

indexing programs: ITO, TREOR90, DICVOL, KOHL, TAUP, FJZN, and LZON. The atomic coordinates obtained by Monte Carlo methods were used to initialize the Rietveld refinements, which were performed using the FULLPROF program [2].

In both cases, NA ligand "organizes" the packing by strong amide-amide hydrogen bonds forming a 3D network with four complexes around each other.

[1] T. Roisnel and J. Rodríguez-Carvajal, *Mater. Sci. Forum.* **2001**, *118*, 378 [2] J. Rodríguez-Carvajal, FULLPROF, V. 1.9c. LLB, CEA/Saclay, France, **2001**.

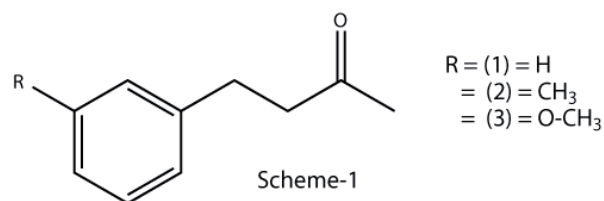
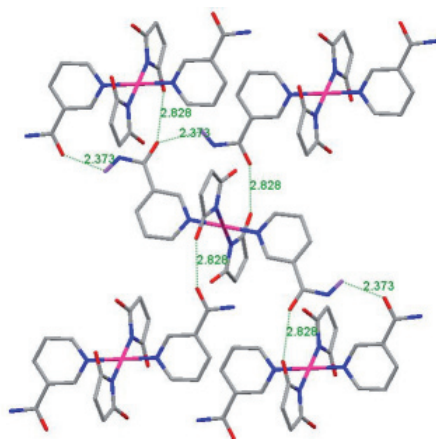
**Keywords:** synchrotron, rietveld, palladium

## MS10.P05

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**Crystal structure from X-ray powder diffraction data with  $Z'=2$**   
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Phenylpropionic acid derivatives exhibit a strong binding ability to peroxidases, which catalyze the oxidation of a number of organic and inorganic substrates. Structural studies of phenylpropionic acid derivatives carried out by our group revealed that the crystal structures are predominantly built up by carboxylic acid dimers forming  $R_2^2(8)$  synthons. In the course of our ongoing program of structural characterization of organic compounds from X-ray powder diffraction data, we came across 3-phenylpropionic acid (**1**), 3-(3-methylphenyl)propanoic acid (**2**) and 3-(3-methoxyphenyl)propanoic acid (**3**) [scheme 1]. Crystal structures of three compounds have been solved from laboratory X-ray powder diffraction data using direct-space approaches and refined by Rietveld method using the program GSAS package with an EXPGUI interface. Hirshfeld surface analysis of compounds were also performed to visualize and discriminate the features of molecular interactions in the compounds. The essential difference between the 3-phenylpropionic acid (**1**) and the compounds **2** and **3** is the presence of different substituent at the 2 positions (methyl group in **2** and methoxy in **3**). The asymmetric unit of compounds **1-3** contains two molecules ( $Z'=2$ ). The carboxylic acid group in **1-3** forms O-H...O hydrogen bonded dimer with O1...O2 distances of 2.683(5) - 2.902(3) Å in an  $R_2^2(8)$  graph-set motif. The interconnection of  $R_2^2(8)$  rings via C-H...O hydrogen bonds generates a ladder-like one dimensional architecture based on fused  $R_2^2(14)$  and  $R_4^4(20)$  synthons in **1**. Pairs of molecules forming  $R_2^2(8)$  rings are further connected through intermolecular C-H...O hydrogen bonds to generate three dimensional structures in compound **2**. In **3**, however, the interconnection of  $R_2^2(8)$  rings via C-H...O hydrogen bonds generates a two dimensional architecture based on edge fused  $R_4^4(32)R_2^2(14)$  synthon. Although crystal structures of molecular compounds can now be accomplished from X-ray powder diffraction data, structure solution of compounds with  $Z'>1$  is not very common.



**Keywords:** Powder diffraction,  $Z$  prime>1, Hirshfeld surface.

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**TALP: A L.S. structure solution program of molecular compounds from powder data**

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In recent years, global optimization methods are increasingly important in crystal structure determination of molecular compounds from powder diffraction data. Most procedures make extensive use of simulated annealing or other more or less exotic optimization algorithms [1]. Here a general easy-to-implement method based on the well-known L.S. algorithm is presented which allows solving crystal structures of a wide variety of relatively complex compounds. TALP structure solution program is based on a global optimization technique which combines a random/incremental iteration strategy for positioning the molecule with an ultra-fast Rietveld refinement. The geometry of the molecule is fixed by restraints. Unlike other structure solution programs, atom coordinates but not torsion angles are refined. Torsion angles are used only to create initial pseudo-random models.

TALP has been tested on powder diffraction data of molecular compounds of different complexity. For simple compounds with cell volumes up to 1400 Å<sup>3</sup> and 4 torsion angles, the solution is obtained straightforwardly. More complex structures with e.g. cell volumes up to 3500 Å<sup>3</sup>, up to 8 torsion angles, and two independent molecules in the unit cell, have been also solved but longer time is required. Although TALP is focused on organic compounds, also coordination compounds have been successfully solved.

[1] W.I.F. David, K. Shankland, *Acta Cryst.* **2007**, *A64*, 52-64.

**Keywords:** Powder diffraction, molecular compounds, *ab initio* structure solution

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**Crystal structures and humidity-dependent phase transitions of Gly-L-Tyr hydrates**

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Oligopeptides are one of the physiologically active substances and used as medicines, sweeteners, and food additives. They frequently crystallize as hydrates, and crystal structural transformations are induced by hydration and dehydration processes. Under such backgrounds, we aim to carry out *ab initio* crystal structure determination of oligopeptides