformers of the anhydride were predicted. Agreement between theoretical and experimental rotational constants indicate that the non-planar trans conformer with the difluoromethyl alpha hydrogen participating in a hydrogen bond with a C=O oxygen is the form observed. The differences in the hydrogen bonding ability of the alpha hydrogens in the CH_3 and CHF_2 groups are a result of the differences in electron density.