fields such as medical chemistry (drug delivery systems), host-guest chemistry, catalysis and molecular electronics.

[1] Lehn J.-M., *Angew. Chem.,Int. Ed. Engl*., 1988, **27**, 89, *ibid*. 1990, **29**, 1304. [2] Lehn J.-M., Atwood J. L., Davies J. E. D., MacNicol D. D., Vögtle F., *Comprehensive Supramolecular Chemistry*, Eds. Pergamon, Oxford, 1996.
Keywords: supramolecular, noncovalent interactions, coordination compounds

MS38.26.4
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Recognition of Weak Interactions at the Gas-crystal Interface
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Molecular self-assembled materials are promising in several fields such as gas storage, selective recognition, separation and modulation of the functions of active molecules. The application of the principles of self-assembly and crystal engineering permit the shaping of specific nanoscale environments where guest molecules, through new weak interactions, are entrapped. We could obtain an empty-pore hexagonal structure (solved by single-crystal analysis) held together by a network of weak interactions and fabricate supramolecular architectures that cooperatively stabilize gases that diffuse in. The molecular crystal can store large amounts of carbon dioxide and methane selectively over nitrogen, oxygen and hydrogen [1]. NMR spectroscopy could measure intermolecular distances and recognize the specific interactions that contribute to the overall stabilization. The impressive upfield shifts caused by the aromatic ring currents on gas molecules at the van der Waals contacts provide a tool for understanding the preferred topology of the gases interacting with the inner surface of the porous crystal. A variety of conjugated molecules can be encapsulated in the infinite nanochannels of 0.5 nm of the host matrix. Weak host-guest CH···π and π···π interactions form collectively a stable architecture with all the active molecules aligned along the crystallographic *c* axis in thermally stable single crystals.

[1] Sozzani P., Bracco S., Comotti A., Ferretti L., Simonutti R., *Angew. Chem. Int. Ed.*, 2005, **44**, 2. [2] Sozzani P., Comotti A., Bracco S., Simonutti R., *Angew. Chem. Int. Ed.*, 2004, **43**, 2811.
Keywords: molecular crystals, intermolecular interactions, NMR spectroscopy

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Peptide-Based Organic Microporous Materials
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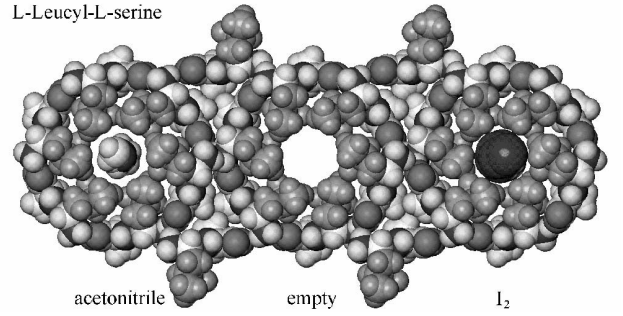
In the last few years, small peptides have emerged as an unexpected source of microporous materials. Uniquely among organic molecules, these compounds may not only form crystal structures with nanotubes with der Waals' diameter from 3.2 to 10 Å, but cocrystallized solvent molecules located in the channels can often be removed with full retention of the peptide scaffold. Subsequently, absorption of other organic or inorganic molecules can take place.



This presentation gives an overview of the known microporous peptide structures, with special emphasis on recent experimental results, as for the dipeptide L-leucyl-L-serine (see illustration).
Keywords: nanotubes, peptides, supramolecular structures

MS39 POWDER DIFFRACTION OF PROTEINS
Chairpersons: Robert H. Blessing, Jeremy Cockcroft

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Recent Developments in Protein Structure Analysis from Powder Diffraction Data
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The central problem in using powder diffraction data for the solution of crystal structures is that the structure factor information is severely limited relative to that obtained from a single crystal covering the same region of reciprocal space. The scattering from a single crystal is represented in reciprocal space by an array of slightly broadened delta functions; their intensity measurement is a simple integration of the peak intensity above background. For a powder diffraction experiment, the reciprocal space picture is of a nested series of spherical shells broadened by sample and instrumental effects; the density of these shells increases cubically with distance from the reciprocal space origin. Their intensity corresponds to that of the structure factor responsible for the shell and its multiplicity. Extraction of the individual structure factor intensities that form the powder pattern is then compromised by the increasing overlap of these shells. This is particularly acute for proteins as the diffraction patterns are made from a very large number of structure factors. However, the unprecedented sharpness of protein powder pattern peaks and their position sensitivity to sample environment provides a means of overcoming the loss of information. This talk will present some recent results on the problem of extracting structure factors and the improvement possible from using combinations of protein powder patterns.
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Keywords: powder diffraction, proteins, structure determination

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Molecular Replacement with Powder Diffraction Data
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As more and more protein folds become known, the molecular replacement (MR) method[1] becomes a more attractive method for structure solution. We will demonstrate that synchrotron powder data are sufficient to solve the simple MR problem of finding the position and orientation of the origin of the unit cell with respect to a single protein molecule. A series of examples of small proteins (including lysozyme, trypsin, myoglobin, thaumatin and apoferritin) that cover symmetries from cubic down to monoclinic will be described.

The challenges encountered in more complex molecular replacement problems depend on both the quality of the search model and experimental data. For single-crystal experiments, the data are effectively error free and this essentially reduces to a question of model quality. The peak overlap problem can be so severe for powder experiments that significant gains are possible when peak overlaps are accounted for. The effects of both counting statistics and instrumental resolution on the likely success of a molecular replacement approach with powder data will also be discussed. While the finding that powder data are sufficient for simple molecular replacement problems is not surprising in view of the complexity of small molecule structures that are now be solved from such data, the routine applicability to macromolecular structures remains to be established.

[1] Rossman M. G., *Acta.,Cryst.*, 1990, **A46**, 73-82.
Keywords: powders, proteins, molecular replacement