SURPRISING DONOR-ACCEPTOR PREFERENCES IN ALCOHOL DIMERS: A JET-FTIR STUDY

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When two alcohol molecules pair to form a hydrogen-bonded dimer, one of them will be the hydrogen bond donor, while the other one acts as the hydrogen bond acceptor. From an energetical standpoint, the preferences are often intuitive and can be confirmed by quantum-chemical calculations. A study of OH-stretching fundamentals for a range of alcohol dimers using the ragout-jet FTIR technique[a] [b] reveals surprising deviations from such energetical expectations. Pairings including methanol, ethanol, tert.-butanol, perfluoro-tert.-butanol, phenol, cresols and silanols are presented and possible explanations are discussed. For ethanol dimers, the most strongly shifted OH stretching band persists when Ar is added to the expansion. It is therefore due to the most stable dimer conformations and there is evidence that they involve two gauche monomers, although ethanol monomer prefers the trans conformation.

[a] T. Häber, U. Schmitt, M.A. Suhm, Phys. Chem. Chem. Phys. 1 (1999) 5573

[b] T. Häber, U. Schmitt, C. Emmeluth, M.A. Suhm, Faraday Discuss. 118 (2001) 331