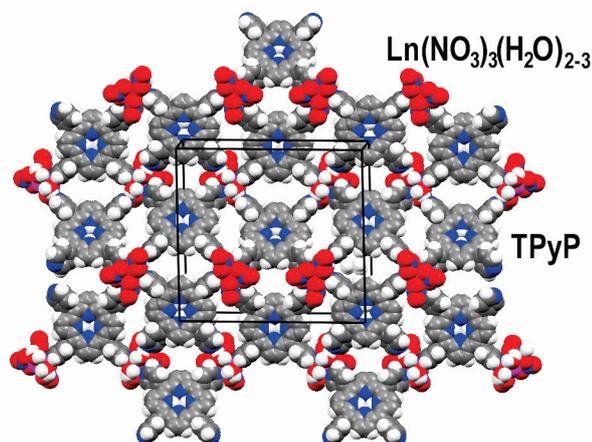


sphere. In addition, partial protonation of the pyridyl substituents of TPyP may also induce self-complementary hydrogen bonding between the pyridinium and pyridyl functions of the porphyrin scaffolds. In this work we explore the networking capacity of TPyP with aqua nitrates of various lanthanide ions, while taking advantage of coordination as well as hydrogen bonding features of the porphyrin entity [2]. Details of the supramolecular assembly modes of these materials will be presented.



[1] Lipstman, S., Muniappan, S., George, S., Goldberg, I., *Dalton Trans.*, 2007, 3273; Muniappan, S., Lipstman, S., George, S., Goldberg, I., *Inorg. Chem.*, 2007, 46, 5544. [2] Lipstman, S., Goldberg, I., *Cryst. Growth Des.* 2010, 10, 1823.

Keywords: crystal engineering, porphyrin networks, supramolecular structures

FA4-MS31-T04

Fantastic Voyage: Molecular Recognition Viewed Through Macroscopic Properties. Alessia Bacchi, Giulia Cantoni, Davide Cremona, Paolo Pelagatti. *Dipartimento di Chimica GIAF, Parma University, Italy.*

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One of the most appealing skills of the chemist is being able to tinker with invisible molecules and evanescent forces in order to create sizable objects. Crystal engineering deals with elaboration of concepts at the molecular scale in order to act on macroscopic properties. Here we explore the fascination of the reverse approach: we analyze and measure macroscopic morphologies obtained by crystallizing from different solvents an organometallic molecule $\text{Ru}(\text{p-cym})\text{Cl}_2(\text{LOH})$ that contains functions potentially able to give many supramolecular synthons, and derive from these measures a ranking of the intermolecular forces responsible for molecular self recognition. We also test and quantify how different functional groups interact with different solvents. The model of Periodic Bond Chains (PBC) is generally used to predict the growth morphology of minerals or of organic compounds by estimating the most relevant interaction energies [1]. By reversing the approach, here we identify the supramolecular synthons active in the packing through the analysis of the growth morphology, by using the argument that the most developed faces must contain two non parallel PBCs. This allows to single out the supramolecular pairs linked by the

main PBCs and stabilized by the principal supramolecular synthons. In addition, the comparison of the the growth rates along the different PBCs depending on the solvent allows to estimate the degree of interaction between the solvent and the different functional groups exposed on the faces.

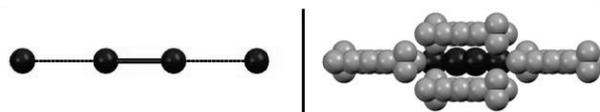
[1] Hartman P.; Perdok W.G. *Acta Cryst.* 1955, 8, 49.

Keywords: Crystal Engineering, Molecular Recognition, Periodic Bond Chains

FA4-MS31-T05

Size Matching of Interacting Moieties: A Design Principle in Crystal Engineering. Giuseppe Resnati^{a,b,c}, Antonio Abate^a, Manu Lahtinen^d, Pierangelo Metrangolo^{a,b}, Tullio Pilati^c, Kari Rissanen^d, Giancarlo Terraneo^{a,b}. ^aNFMLab - D.C.M.I.C. "Giulio Natta", Politecnico di Milano, Via L. Mancinelli 7, 20131 Milan, Italy. ^bCNST - IIT@POLIMI, Politecnico di Milano, Via G. Pascoli 70/3, 20133 Milan, Italy. ^cC.N.R. - I.S.T.M., University of Milan, Via C. Golgi 19, 20133 Milan, Italy. ^dDepartment of Chemistry, Nanoscience Center, University of Jyväskylä, Post Office Box 35, Jyväskylä FI-40014, Finland. E-mail: giuseppe.resnati@polimi.it

Theoretical investigations proved that the linear I_4^{2-} ion is unstable. A search in the Cambridge Structure Database (CSD), in fact, reveals that there are only eight crystal structures containing the symmetric polyiodide I_4^{2-} as a discrete unit. The symmetric I_4^{2-} species may be described as an I_2 molecule bound at both ends each to one Γ ion through linear halogen bonding, that is the intermolecular interaction involving halogen atoms as electrophilic species [1]. We reasoned that matching the symmetric I_4^{2-} polyiodide species with a dication wherein the space separation of the two positive charges is similar to the size of the I_4^{2-} dianion, should increase the strength of electrostatic interactions in the ionic lattice, thus driving forcefully the selective formation of the target polyiodide species. In this communication, we show that bis(trimethylammonium)hexane diiodide encapsulates iodine from solution and through a gas/solid reaction yielding in a predictable and controllable manner the selective formation of the rare polyiodide species $\Gamma \cdots \text{I}-\text{I} \cdots \Gamma$, which matches in length the chosen dication [2]. The size matching method is general and can be extended to the predictable obtainment of other uncommon polyhalide species. This has the potential for significantly augmenting our knowledge of polyhalide species, as well as providing a novel approach to the field of their design and synthesis.



[1] P. Metrangolo, G. Resnati, *Science* 2008, 321, 918. [2] A. Abate, M. Brischetto, G. Cavallo, M. Lahtinen, P. Metrangolo, T. Pilati, S. Radice, G. Resnati, K. Rissanen, G. Terraneo, *Chem. Commun.* 2010, 46, 2724-2726 (Front Cover).

Keywords: Halogen Bonding, Polyiodides, Crystal Engineering