CHIRAL SELF-RECOGNITION: DIRECT ROTATIONAL SPECTROSCOPIC DETECTION OF 2-FLUOROETHANOL DIMERS AND TRIMERS IN THE GAS PHASE

XUNCHEN LIU, NICOLE BORHO, YUNJIE XU, *Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada, T6G 2G2*.

The 2-fluoroethanol (FE) monomer has five conformers and exists predominately in the all-*gauch* conformation which is stabilized by an intra-molecular O-H···F bond. When interacting with another molecule through hydrogen bonding, FE exhibits transient chirality.[a] In this study, we examine the competition between the intra- and inter-molecular hydrogen bonds when two FE form a dimer using rotational spectroscopy and *ab initio* calculations. Three pairs of the homo- and heterochiral binary conformations are predicted to be local minima at the MP2/aug-ccpVTZ//MP2/6-311++G(d,p) level of theory. Jet-cooled rotational spectra of the four out of six binary conformers were measured and unambiguously assigned for the first time. All four observed binary conformers are in the *compact* conformation, where two binding subunits have large contact area. The four conformers have very similar binding energies. These observations are in agreement with the previous jet-cooled low resolution infrared study by Suhm and co-workers.[b] The FE trimers, on the other hand, show strong preference for the homochiral trimers where FEs can form cooperative O-H···O and C-H···F rings. *Ab initio* calculation shows that the C_3 symmetric trimer of the all-*gauch* conformation is the most stable form. The comparison between the binary and ternary FE systems will be discussed.

[a] a) Paul Hearn, Rachel Cobley, Brian Howard, J. Chem. Phys. 2005, 123, 134324; b) Nicole Borho, Yunjie Xu, Angew. Chem. Int. Ed. 2007, 46, 2276-2279.

[b] a) Tina Scharge, Corinna Emmeluth, Thomas Haber, Martin A. Suhm, J. Mol. Struct. 2006, 786 86-95. b) Nicole Borho, Martin A. Suhm, Org. Biomol. Chem., 2003, 1, 4351-4358.