

5.3. SYNTACTIC UTILITIES FOR CIF

_atom_site_label	_atom_site_type_symbol	_atom_site_fract_x	_atom_site_fract_y
N21	N	0.277(3)	0.966(8)
C22	C	0.236(2)	0.778(9)
N23	N	0.137(3)	0.697(7)
C24	C	0.077(5)	0.8267(9)
N25	N	0.109(3)	1.025(8)

Fig. 5.3.3.12. Representation by the *beCIF* editor of looped data within a category (here ATOM_SITE) in spreadsheet style.

IUCr journals to visualize and prepare for publication complete papers submitted in CIF format. Chapter 5.7 describes the workflow and processing of such submissions. Here is given a brief description of the use of the *printCIF* software from an author's viewpoint.

This application also differs from others discussed in this chapter in that it is rather specific to a particular program environment, being written as Visual Basic macros embedded in a Microsoft *Word* template document. Efforts are under way to provide versions that can run with other word processors. Nevertheless, *Word* is currently sufficiently widespread that the utility is likely to be of use to a large community.

Typically the author begins by double-clicking on the icon associated with the *printcif.dot* template file. The initial macros are loaded and the author is prompted to provide the location of a CIF. As the CIF is imported into the application, the data items that will be used in the publication are extracted and converted into a rich-text format (RTF) representation. For extended text fields, this RTF content may be edited directly in the word-processing environment; this makes it easy for authors to compose and edit continuous text in a familiar way. Numeric and brief textual data items from the CIF are processed and presented in read-only fields in the manner in which they will appear in the journal, often as entries in a table or as a list of brief experimental details. These fields may not be edited within the RTF representation; if it is necessary to change these, the author must modify the data value in the CIF itself. To assist the author, the contents of the CIF are opened in a text-editor window alongside the formatted representation. The CIF and RTF representations are linked; if the author selects text in the RTF window, the corresponding CIF data item is highlighted within the text-editor window (Fig. 5.3.3.13).

The advantages to the author of editing in RTF format are that existing text may be cut and pasted from other applications, and formatting features, such as subscript or superscript text, Greek letters and other special symbols, may be entered through the word-processor's menu-driven interface, rather than by use of the rather unmemorable ASCII codings used in CIF.

The major disadvantage is the need to recognize that two versions of the file, both editable, are accessible at the same time; and care must therefore be taken to ensure that conflicting changes are not made, and that the author is aware of which version is currently the master. The function 'Update CIF using RTF' (in the toolbar of the CIF editing window) will reimport into the CIF all the editable content from the RTF window, replacing any existing data items.

Experimental

A solution containing guanidine dissolved in ethanol was heated to reflux. Cyanothiophene was added and heating was continued for 19h. The solution was allowed to cool to room temperature and the off-white precipitate was filtered and washed with cold ethanol.

Crystals of form A were obtained by dissolution of the title compound (5mg) in dry acetonitrile (2.5ml) with heating. The solution was allowed to stand at room temperature for five days. Suitable crystals of form B were obtained by dissolving the title compound (10mg) in dimethyl sulphoxide (1.5ml). The solution was allowed to stand for 2 weeks and crystals were obtained.

Compound global

Crystal data

$C_{11}H_{12}N_4S_2$
 $M_r = 260.33$
 Monoclinic, $P2_1/n$
 $a = 13.886(16) \text{ \AA}$
 $b = 4.974(6) \text{ \AA}$
 $c = 18.09(2) \text{ \AA}$
 $\beta = 111.021(10)^\circ$
 $V = 1166(2) \text{ \AA}^3$

Data collection

Marresearch Image PI
 95 frames at 2θ intervals
 Absorption correction
 $T_{min} = ?$, $T_{max} = ?$
 3652 measured reflect
 2193 independent refl

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.075$ Calculated $w = 1 / [\sigma^2(F_o^2) + (0.126P)^2 + 1.5803P]$
 where $P = (F_o^2 + 2F_c^2) / 3$

Fig. 5.3.3.13. The dual RTF/CIF editing windows in the *printCIF for Word* application. In this example, the author has selected the word 'Monoclinic' in the read-only table of crystal data; the corresponding CIF data item `_symmetry_cell_setting` is highlighted in the CIF window, where it may be edited.

The complementary function, 'Build preprint', creates a fresh copy of the preprint representation of the document in RTF format.

A number of options are available to modify the preprint that is generated (for example, by printing a complete list of the geometry included in the CIF rather than just the items flagged for publication; or listing the atomic coordinate data). The general style is that of *Acta Crystallographica Section C* and *Section E*; nevertheless, the application may be useful to users who do not intend to submit to these journals but who wish to produce an attractive representation of the content of their CIFs.

Utilities are provided to create tables in the RTF environment suitable for embedding in the CIF, to browse the contents of the CIF core dictionary and to validate the syntax of the CIF. The application is not dictionary-driven, however, and does not carry out detailed consistency checks. It is therefore best considered as an aid to publication, to be used alongside data-centric editors and validation tools such as *enCIFer*.

A particularly useful self-documenting feature of *printCIF for Word* is that the User Guide is automatically opened when the application is started, before a CIF is loaded.

5.3.4. Data-name validation

In a CIF, a data name (a character token beginning with an underscore character, `_`) is an essential handle on an item of data within a data block. Equipped only with knowledge of the data names appearing in a CIF, a user may extract, reorder or query the information content of the file. Such manipulations require no prior knowledge of the semantic content of the data. However, for most practical applications it is important to know the meaning attached to data names, and CIF dictionaries provide the mechanism for associating a data name with its intended meaning for an application. It is therefore valuable to be able to check whether data names in a CIF match those defined in a dictionary file. It is also valuable to check the consistency of the data names listed in the dictionary file itself; since this will be used by external applications to validate data names, it is essential that it be internally consistent.