

5.4. CIFTBX: FORTRAN TOOLS FOR MANIPULATING CIFs

Missing loop_name set as _DUMMY

Missing loop_items set as DUMMY

In processing a loop_, a dummy string has been inserted for a missing header or value.

Output CIF line longer than line_

In outputting a line, the data exceed the limit specified in line_. This occurs only if a single data name or a value exceeds this limit.

Out-of-sequence call to end text block

The termination of a text block has been invoked before a text block has been started. This can only occur with irregular use of the *Ciftbx* routines rather than the standard interface routines.

Output prefix may force line overflow

A prefix string placed in prefix_ exceeds line_ less the allowed length of tags.

Prefix string truncated

A prefix string specified to prefix_ is longer than the maximum line length allowed. The prefix string is truncated and processing continues.

5.4.11.6. Warnings: dictionary checks

Aliases and names in different loops; only using

first alias

If a DDL2 dictionary contains a loop of alias declarations, the corresponding data-name declarations are expected to be in the same loop. Only the first alias name is used.

Attempt to redefine category for item

Attempt to redefine type for item

If a DDL2 dictionary contains a category or type for a data item that conflicts with an earlier declaration, the first is used.

Categories and names in different loops

Types and names in different loops

If a DDL2 dictionary contains a loop of category or type declarations, the corresponding data-name declarations are expected to be in the same loop. Only the first category name or type is used.

Category id does not match block name

In a DDL2 dictionary, the save-frame code is expected to start with the category name. If a category name within the frame is not within a loop, it is checked against that in the frame code and a warning is issued if these do not match.

Conflicting definition of alias

A DDL2 dictionary contains a new declaration of a data-name alias which is in conflict with a previous alias definition. The first alias declaration is used.

Duplicate definition of same alias

A DDL2 dictionary contains a new declaration of an alias for a data name which duplicates a previously defined alias pair.

Item name <name> does not match category name

If category checking is enabled and the category assigned to an item name does not match the initial characters of the item name, this message is issued. This may indicate a typographical error or a deprecated item in the dictionary.

Item type <type-code> not recognised

The DDL2 dictionary type codes are translated to the DDL type codes 'numb', 'char' and 'text'. If an unrecognized type code is found no translation occurs.

Multiple DDL category definitions

Multiple DDL name definitions

Multiple DDL type definitions

Multiple DDL related item definitions

Multiple DDL related item functions

DDL1 and DDL2 declarations for categories, data names, data types and related items are used in the same data block or save frame.

Multiple categories for one name

Multiple types for one name

A dictionary contains a loop of category or type definitions and an unlooped declaration of a single data name. The first category or type definition is used.

No category defined in block <name> and name <name> does not match

A DDL2 dictionary contains no category for the defined data item and it was not possible to derive an implicit category from the block name. This usually indicates a typographical error in the dictionary.

No category specified for name <name>

A dictionary contains categories and category checking is enabled but no category is defined for the named data item.

No name defined in block

No name in the block matches the block name

These messages are issued if a dictionary save frame or data block contains no name definition or if all the names defined fail to match the block name.

No type specified for name <name>

A type code is missing from a dictionary and type checking was requested in the dict_ invocation.

One alias, looped names, linking to first

A DDL2 dictionary may contain a list of data names and a single alias outside this loop. In this case, the correct name to which to link the alias must be derived implicitly. If the save-frame code matches the first name in the loop no warning is issued, because the use of the block name was probably the intended result, but if no such match is found this warning is issued.

5.4.12. Internals and programming style

Ciftbx is programmed in a highly portable Fortran programming style. However, on some older systems, some adaptation may be necessary to allow compilation. Implementors should be aware of the extensive use of variables in common blocks to transmit information and control execution (programming by side-effects), the use of the INCLUDE statement, the use of the ENDDO statement, the names of routines used internally by the package, the use of names longer than six characters and the use of names including the underscore character.

Some aspects of the internal organization of the library to deal with characteristics of CIFs are worth noting. *Ciftbx* copies an input CIF to a direct-access (*i.e.* random-access) file, but writes an output CIF directly. All data names are converted to lower case to deal with the case-insensitive nature of CIF. A hierarchy of parsing routines is used to deal with processing white space.

The major issues of programming style and internals are summarized here. See the *Primer* on the CD-ROM for more information.