

Agriculture and Technology, Higashi Koganei, Tokyo-Japan. E-mail: emmanuel_jp@yahoo.com

University of Frankfurt, Germany. ^bInstitute of Inorganic Chemistry, RWTH Aachen, Germany. E-mail: Chunhua.Hu@chemie.uni-frankfurt.de

Understanding the interactions between two different types of molecules in the complex crystal become important in the study of molecular recognition and crystal engineering. Particularly, the molecular recognition in the complex crystal is a subject of considerable interest because of its applications to separation purposes. A few years ago, it was reported [1] that an interaction between a chiral onium salt (Cinchonidinium Chloride) and racemic compound (Bis- β -naphthol) accomplishes a successful enantiomeric resolution, but many researchers are interested in exploiting economical means of resolving racemic compounds such as probable useage of a non-chiral host molecule. This is a difficult task yet to be achieved.

As an initial approach in our investigations, the crystallization of non-chiral host compound (monoalkyltrimethylammonium halides) with (R)-(+)-1,1'-Bi-2-naphthol (RBNP) and Rac-1,1'-Bi-2-naphthol (BNP) were chosen to investigate the molecular recognition between non-chiral host compound and chiral as well as racemic compound from the viewpoint of crystal structure studies in order to know the feasible interactions, molecular packing structures and space groups of such complexes. The investigations revealed that the hexyltrimethylammonium bromide (6TAB) and octyltrimethylammonium bromide (8TAB) interact with RBNP and BNP to form molecular complexes (6TAB/RBNP, 6TAB/BNP, 8TAB/RBNP and 8TAB/BNP) by crystallization or mixing of powdered samples in a mortar. Both 6TAB/RBNP and 8TAB/RBNP molecules crystallize in monoclinic space group $P2_1$, whilst 6TAB/BNP and 8TAB/BNP crystallize in triclinic space group $P\bar{1}$ and monoclinic space group $P2_1/c$, respectively. Hydrogen bonds and C-H \cdots π interactions stabilize the crystal structures and also contribute to the different packing modes observed in the complexes.

[1] Toda F., Tanaka T., *Chem. Commun.*, 1997, **12**, 1087.

Keywords: molecular recognition, crystal engineering, molecular compounds

P.09.02.7

Acta Cryst. (2005). A61, C355

Spontaneous Resolution of *N*-sulfonylpyrimidine Compounds Induced by Chemical Modifications

Aleksandar Višnjevac, Marija Luić, Mladen Žinić, Biserka Žinić, "Ruđer Bošković" Institute - ZFK, P.O.B. 180, HR-10002 Zagreb, Croatia. E-mail: aleksandar.visnjevac@irb.hr

The title compounds belong to a novel series of pyrimidine nucleobase derivatives, some of which exhibit significant anticancer activity *in vitro*. [1] The crystal structures of 1-tosylthymine (**1**), 1-tosyluracil (**2**), α -naphthyl derivatives of thymine (**3**) and uracil (**4**) are presented. The conformational chirality was encountered in all compounds, as the consequence of the S-N single bond free rotation hindrance in solid state (*atropisomerism*). [2]

The spontaneous resolution (*à la Pasteur*) of *P* and *M* conformational enantiomers occurred during the crystallization of **2** and **4**, whereas their 5-methyl analogues, **1** and **3**, crystallized as racemic mixtures. Moreover, spontaneous resolution in the case of **2** was accompanied by a formation of racemically twinned crystals regardless of the solvent used. Obviously, substituents at C-5 position of pyrimidine base as well as in -SO₂-R group dictate the occurrence (or absence) of spontaneous resolution.

[1] Žinić B., Žinić M., Krizmanić I., *Ruđer Bošković Institute*, EP 0 877 022, 2003. [2] Cunningham I.D., Cooles S.J., Hursthouse M.B., *Chem. Comm.*, 2000, 61-62.

