

Poster Presentations

[MS14-P02] **Pushing the limits: determining the average structure in the presence of strong diffuse scattering**
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β -Pigment Red 170, an important industrial pigment, has a structure with severe layer stacking disorder. The single-crystal diffraction pattern shows a difficult-to-disentangle mix of Bragg diffraction and strong streaks of diffuse scattering which pass through and therefore interfere with the estimation or even the detection of the Bragg intensities. We have been attempting to derive the average structure from the Bragg intensities in preparation for a more thorough analysis and modeling of the total scattering. However, the intersection of the diffuse scattering with the Bragg intensities limits what one can do using available tools to accurately integrate the Bragg reflections and leads to ambiguity in the derivation of the unit cell parameters; two unit cell choices initially seem plausible. If the rods of diffuse scattering are kept parallel to \mathbf{a}^* , these unit cells yield the space groups $P2_1/a$, $Z' = 4$ and the non-conventional $B2_1/d$, $Z' = 2$. The differences in the disordered average structure models in these two unit cells are subtle and it is not immediately clear which is correct, requiring extensive analysis of the models, including investigating all subgroups of these two space groups. The differences revolve around whether or not the symmetries displayed within and between the layers in each space group are crystallographic or non-crystallographic. We conclude that the $B2_1/d$ model is likely the best representation of the average structure, but, given the limitations in data processing, it is advisable not to reject the $P2_1/a$ model until the total scattering

pattern has been analyzed, which is currently underway. This presentation will describe our efforts to derive the average structure for β -Pigment Red 170 and show the limitations of conventional structure determination practices in such cases.

Keywords: disorder; diffuse_scattering; pigment