

P22.03.10*Acta Cryst.* (2008). A64, C622**Incommensurately modulated structure of malayamycin A**Andreas Schoenleber¹, Trixie Wagner², Olivier Loiseleur³, Vaclav Petricek⁴¹University of Bayreuth, Laboratory of Crystallography, BGI Building, Universitaetsstrasse 30, Bayreuth, State of Bavaria, 95440, Germany,²Novartis Institutes for BioMedical Research, 4002 Basel, Switzerland,³Research Chemistry, Syngenta Crop Protection AG, 4002 Basel, Switzerland, ⁴Institute of Physics, Academy of Science, 18121 Praha 8, Czech Republic, E-mail: andreas.schoenleber@uni-bayreuth.de

The bicyclic C-nucleoside Malayamycin A, C₁₃H₁₈N₄O₇, is a potent fungicide from the soil organism *Streptomyces malaysiensis* and was discovered at the Syngenta Crop Protection Laboratories [1]. In the solid state the compound exists in two different polymorphs. One consists of a regularly ordered three-dimensional arrangement which can be described in the monoclinic space group $P2_1$ with three independent malayamycin entities and five water molecules in the asymmetric unit. The other shows a modulated structure with a monoclinic basic cell and satellite reflections along the \mathbf{b}^* direction. The structure can be described in the (3+1)-dimensional superspace group $B' 2_1(0\sigma_20)$ with B' describing the additional lattice centring ($\frac{1}{2} 0 \frac{1}{2} \frac{1}{2}$). The modulation wave vector is $\mathbf{q} = (0, 0.257, 0)$. For the description of the modulated structure, the malayamycin entity is divided into several moieties, each one with its own modulation functions. While the rest of the molecule has a continuous modulation described by harmonic functions, the modulation of the urea moiety shows a discontinuous character, described by saw-tooth functions and causing a break of hydrogen bonds as function of the phase of the modulation t . The positions of the crystal water molecules are described by discontinuous crenel functions. In our presentation we will discuss the structure of the modulated phase and the resulting hydrogen bonding motive. We will also analyze the conformation of the molecule in the modulated structure as function of the phase of the modulation t and we will compare it with the conformations of the molecules in the non-modulated structure.

[1] S. Hanessian, G. Huang, C. Chemel, R. Machaalani, O. Loiseleur, *J. Org. Chem.* **70**, 6721-6734 (2005).

Keywords: molecular compound, modulated structure, superspace

P22.03.11*Acta Cryst.* (2008). A64, C622**Distinct band gaps and isotropy combined in icosahedral band gap materials**Walter Steurer¹, Daniel Sutter-Widmer¹, Pedro Neves¹, Patrick Itten¹, Rebecca Sainidou²¹ETH Zurich, Materials Science, Wolfgang-Pauli-Strasse 10, Zurich, Zurich, 8093, Switzerland, ²Instituto de Optica-CSIC, Serrano 121, 28006 Madrid, Spain, E-mail: steurer@mat.ethz.ch

Phononic (photonic) crystals are artificial composite materials which strongly interact with elastic (electromagnetic) waves. The sizes of the unit building blocks (scatterers) constituting these mesostructures, i.e., spheres, rods, or sheets embedded in a different matrix material, are chosen to match any wavelength of interest. Bragg scattering and resonances of the single scatterers both allow the formation of bands and gaps just as for electrons in crystals. Defect modes open the way for applications such as waveguides or cavities. Band gap materials (BGMs) have therefore been intensively studied in the last years.

The inherent structural anisotropy of periodic BGMs, which show at best cubic symmetry, hinders the formation of omnidirectional band gaps. This has been the motivation for the study of the higher-symmetric quasiperiodic BGMs (for a review, see [1]). Icosahedral BGMs optimally combine the distinct band gaps of periodic BGMs with the high rotational symmetry of quasiperiodic structures. This is shown experimentally for longitudinal and transverse polarized elastic waves in a phononic crystal based on the three-dimensional Penrose tiling (3D-PT) and applies equally to photonic crystals. The ability of icosahedral BGMs to form Bragg-type band gaps follows from the similarity between the 3D-PT and the fcc structure, which is its periodic average structure (PAS). 3D quasiperiodic BGMs lack bands of strong transmission like random or disordered BGMs but shows clear band gaps like periodic BGMs. Our investigation demonstrates the usefulness of PAS for the prediction of Bragg gaps in 3D phononic quasicrystals and explains the similarity between the reflection properties of icosahedral and fcc PNCs.

[1] W. Steurer and D. Sutter-Widmer, *J. Phys. D* **40**, R229 2007.

Keywords: quasicrystals, photonic crystals, ultrasonics

P22.02.12*Acta Cryst.* (2008). A64, C622**Structure analysis of layered sodium cobalt oxide hydrates based on composite crystal models**Kazunori Takada¹, Mitsuko Onoda¹, Yong-Nam Choi², Dimitri N Argyriou³, Takayoshi Sasaki^{1,4}¹National Institute for Materials Science, Japan, ²Korea Atomic Energy Research Institute, 150 Deokjin-dong, Yuseong-gu, Daejeon 305-353, Korea, ³Hahn-Meitner-Institut, Glienicke Strasse 100, Berlin D-14109, Germany, ⁴International Center for Materials Nanoarchitectonics, 1-1, Namiki, Tsukuba, Ibaraki 305-0044, Japan, E-mail: takada.kazunori@nims.go.jp

Structure analysis of sodium cobalt oxides with bilayer-hydrate structure using powder neutron diffraction data has showed that they are very unique not only in their superconductivity but also in the crystal structure. Two superconducting phases have been found: one has 2H stacking of the CoO₂ layers and the other has 3R. In spite of the different host structures, they gave very similar diffuse patterns indicating that the interpenetrated guests are common in the arrangement between the two phases. Pattern simulation based on an incommensurate composite structure model with stacking faults revealed the following guest arrangement. The guests are ordered in the galleries to form a $(2/\sqrt{3})a \times (2/\sqrt{3})a$ trigonal lattice, where a is an in-plane lattice constant for the CoO₂ layers. On the other hand along the c -direction, the stacking of a guest layer onto another is accompanied by lateral shifts to $(1/2, 0)$, $(1/2, 1/2)$, and $(0, 1/2)$ with the same probability of $1/3$ each. The cell dimension of $(2/\sqrt{3})a$ for the guest layers suggests that the host and guest subsystems may be commensurate. In fact, the commensurate model constructed by unfolding the host and guest layers into a $2a \times 2a$ superlattice, improved the fitting significantly to support the conclusion that they are commensurate.

Keywords: composite crystal, incommensurate structures, ordering