

## 3.6. CLASSIFICATION AND USE OF MACROMOLECULAR DATA

```

_citation.page_last
_citation.details (~ _citation_special_details)
_citation.title
_citation.year

```

## (b) CITATION\_AUTHOR

```

• _citation_author.citation_id
  → _citation.id
_citation_author.name
_citation_author.ordinal

```

## (c) CITATION\_EDITOR

```

• _citation_editor.citation_id
  → _citation.id
_citation_editor.name
_citation_editor.ordinal

```

The bullet (•) indicates a category key. The arrow (→) is a reference to a parent data item. Items in italics have aliases in the core CIF dictionary formed by changing the full stop (.) to an underscore (\_).

The original core CIF dictionary contained the data item `_publ_section_references` for citations of journal articles, book chapters and monographs. The authors of the mmCIF dictionary felt that a more detailed and structured approach to literature citations was required. This is provided by the mmCIF categories `CITATION`, `CITATION_AUTHOR` and `CITATION_EDITOR`. These categories were subsequently included in the core CIF dictionary and are used in the same way in both dictionaries. Section 3.2.5.1 may be consulted for details. Although `_publ_section_references` remains a valid mmCIF data item, it is expected that the `CITATION`, `CITATION_AUTHOR` and `CITATION_EDITOR` categories will be used for literature citations in mmCIFs.

## 3.6.8.2. Citation of software packages

The categories describing software citations are as follows:

```

COMPUTING group
  COMPUTING
  SOFTWARE

```

It is expected that citations of software packages in an mmCIF will be made using data items in the `SOFTWARE` category. However, in some cases, a particular publisher or database may require that this information is given using data items in the `COMPUTING` category instead (see Section 3.2.5.2 for details).

Data items in these categories are as follows:

## (a) COMPUTING

```

• _computing.entry_id
  → _entry.id
_computing.cell_refinement
_computing.data_collection
_computing.data_reduction
_computing.molecular_graphics
_computing.publication_material
_computing.structure_refinement
_computing.structure_solution

```

## (b) SOFTWARE

```

• _software.name
• _software.version
  _software.citation_id
    → _citation.id
_software.classification
_software.compiler_name
_software.compiler_version
_software.contact_author
_software.contact_author_email
_software.date
_software.dependencies
_software.description
_software.hardware
_software.language
_software.location
_software.mods

```

```

_software.os
_software.os_version
_software.type

```

The bullet (•) indicates a category key. Where multiple items within a category are marked with a bullet, they must be taken together to form a compound key. The arrow (→) is a reference to a parent data item. Items in italics have aliases in the core CIF dictionary formed by changing the full stop (.) to an underscore (\_).

The data item `_computing.entry_id` has been added to the `COMPUTING` category to provide the formal category key required by the DDL2 data model.

The data items in the `SOFTWARE` category are used to cite the software packages used in the structure analysis. The software can be described in great detail if necessary. However, for most applications a small subset of these data items, for example just `_software.name` and `_software.version`, could be used (see Example 3.6.8.1).

Most data items in the `SOFTWARE` category are self-explanatory, but a few require further comment. The data item `_software.citation_id` provides a way to link the details of a program to the citation of an article in the literature that describes the program; this data item must match a value of `_citation.id` in the `CITATION` category. The name and e-mail address of the author of the software can also be given using `_software.contact_author` and `_software.contact_author_email`, respectively. (This may be the original author or someone who subsequently modifies or maintains the software; these data items would generally refer to the person most closely associated with the maintenance of the code at the time it was used.) The release date of the software may be recorded in `_software.date`. As far as possible, the date should be that of the version recorded in `_software.version`. The data item `_software.location` may be used to supply a URL from which the software may be downloaded or where it is described in detail.

## 3.6.8.3. Citation of related database entries

Categories describing related database entries are as follows:

```

DATABASE group

```

*Related database entries* (§3.6.8.3.1)

```

DATABASE
DATABASE_2

```

Example 3.6.8.1. *The refinement program Prolsq described with data items in the SOFTWARE category.*

```

_software.name
_software.version
_software.date
_software.type
_software.contact_author
_software.contact_author_email
_software.location
_software.classification
_software.citation_id
_software.language
_software.compiler_name
_software.compiler_version
_software.hardware
_software.os
_software.os_version
_software.dependencies
_software.mods
_software.description
Prolsq unknown . program
'Wayne A. Hendrickson' ?
'ftp://rosebud.sdsc.edu/pub/sdsc/xtal/CCP4/ccp4/'
refinement ref5 Fortran
'Convex Fortran' v8.0 'Convex C220' ConvexOS v10.1
'Requires that Protin be run first' optimized
'restrained least-squares refinement'

```