therefore extremely fast, enabling thousands of comparisons to the carried out per second on a standard PC.

[1] Morris R.J., Najmanovich R.J., Kahraman A., Thornton J.M., *Bioinformatics*, 2005, *in press*.

Keywords: bioinformatics, function prediction, active-site recognition

P.02.11.1

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Powder Struture Resolution of 1,7-Dioxaspiro[4.4]nonane

Bruno Dacunha[a], Francisco Alonso[b], Jaisiel Meléndez[b], Miguel Yus[b], [a]*RIAIDT, Edificio CACTUS, Universidade de Santiago de Compostela, Spain.* [b]*Facultad de Ciencias, Instituto de Síntesis Orgánica (ISO), Universidad de Alicante, Spain*. E-mail: raiosxp@usc.es

Different attempts to crystallise compound 1,7-dioxaspiro[4.4]nonane, led to very small and irregular crystals which were not good enough to be analysed by the single-crystal X-ray diffraction technique. Moreover, the data collected with powder diffraction technique, was very poor to work with conventional direct methods for the structure solution.

The powder pattern was indexed using the program suite Crysfire. We have modeled different configurations in agreement with the other experimental analyses in order to test them with the powder diffraction data. We have located the different modeled solutions into the refined unit cell with the F.O.X. program. The Rietveld method was used for the refinement of the positions of non H atoms using the Bruker AXS Topas program.

Based on the results of the above mentioned method, it is possible to conclude that the technique of structural resolution by powder diffraction data is sensitive to changes of the atomic positions, or on the nature of atoms of the modeled molecule, and that this technique has allowed the confirmation of the structure of mentioned compound as it was suggested by means of spectroscopic techniques.

Keywords: powder structure resolution, organic structure determination, 1,7-dioxaspiro[4.4]nonanes

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The Structure Determination of Single-component Molecular-metal

Eiji Nishibori[a], Yuichi Fujishiro[a], Makoto Sakata[a], Akiko Kobayashi[b], Masaki Takata[c], Hayao Kobayashi[d], [a]*Department of Applied Physics, Nagoya University, Nagoya, Japan.* [b]*Research Centre for Spectrochemistry, Graduate School of Science, The UniVersity of Tokyo, Hongo, Japan.* [c]*Japan Synchrotron Research Institute and CREST, Kouto, Japan.* [d]*Institute for Molecular Science and CREST, Okazaki , Japan.* E-mail: eiji@mcr.nuap.nagoya-u.ac.jp

The single-component molecular metals, $Ni(tmdt)_2$ [1] and related materials, have attracted much interests due to their characteristic properties. Many other related materials have been produced by changing the metal atom and extended-TTF ligands. The crystal structure determination of newly produced materials is often very difficult due to only small amount of powder sample being available.

In this study, we determined 5 crystal structures of $Ni(tmdt)_2$ related materials, which are $Ni(dt)_2$, $Pd(dt)_2$, $Au(tmdt)_2$, $Pd(tmdt)_2$, and $Pd(dmdt)_2$, by Genetic Algorithm combined with MEM/Rietevled method using synchrotron radiation X-ray powder diffraction data measured at SPring-8, BL02B2. The reliability factors, Rwp and RI, of Rietveld refinements are in the the range of 2~4% and 3~7%, respectively. It was found that the molecular stacking is different by the length of extended-TTF ligands. It is found that the positional relation of neighboring layers is closely related to the conductivity of materials.

[1] Tanaka H., et al., *Science*, 2001, **291**, 285-287.

