

## MS29-P4 Structure factor for generalized Penrose tiling

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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 ( $nD$ ) 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

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## MS30. Structure and function in coordination compounds

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

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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  $[\text{MoO}_2(\text{HL}^R)(\text{MeOH})]\text{Cl}$  (**1-3**), was carried out using  $\text{MoO}_2\text{Cl}_2$  and the corresponding aroylhydrazone ligand  $\text{H}_2\text{L}^R$  (salicylaldehyde isonicotinoylhydrazone ( $\text{H}_2\text{L}^{\text{SIH}}$ ), 2-hydroxy-naphthaldehyde isonicotinoylhydrazone ( $\text{H}_2\text{L}^{\text{NIH}}$ ), or *p*-(*N,N'*-diethylaminosalicylaldehyde isonicotinoylhydrazone ( $\text{H}_2\text{L}^{\text{Et2NSIH}}$ ) in methanol. Compounds  $[\text{MoO}_2(\text{HL}^R)(\text{H}_2\text{O})]\text{Cl}$  (**1a-3a**) obtained upon exposure of the corresponding mononuclear complexes **1-3** to moisture were also investigated. Deprotonation of the mononuclear complexes  $[\text{MoO}_2(\text{HL}^R)(\text{MeOH})]\text{Cl}$  (**1-3**), was performed using  $\text{Et}_3\text{N}$  as a base (by conventional solution based-method and mechanochemical approach) as well as by UV-light assisted reactions yielding  $[\text{MoO}_2(\text{L}^{\text{SIH}})(\text{MeOH})]$  (**4**) [4],  $[\text{MoO}_2(\text{L}^{\text{NIH}})(\text{MeOH})]$  (**5**) and  $[\text{MoO}_2(\text{L}^{\text{Et2NSIH}})]$  (**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*- $\text{MoO}_2^{2+}$  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 isonicotinyl 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.

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