

orientation matrix and re-indexing of the corresponding reflection lists (Smart, XDS). The complete range of programs is freely available as Linux- or Windows-version upon contacting the authors.

Keywords: reciprocal space mapping; software; diffuse X-ray scattering

FA4-MS01-P08

Modeling of Decagonal Quasicrystals. Sofia Deloudi^a, Walter Steurer^a. ^aLaboratory of Crystallography, ETH Zurich, Switzerland.
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Quasiperiodic phases seem to naturally withstand the quantitative description we use for most periodic structures (for an overview of the field, see [1]). Providing good models is therefore crucial in order to understand quasiperiodic structures. They have to bring down the geometric principles of quasiperiodic structures to a few simple concepts, while closely resembling the real structures. Furthermore, they are useful tools for physicists in order to provide a good starting point for simulations. These demands can be fulfilled by the well-established technique of cluster-based modeling.

Among the axial quasicrystal structures, the system Al-Co-Ni is the best studied, but the discussion about the structures within this system is still ongoing. Its suitability as a model system is excellent because of several reasons. The phase diagram is well investigated and shows a wide range of modifications of the decagonal phase as a function of composition and temperature. Large single crystals can be easily grown, and electron-microscopic and surface-imaging methods can be used due to the short translation period along the tenfold axis.

In a previous work [2] we have presented a fundamental cluster with 20 Å diameter which makes it possible to model all decagonal phases in the system Al-Co-Ni (including the approximants) systematically, with small changes in the atomic structure.

We have now extended the modeling to the systems Al-Co-Cu and Al-Fe-Ni, showing that it is possible to derive all these complex phases from only one building principle. Furthermore, it was even possible with this approach to predict and explain atomic flip positions within the structures of all phases.

Here, we will concentrate on the discussion of geometrical aspects of the models for Al-based decagonal QCs with a four-layer periodicity, such as the generation of flip positions and superstructures, and we will discuss the agreement of our models with experiment.

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Keywords: quasicrystal; decagonal; modeling

FA4-MS01-P09

For Some Commensurately Modulated Structure, Different Index Conditions Can See Different

Average Structures. A. David Rae. *The Research School of Chemistry, the Australian National University, Canberra, ACT 0200, Australia.*
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Layer stacking may allow alternative origins or orientations for adjacent layers. A different sequence may give a different origin or orientation of a structure, but different unit cells and space groups are also possible. When different sequences coexist we need to upgrade the refinement model, especially when the prototype layer adjusts for different layer sequences.

Crystals of Bi(SPh)₃ are a case in point. Reflections for k even, $h+k = 4N$ define a 1:1 disordered parent structure in space group $C2/c$, $\mathbf{a}_p = \frac{1}{2} \mathbf{a}$, $\mathbf{b}_p = \frac{1}{2} \mathbf{b}$, $\mathbf{c}_p = \mathbf{c}$ in which only the S are resolved. Disordered layers perpendicular to \mathbf{a}^* of $P2_1/c$ symmetry can only be ordered by doubling b to create a $Z=4$ layer of $P2_1/c$ symmetry. The Bi is near a screw axis. Ordered stacking chooses between layer origins $\frac{1}{2} \mathbf{b}$ apart, implying 4 parameters, but 8 possible layer sequences after fixing the origin of the first layer. Four of these have $P2_1/n$ symmetry modulo $\mathbf{a}, \mathbf{b}, \mathbf{c}$, but different origins. The other 4 can be formed as linear combinations of the previous 4 and have $P2_1/n$ symmetry modulo $\frac{1}{2} \mathbf{a}, \mathbf{b}, \mathbf{c}$ (two origins) and $P-1$ modulo $\frac{1}{4}(\mathbf{a} \pm \mathbf{b}), \mathbf{b}, \mathbf{c}$ (two orientations). Observed intensity for reflections with k even, $h+k \neq 4N$ means the layers relax after ordering. The loss of $2/m$ diffraction symmetry for h odd, k odd reflections implies there is an unequally twinned triclinic component. Observation of reflections excluded by the ordered $P-1$ options means other component structures are present. Refinement of a twin of a prototype structure of $P2_1/n$ symmetry modulo $\mathbf{a}, \mathbf{b}, \mathbf{c}$ disordered over different origins is unsatisfactory. This refinement scales symmetrized components of the prototype structure and these scales vary with index condition. Excluding certain index conditions from refinement allows the remaining reflections to improve but then omitted reflections fit worse. The coexistence of different prototype structures is a necessary model extension.

I wish to thank Professor P.A.W. Dean of the University of Western Ontario for the diffraction data for this structure.

