

Poster Presentations

[MS14-P09] [MS14 – 04] Molecular Modulated Structures: Rare Today, Ubiquitous Tomorrow? K. E. Christensen E. J. Mckinley & A. L. Thompson

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Until recently modulated molecular crystals have largely been ignored by small-molecule crystallographers. Interest in solving and refining modulated molecular structures was driven by the pharmaceutical industry [1, 2]. However, although chemical crystallographers are now becoming increasingly aware of the Devil that can lurk in the detail of the diffraction pattern [3], the majority of chemical crystallographers still either close their eyes (i.e. solve the average structure) or throw the crystals away when faced with the indications of an aperiodic structure.

With new higher intensity in-house X-ray sources and easier access to synchrotron radiation, more and more molecular structures are showing features beyond the realms of conventional crystallography. These effects include, superlattice reflections, incommensurate satellite peaks and diffuse features which can affect everything from the smallest molecules, to large macrocycles and even proteins.

In these examples, the additional features are intrinsic to the material, however, their presence can also be induced using external stimuli. For example, routine investigations into the structure of Barluenga's Reagent (bis(pyridine) iodonium(I) tetrafluoroborate, $[\text{IPy}_2]^+[\text{BF}_4]^-$) [4], demonstrated the presence of a phase transition. However to characterise it and study the structures associated with each phase, a transient phase was observed. Structure solution of the high and low temperature structures allowed a comparison to be made which suggested that the order-disorder behaviour of the BF_4^- ion is responsible for the transition observed and the formation of the lock-in phase.

These structures together with others arising from the Chemical Crystallography Service in Oxford will be discussed, together with reasons why chemical crystallographers often prefer to turn a blind eye and why this may not be possible in the future.

[1] T. Wagner and A. Schönleber, *Acta Cryst.* B65, 249 (2009).

[2] A. Schönleber, *Z. Kristallogr.* 226, 499 (2011).

[3] A. D. Bond, *CrystEngComm.* 14, 2363 (2012).

[4] J. M. Chalker, A. L. Thompson & B. G. Davis, *Organic Syntheses.* 87, 288 (2010).