

Typographical conventions used in this volume

Example	Use
<code>_atom_site_label</code>	Bold monospaced type is used for data names and in example listings representing extracts from data files. If a data name has had to be broken at the end of a line, the break follows an underscore (<code>_</code>) or full point (<code>.</code>) character. Data names broken in this way are <i>not</i> hyphenated.
<code>*_max</code>	Wildcard construction used to indicate related data names sharing a common root prefix.
<code>_diffrn_ , _diffrn_ *</code>	All related data names sharing the specified prefix (the asterisk is used where it may not be apparent that a general class of items is indicated).
<code>data_code</code>	Sloping monospaced type (as in <code>code</code>) is used to indicate variable components of a data name or other character literal string.
<code><DataBlock></code>	Monospaced type is used in formal grammars, to indicate individual tokens in the parsing of a byte stream and to indicate the verbatim value of text strings.
<code>ATOM_SITE</code>	Small capitals are used for categories of CIF data items.

Layout of the CIF dictionaries

The data dictionaries included on the CD-ROM and represented in print in Part 4 are machine-readable ASCII files. The relations between the printed (column 1) and native ASCII (column 2) representations of the dictionaries are illustrated on the facing page for DDL1 dictionaries and inside the back cover for DDL2 dictionaries.

Layout of DDL1 dictionaries

Description of a category

DDL1 does not formally describe data categories (all data items in a looped list must belong to the same category). However, pseudo data names of type 'null' ⑤ are defined to allow textual descriptions of categories and to provide examples. All such pseudo data names themselves belong to the category CATEGORY_OVERVIEW. ⑥ This assignment and the null data type are not listed in the printed version.

The printed category descriptions are boxed to make them more conspicuous. Headwords for navigation in the top line of the dictionary chapters indicate the current category at the start of a left-hand page or the close of a right-hand page.

①	EXPTL
②	Data items in the EXPTL category record details about the experimental work prior to the intensity measurements and details about the absorption-correction technique employed.
③	<i>Example 1 - based on a paper by Steiner [Acta Cryst. (1996), C52, 2554-2556].</i>
④	<pre>_exptl_absorpt_coefficient_mu 0.962 _exptl_absorpt_correction_type psi-scan _exptl_absorpt_process_details 'North, Phillips & Mathews (1968)' _exptl_absorpt_correction_T_min 0.929 _exptl_absorpt_correction_T_max 0.997</pre>

```
data_exptl []
① _name                '_exptl []'
⑥ _category            category_overview
⑤ _type                null
④ loop__example
③   _example_detail
# -----
; _exptl_absorpt_coefficient_mu      0.962
  _exptl_absorpt_correction_type     psi-scan
  _exptl_absorpt_process_details
    'North, Phillips & Mathews (1968)'
  _exptl_absorpt_correction_T_min    0.929
  _exptl_absorpt_correction_T_max    0.997
;
; Example 1 - based on a paper by Steiner [Acta
  Cryst. (1996), C52, 2554-2556].
;
# -----
② _definition
; Data items in the EXPTL category record
  details about the experimental work prior
  to the intensity measurements and details
  about the absorption-correction technique
  employed.
;
```

Description of a simple physical quantity

A typical definition takes the `_name` as headword ①, with data type and associated conditions in parentheses ranged right. The textual definition is given in a large clear type. Permitted numerical ranges are indicated (the open interval in the dictionary is explicitly indicated in print by $\rightarrow \infty$) and the category is listed in square brackets at the end of the entry. By convention, physical units ⑦⑧ are specified in the textual description and not otherwise printed, although they are indicated explicitly in the dictionary.

① **`_diffrn_ambient_temperature`** (*numb, su*) ②③

④ The mean temperature in kelvins at which the intensities were measured.

The permitted range is 0.0 $\rightarrow \infty$. ⑤

⑥ [`diffrn`]

```
data_diffrn_ambient_temperature
① _name                '_diffrn_ambient_temperature'
⑥ _category            diffrn
② _type                numb
③ _type_conditions     esd
⑤ _enumeration_range   0.0:
⑦ _units               K
⑧ _units_detail        kelvin
④ _definition
; The mean temperature in kelvins at which the
  intensities were measured.
;
```

Description of a looped item with discrete enumerated values

Here, the permitted discrete values ⑧ are listed under the legend 'The data value must be one of the following'. Any annotations to the enumerated values (using `_enumeration_detail`) appear in a parallel column.

