Poster Presentation

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Interpreting the effect of de-solvation on structure of molecular crystals.

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The structure effects of varying hydration/solvation levels in molecular crystals can sometimes be difficult to characterize with analytical techniques based solely on Bragg diffraction or other more common methods such as thermal analysis or spectroscopy. It can be demonstrated that supplementary scattering features such as diffuse and satellite intensities can provide insight into these processes even just from a qualitative standpoint. Understanding the nature of these processes is of great importance to many industrial applications (e.g. pharmaceuticals, bulk characterization). One previous caveat is that interpretations for these features are often restricted to experts, yet our work demonstrates this is not the case. For our examples, real-space models can be used to calculate both diffuse diffraction and inter-modulation satellite features. In one case study what we observe when the water leaves the crystal is an incomplete phase transformation and each crystallite in the bulk can be explained as being made up of disordered layers of the different structure phases with an intermediate phase layer resulting in satellite reflections. Another example demonstrates how in a crystal which has one solvent replaced for another, temperature sensitive phase transitional phenomena are induced. Models based on disorder diffraction features not only provide further insight into understanding of the de-solvation process but also could account for observed changes in PXRD from bulk. This can be related to similar material behaviors observed in diffraction patterns from more complex host-guest systems.

Keywords: Diffuse Scattering, Modulated Structure, Phase Transition