

CHIRALITY ASPECTS IN THE DIMERIZATION OF VICINAL DIOLS

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1,2-Ethanediol has been shown by FTIR and Raman spectroscopy in supersonic jets to dimerize preferentially in an S_4 -symmetric structure with a cyclic pattern of four strained hydrogen bonds^a. This forces the two monomers into a heterochiral OCCO helicity. The equally frequent homochiral encounters lead to a rich variety of nearly isoenergetic, but much less stable chain topologies with only three hydrogen bonds. The latter had remained elusive in a previous study but^a are now identified and energetically modulated by chemically freezing the OCCO helicity of the monomers. This is achieved by moving to cyclic diols of different ring sizes. They are explored computationally and in several cases also spectroscopically, exploiting the established complementarities between Raman and IR spectroscopy for hydrogen bonded systems^b.

^aF. Kollipost, K. E. Otto, M. A. Suhm, *Angew. Chem.* **2016**, 128, 4667.

^bThomas Forsting, Hannes C. Gottschalk, Beppo Hartwig, Michel Mons, Martin A. Suhm, *PCCP*, **2017**, 19, 10727