Keywords: single-component molecular-metal, SR powder diffraction, genetic algorithm

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Ab-initio Structure Determination of $C_{18}H_{19}N_4S$ from Powder X-ray Diffraction

Hwo-Shuenn Sheu[a],Ozen Ozgen[a.b], Ying Hsiu Lin[a], Engin Kendi[b], Nesrin Gokhan[c], [a]*National Synchrotron Radiation Research Center, Hsinchu, Taiwan.* [b]*Department of Physics Engineering, Hacettepe University, Ankara, Turkey.* [c]*Department of Pharmacy, Hacettepe University, Ankara, Turkey.* E-mail: hsheu@nsrrc.org.tw

The crystal structure of 1-(N-allythiacarbamoyl)-3-(4-methyl-phenyl)-5-(pyrol-2-yl)-2-pyrazoline, $C_{18}H_{19}N_4S$, has been solved by the method of simulated annealing from synchrotron x-ray powder diffraction data. Pyrazolines are known to display various biological functions, such as fungicidal, antibacterial activities, pharmacological properties such as anti-inflammatory agents and industrial applications. The powder sample was sealed in 1mm capillary and diffraction data was collected with curved imaging plate method using 12KeV x-rays at the BL01C2 beamline in National Synchrotron Radiation Research Center (NSRRC). The structure was determined while following these procedures: (1) determination of the unit cell parameters, (2) determination of the space group, (3) extraction process by Pawley method, (4) structure solution by simulated annealing using DASH (David et al., 1998) and (5) Rietveld refinement by GSAS (Larson &Von Dreele, 1990) programs. The title compound crystallizes in triclinic system with space group, $P\ \bar{1}$, unit cell parameters of a = 12.603(14), b = 9.094(8), c = 8.494(8)Å, α = 70.85(8)°, β = 105.26(8)°, γ = 109.10 (7)°, Volume = 855.7Å^3 and Z=2. The final reliability factors of Rietveld refinement are R_{wp} = 0.039 R_p = 0.029 R_B = 0.118 and S = 1.041.

Keywords: ab-initio structure determination, drug design, synchron powder diffraction

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Structure Determination from Powder Data of two Sub-peptides of Leu-enkephalin

Andy Fitch, Luca Palin, *ESRF, BP220, F-38043 Grenoble Cedex, France.* E-mail: fitch@esrf.fr

The crystal structures of two tripeptides, sub-peptides of leu-enkephalin which belongs to the opiate family of neuropeptides, have been solved from high resolution powder diffraction data using synchrotron radiation. Glycine-phenylalanine-leucine, $C_{13}N_3O_4H_{21}$, is monoclinic, space group $P2_1$, with a = 20.0024(8) Å, b = 4.8738(1) Å, c = 10.2778(2) Å, ß = 103.940(1)°, Z = 2, at room temperature. Glycine-glycine-phenylalanine, $C_{17}N_3O_4H_{24}{\cdot}2H_2O$, recrystalised from water is orthorhombic, space group $P2_12_12_1$, with a = 30.3902(2) Å, b = 10.25972(8) Å, c =4.83972(4) Å, Z = 4. The structures were solved via global optimization, programs TOPAS and FOX, and the use of maximum entropy maps.

Keywords: powder crystallography, peptides, synchrotron X-ray diffraction

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Crystal Structures of 8-Styrylxanthine Analogs from Powder Diffractin Data

Wieslaw Łasocha[1], A. Rafalska-Łasocha[1], P. Talik[2], M. Pawłowski[2], [1]*Faculty of Chemistry,* [2]*Collegium Medicum, Department of. Pharmaceutical Chemistry; Jagiellonian University, Kraków, Poland.* E-mail: lasocha@chemia.uj.edu.pl

Adenosine modulates several physiological functions acting via specific G-protein-coupled receptor subtypes identified as A1, A2a, A2b and A3. Since the discovery that xanthines are the most important class of potent and selective antagonist at adenosine receptors (AR), the interest in this class of compounds has significantly increased. A novel classes of A2aAR antagonists [1] were investigated by means of X-ray powder diffractometry and the crystal structures of some analogs of 8-styrylxanthines: $C_{14}H_{13}N_6O_2Cl$, $C_{14}H_{14}N_6O_2$ (azo-analogs) and $C_{15}H_{14}N_5O_2Br$ (imine-