

ETHANOL DIMER: OBSERVATION OF THREE NEW CONFORMERS BY BROADBAND ROTATIONAL SPECTROSCOPY

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The conformational behaviour of the hydrogen-bonded cluster ethanol dimer has been reinvestigated by chirped pulse Fourier transform microwave spectroscopy in the 2-8 GHz frequency region. Three new conformers (*tt*, *tg+*, and *g-g+*) have been identified together with the three (*g+g+*, *g-t*, and *g+t*) previously observed by Hearn et al. (J. Chem. Phys. 123, 134324, 2005) and their rotational and centrifugal distortion constants have been determined. By using different carrier gases in the supersonic expansion, the relative abundances of the observed conformers have been estimated. The monosubstituted ^{13}C species and some of the ^{18}O species of the most abundant conformers *g+g+*, *g-t*, and *tt* have been observed in their natural abundance, which led to the partial determination of their r_s structures, and the r_0 structure for the *tt* conformer. The six observed conformers are stabilized by the delicate interplay of primary O-H \cdots O and secondary C-H \cdots O hydrogen bonds, and dispersion interactions between the methyl groups. Density functional and ab initio methods with different basis sets are benchmarked against the experimental data.