MS47-P01

Hans Hinterreiter's non-linear transformations.

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Hans Hinterreiter (1902-1989) was a Swiss painter, belonging to the Constructivist movement, who spent most of his life in Ibiza, Spain. Since 1930 he occupied himself with the laws of form and colour. Parallel to Escher, he discovered laws of coloured symmetry before crystallographers started working on them (more about it in [1]). After a period of experimentation with plane groups of symmetry, he moved to a more complex level of geometric abstract art by applying non-linear transformations to the plane-group patterns. His goal was to achieve a more dynamic rendition of the patterns used. My poster illustrates four different cases of this process, starting always with a plane-group pattern and showing both the application of non-linear transformations and coloured symmetry.
In his more complex patterns, two of which are shown on the poster, Hinterreiter created domains of affinely or perspectively distorted motif which were further combined by means of domain boundaries or by the operations of twinning, the latter being frowned upon very much by art specialists when mentioned as one of the analytical concepts. Another means of generalization used by Hinterreiter was a careful mapping of plane-group patterns onto curvilinear nets of different kinds, mostly combined with a skilful application of principles of dichroic or polychromatic symmetry.
Unlike Escher, Hinterreiter strove to achieve the aesthetic ideal of a pure abstract form [2] with its inherent symmetries. His unique, two-step approach that combines plane group patterns with the principles of coloured symmetry and non-linear transformations, his understanding of crystallographic and non-crystallographic symmetry and a meticulous application of these principles even to the most complex patterns produced a legacy close to the heart and mind of every true crystallographer.

[1] Makovicky, E. *Z.Kristallogr.* 1979, 150, 13. [2] Albrecht H.J.; Koella R. *Hans Hinterreiter, a Swiss Exponent of Constructive Art.* Wasser-Verlag Buchs-Zürich.

MS47-P02

Structure Determination of Flufenamic Acid Cocrystals from Laboratory X-ray Powder Diffraction data.

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Recently, cocrystals of an active pharmaceutical ingredient (API) have been attracting attention in the pharmaceutical industry as API cocrystals have possibilities to improve their physicochemical properties such as solubility, dissolution rate, and physical stability, compared with a single-component crystal of APIs.[1]
We have been synthesizing three types of cocrystals of an API flufenamic acid (non-steroidal anti-inflammatory drug) using three different coformers (nicotinamide, salicylic acid and benzoic acid). These cocrystal structures were determined from their laboratory X-ray powder diffraction data.
While the flufenamic acid nicotinamide cocrystal forms infinite one-dimensional chain structure through hydrogen bonds between the API and coformer molecules, in the other two cocrystals the flufenamic acid molecule is connected with the coformer through hydrogen bonds and the pairs of molecules are stacking.
Experimental and structure analysis details will be reported in this presentation.

[1] Takata N., Shiraki K., Takano R. Hayashi Y. Terada K. *Cryst. Growth Des.*, 2008, 8, 3032.

Keywords: X-ray powder diffraction, ab-initio structure determination, cocrystals

MS47-P03

A single instrument, two wavelengths and many applications.

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Increasingly we wish to obtain a much fuller understanding of materials of interest to us, beyond the standard very valuable structure determination. To do this we must use a range of crystallographic techniques and experimental conditions, often with the additional challenge that many of the most interesting samples, unfortunately, often only form very small and/or weakly diffracting crystals. To obtain the high quality results desired we need very powerful and versatile instruments; where we can use both Mo and Cu radiation, work with both small and large unit cell systems and handle these small, challenging samples. The combination of a high brilliance rotating anode dual-wavelength X-ray generator, with the RAPID II curved large area image plate detector provides a single, highly versatile instrument which can be used for a very wide range of applications. For example absolute configuration determination of a light atom compound using Cu radiation and a charge density study requiring high resolution data using Mo radiation are both experiments that this single instrument is very well suited to and which make full use of the very large resolution range and dynamic range collected on a single image. Results of studies illustrating the versatility of this instrument to carry out these experiments and others, including powder diffraction data collection will be presented.

Keywords: instrument development, chemical crystallography, absolute configuration