

## 3. CIF DATA DEFINITION AND CLASSIFICATION

freely used by other publishers who wish to handle articles submitted in CIF format. The JOURNAL and JOURNAL\_INDEX categories are used in the same way in the core CIF and mmCIF dictionaries, and Section 3.2.5.4 can be consulted for details.

## 3.6.8.4.2. Contents of a publication

Data items in these categories are as follows:

## (a) PUBL

- `_publ.entry_id`  
→ `_entry.id`
- `_publ.contact_author`
- `_publ.contact_author_address`
- `_publ.contact_author_email`
- `_publ.contact_author_fax`
- `_publ.contact_author_name`
- `_publ.contact_author_phone`
- `_publ.contact_letter`
- `_publ.manuscript_creation`
- `_publ.manuscript_processed`
- `_publ.manuscript_text`
- `_publ.requested_category`
- `_publ.requested_coeditor_name`
- `_publ.requested_journal`
- `_publ.section_abstract`
- `_publ.section_acknowledgements`
- `_publ.section_comment`
- `_publ.section_discussion`
- `_publ.section_experimental`
- `_publ.section_exptl_prep`
- `_publ.section_exptl_refinement`
- `_publ.section_exptl_solution`
- `_publ.section_figure_captions`
- `_publ.section_introduction`
- `_publ.section_references`
- `_publ.section_synopsis`
- `_publ.section_table_legends`
- `_publ.section_title`
- `_publ.section_title_footnote`

## (b) PUBL\_AUTHOR

- `_publ.author.address`
- `_publ.author.email`
- `_publ.author.footnote`
- `_publ.author.id_iucr`
- `_publ.author.name`

## (c) PUBL\_BODY

- `_publ.body.contents`
- `_publ.body.element`
- `_publ.body.format`
- `_publ.body.label`
- `_publ.body.title`

## (d) PUBL\_MANUSCRIPT\_INCL

- `_publ.manuscript_incl.entry_id`  
→ `_entry.id`
- `_publ.manuscript_incl.extra_defn`
- `_publ.manuscript_incl.extra_info`
- `_publ.manuscript_incl.extra_item`

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 categories PUBL, PUBL\_AUTHOR, PUBL\_BODY and PUBL\_MANUSCRIPT\_INCL are also members of the IUCR group in the mmCIF dictionary. They are used in the same way in the core CIF and mmCIF dictionaries, and Section 3.2.5.5 can be consulted for details.

## 3.6.9. File metadata

As in the core CIF dictionary, information about the source and the revision history of an mmCIF may be given in the AUDIT group

of categories: AUDIT, AUDIT\_AUTHOR, AUDIT\_CONTACT\_AUTHOR and AUDIT\_CONFORM (Section 3.6.9.1). However, the mmCIF dictionary differs from the core CIF dictionary in the way it expresses relationships between data blocks: instead of the core AUDIT\_LINK category, mmCIF has two categories, ENTRY and ENTRY\_LINK, that essentially fulfil the same role but are classified in a distinct category group (Section 3.6.9.2).

## 3.6.9.1. History of a data block

The categories describing the history of a data block are as follows:

- AUDIT group
  - AUDIT
  - AUDIT\_AUTHOR
  - AUDIT\_CONFORM
  - AUDIT\_CONTACT\_AUTHOR

Data items in these categories are as follows:

## (a) AUDIT

- `_audit.revision_id`
- `_audit.creation_date`
- `_audit.creation_method`
- `_audit.update_record`

## (b) AUDIT\_AUTHOR

- `_audit.author.name`
- `_audit.author.address`

## (c) AUDIT\_CONFORM

- `_audit.conform.dict_name`
- `_audit.conform.dict_version`
- `_audit.conform.dict_location`

## (d) AUDIT\_CONTACT\_AUTHOR

- `_audit.contact_author.name`
- `_audit.contact_author.address`
- `_audit.contact_author.email`
- `_audit.contact_author.fax`
- `_audit.contact_author.phone`

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. Items in italics have aliases in the core CIF dictionary formed by changing the full stop (.) to an underscore (\_).

The data items in these categories are used in the same way in the mmCIF dictionary as in the core CIF dictionary (see Section 3.2.6). The data item `_audit.revision_id` has been added to the AUDIT category to provide the formal category key required by the DDL2 data model. The core data item `_audit_block_code` has been replaced by `_entry.id` (see Section 3.6.9.2).

## 3.6.9.2. Links between data blocks

The categories describing links between data blocks are as follows:

- ENTRY group
  - ENTRY
  - ENTRY\_LINK
- AUDIT group
  - AUDIT\_LINK

Data items in these categories are as follows:

## (a) ENTRY

- `_entry.id`

## (b) ENTRY\_LINK

- `_entry_link.entry_id`  
→ `_entry.id`
- `_entry_link.id`
- `_entry_link.details`