

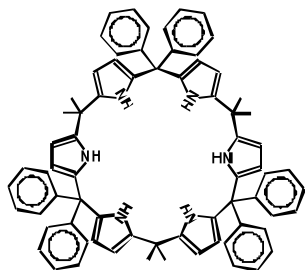
s9.m3.p21 Calixpyrroles and their Complexes. K. Suwinska¹, B. Turner², Y. Eichen³, ¹*Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland,* ²*Technion – Israel Institute of Technology, Haifa, Israel.*

Keywords: molecular interactions, supramolecular assemblies.

Calix[n]pyrroles have recently become the subject of intensive research aimed at the development of novel hosts for molecular inclusion of different species.

Calix[4]pyrroles, a class of tetrapyrrolic macrocyclic molecules are effective and selective receptors for anions such as fluoride and neutral guest species such as alcohols and ketones. The results obtained for calix[4]pyrroles inspired researchers to explore the complexation properties of larger calixpyrroles such as calix[5]pyrroles and calix[6]pyrroles. Such extended cavity receptor molecules should allow the selective binding of aromatic guest molecules as well as large anionic species such as I⁻, substrates that can not be recognized and complexed by the smaller calix[4]pyrrole system.

In this work, a number of calix[4]pyrrole and calix[6]pyrrole complexes with various guest species will be reported, and the conformational differences between the uncomplexed and complexed forms of the host molecule will be shown. The host-guest interactions will be discussed.



calix[6]pyrrole

s9.m3.p22 Crystal Structures of Solvated and Unsolvated Decameric Oxomolybdenum(V,VI) Cluster with Coordinated 3-Methylpyridine B. Modec, J.V. Brencic, L. Golic, *Faculty of Chemistry and Chemical Technology, Askerceva 5, P.O.Box 537, 1001 Ljubljana, Slovenia*

Keywords: crystal structures, oxomolybdenum(V,VI) cluster, solvothermal synthesis.

[Mo₁₀O₂₆L₈] and [Mo₁₀O₂₆L₈].L (L= 3-methylpyridine) are the products of solvothermal reactions between (PyH)₂[MoOCl₅] dissolved in methanol and 3-methylpyridine at 130^oC.

Compact single crystals were obtained after 104 hours.

X-ray structural analysis confirmed the presence of discrete neutral molecules.

[Mo₂O₄]²⁺ unit is a common structural motif in the cluster. Ten molybdenum atoms are grouped into four Mo₂^V pairs with Mo-Mo single bonds in the range 2.56-2.61Å and two Mo(VI) sites. Molybdenum atoms are connected by oxygen atoms which are singly, doubly, triply and quadruply bridging. Mo-O(terminal) bonds are from 1.61-1.71Å. The shortest Mo-O(bridging) bond is 1.79Å. There is no important difference between bonds in solvated and unsolvated compound.

[Mo₁₀O₂₆L₈] is monoclinic: P2₁/c with a= 11.925(3), b= 12.961(3), c= 23.404(7)Å and β=101.56(3)^o. V= 3544(2)Å³.

[Mo₁₀O₂₆L₈].L is monoclinic as well: P2₁/n with a= 12.1956(10), b=12.7373(10), c=22.586(10)Å and β= 92.791(10)^o. V=3504.0(4)Å³.