Organic and Biomolecular Chemistry 2007 vol.5 N9, pages 1472-1478

Nonregular structure-property relationships for inclusion parameters of tert-butylcalix[5]arene

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Abstract

The effect of macrocycle size on the structure-property relationships was studied for inclusion compounds of tert-butylcalix[n]arenes (n = 4,5) with volatile organic guests having various molecular size and group composition. Vapor-sorption isotherms, guest-inclusion stoichiometry and Gibbs energy, thermostability parameters and decomposition enthalpies were determined for host-guest compounds (clathrates) obtained using saturation of solid calixarene powder with guest vapor. The increase of the host macrocycle in the studied calixarene pair changes the observed structure-property relationship from the guest-binding selectivity mostly seen in inclusion Gibbs energy to the high sensitivity for guest structure in inclusion stoichiometry. The host with the larger macrocycle has more clathrates with stepwise formation and decomposition. Specific types of guest binding with solid hosts are discussed. © The Royal Society of Chemistry.

http://dx.doi.org/10.1039/b701082f