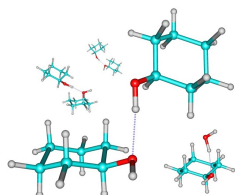


## THE CYCLOHEXANOL DIMER AND THE MONOHYDRATE: INTERNAL ROTATION AND CONVERSION FROM TRANSIENT TO PERMANENT CHIRALITY

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The conformational preferences, molecular structure and intramolecular dynamics of cyclohexanol (CHOL), the cyclohexanol dimer (CHOL<sub>2</sub>) and cyclohexanol-water (CHOL...H<sub>2</sub>O) have been analyzed using rotational spectroscopy in a supersonic jet expansion. The monomer conformation is controlled by ring inversion (equatorial/axial) and alcohol internal rotation (gauche+/gauche- or trans). Both equatorial trans (rigid) and equatorial gauche (tunneling) isomers were observed, but axial cyclohexanol went undetected. The monohydrate CHOL...H<sub>2</sub>O exhibits a single hydrogen bonded equatorial gauche conformation, with tunneling splittings revealing a concerted motion of the hydroxyl and water molecules. The formation of the dimer CHOL<sub>2</sub> stabilizes the transient chirality of the gauche+/gauche- monomer conformations, as different chiral combinations donor-acceptor result in permanent chirality. This molecular dimer represent a larger level of complexity compared with previous studies<sup>ab</sup>, as 36 different donor-acceptor combinations are now possible and the relative orientation of the two rings generates multiple conformations. Finally, six different isomers were observed for the dimer. Accurate rotational parameters for the observed conformations and supporting ab initio and DFT calculations will be reported.

<sup>a</sup>M. S. Snow, B. J. Howard, L. Evangelisti, W. Caminati, *J. Phys. Chem. A* **2011**, 115, 47.

<sup>b</sup>A. K. King, B. J. Howard, *Chem. Phys. Lett.* **2001**, 348, 343.