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Isostructurality and Morphotropism of Published 2,4,6-Triphenoxy-1,3,5-triazines Alajos Kálmán, Petra Bombicz, *Institute of Structural Chemistry, Chemical Research Center, Hungarian Academy of Sciences, Budapest, Hungary*. E-mail: akalman@chemres.hu

Keywords: Isostructurality, morphotropism, polymorphism

The semirigid triphenoxy-1,3,5-triazine (POT) molecule and its 2X-, 3X- and 4X- (mainly *halo*-) substituted derivatives enabled us to demonstrate different morphotropic links (including polymorphism) [1] between the groups of isostructural crystals hallmarked by space groups $R\bar{3}c$, $P6_3/m$, $R\bar{3}$, $P\bar{3}c1$ etc. Since all of these structures have been published to elucidate their ability to form Piedfort complexes (PUs) e.g. [2], no one paid attention to those structural connections which are established between them by non-crystallographic rotations or translations. Our present (supplementary) results demonstrate the power of perception.

(i) The 2D-isostructurality of POT (space group Ia) and 4-FPOT ($P2_1/c$) are related by a turn of C_3 -PUs through 180° sitting on every second c glide plane, around axis b . (ii) Relationship between the $R\bar{3}c$ and $P6_3/m$ dimorphs of 4-BrPOT, the second is isostructural with 4-CIPOT, is established by a turn of every second molecule of the C_3 -PU diads through 180° perpendicular to the trigonal axis. (iii) *Mutatis mutandis*, a turn of 60° between the eclipsed molecules of 4-CIPOT linked by $3/m$ symmetry may result in a novel columnar stacking ($\bar{3}$), if X atoms migrate from para to meta positions. However, space group $R\bar{3}$ is maintained only in 3-IPOT. (iv) In case of the smaller substituents [2], every second C_{3i} -PU diad from the trigonal ($\bar{3}$) columns turns upside down which results in space group $P\bar{3}c1$. In the new columnar array the C_{3i} -PU diads are separated by D_3 -PUs and *vice versa*.

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Supercooled High Spin State in Metallo-supramolecular Assemblies, Ullrich Pietsch^a, Martin Lommel^a, Yves Bodethin^a, Dirk Kurth^b, Guntram Schwarz^b, Helmut Möhwald^b ^a*Solid State Physics Department of Physics, University of Siegen, Germany*. ^b*Imax-Planck-Institute of Colloid and Interface Science, Potsdam, Germany*. E-mail: pietsch@physik.uni-siegen.de

Keywords: Molecular magnetism, supramolecular assemblies, structure analysis

In contrast to the current line of molecular magnetism to synthesize molecules or molecule clusters with large spins, the concept of designing supramolecular assemblies containing small magnetic units is most flexible and tunable. An especially versatile approach relies on metallo-supramolecular polyelectrolyte amphiphile complexes self-assembled from bis-terpyridine ligands and amphiphilic molecules hosting octahedrally

coordinated Fe^{2+} - or other transition metal ions [1,3]. The Fe^{2+} ion can be induced to switch between a low-spin and a high spin electronic state near room temperature. Using experiments of x-ray scattering, x-ray magnetic circular dichroism and magnetic measurements at powdered material the spin transition has been identified as a transition from the diamagnetic $t_{2g}^6e_g^0$ low spin state to the magnetic $t_{2g}^4e_g^2$ high-spin state and is induced by a structural order-disorder transition of the amphiphilic matrix upon heating. The temperature of phase transition can be modified by the number and length of amphiphils attached. In contrast to thin organized films the induced spin transition is not reversible and can be classified as super-cooled high-spin state which might be stabilized by the disorder and interdigitation of amphiphilic molecules. Low temperature measurements may reveal possible anti-ferromagnetic spin coupling between Fe^{2+} ions. The temperature of spin transition and the amount of the magnetic moment can be tuned by mixtures of Ni^{2+} and Fe^{2+} ions [3].

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A Singular Noninterpenetrating Coordination Polymer with the Pt_3O_4 Structure Xavier Solans,^c Ana B. Gaspar,^a Ana Galet,^b M. Carmen Muñoz,^b and José Antonio Real^a, ^a*Universitat de València*. ^b*Universitat Politècnica de València*. ^c*Universitat de Barcelona, Spain*. E-mail: xavier@geo.ub.es

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The homoleptic low-spin complex $[Fe(L)_3]^{2+}$, where L is the bisbidentate ligand 1,10-phenanthroline-5,6-dione, coordinates Na^+ ions via exo-oriented dione groups defining a three-dimensional cationic network $\{[Fe(L)_3]_4Na_3\}^{11+}_n$ with Pt_3O_4 topology. The large volume generated by the network is filled with 11 perchlorate ions, 7 " $NaClO_4$ " ionic pairs, and 9 H_2O molecules. Singular $[Na^+]_4$ units, in which the Na^+ ions are practically uncoordinated, are formed. Crystal data formula $C_{144}H_{90}Cl_{18}Fe_4N_{24}Na_{10}O_{105}$, $M = 4927.18$, cubic, space group $Pm\bar{3}n$ (No. 223), $a = 23.6270(10)$ Å, $V = 13189.42$ Å³, $Z = 2$, $\rho_{calc} = 1.236$ g cm⁻³, $F(000) = 5028$, $\mu(Mo K\alpha) = 5$ cm⁻¹; 2387 reflections observed [$I > 2\sigma(I)$]; $R1 = 0.0656$, $wR2 = 0.1688$.

The X-ray single-crystal structure revealed a cationic polymeric framework composed of mononuclear species $[Fe(L)_3]^{2+}$ assembled by Na^+ cations $[Na(1)]$. The FeII atoms lie in an almost regular octahedral environment defined by six N atoms belonging to three L ligands. Four $[Fe(L)_3]^{2+}$ units with alternating chirality assemble, defining a pseudocubic coordination site for $Na(1)$. The large intraframework spaces which the Na^+ ions can be considered uncoordinated. The cationic covalent network $\{[Fe(L)_3]_4Na_3\}^{11+}$ constitutes a rare example of a (3,4)-connected non-interpenetrated coordination polymer based on the structure of the binary oxide Pt_3O_4 . The $Na(1)$ atoms and the $[Fe(L)_3]^{2+}$ units play the role of the 4-connected Pt