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Solution structure and equilibrium of new calix[4]resorcinarene complexes - Prototype of molecular machines. NMR data

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Abstract

Association properties and molecular machine application of water soluble calix[4]resorcinarene (1) with two aromatic guests (2-naphthol (2) and 1,5-naphthalenediamine (3)) have been investigated by various NMR methods (chemical shift, nOe and diffusion measurements) in aqueous solution at different concentrations and pH range. In neutral solution 1 strongly associates with 2, while only moderately associating with 3. Increase in concentration causes an increase in the stability of 1 + 3 and 1 + 2 + 3 complexes and produces high order complexes. The decrease of pH does not have an influence on 1 + 2 association, but disrupts 1 + 3 assembly. 1 can be used for the separation of 2 + 3 mixture in aqueous solution at moderate concentrations. The pH dependency of the association properties of the 1 + 3 system makes these compounds prime candidates for pH-responsive molecular machines applications. © Springer Science+Business Media B.V. 2007.

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Keywords

DOSY, Host-guest complex, Molecular machine, NMR