

Phage fibre proteins may also find applications in nanotechnology or in recognition of pathogenous bacteria and their elimination (phage therapy).

Bacteriophage T4 contains six short and six long fibres. The long fibres are responsible for initial host cell recognition. They contain a trimer of gp34, a single copy of gp35, a trimer of gp36, and a trimer of gp37. T4 fibre proteins need the chaperone gp57 for correct folding. Gp37 also needs a second chaperone, gp38. We have expressed gp37 by co-expression with gp57 and gp38 and solved the structure of the gp37 receptor-binding needle domain.

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Keywords: virus, fibre, structure

L.A.10

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New copper based MOF's built up from 1,2,3,4-cyclobutanetetracarboxylate ligand.

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One of the areas of solid-state chemistry that has shown remarkable growth over the last two decades concerns the synthesis and characterization of metal-organic magnetic materials (MOFs). As part of our ongoing study of molecular materials, we reported several studies of correlation between crystal structure and magnetic properties in a tetracarboxylate ligand with different metal ions [1]. In this communication we report the current studies with the 1,2,3,4-cyclobutanetetracarboxylate ligand (cbt)⁴⁻. Three new copper(II) metal-organic compounds have been synthesized using the gel technique varying the stoichiometry of the reaction in an effort to prepare low density frameworks [2].

The [Cu₂(cbt)(H₂O)₄].2H₂O (**1**) complex is built up by two different inorganic tapes: one formed by dinuclear copper(II) assemblies, and a second one formed by triple-bridge copper(II) regular chains. These inorganic tapes are kept together through the cbt that acts as a connector in a hexakis-monodentate way, giving rise to a 2D structure. The [Cu₂(cbt)(H₂O)₄].2H₂O (**2**) compound presents a 3D structure where the cbt acts as pentakis-monodentate, giving rise to a porous structure with two different types of square channels running along the *c*-axis. Crystallization and coordination water molecules are allocated in the bigger channels, while in the small ones there are only coordination water molecules. The [Cu₃(cbt)₂(OH)₂(H₂O)₈].8H₂O (**3**) compound presents a crystallographically independent cbt acting simultaneously as hexakis-monodentate and bidentate. This intricate coordination mode produces a 3D porous crystal structure, with cavities along the *b*-axis where the crystallization water molecules are allocated.

Here we present the X-ray single-crystal diffraction studies, the thermogravimetric analysis, and the magnetic studies of this new family of MOFs that opens new possibilities in the field of multifunctional materials.

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Preparation and molecular structure of the complex [Sn^{IV}(C₄₄H₂₈N₄)(OCN)(OH)]

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For a review of porphyrin complexes [1] and For the synthesis of tin(IV) porphyrin species [2].

The title complex, [Sn^{IV}(C₄₄H₂₈N₄)(OCN)(OH)], exhibits substitutional disorder of the OH⁻ and OCN⁻ axial ligands. The Bis[(cyanato-*O*)(hydroxo)(0.5/0.5)][(5,10,15,20-tetraphenylporphyrinato-κ⁴N)tin(IV)] has been synthesized and characterized by UV-vis, IR and proton NMR and the tin ion presents the oxidation state IV, Thus, the cyanato-*O* ligand and the hydroxyl group bonded to the central Sn^{IV} atom share statistically the axial position. The X-ray molecular structure shows that the Sn^{IV} ion is hexacoordinated by the four N atoms of the pyrrole rings of the tetraphenylporphyrin (TPP) and the O atoms of the two disordered OCN⁻ and OH⁻ axial ligands. The equatorial tin-pyrrole N atom distance (Sn—Np) is 2.100 (2) Å and the axial Sn—O(OCN) or Sn—O(OH) bond length is 2.074 (2) Å. The complex [Sn^{IV}(C₄₄H₂₈N₄)(OCN)(OH)] crystallizes in the monoclinic space group *P2₁/c* with unit cell dimensions a=11.2943(6) Å, b=12.6972(7) Å, c=13.0711(8) Å, β=114.251(2)°. The structure was refined to R=3.9%, WR2=9.7% and S=1.13.

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Keywords: Sn-porphyrin, cyanato-*O* ligand

L.A.12

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Development of Cubic Anvil Type High Pressure Apparatus for Neutron Scattering at Low Temperature Koji Munakata^{a,b}, Hideki Ishida^b, Kittiwit Mathan^b, Soushi Ibuka^b, Taku J Sato^b, Masakazu Nishi^b, Kazuyuki Matsubayashi^b, Yoshiya Uwatoko^b, Hiroyuki Kagi^c, ^aResearch Center for Neutron Science & Technology, Comprehensive Research Organization for Science and Society (CROSS), Tokai, Japan. ^bThe Institute for Solid State Physics (ISSP), The university of Tokyo, Kashiwa, Japan. ^cGraduate School of Science, The University of Tokyo, Tokyo, Japan. E-mail: k_munakata@cross.or.jp

In recent years, as an important physical measurement device, various types of high pressure apparatus have been developed for each experimental purposes [1]. Among them, cubic (multi) anvil type apparatus is more suitable for good-hydrostatic pressure [2]. Another merit of this apparatus is that which has relatively large sample space. On the other hands, in the field of neutron experiments, high pressure technique is less common compared to other experiments due to the inevitable difficulty, such is a significant decrease in intensity by absorption and scattering when the neutrons pass through a pressure device which surrounds the sample: it is difficult to conduct experiments with reliability and accuracy.

Recently, we have developed small and/or compact high pressure apparatus for transport and magnetic measurements, a clamp type Palm Cubic Anvil Cell (PCAC) [3] (Fig. 1). PCAC can generate superior hydrostatic pressure than other high pressure apparatus at low temperature.

