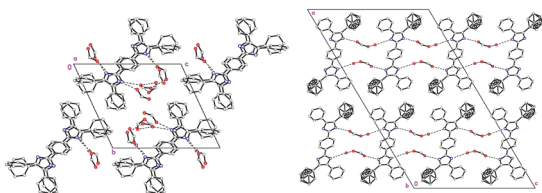


FA4-MS31-P11

Supramolecular associations in bisimidazole derivative/formic acid solvates. L. Izotova⁽²⁾, J. Ashurov⁽²⁾, S. Talipov⁽²⁾, B. Ibragimov⁽²⁾, E. Weber⁽¹⁾, ¹Institute für Organische Chemie, TU Bergakademie Freiberg, Germany. ²Institute of Bioorganic Chemistry, Tashkent, Uzbekistan
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Recently, heterocyclic imidazole derivatives (especially phenylimidazoles) have attracted considerable attention because of their unique optical properties [1]. From solution of formic acid have been obtained two types solvates of 1,4-bis(4',5'-diphenylimidazol-2-yl)benzene with formic acid – unstable and stable forms. The first unstable form – yellow plate, Sp.gr.P-1, cell parameters: $a=10.420(2)\text{\AA}$ $b=13.804(3)\text{\AA}$, $c=15.251(3)\text{\AA}$, $\alpha=63.86(3)^\circ$, $\beta=82.23(3)^\circ$, $\gamma=70.58(3)^\circ$, $V=1857.1(7)\text{\AA}^3$, the host/guest ratio is 1:5. Five formic acid molecules form the glue between two molecules of bisimidazole derivative through hydrogen bonding, thus forming 0D supramolecular arrangement. The second stable form –yellow bulk needles, crystallized in C2/c space group and have following cell parameters: $a=35.395(7)\text{\AA}$, $b=5.1576(10)\text{\AA}$, $c=20.607(4)\text{\AA}$, $\beta=120.85(3)^\circ$, $V=3229.7(11)\text{\AA}^3$. Host/guest ratio is 1:2:2H₂O. In this structure host and guest molecules *via* H-bonds are associated in 1D chain in the *c*-axis direction. A proton from the formic acid was transferred to one of the imidazole rings. Therefore one nitrogen of the imidazole ring is positively charged.



[1] P.T. Chou, M.L. Martinez, Radiat. Phys. Chem. 41 (1993) 373.

Key words: crystal engineering, hydrogen bonding, supramolecular assemblies

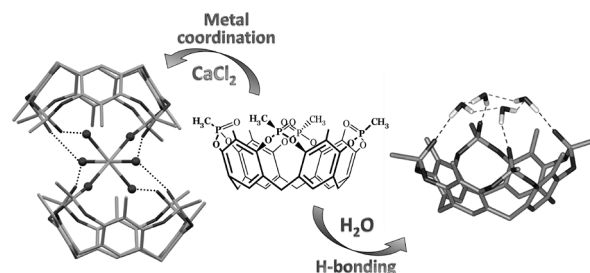
FA4-MS31-P12

Interplay between H-bonding and Metal Coordination in Tetrphosphonate Cavitands. Chiara Massera^a, Monica Melegari^b, Enrico Dalcanale^b, Franco Ugozzoli^a, ^a Department of General and Inorganic Chemistry, University of Parma, Italy, ^b Department of Industrial and Organic Chemistry, University of Parma, Italy
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Phosphorylated cavitands are an emerging class of versatile synthetic receptors, whose complexation properties span from neutral molecules like alcohols to positively charged species like ammonium and pyridinium salts [1]. In all these cases the molecular recognition phenomena depend on the synergistic effect of a π -basic cavity and of P=O groups at the upper rim which are effective H-bond acceptors. Here we report an innovative approach to the generation of a single tetrameric

water cluster in the solid state by using the tetraphosphonate cavitand template Tiiii[H₂CH₃,CH₃].

The specific H-bond interaction pattern induced by the host *via* its rigidly preorganized four P=O acceptor groups leads to the exclusive formation of a cyclic water tetramer of C₄ symmetry [2]. The four P=O units form an array of H-bonding with the cluster, controlling the orientation of the free hydrogens below the molecular plane of the tetramer. This water cluster is maintained also if competitive alcoholic guests like methanol or ethylene glycol are added to the crystallization mixture. Considering the affinity of this class of receptors towards cationic species and water, we have decided to investigate their behavior in the presence of both components.



The rigidity and the preorganized geometry of the organic hosts are ideal to discriminate the differences in size and coordination propensity of metallic cations and thus to control the formation of the corresponding organometallic complexes. Three novel dimeric capsules formed by Tiiii[H₂CH₃,CH₃] with barium, calcium and zinc salts have been synthesized and structurally characterized [3]. The role of cation dimensions and of coordinated water molecules in determining different architectures is also described.

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Keywords: Cavitands, Metal coordination, H-bonding

FA4-MS31-P13

Disorder in Self-assembled Halogen-bonded Perfluoroalkyl Onium Salts. Tullio Pilati^a, Antonio Abate^b, Gabriella Cavallo^b, Pierangelo Metrangolo^{b,c}, Giuseppe Resnati^{a,b,c}, Giancarlo Terraneo^{b,c}, ^aC.N.R. - I.S.T.M., University of Milan, Via C. Golgi 19, 20133 Milan, Italy, ^bNFMLab - D.C.M.I.C. "Giulio Natta", Politecnico di Milano, Via L. Mancinelli 7, 20131 Milan, Ital, ^cCNST - IIT@POLIMI, Politecnico di Milano, Via G. Pascoli 70/3, 20133 Milan, Italy
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In the last decade new families of liquid-crystalline materials based on non-covalent interactions such as hydrogen bonding, quadrupolar and charge-transfer interactions have been developed. Halogen bonding, namely any noncovalent interactions involving halogens as electrophilic species [1], has proven successful in driving self-assembly processes in supramolecular chemistry, crystal engineering, and materials