MS29-P4 Structure factor for generalized Penrose tiling

Maciej Chodyn[1], Pawel Kuczera[1,2], Janusz Wolny[1]

1. Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Krakow, Poland
2. Laboratory of Crystallography, ETH Zurich, Zurich, Switzerland

email: maciej.chodyn@gmail.com

The Generalized Penrose Tiling (GPT) [1,2] can be considered a promising alternative for Penrose Tiling (PT) as a model for decagonal quasicrystal refinement procedure, particularly in the statistical approach (also called the Average Unit Cell (AUC) approach) [3].The statistical method using PT has been successfully applied to the structure optimization of various decagonal phases [4]. The application of the AUC concept to the GPT will be presented.

In the higher dimensional (*n*D) approach, PT is obtained by projecting a 5D hypercubic lattice through a window consisting of four pentagons, called the atomic surfaces (ASs), in the perpendicular space. The vertices of these pentagons together with two additional points form a rhombic icosahedron. The GPT is created by projecting the 5D hypercubic lattice through a window consisting of five polygons, generated by shifting the ASs along the body diagonal of the rhombic icosahedron. Three of the previously pentagonal ASs will become decagon, one will remain pentagonal and one more pentagon will be created (for PT it is a single point). The structure of GPT will depend on the shift parameter, its building units are still thick and thin rhombuses, but the matching rules and the tiling changes. Diffraction pattern of GPT have peaks in the same positions as regular PT, however their intensities are different.

Binary decagonal quasicrystal structure with arbitrary decoration for a given shift value was simulated. Its diffraction pattern was calculated using AUC method [5,6]. Generated diffraction pattern were used as "experimental data set" in structure refinement algorithm made to test the refining of shift parameter.

Literature

[1] K. N. Ishihara, A. Yamamoto, Acta Cryst. (1988), A44, 508-516

[2] A. Pavlovitch, M. Kleman, J Phys a-Math Gen. (1987), 20, 687-702

[3] J. Wolny, Phil. Mag. (1998), 77, 395-414

[4] P. Kuczera, J. Wolny, W. Steurer, Acta Cryst. (2012), B68, 578–589

[5] B. Kozakowski, J. Wolny, Acta Cryst. (2010), A66, 489-498

[6] M. Chodyn, P. Kuczera, J. Wolny, Acta Cryst. (2015), A71, 161–168

Keywords: quasicrystals, structure factor, Generalized Penrose Tiling

---

MS30. Structure and function in coordination compounds

Chairs: Marijana Đaković, Janusz Lipkowski

MS30-P1 Synthesis and structural studies of dioxomolybdenum(VI) complexes with isoniazid-related hydrazones

Biserka Prugovečki[1], Višnja Vrdoljak[1], Marina Cindrić[1], Ivana Pulić[1], Dubravka Matković-Čalogović[1]

1. Division of General and Inorganic Chemistry, Department of Chemistry, Faculty of Science, University of Zagreb, Croatia

email: biserka@chem.pmf.hr

The chemistry of hydrazones is continuing to be an interesting area of research because of their modularity, easiness of synthesis and stability towards hydrolysis.[1–3] Synthesis of the dioxomolybdenum(VI) complexes $[MoO_2(HL^R)(MeOH)]Cl$ (**1**–**3**), was carried out using MoO_2Cl_2 and the corresponding aroylhydrazone ligand H_2L^R (salicylaldehyde isonicotinoylhydrazone (H_2L^{SIH}), 2-hydroxy-naphthaldehyde isonicotinoylhydrazone (H_2L^{NIH}), or *p*-(*N*,*N'*-diethylaminosalicylaldehyde isonicotinoylhydrazone ($H_2L^{Et2NSIH}$) in methanol. Compounds $[MoO_2(HL^R)(H_2O)]Cl$ (**1a**–**3**a) obtained upon exposure of the coresponding mononuclear complexes **1**-**3** to moisture were also investigated. Deprotonation of the mononuclear complexes $[MoO_2(HL^R)(MeOH)]Cl$ (**1**–**3**), was performed using Et_3N as a base (by conventional solution based-method and mechanochemical aproach) as well as by UV-light assisted reactions yielding $[MoO_2(L^{SIH})(MeOH)]$ (**4**) [4], $[MoO_2(L^{NIH})(MeOH)]$ (**5**) and $[MoO_2(L^{Et2NSIH})]_n$ (**6**), respectively. Crystal and molecular structures of all complexes were solved by the single-crystal X-ray diffraction method. In all complexes the ligand coordinates the metal centre of the *cis*-MoO_2^{2+} core tridentately *via* phenolic-oxygen, azomethine-nitrogen and ketohydrazone oxygen forming five and six member chelate rings. The remaining sixth coordination site of the distorted octahedron is occupied by the oxygen atom of the solvent molecule (methanol in **1**-**3** and **5**, water in **1a**–**3a**) or nitrogen atom of the bridging izonicotinyl moiety of the neighboring complex (in **6**). We were interested to investigate importance of nonbonding interactions in the structures, especially the ability of these complexes to form different hydrogen bonding motifs depending on the protonation state of the complexes.