In this work, for neutron scattering experiments, we optimized the anvil material of PCAC from tungsten carbide (WC) to zirconia (ZrO_2) which has relatively strong material strength and relatively transparent to neutron beams. Pressurization test was carried out at room temperature. Duralumin (A7075), aluminium-based hard material, was used for a gasket. Deuterated glycerol was chosen as a pressure transmitting medium because of its good hydrostatic property. A single crystal of NaCl, about $1.5 \times 1.5 \times 1.5 \text{ mm}^3$ in size, was set in the gasket and pressurized with a hydraulic press. Generated pressures in the gasket were estimated from a compressibility of NaCl by determining a lattice constant from (200) reflection at each external load. We confirmed that a generating pressure was about 7 GPa when a load of 80 ton is applied. For low temperature measurement, 4 K closed-cycle refrigerator was used together with PCAC. We expect that PCAC will be useful apparatus in the field of high pressure and low temperature neutron experiments.

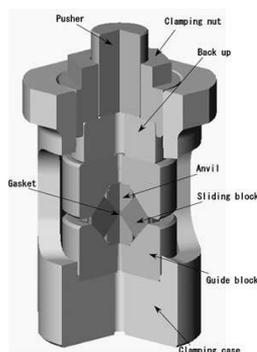


Fig. 1 Schematic cross sectional view of clamp type PCAC.

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Keywords: high pressure, low temperature, neutron scattering

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Protein Tectonics Platform That Facilitates Synchrotron Radiation Life Science Hajime Saburi, Hisashi Naitow, Katsuhide Yutani, Michihiro Sugahara, Tomoyuki Tanaka, Yoshinori Matsuura, Tetsuya Ishikawa, Naoki Kunishima, *Protein Crystallography Research Group, RIKEN SPring-8 Center, Harima Institute*. E-mail: hajime_saburi@spring8.or.jp

To understand rationally the function of protein that supports life activities, it is necessary to determine its 3D-structure at atomic level. The X-ray crystallography analysis had previously been the most efficient and popular way to determine protein 3D-structures at atomic level. However, as a result of structural genomics on the hyperthermophile *Thermus thermophilus* HB8, it was revealed that proteins yielding analyzable crystals were only 20% in the genome. To construct a high-throughput framework for the structure determination of challenging targets such as membrane proteins and supramolecular complexes, and to contribute to relevant industrial applications such as structure-based drug design, we launched the Protein Tectonics Platform (PTP) at the SPring-8 campus, Japan, on the basis of synchrotron radiation protein crystallography resources

that had been built in the national structural genomics project of Japan's "Protein 3000" initiative (FY 2002-2006).

The PTP at the RIKEN SPring-8 Center enables beamline users to conduct efficient and complete protein science experiments within the SPring-8 campus. The PTP acts as an integrated hub by taking advantage of its location, just 5 minutes from the SPring-8 beamlines. The PTP's technical staff gained experience managing the state-of-the-art platform for the synchrotron radiation protein crystallography with the Protein 3000 project. The combination of the SPring-8 beamlines, the high-performance facility, and the experienced technical staff will promote innovative bio-science in the SPring-8 campus.

In order to disseminate Protein 3000 results for the benefit of society, the PTP is now available to various research groups inside and outside RIKEN. In this poster, detailed contents of the PTP and its availability will be introduced.

Keywords: PTP, SPring-8, Protein 3000

L.A.14

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The Influence of Apatite-Plate Orientation on the Behaviour of Living Cells Marzena Suder,^a Małgorzata Tyszcza-Czochara,^b Katarzyna Stadnicka,^a *Department of Crystal Chemistry and Crystal Physics, Faculty of Chemistry, Jagiellonian University, Kraków.* ^b*Faculty of Pharmacy, Jagiellonian University Medical College, Kraków (Poland)*. E-mail: suderm@chemia.uj.edu.pl

The adsorption of acidic non-collagenous proteins like phosphophoryn and osteonectin on faces of synthetic single-crystal hexagonal hydroxyapatite, $Ca_5(PO_4)_3(OH)_2$ was found to be preferential for (10-10) face [1]. It has also been shown *in silico* studies that the adsorption of three amino acids: glycine, proline and hydroxyproline, the major components of the collagen type I, is preferential at monoclinic hydroxyapatite (01-10) face [2]. The adsorption of proteins at (10-10) affects the crystal morphology of bone apatite so the crystals are elongated in c-direction. Since adhesion of living cells to surface of biomaterials is mediated by protein layer, the different faces of apatite may cause different cellular behaviour. The representative minerals of apatite family, with the general chemical formulae $[A(1)_2][A(2)_3](BO_4)_3X$ [3] and $P6_3/m$ space-group symmetry, were investigated in respect of the influence of crystallographic orientation on the fibroblast cells. The number of living cells proliferating on the single-crystal mineral plates with crystallographic orientations (10-10), (10-11) and (0001) was evaluated by direct counting, and by the measurement of formazan absorbance and by the luminescence assay for ATP detection. The cytotoxicity of the mineral samples was excluded in MTT test. Single-crystal X-ray diffraction was used to determine the crystal structure of the mineral apatites confirming their chemical formula: $Ca_5(PO_4)_3F_{0.69}(OH)_{0.31}$, $Ca_5(PO_4)_3F_{0.55}(OH)_{0.43}Cl_{0.02}$ and $Ca_{4.74}(PO_4)_3F_{0.24}(OH)_{0.24}Cl_{0.05}$. Our results clearly indicate the preferential interaction of the fibroblast cells with the (10-10) plates.

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