

CIFFOLD: Managing Long Lines in CIF

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Until recently, information in Crystallographic Information File (CIF) format [1] was limited to 80 characters per line and there was no way to represent longer data items and comments faithfully. With the release of CIF version 1.1 [2], the maximum line size has been increased to 2048 characters and a protocol has been specified for folding and unfolding text fields and comments that exceed any given maximum line size. The C/C++ program CIFFOLD implements this line folding/unfolding protocol without loss of the semantic information in the files. This allows new, long-line CIF 1.1 files to be converted to a form suitable for processing by existing software for 80-character line CIF 1.0 files and to recover long-line CIF 1.1 files from CIFs produced by CIF 1.0 software. In addition to folding and unfolding, the software performs logical integrity checks and allows the user to set a variety of options providing control over the tradeoff between faithful versus compact representations. CIFFOLD is part of a package of CIF software for managing IUCr publications that is being upgraded from CIF 1.0 to CIF 1.1 specifications. All the new software in this package will be released under open-source software licenses. Parsers for CIF 1.1 written in C and in Fortran are included in this package.

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[1] Hall S.R., Allen F.H., Brown I.D., *Acta Cryst.*,1991, A47, 655-685. [2] <http://www.iucr.org/iucr-top/cif/spec/version1.1>

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