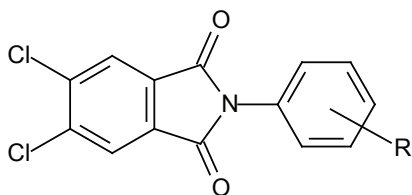
Keywords: problem structure; refinement; modulated structure

FA4-MS01-P10

Structures of Some 4,5-Dichlorophthalimide Derivatives. Orhan Büyükgüngör^a, Mustafa Odabaşoğlu^b. ^aOndokuz Mayıs University, Department of Physics, Samsun-Turkey. ^bPamukkale University, Chemistry Programme, Denizli-Turkey.
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Phthalimide derivatives have been gaining considerable interest since 1979, after recognized the hypolipidemic activity of N-substituted phthalimide derivatives [1]. Later on, researchers reported the antihyperlipidemic [2], hypolipidemic [3], anticonvulsant [4] activity and other interesting aspects [5] of phthalimide derivatives. In view

of importance of the phthalimides, we herein report the structures of (I), (II) and (III) compounds.



(I) R= 2-F; (II) R= 2-OH; (III) R= 3-OMe

The crystal structure of the (I) exhibit C-H... π , and π - π interaction. The compound (II) has C-H...O, O-H...O hydrogen bonds and C-Cl...O hetroatom interactions and the crystal structure of (III) is stabilized by aromatic π - π stacking interactions. The dihedral angle between the isoindoline units and phenyl rings in (I), (II) and (III) are 58.63(18) $^\circ$, 75.55(3) $^\circ$ and 77.63(3) $^\circ$, respectively.

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Keywords: dichlorophthalimide derivatives; X-ray analysis

FA4-MS01-P11

2- { 1- [(4-Methoxyphenyl)Imino]Ethyl} -4-Nitrophenol. Tufan Akbal^a, Ahmet Erdönmez^a, Erbil Ağar^b, Ferda Erşahin^b. ^aDepartment of Physics, Ondokuz Mayıs University, Samsun, Turkey. ^bDepartment of Chemistry Ondokuz Mayıs University, Samsun, Turkey.

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The title compound, C₁₅N₂O₄H₁₄, crystallizes in a enol amine tautomeric form.

The structure is stabilized by O-H...N intramolecular hydrogen bonds and the molecules are linked by intermolecular C-H...O hydrogen bonds. The two benzene rings are not coplanar and dihedral angle them is 68,15(5) $^\circ$. The C6-O1 and C7-N2 bond lengths verify the enol-imine tautomeric form. These distances agree with the literature [1]. The C3-N1 bond length in is also in a good agreement with the corresponding distances in the literature [2] and [3].

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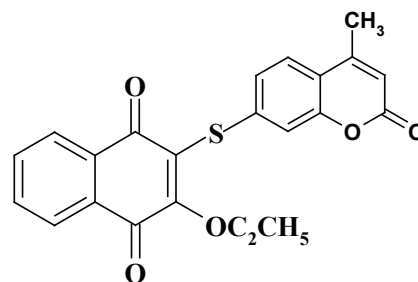
Keywords: tautomerism; crystal and molecular structure; organic compound

FA4-MS01-P12

Synthesis and Crystal Structure of 2-(7-sulfanyl-4-methyl-coumarinyl)-3-(1-ethoxy)-1,4-Naphthoquinone. N. Gulsah Deniz^a, Cemil Ibis^a. ^aIstanbul University, Engineering Faculty, Department of Chemistry, Division of Organic Chemistry, Avcılar Istanbul, Turkey.

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Quinonic compounds are of great importance to understand different processes that are related to biology. The ability to carry electrons makes them an important component of photosynthetic and respiratory electron transfer chain [1]. Naphthoquinones have been used to treat burns, cuts and all sorts of skin diseases worldwide. Sulfur containing naphthoquinones have been the subject of much interest for a number of years due to anti-inflammatory [2], anti-bacterial, anti-fungal and anti-viral biological activities [3]. In the title compound, C₂₂H₁₆O₅S, crystallizes in the triclinic space group P-1, a = 8.4474(2) Å, b = 9.1257(1) Å, c = 11.9197(2) Å, α = 84.474(4) $^\circ$, β = 84.506(4) $^\circ$, γ = 80.473(4) $^\circ$, V = 899.00(3) Å³, Z = 2, R₁ = 0.056 and wR₂ = 0.098.



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Keywords: organic structures; aromatic organic compounds; biologically important compounds

FA4-MS01-P13

Structures of Some Isoindolo-Benzoxazine Derivatives. Mustafa Odabaşoğlu^a, Orhan Büyükgüngör^b. ^aPamukkale University, Chemistry Program, Denizli-Turkey. ^bOndokuz Mayıs University, Department of Physics, Samsun-Turkey.

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Isoindolin-1-one and 2,4-dihydro-1H-benzo[d][1,3]oxazine units are commonly present in synthetic and natural products as simple structures or as a part of complex systems. A search of the literature revealed that some isoindolin-1-one derivatives have important biological properties, such as anti-microbial, anti-bacterial, anti-diarrheal, anti-inflammatory [1], anti-angiogenic [2], anti-hipertansiv, anti-fungal, anti-tumor [3], and anti-HIV [4] activities.