

The Role of Data Ontologies in CIF Deposition and Access

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For well over a decade crystallographic data have been routinely submitted to journals and databases as CIFs. During the deposition process, data contained within a CIF can be automatically checked and validated using electronic CIF dictionaries that contain the precise definitions of individual data items. When employed, these ontologies also serve an important role when archiving or accessing deposition data, and within or between crystallographic software applications.

This talk will describe how existing ontologies are employed in CIF deposition and access processes, and what software is currently available to utilize the DDL1 and DDL2 dictionaries during the reading and writing of CIFs. We will describe how the concept of ontological definitions can be extended to automatically provide executable functionality to validation and evaluation processes.

Many aspects of this talk are covered in detail in *International Tables for Crystallography Volume G*[1], which is being launched at this congress.

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

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