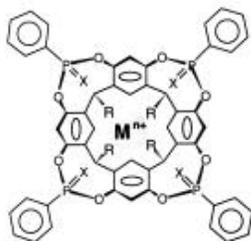


s9.m3.p9 A Novel Thiophosphorylated Cavitand and its Complex with Silver Picrate. B. Tinant^a, J.-P. Declercq^a, B. Bibal^b, and J.-P. Dutasta^b, ^aUniversité Catholique de Louvain, Unité CPMC, 1 Place Pasteur, B-1348 Louvain-la-Neuve, ^b Ecole Normale Supérieure de Lyon, 46 Allée d'Italie, F-69364 Lyon Cedex 07, France. Keywords: molecular interactions, supramolecular assemblies.

The phosphoryl and thiophosphoryl groups have been introduced into the preorganised structure of the calix-4-resorcinarene. We recently reported the synthesis of the phosphorylated cavitands, their high affinity for cationic species and the X-ray structures of the complexes with Cs⁺ and MeNH₃⁺ [1,2].

The amphiphilic thiophosphoryl derivative **1** was synthesised. The long R chain substituent at the lower rim was introduced in order to increase the lipophilicity of the ligand. The *iiii* isomer with the four P=S groups pointing inward (*i*) the molecular cavity was obtained.

The complexing properties of these ligands for Mⁿ⁺ and ammonium cations have been characterized by liquid-liquid extraction experiments: cavitand **1** extracts Ag⁺ in a very selective way.



1 X=S, R=C₁₁H₂₃

2 X=S, R=C₁₁H₂₃,
M= Ag⁺

The ligand **1** and its complex with silver picrate **2** were crystallized and their structures refined using data collected with a MAR345 image plate at 100K. In the complex four Ag⁺ cations link two ligands by P=S...Ag...S=P bonds. The geometry of the free ligand and the complex will be discussed in details.

s9.m3.p10 Derivatives of 5-Morpholine-2-phenyl-3-pyridazinone. A. Katrusiak¹, S. Baloniak¹, A. Katrusiak², ¹Department of Organic Chemistry, School of Medicine, Grunwaldzka 6, 60-780 Poznan, ²Department of Crystal Chemistry, Adam Mickiewicz University, Grunwaldzka 6, 60-780 Poznan, Poland. Keywords: pyridazinone, conformational analysis, polymorphism.

Derivatives of pyridazine, pyridazinone and maleic hydrazide attract considerable attention for their biological activities [P.D.Cradvick, Nature 258 (1975) 774; D. Becker et al., Acta Cryst. B54 (1998) 671]. Structures of a series of 5-morpholine-2-phenyl-3-pyridazinone derivatives have been determined by X-ray diffraction. The distortions of the pyridazinone ring will be analysed and discussed. It is shown that pyramidal distortions of the pyridazine nitrogens facilitate accommodation of the ring substituents. Directions of intermolecular interactions of the pyridazine nitrogens will be analysed for the polymorphic structures of maleic hydrazide [A. Katrusiak, Acta Cryst. C49 (1993) 36].

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[2] Tinant, B., Declercq, J.P., Bibal, B., Delangle, P., Dutasta, J.P. "Novel (thio)phosphorylated cavitands" 1st Belgian Crystallographic Symposium (1999) poster nr 4.01.