**Can a Computational Search Predict Complications in Single Crystal Growth?**

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To study the variation in possible crystal packing of structures with respect to the relative positions of functional groups, five dichloronitrobenzenes have been studied both experimentally and computationally. A manual polymorph screen has been carried out for each compound using a variety of solvent methods and sublimation to grow crystals.

The experimental search found considerable difficulty in growing crystals suitable for single crystal X-ray diffraction with many exhibiting multiple domains and plate-like morphologies. Redeterminations have been carried out at low temperature but have not shown a marked improvement on the published refinements.

The computational searches found the known structures as the global minimum in a few cases. For each compound, though, there were many hypothetical structures within a small energy range of that minimum with many of these being variants on the experimentally observed sheet structures.

The predicted low energy structures illustrate variations in the sheet packing which could be indicative of, for example, slippage between the layers or disorder in the stacking. A possible link between this phenomenon and the problems associated with crystal growth and structure determination will be discussed.

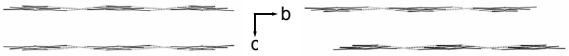


Figure 1. Two variations on the stacking of sheets related by slippage along c.

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