Weak Intermolecular Interactions in Cavitands as Receptors for Mass Sensors

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Cavitands, synthetic organic compounds with enforced cavities of molecular dimensions, are extremely interesting and versatile molecular receptors whose complexation properties mainly derive from H-bonding, CH- π and dipole-dipole interactions [1].

The rational design of organic hosts is particularly appealing to chemical sensor technology, which requires selective, sensitive and stable receptors. The use of supramolecular structures coated as thin layers on quartz crystal microbalances (QCM) has proved to be one of the best approaches to generate new materials with molecular specificity for chemical sensing [2].

Following these studies, convenient phosphorus-bridged cavitands were designed and synthesized to investigate their complexation properties towards linear alcohols [3]. X-ray diffraction on single crystals has been widely used to study the multiple binding interactions in these phosphonate cavitands (hydrogen bonds involving the PO groups and CH- π interactions with the π -basic cavity). It has been thus evidenced that the synergistic behaviour of an increasing number of convergent PO groups enhances the complexation of the guests, giving rise to entropically favoured complexes.

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