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], [a]*K.F. University Graz, Austria.* [b]*Center 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 thermostabiliy 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, nitrobezaldehydes and nitrobenzoic acids. The prediction was carried out using the *Polymorph Predictor*, module of *Cerius*[2] 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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