CONFORMATION AND AGGREGATION OF FLUORINATED ALCOHOLS

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Replacement of hydrogen by fluorine in aliphatic alcohols leads to rich isomerism in the associated clusters, involving conformation, hydrogen bond topology and chiral recognition issues.^{*a*} Besides the classical OH···O hydrogen bond the aggregates are stabilized by two weaker interactions: OH···F and CH···F. The aggregates are formed in a jet expansion and characterized by FTIR spectroscopy, based on their stagnation pressure dependence and on argon coating effects. The experimental data are supported by quantum chemical calculations.

^aT. Scharge, C. Emmeluth, T. Häber, M. A. Suhm, Competing hydrogen bond topologies in 2-fluoroethanol dimers, J. Mol. Struct., (2006), in press.