

s8.m28.o2 **Dipeptide Nanotubes: Towards a Functionalized Channel Interior.** Carl Henrik Görbitz, Department of Chemistry, University of Oslo, Norway. E-mail: c.h.gorbitz@kjemi.uio.no

Keywords: Peptides; Nanotubes; Crystal Engineering

A systematic survey of the crystal structures of dipeptides constructed from the five hydrophobic amino acid residues L-Ala, L-Val, L-Ile, L-Leu and L-Phe has unexpectedly revealed that certain of them form nanotubes [1-3]. Depending on the nature of the pores and the hydrogen bond network, these structures fall into two distinct families: A) Crystals of compounds with two small side chains have hexagonally symmetric (space group $P6_1$), hydrophobic pores with van der Waals' diameter between 3.2 and 5.3 Å. The common hydrogen bond network is three-dimensional. This group is called the **VA**-class after L-Val-L-Ala [1], and includes also L-Ala-L-Val, L-Val-L-Val, L-Ala-L-Ile, L-Ile-L-Ala, L-Val-L-Ile and L-Ile-L-Val [2]. B) Crystals of compounds with two large side chains have hydrophilic pores and size range from rectangular 2.5 x 6.0 Å to circular with diameter 10 Å. This structural family has been referred to as the **FF**-class after L-Phe-L-Phe [3]. Other members are L-Leu-L-Leu, L-Leu-L-Phe, L-Phe-L-Leu, and L-Ile-L-Leu. The work presented here is focused on L-Ile-L-Ile (**II**). From an aqueous solution, **II** is easily crystallized as an orthorhombic dihydrate without pores [4]. Crystallization from trifluoroethanol (TFE), on the other hand, yielded the spectacular structure of **II** hydrate TFE solvate, which is related to, but not a member of the **VA**-class. It is unique among nanoporous peptide structures not only due to the share size of the pores, with diameter about 10 Å, but also by the fact that the cocrystallized TFE solvent molecules occupy "alcohol sites" on the interior walls of the channels. The potential substitution of TFE with designed alcohols after crystallization sets the path for obtaining nanotubes with a functionalized interior. Potential applications include use as chiral containers and separators, in catalysis and more.

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- [4] Görbitz C.H., *Acta Crystallogr.*, 2004, **B60**, submitted.

s8.m28.o3 **Whole Profile Fitting to Electron Diffraction Patterns from Nanocrystalline Powders.** János L. Lábár, Research Institute for Technical Physics and Materials Science, Budapest, Hungary. E-mail: labar@mfa.kfki.hu

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Extraction of individual line intensities without using an explicit structure model can be done in the ProcessDiffraction program (Lábár, 2000), which is available free from the internet: <http://www.mfa.kfki.hu/~labar/ProcDif>. Part of the distortions introduced by lenses is compensated by averaging the intensity along ellipses in contrast to perfect circles. Eccentricity of about 2% is not uncommon in electron diffraction and it is difficult to detect by the naked eye. It is generally identified by comparing the measured rings to reference circles on the screen, or alternatively, by making measurements of ring diameters in different directions. An automatic peak search (using first and second derivatives) locates the (overlapping) peaks. The list of automatically detected peaks can be edited manually. In case of preliminary identified phases, peak positions can also be taken from a list of peaks, calculated for the identified phases.

Quantitative pattern decomposition uses an empirical model for the background and the peak positions taken from the above list. Presence of broad, diffuse peaks under the interesting (narrower) peaks can also be identified manually. Parameters in the model are determined from a least square fit of the model pattern to the measured pattern. The primary parameters to optimize during the least square fit are the peak shape parameters and the peak area for each individual peaks. Optionally, background parameters and the parameters describing the amorphous components can also be optimized within the same iteration. At present, three different shape functions can be selected for the background (Gaussian, called "normal", log-normal and polynomial) and also three functions (Gaussian, Lorentzian and Pseudo-Voigt) can be selected for peak shapes. Peak width parameters can (optionally) be optimized individually or connected through a simple formula as a function of peak position. This is similar, but not identical to the approach introduced for XRD (Caglioti *et al.*, 1958). Parameters can be switched on and off during consecutive steps of iteration, while tolerance for detecting convergence can also be adjusted. Probing of the parameter-space for the global minimum is done by using a downhill SIMPLEX method (Nelder and Mead, 1995). Alternative functions for the background and for the peak shapes, furthermore alternative approaches for locating the global minimum are planned to be introduced in later versions of the program.

Poor resolution of electron diffraction restricts pattern decomposition to systems with higher symmetry. Modification of the program to perform a Rietveld-type refinement is planned in coming versions.

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