**Classification and use of topological data**

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**1. Introduction**

Raw crystallographic data obtained from experiment or theoretical modeling contain no information on the crystal structure connectivity. However, this information, which might describe all sorts of interatomic bonding, is crucial for many tasks of crystal chemistry and materials science, such as classification, comparative analysis, modeling of crystal growth and assembling, as well as search for correlations among crystal composition, structure and properties. Similar to molecular graphs, which are widespread in organic chemistry, crystal structure can be represented as a three-periodic graph, which is usually called a *net* (Delgado-Friedrichs & O’Keeffe, 2005; Delgado-Friedrichs *et al*., 2005). Unlike molecular graphs, nets are infinite and require special methods of description. Such descriptions have become increasingly common in routine crystal structure determinations and usually follow the conventional crystallographic description, which includes atomic coordinates, space group, unit cell dimensions, and other geometrical information, but does not concern the structure connectivity. Many topological descriptors have been proposed for nets; all of these descriptors are determined from the initial crystallographic data using algorithms. Software implementing these algorithms (Delgado-Friedrichs & O’Keeffe, 2003; Blatov *et al*., 2014) has made topological analysis available for the general crystallographic community and has already led to the development of special databases (O'Keeffe *et al*., 2008; Blatov *et al*., 2014) that collect the topological parameters of crystal structures. This work will be facilitated by an extension of the CIF format that makes it possible to store topological information along with a crystal structure and to describe the crystal architecture at different levels of organization.

Although the core CIF dictionary contains some topological information in the CHEMICAL\_CONN, GEOM\_BOND, and GEOM\_CONTACT categories, this information is limited and does not cover all topological aspects of a crystal. The core CIF dictionary does not have the ability to describe a plethora of non-valence intra- or intermolecular interactions (hydrogen bonds, halogen and other specific bonds, van der Waals interactions, *etc*.). Moreover, structures that contain polyatomic building units, such as molecules, metal complex groups, clusters, *etc*., can be simplified to underlying nets, which bear the general topological motif of these units, and these nets should also be formalized in an appropriate format. The topoCIF dictionary solves all of these issues, making the exchange of the topological information easier.

**2. Dictionary design considerations**

**2.1 Overall format** The topoCIF dictionary can be expressed in either CIF 1 or CIF 2 format. Where there is a difference, it is in the use of CIF 2 lists for just a few data items. The discussion below lists the CIF 2 data keys; ⱡ indicates the availability of CIF 1 equivalents, which are discussed where appropriate.

**2.1 Categories and scope**

The topoCIF dictionary contains categories for the description of connectivity and topological properties of periodic nets. Since the corresponding terminology is still under development, only conventional terms and descriptors defined by Delgado-Friedrichs & O’Keeffe (2005) and Blatov *et al*. (2010) are included. The TOPOL\_ENTANGL category has been left empty until the terminology on entanglements gains consistency. The categories can be divided into two groups: (i) descriptors of crystal structure connectivity, and (ii) descriptors of topological properties of a periodic net. The descriptors of the first group can be computed directly from the initial crystallographic data; the descriptors of the second group are determined based on that connectivity information. Thus, the topoCIF dictionary enables one to generate two new levels of the crystal structure description: a connected net without any further detailing and a topological description of that connected net.

**3. Classification of data definitions**

**3.1. Underlying net description**

The *underlying net* is the net of centroids of structural units. The edges of the net represent the links between these units. The underlying net describes the topology of a particular representation of a crystal structure. This representation is said to be *complete* if the underlying net coincides with the initial structure (that is, maps all atoms in the ATOM\_SITE block), and partial if not. For example, diamond and SiO2 (cristobalite) can be represented by the same underlying net **dia**. For diamond, this net is complete, because all the bonding we would normally associate with the diamond structure are represented by the net. But for cristobalite, **dia** is only a partial net, since it only represents the silicon atoms. The oxygen atoms can be considered to be bridges (links) between silicon atoms, but those links are represented just by edges of the **dia** net. In the discussion below, bullet (∙) indicates the category key, typically an integer, and arrow (→) indicates a reference to another category’s key having the same value.

TOPOL\_LINK

A basic net that only references nodes that are single crystallographic atoms requires only the TOPOL\_LINK category.

