5.4. *CIFtbx*: Fortran tools for manipulating CIFs

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5.4.1. Introduction

CIFtbx is a function library for programmers developing CIF applications. It is written in Fortran and is intended for use with Fortran programs. The first version was released in 1993 (Hall, 1993*b*) and was extended (Hall & Bernstein, 1996) to accommodate subsequent CIF applications and DDL changes. The *CIFtbx* library is for novice and expert programmers of CIF applications. It has been used to develop CIF manipulation programs such as *CYCLOPS* (Bernstein & Hall, 1998), *CIFIO* (Hall, 1993*a*), *cif2cif* (Bernstein, 1997), *pdb2cif* (Bernstein *et al.*, 1998) and *cif2pdb* (Bernstein & Bernstein, 1996). Programmers writing in C, C++ and mixed Fortran–C should consider alternative approaches, as discussed in Chapter 5.1 or in the work on *CCP4* (Keller, 1996).

The description of library functions below assumes familiarity with the STAR, CIF and DDL syntax described in Part 2. A complete *Primer and reference manual* for *CIFtbx* is provided on the CD-ROM accompanying this volume.

Fortran is a very general and powerful language, and many compilers allow programming in a wide variety of styles. However, there is a traditional Fortran programming style that ensures portability to a wide variety of platforms. *CIFtbx* conforms to this style and has been ported to many platforms. The internals of *CIFtbx* and the style chosen are discussed at the end of this chapter and in more detail in the *Primer*.

5.4.2. An overview of the library

The *CIFtbx* library is made up of functions, subroutines and variables that can be added to application programs as 'commands' to read and write CIF data. They may also be used to automatically validate incoming and outgoing CIF data. The self-checking aspects of some functions ensure that data are syntactically correct and, when used with DDL dictionaries, that individual items conform to their formal definitions.

The *CIFtbx* commands are invoked in user software as standard Fortran function or subroutine calls. For example, to open the dictionary file 'core.dic' one uses the *logical* function `dict_` as follows.

```
FN = dict_('core.dic','valid')
```

The argument `'core.dic'` is the local file identifier for the relevant dictionary. The argument `'valid'` signals that checking should be done against the data definitions in this dictionary. The local *logical* variable `FN` is returned as `.true.` if `dict_` opens the file core.dic correctly; otherwise the function is returned as `.false.`.

Some *CIFtbx* commands are issued as subroutine calls. For example, to clear the internal data tables the programmer inserts the command

```
call purge_
```

The arguments in *CIFtbx* commands have been kept to a minimum. Most of the parameter setting is handled automatically by reading and setting variables held in common blocks supplied as the file ciftbx.cmn. The type declarations for all the commands are also provided in the file ciftbx.cmn, and the programmer must '`include`' this file in each application program, function or subroutine invoking *CIFtbx* commands.

The flexibility of the CIF syntax can present some challenges to an author of applications reading or writing CIF data. This is because the information in a CIF may be in any order, have data names as either upper or lower case, and have an arbitrary spacing between data items. For example, one may extract the cell parameters from the front of a CIF and place them at the end, change all the data names from lower case to upper case, and introduce a blank line between each data name and its value, and yet the data (value) content of the output CIF will be identical to that input. *CIFtbx* provides the application writer with the tools to handle such presentation details seamlessly without altering the basic information content.

Most importantly, *CIFtbx* allows applications to be 'object-oriented', in that data items are simply requested by name without prior knowledge of the file structure. It also allows for more advanced data processing in which data items are parsed sequentially, and typed and validated *via* the dictionary. This enables items to be read independently of the names, and the data typing is automatically determined and returned. In this way, where needed, applications can go beyond the position-independent context of a CIF.

The main purpose of *CIFtbx* is to manipulate CIF data. However, there is much in common between CIF and the Extensible Markup Language XML (Bray *et al.*, 1998), and facilities have been added to *CIFtbx* to facilitate writing output in XML as well as CIF format.

CIFtbx provides four basic kinds of facilities for programmers:
(i) commands to *initialize* later handling;
(ii) commands to *read* CIF data;
(iii) commands to *write* CIF data;
(iv) variables for *monitor* and *control* signals.
These commands are described in detail below.

5.4.3. Initialization commands

Initialization commands are applied at the start of a program to set global conditions for processing CIF data. There are only two commands of this type.

```
logical function init_
  (devcif, devout, devdir, deverr)
  integer devcif, devout, devdir, deverr
logical function dict_ (fname, checks)
  character fname*(*), checks*(*)
```

`init_` is an optional command that specifies the device number assignments for the input CIF *`devcif`*, the output CIF *`devout`*, an internal scratch file *`devdir`* and the file containing error messages *`deverr`*. The internal scratch file *`devdir`* is used to hold a copy of

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references