

Oral Contributions

[MS11-03] Homometric Structures that Result from Data Collection using Powder Diffraction A David Rae,

Research School of Chemistry, Australian National University, Canberra, ACT 0200, Australia.

E-mail: rae@rsc.anu.edu.au

In powder diffraction correlations between the structure factors for symmetrized components of the structure are lost. This allows structure alternatives that would be distinguished using single crystal data to become indistinguishable using powder diffraction data or data from an equally twinned crystal. It will be shown how to create these alternative structures.

Many important structures can be described as modulations of a parent structure of higher symmetry. They can be described as a displacive modulation of an idealized parent structure of higher symmetry but equally well as an occupancy modulation of an equally disordered parent structure of higher symmetry that is constructed from the actual structure. The symmetrized components can then be described as a linear combination of the actual structure transformed by the various symmetry elements of the parent symmetry and the structure can be described as a linear combination of these symmetrized components.

If the actual structure can be described relative to a lattice in three or more ways that are not related by translation then alternative structures exist that are not the actual structure or its inverse in a different orientation and fit the diffraction data equally well. Consequently other considerations must be used to select the correct structure option.

Keywords: homometric structures, twinning, powder diffraction