List membership is indicated by phrases such as 'Appears in list' (when the `_list` attribute has the value 'yes') or 'May appear in list' (as here, where `_list` is 'both') ④. A mandatory list element (`_list_mandatory` appears and has the value 'yes') is indicated with the phrase '... as essential element of loop structure.' One or more items that identify the list (`_list_reference`) are introduced by the word 'containing' ⑤.

Related items are listed with the relationship (the value of `_related_function` ⑦) in parentheses, except where it is 'replace'. Then the entire entry is italicized to emphasize that an alternative data item is preferred.

① **`_exptl_crystal_colour_lustre`** (*char*) ②

③ The enumeration list of standardized names developed for the International Centre for Diffraction Data ...

May appear in list ④ containing `_exptl_crystal_id` ⑤

Related item: `_exptl_crystal_colour` ⑥ (alternate). ⑦

The data value must be one of the following:

⑧ metallic

dull

clear

⑨ [`exptl_crystal`]

```
data_exptl_crystal_colour_lustre
① _name                '_exptl_crystal_colour_lustre'
⑨ _category            exptl_crystal
② _type                char
④ _list                both
⑤ _list_reference      '_exptl_crystal_id'
⑧ loop__enumeration
    metallic
    dull
    clear
⑥ _related_item        '_exptl_crystal_colour'
⑦ _related_function    alternate
③ _definition
; The enumeration list of standardized names
  developed for the International Centre for
  Diffraction Data ...
;
```


Description of an identifier as a category key

Category keys have important roles in ensuring the integrity of the data structure in DDL2 dictionaries. They are mandatory elements, flagged by the marginal asterisk * ①. In some cases, although the item is formally necessary, its value may be derived from context. This is indicated by assigning a value of 'implicit' to `_item.mandatory_code`. In such a case the asterisk appears in parentheses (*).

Formally a single save frame may be used in a DDL2 dictionary to define all occurrences of the same identifier in different categories (indicated by the looping of `_item.name`, `_item.category_id` and `_item.mandatory_code`). To make the printed dictionary easier to read, only the primary instance ⑧ is defined in a single listing. The other instances (indicated by `_item_linked.child_name` ⑤) are defined tersely in abbreviated listings within the relevant categories.

*①② `_citation.id` (code)③

`_citation_id` (cif_core.dic 2.0.1)

④ The value of `_citation.id` must uniquely identify a record in the CITATION list. The `_citation.id` 'primary' should be used to indicate the citation that the author(s) consider to be the most pertinent to the contents of the data block. Note that this item need not be a number; it can be any unique identifier.

The following item(s) have an equivalent role in their respective categories:

`_citation_author.citation_id` ⑤,

`_citation_editor.citation_id`,

`_software.citation_id`.

⑥ Examples: 'primary', '1', '2'.

⑦ [citation]

```
save_citation.id
④ _item_description.description
; The value of _citation.id must uniquely identify a
record in the CITATION list. The _citation.id
'primary' should be used to indicate the citation
that the author(s) consider to be the most
pertinent to the contents of the data block.
Note that this item need not be a number; it can be
any unique identifier.
;
loop_
② _item.name
⑦ _item.category_id
① _item.mandatory_code
'_citation.id' citation yes
'_citation_author.citation_id' citation_author yes
'_citation_editor.citation_id' citation_editor yes
'_software.citation_id' software yes
_item_aliases.alias_name '_citation_id'
_item_aliases.dictionary cif_core.dic
_item_aliases.version 2.0.1
loop_
⑤ _item_linked.child_name
⑧ _item_linked.parent_name
'_citation_author.citation_id' '_citation.id'
'_citation_editor.citation_id' '_citation.id'
'_software.citation_id' '_citation.id'
③ _item_type.code code
loop_
⑥ _item_examples.case 'primary' '1' '2'
save_
```