* \_topol\_link.id

\_topol\_link.atom\_label\_1 → \_atom\_site.label

\_topol\_link.atom\_label\_2 → \_atom\_site.label

\_topol\_link.symop\_1 → \_space\_group\_symop.id

\_topol\_link.translation\_1ⱡ

\_topol\_link.symop\_2 → \_space\_group\_symop.id

\_topol\_link.translation\_2ⱡ

\_topol\_link .id is the unique category key, an integer, typically starting with 1. It is only required if TOPOL\_ATOM is present, as that is where it is referenced. Similar to the GEOM\_BOND category, TOPOL\_LINK allows for a general reference to an ATOM\_SITE atom along with a symmetry operation and a translation to be applied to that atom’s reference position. The syntax, however, is slightly different. Like \_geom\_bond.symmetry\_\*, \_topol\_link.symop\_\* references \_space\_group\_symop.id, but the added translational component is indicated as a list [ i j k ] with [1 0 0] representing a unit translation along the *a* axis. (This allows for a more general representation than the “555” notation used in \_space\_gorup\_symop.id.) Both the identity operation (*x,y,z*, always 1), and no translation, [0 0 0], can be represent using the CIF “default” indicator, an unquoted full stop (period) character. The CIF 1 equivalents for \_topol\_link.translation\_\* are \_topol\_link.translation\_\*\_x, \_topol\_link.translation\_\*\_y, and \_topol\_link.translation\_\*\_z, where \* is 1 or 2. Thus, the simplest of nets, for diamond, can be described simply with:

loop\_

\_topol\_link.atom\_label\_1

\_topol\_link.atom\_label\_2

\_topol\_link.symop\_1

\_topol\_link.translation\_1

\_topol\_link.symop\_2

\_topol\_link.translation\_2

C1 C1 1 . 13 .

where the only data record in atom\_site is for atom\_site.label = C1. When the TOPOL\_NODE category is present, two additional items referencing those nodes are required:

\_topol\_link.node\_id\_1 → \_topol\_node.id

\_topol\_link.node\_id\_2 → \_topol\_node.id

Additional items describing links include

\_topol\_ link.net\_id → \_topol\_net.id

\_topol\_link.distance

\_topol\_link.distance

\_topol\_link.type

\_topol\_link.order

\_topol\_link.multiplicity

\_topol\_link.special\_details

\_topol\_link.Voronoi\_solidangle

These items are described more fully in the dictionary descriptions. \_topol\_link.net\_id is only required if the TOPOL\_NET category is present and more than one net is listed. topol\_link.Voronoi\_solidangle item designates the solid angle of an interatomic contact A-X, which corresponds to a common face of the Voronoi polyhedra of A and X atoms (Blatov, 2004; Fig. 1).



**Figure 1:** The solid angle of the shaded Voronoi polyhedron face in the body-centered cubic lattice is equal to the shaded segment of the unit sphere being cut off by the pyramid with the Voronoi polyhedron atom A at the vertex and the face in the base. The shaded face is shared between Voronoi polyhedra of A and X atoms and corresponds to the bond A-X.

TOPOL\_NODE

A succinct alternative to directly describing the atoms and symmetry in the TOPOL\_LINK category is to move that information to a TOPOL\_NODE loop and simply point to nodes involved in the link. This provides a better separation between the mathematical abstraction of a net of links and nodes and the geometry associated with that net. Thus, the above diamond example could be described as follows, where the TOPOL\_LINK section reduces to a simple n x 2 matrix:

loop\_

\_topol\_link.node\_id\_1

\_topol\_link.node\_id\_2

1 2

loop\_

\_topol\_node.id

\_topol\_node.atom\_label

\_topol\_node.symop

\_topol\_node.translation

1 C1 1 .

2 C1 13 .

And a mix of these two modes is also possible:

loop\_

\_topol\_link.node\_id\_1

\_topol\_link.node\_id\_2

\_topol\_link.symop\_1

\_topol\_link.translation\_1

\_topol\_link.symop\_2

\_topol\_link.translation\_2

1 1 . . 13 .

loop\_

\_topol\_node.id

\_topol\_node.atom\_label

1 C1

More generally, the TOPOL\_NODE category involves the following primary keys:

