

FA4-MS03-P01**The Supramolecular Assemblies of a Selection of Imidazole Derivative and Dicarboxylic Acid Salts.**

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Although recrystallisation of a heteromeric solution is commonly used as a method of purification, it may also result in the formation of a salt. Salt formation is a technique often used by the pharmaceutical industry to enhance the physicochemical, formulation, biopharmaceutical, and therapeutic properties of a drug without modifying the basic chemical structure[1]. It would be of great benefit to chemists and formulators to be able to predict the effect various salt formers have on a drug. As the properties of the salt are derived from its crystal structure, we have performed a systematic study of solid forms consisting of simple organic molecules with weakly interacting functional groups in order to gain more understanding of the process of salt formation.

This study involved reacting a large number of simple nitrogen-containing compounds with α,ω -dicarboxylic acids (diacids), including alkane, alkene and hydroxy diacids. The work presented here describes sixteen salts (twelve synthesised and four obtained from the literature[2]) containing imidazole, 1-methylimidazole, 2-methylimidazole, 4-methylimidazole or 1,2-dimethylimidazole. The products were characterised by single crystal X-ray diffraction and the intermolecular interactions between the functional groups in each of the crystal structures were compared. It was found that these sixteen salts all formed similar sheet structures which could be depicted schematically, incorporating the direction of the anion chains, and the orientation of the imidazole methyl group within the sheet. The deprotonation patterns of the diacids, the effect of the methyl group together with its position on the imidazole ring, and the importance of C-H...O hydrogen bonding interactions in the sheet structures are assessed.

[1] P. H. Stahl, C. G. Wermuth (Eds.), *Handbook of Pharmaceutical Salts Properties, Selection and Use*, Wiley-VCH, Zürich, 2002. [2] J.C. MacDonald, P.C. Dorrestein, M.M. Pilley, *Cryst. Growth Des.*, 2001, 1, 29-38.

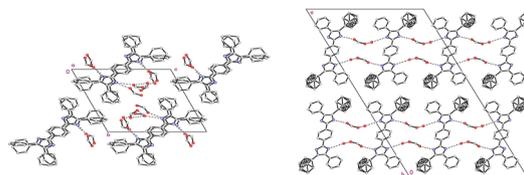
Keywords: salt; supramolecular; hydrogen bonding

FA4-MS03-P02

Supramolecular Associations in Bisimidazole Derivative/formic Acid Solvates. Lidiya Izotova^a, Jamshid Ashurov^a, Samat Talipov^a, Bakhtiyar Ibragimov^a, Edwin Weber^b. ^a*Institute of Bioorganic Chemistry, Tashkent, Uzbekistan.* ^b*Institute für Organische Chemie, TU Bergakademie Freiberg, Germany.*

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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.

Keywords: crystal engineering; hydrogen bonding; supramolecular assemblies

FA4-MS03-P03**The Crystal Structure, Substructure and Properties of Langatate.**

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Langatate crystals ($\text{La}_3(\text{Ga}_{0.5}\text{Ta}_{0.5})\text{Ga}_5\text{O}_{14}$ – LGT, sp.gr. P321) are the most promising materials for making both bulk acoustic and surface acoustic waves devices. The aim of this paper is to exhibit a role of some growth conditions in a property peculiarities and structural perfection of LGT. Crystals with dimensions 3" have been grown in $\langle 0001 \rangle$

(Z-crystals) and $\langle 01\bar{1}1 \rangle$ (Y54°-crystals) directions by Czochralski technique. They were analyzed by X-ray (CAD-4 and Xcalibur diffractometers, MoK_α) and neutron (TriCS diffractometer, $\lambda=1.18\text{\AA}$; diffractometer located at the channel 5C2, $\lambda=0.83\text{\AA}$) diffraction methods. The refinement of the crystal structure was carried out using