GAS PHASE CHIRAL RECOGNITION: AN FTMW AND AB INITIO STUDY OF THE ETHANOL DIMER

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Ethanol dimer is probably the simplest system in which chiral self recognition occurs. Chiral recognition is a possibility because the two gauche forms of the ethanol monomer are non-superimposable mirror images; the microwave spectrum of the gauche form of the monomer displays a 96 GHz tunnelling splitting. On dimerization this motion is quenched. Hence, differing dimer structures arise depending on which of the three possible monomer conformations, trans (t) and two gauche (g and g'), are present. In all there are eighteen ways of combining the hydroxyl rotamers of the ethanol molecule in pairs. Nine of these combinations are spectroscopically distinct.

The microwave spectra of two conformations of the ethanol dimer have been recorded between 6 and 18 GHz with a supersonic jet Fourier transform microwave spectrometer. By comparison with *ab initio* calculations we believe that both dimers are hydrogen bonded such that an ethanol molecule in the trans conformation accepts a proton from a molecule in the gauche conformation (tg and tg'). Detailed results will be presented.