A Parametric Approach to Single Crystal Diffraction Data Analysis

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Snapshots of molecular crystal structures using single crystal diffraction at a single temperature yield a determination that is sufficient for many purposes. However, for systems that are undergoing change, characterisation of the structure at a series of temperatures is vital. There has been a recent increase in the number of such variable temperature studies being undertaken; however, measurements have been traditionally performed at rather few temperatures. There is relatively little evidence to date of single crystal diffraction studies involving the exploitation of data sets of an evolving molecular structure at many temperatures (say, for example, 50-100) in the more parametrically challenging regime.

We have been developing novel ideas regarding both experimental protocol and data analysis which could maximise the information content available from laboratory single crystal X-ray diffraction data. The basic idea behind the approach is that, when analysing variable temperature data, one is not examining sets of unrelated parameters at individual different temperatures, but the evolution of the fundamental parameters throughout the whole experimental period. One can thus treat the data as an ensemble and, by defining the temperature evolution of a parameter by a suitable function, fit all the data simultaneously to a single continuously evolving structural model. The approach will be outlined and selected examples of its application given.

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