



# International Tables for Crystallography, Volume G, Definition and Exchange of Crystallographic Data

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## DESCRIPTION

International Tables for Crystallography is the definitive resource and reference work for crystallography and structural science.

Each of the volumes in the series contains articles and tables of data relevant to crystallographic research and to applications of crystallographic methods in all sciences concerned with the structure and properties of materials. Emphasis is given to symmetry, diffraction methods and techniques of crystal-structure determination, and the physical and chemical properties of crystals. The data are accompanied by discussions of theory, practical explanations and examples, all of which are useful for teaching.

Volume G deals with methods and tools for organizing, archiving and retrieving crystallographic data. The volume describes the Crystallographic Information File (CIF), the standard data exchange and archival file format used throughout crystallography.

The volume is divided into five parts:

**Part 1** – An introduction to the development of CIF.

**Part 2** – Details concepts and specifications of the files and languages.

**Part 3** – Discusses general considerations when defining a CIF data item and the classification and use of data.

**Part 4** - Defines all the data names for the core and other dictionaries.

**Part 5** - Describes CIF applications, including general advice and considerations for programmers.

The accompanying software includes the CIF dictionaries in machine-readable form and a collection of libraries and utility programs.

Volume G is an essential guide for programmers and data managers handling crystal-structure information, and provides in-depth information vital for recording or using single-crystal or powder diffraction data in small-molecule, inorganic and biological macromolecular structure science.

More information on the series can be found at: <http://it.iucr.org>

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## ABOUT THE AUTHOR

Sydney Hall and Brian McMahon are the authors of International Tables for Crystallography, Volume G, Definition and Exchange of Crystallographic Data, published by Wiley.

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