Keywords: conformational chirality, racemic twinning, pyrimidine nucleobases

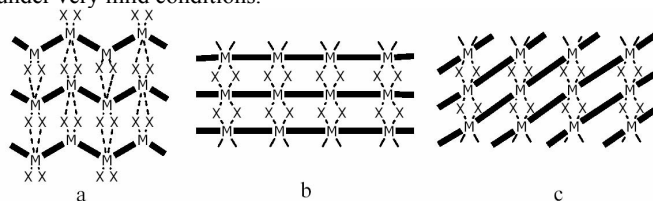
P.09.03.1

Acta Cryst. (2005). A61, C355

Single-Crystal to Single-Crystal Reactions

Chunhua Hu^a, Ulli Englert^b, ^a Institute of Inorganic Chemistry,

Single-crystal to single-crystal (SCSC) reaction represents the most fascinating field of solid-state chemistry [1-2], which in nature demands to make or break strong chemical bonds. Such transformation involves cooperative atomic movement between reactant and product (both are single crystals) in solids. In this contribution we wish to present two thermal-induced reversible SCSC reactions, in which unprecedented changes in network topology occur under very mild conditions.



1) Topotactic phase transformation between 1D tetrahedral chain polymers $[Zn(\mu-Cl)_2(4,4'-bpy)]_\infty^1$ (**1a** and **1b**, structure a) and 2D network $[Zn(\mu-Cl)_2(\mu-bpy)]_\infty^2$ (**2**, b) [3]; 2) between two 2D networks b and c on the polymer $[Pb(\mu-Cl)_2(\mu-bpy)]_\infty^2$ (**3**).

[1] Tanaka K., Toda F., *Chem. Rev.*, 2000, **100**, 1025. [2] Braga D., Grepioni F., *Angew. Chem. Int. Ed.*, 2001, **40**, 4002. [3] Hu C., Englert U. E., *Angew. Chem.*, 2005, *in press*.

Keywords: crystal engineering, topotactic phase transformations, crystal chemistry and reactions in solids

P.09.03.2

Acta Cryst. (2005). A61, C355

Crystal Engineering of Metal-organic Frameworks Using 4,4'-Dipyridyl-N,N'-Dioxide

Lesego J. Moitsheki, Susan A. Bourne, Luigi R. Nassimbeni, Department of Chemistry, University of Cape Town, Rondebosch, 7701, Cape Town, South Africa. E-mail: mlesego@science.uct.ac.za

Hybrid organic-inorganic materials provide the possibility of combining the advantages of organic and inorganic substances [1]. Schröder *et al* reported [2] that several terbium (III) coordination polymers of differing stoichiometry can be prepared by means of diffusion solvent mixtures using 4,4'-dipyridyl-N,N'-dioxide (dpdo). We have been investigating the coordination polymers of gadolinium (III) and thallium (III). Crystal structures acquired had either zigzag diamondoid or ladder shapes.

The study of metal-organic frameworks (MOF) has been extended to transition elements such as CuCl₂, ZnBr₂, Zn(NCS)₂ and PbCl₂. We have found that changing the metal geometry, while using the same spacer ligand (dpdo), has a significant effect on the type of MOF obtained. The effect of the metal salt anion is also examined. Crystal structures show that the materials we obtain are either polymeric or discrete molecules, which form a 2D or 3D network by means of supramolecular interactions.

Compounds synthesized were characterized by x-ray diffraction and thermal analysis {thermogravimetry (TG), differential scanning calorimetry (DSC) and hot stage microscopy}. Microanalysis was used to confirm the elemental composition.

[1] Mitzi D.B., *J. Chem.Soc., Dalton Trans.*, 2001, 1-12. [2] De-Liang., Blake A.J., Champness N.R., Wilson C., Schröder M., *Chem. Eur.J.*, 2002, **8**, 2026-2033.

Keywords: crystal engineering, metal-organic framework, X-ray diffraction

P.09.03.3

Acta Cryst. (2005). A61, C355-C356

MOFs of Phenylamine and Pyridine Derivatives: Structure and Thermal Analysis

Susan A Bourne, Lesego J Moitsheki, Zelo Mangombo, ^aDepartment