MOLECULAR RECOGNITION IN HYDROGEN-BONDED COMPLEXES OF ETHANOL AND OXIRANE DERIVATIVES - A ROTATIONAL SPECTROSCOPIC STUDY

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High resolution microwave spectroscopy complimented by ab initio calculations has been used to elucidate the diastereomeric interactions in a set of small model complexes. Ethanol, a transient chiral alcohol, was combined with oxirane (achiral), methyl-oxirane[a] (1 stereocenter) and trans-2,3-dimethyloxirane (2 stereocenters) to form hydrogen-bonded 1:1 complexes. The rotational constants of two conformers of ethanol· · ·oxirane, six conformers of ethanol· · ·methyl-oxirane and three conformers of ethanol· · ·trans-2,3-dimethyloxirane have been determined and the relative stability order of the conformers has been established. The dependence of the observed intensity on pressure, nozzle temperature and different carrier gases has been investigated for the case of ethanol· · ·trans-2,3-dimethyloxirane to give a first insight into the kinetical and thermodynamical influence on the formation of different conformers. The step-by-step methyl addition to oxirane helps to unravel the diastereomeric interactions at play via analysis of the subtle energy differences between each set of conformers, allowing for a detailed understanding of molecular recognition in this benchmark system.

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