MOLECULAR RECOGNITION OF CHIRAL CONFORMERS: A ROTATIONAL STUDY OF THE DIMERS OF GLYCIDOL

ASSIMO MARIS, BARBARA M. GIULIANO, DARIA BONAZZI and WALTHER CAMINATI , *Dipartimento di Chimica "G. Ciamician" dell'Università, Via Selmi 2, I-40126 Bologna, Italy*.

We report for the first time the rotational spectra of dimers deriving from the combinations of different conformers of a chiral alcohol, glycidol. Its MW spectra has been reported, and two hydrogen bonded conformers, 1 and 2 have been identified.[a] Conformer 1 is more stable by 3.4 (4) kJ/mol. A pure chiral species (either R or S) can form seven hydrogen bonded homo - dimers, identified with the label Hom. They can be divided into two groups: one group where the hydrogen bonds form a ring involving 8 heavy atoms and another group where this ring involves only 5 heavy atoms, called 8Hom and 5Hom. Six (three Hom and three Het) conformers have the 8-heavy-atom-frame while eight (four Hom and four Het) conformers have the 5-heavy-atom-frame. Only the rotational spectra of species 8Hom-11 and 8Hom-12 have been observed. We recorded the FTMW spectra in a supersonic expansion. The relative energies and dynamics of formation of the dimers in the supersonic expansion will be discussed.

[a] K.-M. Marstokk, H. Möllendal and Y. Stenström,Acta Chem. Scand. 1992, 46, 432