

Two enantiomeric molecules of (I) are linked by N-H...O hydrogen bonds. These N-H...O hydrogen bonds generate $R_2^2(12)$ rings, which also have two edge-fused S(5) rings, resulting in an S(5)[$R_2^2(12)$]S(5) motif [1]. The structure (II) is stabilized by N-H...O, C-H...O and C-H... π interactions. The N-H...O hydrogen bonds generate two C(6) chains one within the other and these chains are linked by C-H...O hydrogen bonds generating and $R_2^2(21)$ ring motif. Two inversion-related molecules of (III) are linked by N-H...O hydrogen bonds generating an $R_2^2(12)$ ring motif. There are no direction specific aromatic π - π interactions between adjacent rings in of (III), but two C-H... π interactions link parallel phthalide rings [2]. The phthalide part of the molecules are planar in all three compounds and the dihedral angles between the phthalide group and the benzene ring are 63.26 (8)°, 62.81(8)° and 71.18 (5)° for I, II and III, respectively.

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MS19 P14

First atomic structure of bacterial S-layer protein reveals a novel protein architecture Tea Pavkov^a, Eva M. Egelseer^b, Margit Sara^{b†}, Walter Keller^a, ^aK.F. University Graz, Austria. ^bCenter for Nanobiotechnology, University of Natural Resources and Applied Life Sciences, Vienna, Austria. [†]deceased May 2006
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Keywords: 3D-structure, bacterial S-layer, SAXS

Surface layer (S-layer) proteins are one of the most abundant cellular proteins with the ability to form a very uniform surface on the prokaryotic cell. Different functions, from protection to recognition, are proposed. In spite of their biological importance for the functionality of prokaryotic cells, high resolution structural information of S-layer proteins is very scarce. The main reason for the absence of 3-D structural information resides in the tendency of S-layer proteins to self-assemble into 2-D crystalline lattices, thereby preventing the formation of 3-D crystals.

For obtaining 3D-crystals and determining the structure-function relationship of SbsC, the S-layer protein from *G. stearothermophilus*, deletion mutants were produced. It was shown that the N-terminal part is responsible for binding of the secondary cell wall polymer (SCWP) and that the C-terminal part is essential for self-assembly [1].

We present here the first structure of a bacterial S-layer protein. The C-terminally truncated form rSbsC₍₃₁₋₈₄₄₎ was crystallized [2] and the structure was solved by MIRAS to 2.9Å. It revealed a novel ring-like architecture with an interesting fold at the N-terminus and disordered second part of the molecule. Since the structure was difficult to refine the approximate domain boundaries were determined and new truncation mutants designed. The structure of another truncation mutant was solved to 2.4Å using the well defined domains from rSbsC₍₃₁₋₈₄₄₎ structure as a starting model. The structures were compared and flexibility between the domains could be observed. In order to investigate the behaviour of the truncated mutants in solution, SAXS experiments were performed. Surprisingly, the protein behaves differently in the solution showing an elongated conformation. This finding confirmed the large inter-domain flexibility of the protein.

Furthermore, the thermostability of truncation mutants was investigated in presence and absence of SCWP. A drastic stabilization of the protein was observed when SCWP is bound.

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MS19 P15

Predicted and experimental crystal structures of nitroanilines and nitrophenols Grażyna Wójcik and Izabela Mossakowska, *Institute of Physical & Theoretical Chemistry, Wrocław University of Technology, 50-370 Wrocław, Poland.*

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Keywords: crystal structure prediction, polymorphism, nitrobenzenes

The crystal structure prediction experiment has been performed for several single-substituted nitrobenzenes, i.e. ortho-, meta and para-isomers of nitro-, halogeno-, nitrilo-, isonitrilo- and methyl derivatives, as well as nitrophenols, nitroanilines, nitrobenzaldehydes and nitrobenzoic acids. The prediction was carried out using the *Polymorph Predictor*, module of *Cerius²* program [1, 2]. The Monte Carlo simulated annealing was used for searching crystal structures corresponding to global minimum in the lattice energy for several chosen space groups [3]. An intermolecular force field was used to calculate intermolecular energy, which consisted of coulombic, polarisation, dispersion and repulsion terms [1]. The lattice energy was calculated as a sum of interactions using the atom-atom potential approach. The molecular geometries were minimized using three different methods: a force-field or semiempirical quantum methods, or *ab initio* RHF/6-31g^{**}.

The results of the prediction procedure concerning dinitrobenzenes, halogenonitrobenzenes, nitrilo- and isonitrilobenzenes, and methylnitrobenzenes were satisfying. The structures predicted successfully (i.e. very similar to the known experimental crystal structures) were found among ten predicted structures of lowest energies.

The results of prediction of anilines, phenols, aldehydes and acids were far worse. The crystal structures of 3 isomers of nitroanilines have not been found. The reason for that may consist in an improperly determined charge distribution in those highly polarizable molecules. In case of nitrophenols only the low-temperature polymorphs of m- and p-nitrophenol have been found. The negligence of temperature and entropic effects may be the reason for that. The crystal structure of o-nitrophenol have not been found. However, the density of the real crystal of o-nitrophenol is far smaller than the densities of the predicted crystal structures of lowest energies. This result suggests that the known crystal structure may correspond to a high-temperature polymorph. Search for another polymorph is at the moment in progress. The predicted crystal structures will be presented and discussed in terms of important interactions and possible molecular synthons in the crystals.

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MS19 P16

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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MS19 P17

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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MS19 P18

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*.

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Keywords: iron complex, crystal structure, inclusion compound

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