# Typographical conventions used in this volume

| Example | Use |
| --- | --- |
| **\_atom\_site\_label** | 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 (\_) or full point (.) character. Data names broken in this way are *not* hyphenated. |
| **\*\_max** | Wildcard construction used to indicate related data names sharing a common root prefix. |
| **\_diffrn\_, \_diffrn\_\*** | 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). |
| **data\_*code*** | Sloping monospaced type (as in ***code***) is used to indicate variable components of a data name or other character literal string. |
| `<DataBlock>` | 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. |
| ATOM_SITE | 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**
>
> ②Data 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 *Example 1 - based on a paper by Steiner [Acta Cryst. (1996), C52, 2554–2556].*
>
> ④
> ```
> _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
> ```

```
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 units⑦⑧ 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

④The 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

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

May appear in list④ containing **`_exptl_crystal_id`**.⑤

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

The data value must be one of the following:

⑧metallic
  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 ...
;
```

# Layout of DDL2 dictionaries

## Description of a category

DDL2 dictionaries have explicit definitions of data categories. Category descriptions are boxed to make them 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.

Category keys are listed, together with the category groups of which the current category is a member. Categories considered mandatory (`_category.mandatory_code` has a value of 'yes') are indicated by the phrase 'Mandatory category' in bold type at location ⑦.

---

① **EXPTL**

②Data items in the EXPTL category record details about the experimental work prior to the intensity measurements and details about the absorption-correction technique employed.

⑦

Category group(s): `inclusive_group` ③
        `exptl_group`

Category key(s): `_exptl.entry_id` ④

---

⑤ *Example 1 - based on laboratory records for Yb(S-C$_5$H$_4$N)$_2$(THF)$_4$*

⑥

```
_exptl.entry_id                    datablock1
_exptl.absorpt_coefficient_mu      1.22
_exptl.absorpt_correction_T_max    0.896
_exptl.absorpt_correction_T_min    0.802
_exptl.absorpt_correction_type     integration
```

---

```
save_exptl
②  _category.description
;   Data items in the EXPTL category record details
    about the experimental work prior to the ...
;
①  _category.id                      exptl
⑦  _category.mandatory_code          no
④  _category_key.name                '_exptl.entry_id'
    loop_
③  _category_group.id                'inclusive_group'
                                      'exptl_group'
    loop_
⑤  _category_examples.detail
⑥  _category_examples.case
# - - - - - - - - - - - - - - - - - - - - - - - - -
;   Example 1 - based on laboratory records for ...
;
;   _exptl.entry_id                   datablock1
    _exptl.absorpt_coefficient_mu     1.22
    _exptl.absorpt_correction_T_max   0.896
    _exptl.absorpt_correction_T_min   0.802
    _exptl.absorpt_correction_type    integration
;
# - - - - - - - - - - - - - - - - - - - - - - - - -
    save_
```

## Description of a simple physical quantity

A typical definition takes the `_item.name` as headword, with data type and associated conditions in parentheses ranged right. Aliases to other data names are listed below the headword, with the name and version of the dictionary in which they are defined.

The textual definition is given in a large clear type. Permitted numerical ranges are indicated. DDL2 dictionaries distinguish closed intervals (where the boundary value appears as both `_item_range.maximum` ⑧ and `_item_range.minimum` ⑨) from open intervals. In print, closed intervals are enclosed in square brackets, open intervals in parentheses. The example is closed at zero, but open with an unbounded upper value.

Related items are listed with the relationship (the value of `_item_related.function_code` ⑪) in parentheses. The category is listed in square brackets at the end of the entry.

By convention, physical units ⑬ are specified in the textual description and not otherwise printed, although indicated explicitly in the dictionary. No special marking indicates data items where `_item.mandatory_code` ⑭ is 'no' (see the `_citation.id` example opposite for a different case).

①**`_diffrn.ambient_temp`**        *(float, su)*②③
*`_diffrn_ambient_temperature`*④ *(cif_core.dic*⑤ *2.0.1*⑥*)*

⑦The mean temperature in kelvins at which the intensities were measured.

The permitted range is [0.0, ∞)⑧⑨.

Related item: `_diffrn.ambient_temp_esd`⑩ (associated esd)⑪.    ⑫ **[diffrn]**

```
save__diffrn.ambient_temp
⑦  _item_description.description
;   The mean temperature in kelvins at which the
    intensities were measured.
;
①  _item.name                     '_diffrn.ambient_temp
⑫  _item.category_id               diffrn
⑭  _item.mandatory_code            no
④  _item_aliases.alias_name
                                   '_diffrn_ambient_temperature
⑤  _item_aliases.dictionary        cif_core.dic
⑥  _item_aliases.version           2.0.1
    loop_
⑧  _item_range.maximum
⑨  _item_range.minimum                    .    0.0
                                          0.0   0.0
⑩  _item_related.related_name
                                   '_diffrn.ambient_temp_esd'
⑪  _item_related.function_code     associated_esd
②  _item_type.code                 float
③  _item_type_conditions.code      esd
⑬  _item_units.code                kelvins
    save_
```

## Description of an item with discrete enumerated values

The permitted discrete values ④ are listed under the legend 'The data value must be one of the following'. Annotations to the enumerated values ⑤ appear in a parallel column.

①**`_chem_comp_chir.atom_config`**        *(ucode)*②

③The chiral configuration of the atom that is a chiral centre.

The data value must be one of the following:

④R          absolute configuration *R*⑤
 S          absolute configuration *S*

                      ⑥ **[chem_comp_chir]**

```
save__chem_comp_chir.atom_config
③  _item_description.description
;   The chiral configuration of the atom that is a
    chiral centre.
;
①  _item.name              '_chem_comp_chir.atom_config'
⑥  _item.category_id               chem_comp_chir
    _item.mandatory_code            no
②  _item_type.code                 ucode
    loop_
④  _item_enumeration.value
⑤  _item_enumeration.detail
                            R  'absolute configuration R'
                            S  'absolute configuration S'
    save_
```

# 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)

④The 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_
```