MOLECULAR RECEPTORS BASED ON HETEROCYCLE CONTAINING CALIX[4]ARENES

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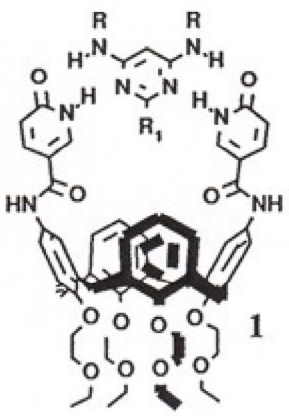
The rational design of specific receptors for the selective binding of (neutral) guests is a rapidly growing field of interest in supramolecular chemistry. Therefore, it is important to develop three-dimensional building blocks for the attachement of functional groups that can be oriented in space in such a way that they can form a suitable binding site. In particular, calix[4]arene, a cyclic tetramer composed of phenolic units which are linked via the ortho position by methylene bridges, is recognized to be such an important molecular building block.

The preliminary results of several approaches of heterocycle containing calix[4]arene based molecular receptors will be discussed. E.g. receptor **1** is based on a calix[4]arene moiety in the cone conformation bearing two divergent pyridone groups. CPK models suggest that complexation with diaminopyrimidines should be possible. Compound **1** could easily be prepared starting from the corresponding dinitrocalix[4]arene. Receptor **1** already shows intermolecular selfassociation in solution; the FAB mass spectrum exhibits distinct peaks of the corresponding double and even triple calix[4]arenes.

Another receptor (**2**) consists of a calix[4]arene in the cone conformation bearing two diaminotriazine units. This compound could be synthesized by reaction of the corresponding diaminocalix[4]arene with cyanuric chloride and subsequent substitution of the remaining chloro atoms with butylamine. Compound **2** has a cleft in which barbiturates fit in. Upon complexation the conformation of the calix[4]arene changes to a distorted cone conformation, as was confirmed by molecular mechanics calculations. Both the synthesis and complexation behavior of the receptors will be presented.



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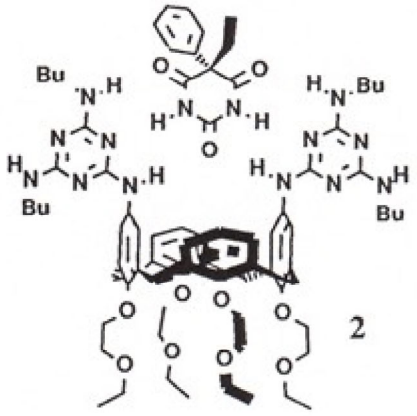

2