[1] S. Banerjee, A. Ray, S. Sen, S. Mitra, D. L. Hughes, R. J. Butcher, S. R. Batten and D. R. Turner, *Inorg. Chim. Acta.,* 2008, **361**, 2692.

[2] J. G. Vos and M. T. Pryce, *Coord. Chem. Rev.*, 2010, **254**, 2519.

[3] A. Kobayashi, D. Yamamoto, H. Horiki, K. Sawaguchi, T. Matsumoto, K. Nakajima, H.-C. Chang and M. Kato, *Inorg. Chem.*, 2014, **53**, 2573.

[4] S. Gao, L.-H. Huo, H. Zhao and S. W. Ng, *Acta Cryst.* 2004, **E60**, m1757.

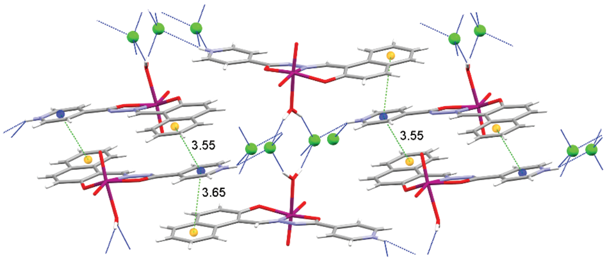

Figure 1. Layers of complex ions in 2a. Hydrogen bonds are shown by blue dotted lines and $\pi \bullet\bullet\bullet \pi$ interactions by green dashed lines. The distance between centroids is given in Å.

Keywords: dioxomolybdenum(VI) complexes, deprotonation, structural studies, hidrazones

MS30-P2 Oxo-bridged dinuclearCr^{III}-Ta^{V} complex: structural and spectroscopic characterization

Lidija Androš Dubraja[1], Marijana Jurić[1]

1. Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia

email: Lidija.Andros@irb.hr

The oxo-bridged metal units are interesting intramolecular motifs appearing in several bioinorganic molecules such as metalloproteins (Fe–O–Fe core) and in various inorganic systems, especially as polyoxometallates, materials with outstanding properties and functions.[1,2] Recently, unusual behaviour that causes the changes in material color and magnetic properties has been observed in structures with Cr–O–Cr bridges, referred as metal-to-metal-charge transfer (MMCT).[3] Even though there are several reports of light- and heat-induced MMCT, the occurrence of this intriguing phenomena is hard to predict and the relationship between electron transfer and molecular structure is not jet understood.[4]

In the recent years our research group has been involved in intensive studies related to tris(oxalato)oxotantalate(V) anion, with the aim of obtaining new metal-organic coordination systems with specific (electrical, optical, catalytic and/or magnetic) properties. It was found that this type of anion is prone to form heterometallic complexes with different topologies and nuclearities.[5] Depending on reaction conditions and reagents, the oxo group in $[TaO(C_2O_4)_3]^{3-}$ can be protonated or replaced with other ligand in the coordination sphere of tantalum.[6] Reaction of water solutions of complex $[Cr(bpy)_2(OH_2)]^{3+}$ cations and $[TaO(C_2O_4)_3]^{3-}$ anions yielded compound with new bonding topology of this anion – dinuclear oxo-bridged complex $[Cr(bpy)_2(OH_2)(\mu\text{-O})Ta(C_2O_4)_3]_2\cdot 7H_2O$ (**1**) (bpy = 2,2´-bipyridine). Compound **1** was characterized by single-crystal X-ray diffraction, IR and UV/Vis spectroscopy. Figure 1 shows dinuclear $[Cr(bpy)_2(OH_2)(\mu\text{-O})Ta(C_2O_4)_3]$ unit, with chromium in octahedral geometry and tantalum in distorted pentagonal bipyramidal geometry. Single crystal measurements at room temperature and at 100 K have shown some differences in the unit cell parameters, as well as in the M–(O, N) bond lengths, which my indicate the change of oxidation state of metal centres. Further magnetic and MMCT studies of **1** are in progress.

[1] J. B. Vincent *et al.*, *Chem. Rev.*, 1990, **90**, 1447–1467; [2] D.-L. Long *et al.*, *Angew. Chem. Int. Ed.*, 2010, **49**, 1736–1758; [3] T. J. Morsing *et al.*, *Inorg. Chem.*, 2014, **53**, 2996–3003; [4] E. S. Koumousi *et al.*, *J. Am. Chem. Soc.*, 2014, **136**, 15461–15464; [5] a) L. Androš *et al.*, *Inorg. Chem.*, 2013, **52**, 14299–14308; b) L. Androš Dubraja *et al.*, *CrystEngComm*, 2015, **17**, 2021–2029; [6] L. Androš *et al.*, *CrystEngComm*, 2013, **15**, 533–543.