

Abstract

Spectroscopic Study of (*all-R,R*)-cyclohexanohemicucurbit[8]uril and Its Host-Guest Supramolecular Hexafluorophosphate Complexes [†]

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(*all-R,R*)-Cyclohexanohemicucurbit[8]uril (cycHC[8]) is a chiral macrocycle binding anions [1] with 1:1 stoichiometry in protic solvents with the association constant of $K_a = 3 \times 10^4 \text{ M}^{-1}$ in the case of the PF_6^- anion. Spectroscopic properties of cycHC[8] have been analysed by ultraviolet and circular dichroism spectroscopy exhibiting the corresponding electronic absorption. Host-guest complexation of cycHC[8] with the hexafluorophosphate anion containing chromophores was studied in different solvents. It was found that using ultraviolet, fluorescence and circular dichroism spectroscopies, it is possible to follow the supramolecular interaction between cycHC[8] and chromophore containing the hexafluorophosphate anion in methanol through the spectral changes of its cationic moiety. Furthermore, it was shown with circular dichroism that the cycHC[8] host uptakes the achiral hexafluorophosphate anion into its cavity, whilst the remaining chromophoric cation binds the cycHC[8]—anion complex via the corresponding electrostatic interactions. In the case of the chiral chromophoric guest, the effect of chiral discrimination is observed. The scope of chiral cations for enantio selectivity and achiral cations for chirality induction will be discussed.

Reference

1. Kaabel, S.; Adamson, J.; Topić, F.; Kalenius, A.K.E.; Öeren, M.; Reimund, M.; Prigorchenko, E.; Lõokene, A.; Reich, H.J.; Rissanen, K.; et al. Chiral hemicucurbit[8]uril as an anion receptor: Selectivity to size, shape and charge distribution. *Chem. Sci.* **2017**, *8*, 2184–2190.



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