

3. CIF DATA DEFINITION AND CLASSIFICATION

Example 3.2.6.3. List of linked data blocks in a CIF.

```

data_global
_audit_block_code      global
loop_
_audit_link_block_code
_audit_link_block_description
.      'text of paper with two structures'
morA_ (1)  'structure 1 of 2'
morA_ (2)  'structure 2 of 2'

```

Example 3.2.6.4. Complementary list of linked data blocks in a secondary block.

```

data_morA_ (1)
_audit_block_code      morA_ (1)
loop_
_audit_link_block_code
_audit_link_block_description
global      'text of paper with two structures'
.      'structure 1 of 2'
morA_ (2)  'structure 2 of 2'

```

For many applications, it is enough for a statement of the links between the data blocks in a CIF to be included once only in the file, normally in the initial data block. However, for completeness and to permit consistency checking, it is best if the other data blocks in the file have complementary declarations (Example 3.2.6.4).

Current practice as described in the core dictionary restricts this reporting of links between data blocks to the contents of a single file. In principle, if `_audit_block_code` were known to have globally unique values in each distinct data block, the mechanism could be extended to permit inter-file linkage.

Appendix 3.2.1

Category structure of the core CIF dictionary

Table A3.2.1.1 provides an overview of the structure of the core CIF dictionary by informal category group and categories.

Table A3.2.1.1. Categories in the core CIF dictionary

Numbers in parentheses refer to the section of this chapter in which each category is described in detail.

ATOM group (§3.2.4.1)	DIFFRN_SCALE_GROUP (§3.2.2.2.5(d))
ATOM.SITE (§3.2.4.1.1)	DIFFRN_SOURCE (§3.2.2.2.2(d))
ATOM.SITES (§3.2.4.1.2)	DIFFRN_STANDARD_REFLN (§3.2.2.2.5(e))
ATOM.TYPE (§3.2.4.1.3)	DIFFRN_STANDARDS (§3.2.2.2.5(f))
AUDIT group (§3.2.6)	EXPTL group (§3.2.2.3)
AUDIT (§3.2.6(a))	EXPTL (§3.2.2.3(a))
AUDIT_AUTHOR (§3.2.6(b))	EXPTL_CRYSTAL (§3.2.2.3(b))
AUDIT_CONFORM (§3.2.6(c))	EXPTL_CRYSTAL_FACE (§3.2.2.3(c))
AUDIT_CONTACT_AUTHOR (§3.2.6(d))	GEOM group (§3.2.4.3)
AUDIT_LINK (§3.2.6(e))	GEOM (§3.2.4.3.1(a))
CELL group (§3.2.2.1)	GEOM_ANGLE (§3.2.4.3.1(b))
CELL (§3.2.2.1(a))	GEOM_BOND (§3.2.4.3.1(c))
CELL_MEASUREMENT_REFLN (§3.2.2.1(b))	GEOM_CONTACT (§3.2.4.3.1(d))
CHEMICAL group (§3.2.4.2)	GEOM_HBOND (§3.2.4.3.1(e))
CHEMICAL (§3.2.4.2.1(a))	GEOM_TORSION (§3.2.4.3.1(f))
CHEMICAL_CONN_ATOM (§3.2.4.2.2(a))	JOURNAL group (§3.2.5.4)
CHEMICAL_CONN_BOND (§3.2.4.2.2(b))	JOURNAL (§3.2.5.4(a))
CHEMICAL_FORMULA (§3.2.4.2.1(b))	JOURNAL_INDEX (§3.2.5.4(b))
CITATION group (§3.2.5.1)	PUBL group (§3.2.5.5)
CITATION (§3.2.5.1(a))	PUBL (§3.2.5.5(a))
CITATION_AUTHOR (§3.2.5.1(b))	PUBL_AUTHOR (§3.2.5.5(b))
CITATION_EDITOR (§3.2.5.1(c))	PUBL_BODY (§3.2.5.5(c))
COMPUTING group (§3.2.5.2)	PUBL_MANUSCRIPT_INCL (§3.2.5.5(d))
COMPUTING (§3.2.5.2)	REFINE group (§3.2.3.1)
DATABASE group (§3.2.5.3)	REFINE (§3.2.3.1(a))
DATABASE (§3.2.5.3)	REFINE_LS_CLASS (§3.2.3.1(b))
DIFFRN group (§3.2.2.2)	REFLN group (§3.2.3.2)
DIFFRN (§3.2.2.2.1)	REFLN (§3.2.3.2.1)
DIFFRN_ATTENUATOR (§3.2.2.2.2(a))	REFLNS (§3.2.3.2.2(a))
DIFFRN_DETECTOR (§3.2.2.2.4)	REFLNS_CLASS (§3.2.3.2.2(b))
DIFFRN_MEASUREMENT (§3.2.2.2.3(a))	REFLNS_SCALE (§3.2.3.2.2(c))
DIFFRN_ORIENT_MATRIX (§3.2.2.2.3(b))	REFLNS_SHELL (§3.2.3.2.2(d))
DIFFRN_ORIENT_REFLN (§3.2.2.2.3(c))	SYMMETRY group (§3.2.4.4)
DIFFRN_RADIATION (§3.2.2.2.2(b))	SPACE_GROUP (§3.2.4.4.2(a))
DIFFRN_RADIATION_WAVELENGTH (§3.2.2.2.2(c))	SPACE_GROUP_SYMOP (§3.2.4.4.2(b))
DIFFRN_REFLN (§3.2.2.2.5(a))	SYMMETRY (§3.2.4.4.1(a))
DIFFRN_REFLNS (§3.2.2.2.5(b))	SYMMETRY_EQUIV (§3.2.4.4.1(b))
DIFFRN_REFLNS_CLASS (§3.2.2.2.5(c))	VALENCE group (§3.2.4.5)
	VALENCE_PARAM (§3.2.4.5(a))
	VALENCE_REF (§3.2.4.5(b))

References

- Busing, W. R. & Levy, H. A. (1967). *Angle calculations for 3- and 4-circle X-ray and neutron diffractometers*. *Acta Cryst.* **22**, 457–464.
- Hall, S. R. (1981). *Space-group notation with an explicit origin*. *Acta Cryst.* **A37**, 517–525; erratum (1981), **A37**, 921.
- Hall, S. R. & Grosse-Kunstleve, R. W. (2001). *International tables for crystallography*, Vol. B, *Reciprocal space*, edited by U. Shmueli, 2nd ed., Appendix A1.4.2.3. Dordrecht: Kluwer Academic Publishers.
- Klyne, W. & Prelog, V. (1960). *Description of steric relationships across single bonds*. *Experientia*, **16**, 521–523.