MS43-P01 | Cooking Crystals: Radiation Damage in Molecular Modulated Materials

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Single-crystal X-ray diffraction is a maturing technique; with structure determination becoming more routine, there are an increasing number of non-expert users collecting data, solving and refining structures. As the technique improves, easier access to synchrotron radiation and more sensitive detectors means that more data collections are showing features beyond the realms of conventional crystallography. The concept of non-Bragg diffraction is well understood in solid state chemistry, however, the phenomena of diffuse scattering and modulation have been studied less in molecular materials.

Barluenga's reagent, IPy_2BF_4, has been shown to exhibit a transient modulated phase on cooling from a dynamic room temperature phase to an ordered low temperature structure. Systematic studies on the derivatives of Barluenga's reagent have been carried out in which iodine with bromine, the BF_4 anion is replaced with other small anions including ClO_4 and PF_6 and the pyridine is replaced with 2,4,6-trimethyl pyridine (collidine). While attempting to map the phase behaviour of these materials we discovered that the intense radiation at synchrotron facilities can interact with the satellite reflections indicative of the modulated phase. Understanding these effects could, not only improve our knowledge of the causes of modulation in molecular materials, but also further our understanding of the causes of radiation damage.