

## MS36. Molecular crystals offering new insight into intermolecular interactions

Chairs: Paola Gilli, Carl Henrik Gørbitz

### MS36-O1 Tailoring host-guest interactions for sensing with cavitands

Chiara Massera<sup>1</sup>

1. Dipartimento di Chimica, Parco Area delle Scienze 17/A, 43124 Italy

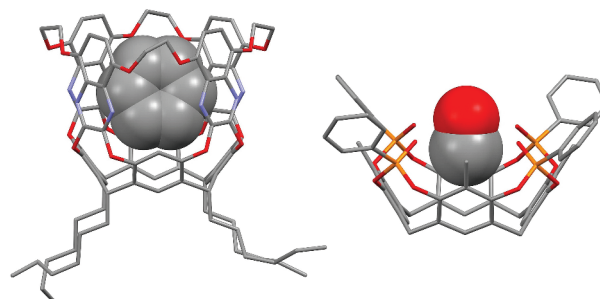
email: chiara.massera@unipr.it

Cavitands, synthetic organic compounds with enforced cavities of molecular dimensions, represent a very important class of receptors for chemical and biochemical sensing [1]. Particularly attractive is the possibility of designing and decorating these receptors to tailor the supramolecular interactions responsible for the recognition of different analytes, thus tuning their selectivity towards desired classes of chemical species in presence of interferents [2]. In the case of aromatic guests, quinoxaline-bridged and linked quinoxaline-bridged cavitands have proved to be extremely effective receptors through the formation of  $\pi$ - $\pi$  stacking and CH- $\pi$  interactions, while the H-bond active tetraphosphonate cavitands are well-known for their ability to complex positively charged species and neutral molecules [3, 4].

We present our recent investigations in the field of supramolecular sensing with cavitands carried out by means of single-crystal X-ray analysis, studies in solution and theoretical calculations.

#### References

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**Figure 1.** Molecular structure of the complex formed between a linked quinoxaline-bridged cavitand and benzene (left) and a tetraphosphonate cavitand and methanol (right).

**Keywords:** cavitands, molecular recognition, weak interactions