Computations and 1H NMR Spectroscopy of the Imide Region Can Distinguish Isomers of Hydrogen-Bonded Aggregates. Chin, Donovan N.; Simanek, Eric E.; Li, Xinhua; Wazeer, Mohammed I. M.; Whitesides, George M. Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, USA. Journal of Organic Chemistry (1997), 62(6), 1891-1895. Publisher: American Chemical Society.

Abstract

General rules for the assignment of isomers of the aggregates of Hub(M)3 (I), a sym. triimide based on a tris(melamine coupled triphenylamine) condensed to a 1,3,5-benzenetricarboxylic acid (the Hub) deriv., with cyanuric acid (CA) derivs. using mol. modeling of the I·i-Prbenz(CA)2 and I·i-Prfuran(CA)2 complexes. A simple modification to a noncovalent aggregate can translate into addnl. structural simplicity (due to, in the case of the I complexes, steric repulsion between groups along the periphery of the aggregate). I.e., the use of i-Prbenz(CA)2 instead of i-Prfuran(CA)2 results in fewer isomers. The rules for interpreting the imide region of the 1H NMR apply to these more complicated aggregates: the suggest the no. and symmetries of isomers in soln. Aggregates incorporating C3 sym. Hub(M)3 groups are more stable than those that incorporate asym. Hub(M)3 groups. The use of the deviation from planarity (DP) as a computational surrogate for the assignment of relative stability is discussed.