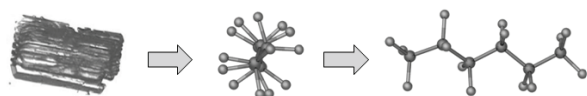


science [2]. We have used this interaction to realise the self-assembly of new families of liquid-crystalline materials based on perfluoroalkyl onium salts. An accurate choice of the starting components allowed us to produce superfluorinated ionic liquid crystalline materials with relatively high clearing points; some of those gave crystals of sufficiently good quality to be studied by single crystal X-ray diffraction. These compounds present an extensive disorder, mainly in the perfluorinated chains. In this contribution we present how to model the disorder, essential for a reasonable refinement of the structure, and which choices have driven our hands in selecting a good crystal for data collection. They are normally 'buttery' or at least very easily deformable, or extremely thin, or curved, twinned and often undergo phase transition at low temperatures.



[1] P. Metrangolo, G. Resnati, *Science* 2008, 321, 918. [2] P. Metrangolo, F. Meyer, T. Pilati, G. Resnati, G. Terraneo, *Angew. Chem. Int. Ed.* 2008, 47, 6114.

Keywords: Perfluoroalkyl Chains, Liquid Crystals, Disorder Modelling

FA4-MS31-P14

Synthesis and Crystal structure of Diethyltin bis-dihydrogenphosphate, (Et₂Sn)(H₂PO₄)₂ *Martin Reichelt^a, Hans Reuter^a,*
aInstitute of Chemistry, University of Osnabrück, Germany

E-mail: mareiche@uos.de

The title compound was synthesized from Et₂SnO and H₃PO₄. Its colourless needle shaped crystals crystallise in the monoclinic space group C2/c (no. 15) with $a = 22.4786(8)$ Å, $b = 9.9382(3)$ Å, $c = 20.3812(7)$ Å, $\beta = 96.922(2)^\circ$, $V = 4519.9(3)$ Å³, $Z = 16$ and $d = 2.180$ g/cm³. For structure solution and refinement 82153 reflections in the θ -range 2.01°–28.00° were collected, resulting in 5450 unique reflections ($R_{int} = 0.0396$) after applying an empirical absorption correction ($T_{min} = 0.6360$, $T_{max} = 0.8309$). In summary 286 parameters (2 restraints) were refined to $R1 = 0.0212$, $wR2 = 0.0453$ for 5450 reflections with $I > 2\sigma(I)$ and $R1 = 0.0252$, $wR2 = 0.0465$ for all reflections.

The asymmetric unit consists of two formula units and contains {Et₂SnO₃} trigonal bipyramids and {PO₄} tetrahedra, which are connected with each other to rings and chains. Via hydrogen bonds an extended three-dimensional framework is built up with channels parallel to the crystallographic b axis filled by the organic groups.

Keywords: tin compounds, phosphates, organic-inorganic hybrid materials

FA4-MS31-P15

The crystal structure of α -sodium stearate NaC₁₈H₃₅O₂ · 0.5 H₂O. *Alexandra Christine Schaap, Walter Frank, Institut für Anorganische Chemie und*

Strukturchemie, Lehrstuhl II, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf

E-mail: wfrank@uni-duesseldorf.de

Sodium soaps are materials with a wide range of industrial applications for example as detergents, greases, lubricants and cosmetics. Hence, the knowledge of the structural behaviour of sodium soaps is of general interest. However, until today crystallography of neutral sodium soaps is restricted to the determination of unit cell parameters [1, 2, 3, 4, 5]. Here we present the results of the first crystal structure determination of a curd soap, α -sodium soap: NaC₁₈H₃₅O₂ · 0.5 H₂O (**1**). Extremely thin platelet crystals of **1** were obtained by slow cooling of a propylglycolic solution that contained 5% of water. Soap **1** crystallizes in the triclinic space group $P\bar{1}$ with unit cell parameters of $a = 7.847(2)$ Å, $b = 9.302(2)$ Å, $c = 51.100(10)$ Å, $\alpha = 91.68(3)^\circ$, $\beta = 92.46(3)^\circ$ and $\gamma = 90.11(3)^\circ$ and with $Z = 2$. The sodium soap can be described as a bilayered structure with a strict separation of hydrophobic and hydrophilic parts that can be considered as an arrangement of model membranes.

[1] Buerger, M.J., Smith L.B., de Bretteville, A., Ryer, F.V., *Proc. Natl. Acad. Sci. USA*, 1942, 28, 526. [2] Buerger, M.J., *Proc. Natl. Acad. Sci. USA*, 1942, 28, 529. [3] Buerger, M.J., Smith L.B., Ryer, F.V., Spike, J.E., *Proc. Natl. Acad. Sci. USA*, 1945, 31, 226. [4] Buerger, M.J., *Am. Mineral.*, 1945, 30, 551. [5] Minor, J.E., Lingafelter, E.C., *J. Am. Chem. Soc.* 1949, 71, 1145.

Keywords: soap, α -sodium stearate, crystal structure determination

FA4-MS31-P16

Engineering Metal Organic Frameworks with a Triazole-Tetrazole Ligand. *Bernard Tinant^a, Anil D. Naik^b, Mathieu Monaux^a, Yann Garcia^a, ^aInstitut de la Matière Condensée et des Nanosciences, Université Catholique de Louvain, Belgium*
E-mail: Bernard.tinant@uclouvain.be

Cavernous solids at the designer's aspiration have found applications in separation science, gas storage technology, sensors, catalysis, drug delivery [1]. In continuation of our modular approach to functional materials of metal-organic frameworks, [2] we now direct our interest to the coordination chemistry of a novel asymmetric tecton (L1H = (5-(4H-1,2,4-triazol-yl)-2H-tetrazole), whose crystal structure was solved. This molecule was designed based on a conceivable transamination method [3] and actually represents the first molecular tecton wherein two flagged motifs of 1,2,4-triazole and tetrazole were brought on the same platform in a conciliation conformation. This unique molecule can behave as bifunctional bridging ligand as well as anion. [Zn(phen)₂(L1)]BF₄ (**1**) crystallises in a centrosymmetric space group (Pnma) with unsymmetrical L1 acting as 'interpolating' pillars and chelating phen as a capping ligand of hexa-coordinated Zn^{II} ions thus affording a robust 2D zig-zag network propagated by π - π interactions from heterocycles. The inclusion complex [Zn(bpy)₃]₂(L1) · (BF₄)₃ · 10H₂O (**2**) crystallises in a non-centrosymmetric space group (P2₁2₁2₁). It is a mononuclear octahedral complex presenting trapped L1 molecules in the water occupied channels by multiple secondary interactions also acting as an anion. TGA-DTA of **1**