

Poster Presentation

MS67.P44

Applications of the Twinning CIF Dictionary 1.0 for Twinned Crystals

V. Young¹, J. Hester², I. Brown³

¹University of Minnesota, Department of Chemistry, Minnesota, USA, ²ANSTO, Bragg Institute, Australia, ³McMaster University, Brockhouse Institute for Materials Research, Ontario, Canada

Version 1.0 of the Twinning CIF Dictionary was posted on the IUCr web site in February 2014.[1] The purpose of this presentation is to illustrate the application of these definitions in many common situations relevant to chemical crystallography. Within these definitions are tools to describe all known twin types as defined by the monograph by Nespolo.[2] Tools are available to describe a single twin law or combinations of unrelated twin laws. These definitions were developed mindful that experimental data should have a set format for deposition and validation through future developments of the web-based IUCr CheckCIF software. Several examples of twins will be presented to illustrate the functionality of these definitions.

[1] *Twinning CIF Dictionary 1.0*, V.G. Young Jr, I. D. Brown, and J. Hester, 18 February 2014, http://www.iucr.org/resources/cif/dictionaries/cif_twinning, **[2]** *International Union of Crystallography Commission on Mathematical and Theoretical Crystallography, Research Themes: Crystal Twinning*, M. Nespolo, 3 February 2009, <http://www.crystallography.fr/mathcryst/twins.htm>

Keywords: Twinning, CIF