Powder Diffraction CIFs: Preparation and Review

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The IUCr now strongly urges authors to submit observed and computed powder diffraction data in CIF format when publishing Rietveld results [1]. This will offer obvious benefits for the archival of data and for the testing of alternative models where structures are in dispute. The most immediate application is likely to be for manuscript review, as the quality of a Rietveld fit is best judged graphically, not from statistical figures of merit, such as profile R-factors or χ^2 values. Figures submitted for publication are seldom sufficient for close examination.

This paper will present some resources for reporting Rietveld results in CIF format, including information on software available for preparation of a CIF from a Rietveld fit. For the review of Rietveld results from a CIF, the pdCIFplot program will also be discussed [2]. This open-source program runs on all common computer platforms (Windows, Macintosh, & Unix) and allows powder diffraction data and fits to be plotted in a variety of formats directly from a CIF.

[1] http://journals.iucr.org/services/cif/powder.html
[2] http://www.ncnr.nist.gov/xtal/software/cif/pdCIFplot.html

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