### Typographical conventions used in this volume

<table>
<thead>
<tr>
<th>Example</th>
<th>Use</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>atom_site_label</em></td>
<td>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.</td>
</tr>
<tr>
<td>_*<em>max</em></td>
<td>Wildcard construction used to indicate related data names sharing a common root prefix.</td>
</tr>
<tr>
<td><em>differn</em>, <em>differn</em>*</td>
<td>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).</td>
</tr>
<tr>
<td>data_code</td>
<td>Sloping monospaced type (as in code) is used to indicate variable components of a data name or other character literal string.</td>
</tr>
<tr>
<td>&lt;DataBlock&gt;</td>
<td>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.</td>
</tr>
<tr>
<td>ATOM.SITE</td>
<td>Small capitals are used for categories of CIF data items.</td>
</tr>
</tbody>
</table>

### 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’ are defined to allow textual descriptions of categories and to provide examples. All such pseudo data names themselves belong to the category CATEGORY_OVERVIEW. 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.

EXPTL

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.


EXPTL

EXPTL_Absorb_Coefficient_Mu 0.962
EXPTL_Absorb_Correction_Type PS: -scan
EXPTL_Absorb_Correction_Process_Details ‘North, Phillips & Mathews (1968)’
EXPTL_Absorb_Correction_T_Mn 0.929
EXPTL_Absorb_Correction_T_Mx 0.997


# A 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, 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 →∞) and the category is listed in square brackets at the end of the entry. By convention, physical units are specified in the textual description and not otherwise printed, although they are indicated explicitly in the dictionary.

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

The permitted range is 0.0 → ∞.

Description of a looped item with discrete enumerated values

Here, the permitted discrete values are listed under the heading ‘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’). 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 ‘contains’.

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

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

May appear in list containing: exptl_crystal_id

Related items: exptl_crystal_colour

The data value must be one of the following:

metallic

dull

Clear

[exptl_crystal]
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 ①.

**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 and _item.range.minimum) and 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) in parentheses. The category is listed in square brackets at the end of the entry.

By convention, physical units [ ] 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 is ‘no’ (see the _citation.id example opposite for a different case).

**Description of an item with discrete enumerated values**

The permitted discrete values ① 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.

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

The data value must be one of the following:

① R absolute configuration R

② S absolute configuration S

③ (chem_comp_chir)
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 (3) 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.

*1,2_ citation.id
   _citation_id(cif.corr.2.0.1)

3 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.


4 [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

2 _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

   _loop

6 _item_examples.case

   'primary' '1' '2'

save_