* \_topol\_node.id

\_topol\_node.label

\_topol\_node.net\_id → \_topol\_net.id

\_topol\_node.atom\_label → \_atom\_site\_label

\_topol\_node.symop

\_topol\_node.translationⱡ

\_topol\_node.fract\_x

\_topol\_node.fract\_y

\_topol\_node.fract\_z

\_topol\_node.symmetry\_multiplicity

\_topol\_node.Wyckoff\_symbol

\_topol\_node.id is a required tag, as it is the category key, referenced by TOPOL\_LINK and TOPOL\_ATOM. Its integer value must be unique and typically the series starts with the value 1. \_topol\_node.label is optional and is used for readability or representational labeling only; it does not have to be unique and therefore should never be referenced by any other category. \_topol\_node.net\_id refers to a particular net described in the TOPOL\_NET category, only required if there is more than one net. Note that any number of nodes may correspond with a given net, but each node must correlate with only one net. \_topol\_node.atom\_label is required only if all nodes correspond to single crystallographic atoms. Otherwise, that reference can be moved to TOPOL\_ATOM (below). In general, when \_topol\_node.atom\_label is present, \_topol\_node.fract\_x, \_topol\_node.fract\_y, and \_topol\_node.fract\_z, \_topol\_node.symmetry\_multiplicity, and \_topol\_node.Wyckoff\_symbol should not be present or indicated as the default ‘.’ value, as that information can be extracted from the corresponding items of the ATOM\_SITE category. However, when a node does not correlate with an atom position in ATOM\_SITE, then these fields can be used, and \_topol\_node.atom\_label should be indicated using ‘.’.

Additional TOPOL\_NODE descriptors include:

\_topol\_node.net\_id

\_topol\_node.chemical\_formula\_iupac

\_topol\_node.chemical\_formula\_moiety

\_topol\_node.chemical\_formula\_sum

\_topol\_node.structural\_formula\_InChI

\_topol\_node.structural\_formula\_SMILES

\_topol\_node.coordination\_sequence

\_topol\_node.coordination\_sequence\_plain

\_topol\_node.point\_symbol

\_topol\_node.extended\_point\_symbol

\_topol\_node.vertex\_symbol

[describe?]

TOPOL\_ATOM

When some of the nodes of a net do not correspond with an atom of the crystal structure, or links themselves are abstractions of atoms or groups of atoms (*building units*, Alexandrov *et al*. 2011; Bonneau *et al.* 2018; Shevchenko & Blatov, 2021) the TOPOL\_ATOM category is required along with TOPOL\_NODE and TOPOL\_LINK. These three categories, then, describe the full chemical constitution and connectivity of the underlying net. The TOPOL\_ATOM category is quite simple:

* \_topol\_atom.id

\_topol\_atom.atom\_label

\_topol\_atom.node\_id → \_topol\_node.id

\_topol\_atom.link\_id → \_topol\_link.id

\_topol\_atom.symop

\_topol\_atom.translationⱡ

\_topol\_atom.elemental\_symbol

Of these items, only \_topol\_atom.atom\_label is absolutely required. Though \_topol\_atom.id is a key, within the current specification it is not referenced. Exactly one of \_topol\_atom.node\_id or \_topol\_atom.link\_id is required, pointing to the node or link that this atom is associated with. Note that this allows any number of atoms to be associated with a give node or link. \_topol\_atom.elemental\_symbol is strongly recommended, as there is no other location in a CIF file where a specific element symbol is required. In the case that for some reason the atom does not relate to a specific element (due to occupational disorder or some other reason), this field should be left as unquoted ‘.’.

Using TOPOL\_ATOM, our simple diamond example could be described as follows:

loop\_

\_topol\_link.node\_id\_1

\_topol\_link.node\_id\_2

1 2

loop\_

\_topol\_node.id

1

2

loop\_

\_topol\_atom.atom\_label

\_topol\_atom.symop

\_topol\_atom.translation

C1 1 .

C1 13 .

