Volume G: Definition and Exchange of Crystallographic Data

Sydney Hall[a], Brian McMahon[b], [a]*School of Biomedical and Chemical Sciences, University of Western Australia, Nedlands, Australia.* [b]*International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.* E-mail: syd.hall@bcs.uwa.edu.au

Volume G[1] will be launched at this congress. The highly data-dependent nature of crystallographic studies places great importance on the need for orderly acquisition and retention of data, and for computational tools that facilitate efficient data handling. To support this data-rich environment, Volume G is dedicated to the precise definition of the most commonly used data items. Although it focuses on the Crystallographic Information File (CIF) representation of data adopted by the IUCr in 1990 for journal submissions, it also considers more recent data-language developments involving XML.

CIF data dictionaries are described for *core*, *macromolecular*, *powder*, *symmetry*, *modulated-structure* and *precision-density* studies. The underpinning dictionary languages are also detailed, as are approaches for defining and storing image (binary) data. In these dictionaries, each data item is defined in terms of attributes that characterise their allowed values and mutual relationships. These provide human-readable and machine-readable descriptions of the data. However, the main use of the definitions is in a computer-software environment, so details of computer programs and libraries used with the electronic dictionaries to validate and exchange data items are also described. A CD-ROM will accompany the volume.

[1] International Tables for Crystallography, 2005, Volume G, *Definition and exchange of crystallographic data*, edited by S.R. Hall & B. McMahon, Heidelberg: Springer.

Keywords: International Tables, CIF dictionaries, data definition