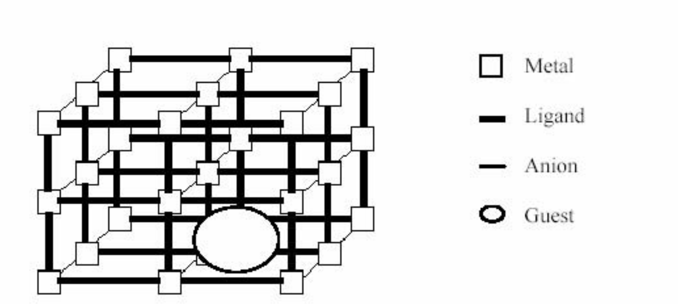
by rational self-assembly using the principles of crystal engineering. Metal ions are usually coordinated to two or more bridging ligands giving a final semi-rigid structure suitable for adsorption, catalysis, etc. Nano-porous materials based on new linear ligands coordinated to metallic centers are presented and have been characterized by physical and chemical methods. These compounds have the general formula $[M(L)A]_n$ where M = Cu^{2+}, Co^{2+}, Ni^{2+}, L = 4,4'-bipyridyl, 4,4′-bipyridyl N,N′-dioxide and A = $S_2O_6^{2-}$, SO_4^{2-} [1].



[1] Neels A., Montse A., González Mantero D., Stoeckli-Evans H., *Chimia*, 2003, 619-622.

Keywords: crystal engineering, nanoporous materials, physical adsorption

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The Interplay between N-H···O Hydrogen Bonding and Cl···Cl Interactions in Arylformamides

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N-H…O hydrogen bonding occurs in both dichlorophenyl- and dimethylphenyl-formamides, regardless of the substitution pattern around the phenyl group (Fig. 1), forming infinite chains of molecules. We have found that while there are significant differences in the crystal structures of 2,6-dichlorophenyl- (**1**) and 2,6-dimethylphenylformamide (**2**) (Fig. 1), **1** undergoes a phase transformation to a phase isomorphous with that of 2,6-dimethylphenyl-formamide. The differences in these structures are rationalized in terms of the presence (2,6-dichoro) or absence (2,6-dimethyl) of Cl…Cl interactions. In addition the presence of a Me or Cl group in both phenyl ortho positions affects the conformation of the formamide group.

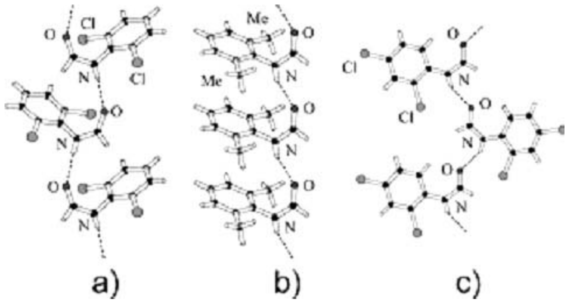

Figure 1. N-H…O hydrogen bonding patterns in (a) **1** (b) **2** (c) 2,4-dichlorophenylformamide.

Keywords: polymorph, phase transition, hydrogen bonding

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New Helical Host System Showing True Self-Inclusion

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Crystal engineering of host/guest systems has been a major field of study for the last couple of decades. Even though recent studies appear to be focusing on coordination polymers, the organic host systems, such as the crown ethers, cavitands, cryptands and calixarenes, have proven to be highly successful. Due to their biological relevance, helical host systems have also been developed. The urea family and the alicyclic diol family are the most well known. The compound 2,7-dimethyl-3,5-octadiyne-2,7-diol [1] was crystallized from several solvents and single crystal X-ray diffraction analysis performed to determine whether encapsulation had occurred. The host system comprises of triple helical tubes formed via hydrogen bonding. The guest is enclathrated inside these tubes. The host shows good selectivity, as it does not encapsulate most solvents. To investigate whether the host system could be porous, crystals were grown by sublimation. The sublimed material was found to have the same host helical structure but with the host compound also inside the channels. The same self-included structure was also found when no encapsulation occurred. To our knowledge this is the first example of a host system having the same basic structure when it includes itself.

[1] Leigh D.A., Moody A.E., Pritchard R.G., *Acta Cryst. C*, 1994, C**50**, 129.

Keywords: materials, supramolecular, self inclusion

P.09.06.2

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Comparative Study of Framework Borates Optical Non-linearities

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One of the pressing problems of modern crystallography and crystal chemistry is construction of noncentosymmetric crystal structures with high with second-order optical susceptibilities. Good solution to the problem may be using of the boron oxide framework matrix as a host for the high-polarizable metal cations. The recently discovered members of the known family of non-centrosymmetric halogen-pentaborates ($M_2B_5O_9Hal$, M = Ca, Sr, Ba, Pb, Eu, Hal = Cl, Br) with hilgardite-type structure are attractive due to their second harmonic generation (SHG) activity. In particular, lead derivative phases demonstrate SHG comparable with well-known BIBO (BiB_3O_6) crystal. The compounds of this family possess zeolite-like framework structures. As it was shown only metals mentioned above stabilize the structural type of hilgardite. Our attempts to obtain other representatives of this family with the same stochiometry lead to producing another structure type of framework halogen borates – boracites stoichiometry $M_3B_7O_{13}Hal$. They are characterized by a zeolite-like 3D non-centro-symmetric structure. We report comparison of our experimental and theoretical results on SHG efficiency for hilgardite and boracite families' members. The experiments show an order less SHG efficiency for boracites relative to hilgartdites. Computational methods developed by Phillips and Van Vechten and approached by Zhang to complex crystals were performed to explain corresponding difference in optical second-order nonlinearities of the crystals. Sequence of compounds in both families according to their SHG efficiencies conforms to the theoretically predicted values.

Keywords: noncentrosymmetric oxides, boron compounds, NLO

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Optical and Pyroelectric Properties and Structure of $2[K^+H(C_4H_5O_5)^-].C_4H_6O_5$

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The semi-organic crystal Bis (Potassium Hydrogen L-Malate) L-Malic Acid, $2[K^+H(C_4H_5O_5)^-].C_4H_6O_5$, shows a large spontaneous polarization (in the range 30-40mC/cm2) in the vicinity of 365K, which is one order of magnitude higher than that of TGS. The title compound also shows a second harmonic generation that is about 70% that of KDP. The crystal structure has been re-determined by single