

5. APPLICATIONS

5.4.12.9. Case sensitivity

A CIF may contain data names in upper, lower or a mixture of cases. Internally, *CIFtbx* does all its name comparisons in lower case, using the function `lower` (see above) to convert. Good style, however, dictates the use of certain case combinations in certain names. Therefore *CIFtbx* does this lower-case conversion as needed, preserving the original case for whatever use may be desired. An application needing maximum speed and which does not need to preserve the cases in the original CIF might consider doing the case conversion once and removing the use of `lower`.

5.4.12.10. Management of white space

CIF does not care about white space. One blank or tab is equivalent to many blanks or tabs or empty lines in separating data names from values and values from one another. The internal routine `getstr` extracts the next white-space-delimited string, using `getline` to deliver input lines from the direct-access file as required. Since Fortran does not provide dynamic memory allocation, this approach presents a problem with multi-line text fields. Rather than allocate a large fixed space that might not hold still larger text fields, the library delivers those strings one line at a time. As with case sensitivity, *CIFtbx* does white-space scanning repeatedly, keeping the original presentation (including tabs) available should an application need access to it. The author of an application needing maximum speed, not needing the original presentation and wishing to conserve disk space might wish to modify the operation of *CIFtbx* to remove all comments and compress all separating white space to single blanks or line terminators in an initial sweep.

5.4.13. Distribution

Version 2.6.4 and an early release of version 3 of *CIFtbx* are included on the accompanying CD-ROM. As later versions are developed they will be available from the IUCr (<http://www.iucr.org/iucr-top/cif>) and authors' (<http://www.bernstein-plus-sons.com/software/cif2cif>) web sites.

The release kit is a compressed C-shell archive `cif2cif.cshar.Z` or a compressed shell archive `cif2cif.shar.Z`. Only one is needed. The uncompressed files `cif2cif.cshar` or `cif2cif.shar` are needed for implementation.

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