For such a simple case, the use of TOPOL\_ATOM and TOPOL\_NODE are clearly unnecessary. But consider the following pair of nets:

         loop\_

         \_topol\_net.id

         \_topol\_net.label

         \_topol\_net.special\_details

         \_topol\_net.overall\_topology\_TOPOS

         1 Net\_1 'Atomic net' 'Unknown'

         2 Net\_2 'Underlying net with carbonyl ligands as nodes' '2,4T3'

We describe the links as a simple topological matrix, with additional descriptive information:

         loop\_

         \_topol\_link.id

         \_topol\_link.net\_id

         \_topol\_link.node\_id\_1

         \_topol\_link.node\_id\_2

         \_topol\_link.distance

         \_topol\_link.type

         \_topol\_link.multiplicity

         1 1 1 2   1.9121 v 4  # Li1 - O1

         2 1 2 3   1.1452 v 4  # O1 - C1

         3 1 2 4   1.7422 v 4  # C1 - Co1

         4 2 5 6   2.4032 v 4  # Li1 - CO

         5 2 6 7   2.3963 v 4  # CO - Co

Adding the nodes, with labels and chemical formulas:

         loop\_

         \_topol\_node.id

         \_topol\_node.net\_id

         \_topol\_node.label

         \_topol\_node.chemical\_formula\_sum

         1 1 Li1 Li

2 1 O1  O

         3 1 C1  C

         4 1 Co1 Co

         5 2 ZA1 Li

         6 2 ZB1 CO

         7 2 ZC1 Co

Note that Node 6 has two atoms associated with, the carbon and oxygen atoms of a carbonyl group. Finally, specifying the positions of those nodes that have special labels:

loop\_

\_topol\_atom.id

\_topol\_atom.node\_id

\_topol\_atom.label

\_topol\_atom.chemical\_formula\_sum

1 5 Li1  Li

2 6 C1   C

3 6 O1   O

4 7 Co1  Co

Scheme I shows the overall relationship among TOPOL\_NET, TOPOL\_LINK, TOPOL\_NODE, and TOPOL\_ATOM. The key category is TOPOL\_LINK, with references to TOPOL\_NET and TOPOL\_NODE. TOPOL\_ATOM provides coordinates for atoms associated with nodes and links. All three categories can reference ATOM\_SITE directly, depending upon the complexity of the net.



For a much more involved example, see the metal-organic framework MOF5 example at GitHub (<https://github.com/COMCIFS/TopoCif/blob/master/more_examples/mof5-v2d-three_nets.cif>), involving three distinct nets, ten links, eleven nodes, and sixty atoms.

**3.2. Underlying net topological properties**

The topological properties of underlying nets described by the TOPOL\_LINK, TOPOL\_NODE and TOPOL\_ATOM categories are collected in the remaining TOPOL categories, namely TOPOL\_NET, TOPOL\_ENTANGL, TOPOL\_TILING (including TOPOL\_TILING\_FACES and TOPOL\_TILING\_TILE), and TOPOL\_OCCURRENCE categories. These categories are discussed below.

TOPOL\_NET

If several nets are described, or additional net-level descriptions are needed, the TOPOL\_NET category is necessary. Its items include:

* \_topol\_net.id

\_topol\_net.name

\_topol\_net.overall\_topology\_EPINET

\_topol\_net.overall\_topology\_RCSR

\_topol\_net.overall\_topology\_SP

\_topol\_net.overall\_topology\_TOPOS

\_topol\_net.period

\_topol\_net.special\_details

\_topol\_net.td10

\_topol\_net.total\_point\_symbol

\_topol\_net.genus

\_topol\_net.occurrence\_total

\_topol\_net.id, again a serial integer, is required if there is more than one net, as it is the key referenced from TOPOL\_LINK and TOPOL\_NODE. \_topol\_net.name allows for an optional arbitrary name for the net. The overall topology of the net can be described in accordance with four known nomenclatures, or given in an arbitrary format. The followingnomenclatures are used to designate the overall topologies of periodic nets:

* RCSR lower-case bold three-letter symbols, see O'Keeffe *et al*. (2008) and http://rcsr.net/ for details. Example: **dia** (see http://rcsr.net/nets/dia)
* EPINET *sqc*XXXXX symbols, see Ramsden *et al*. (2009) and http://epinet.anu.edu.au/ for details.
* SP (sphere packing) symbols *k*/*m*/*fn* as proposed by Koch *et al*. (2006).
* TOPOS symbols N*D*n (Aman *et al*., 2014), where N is a sequence of degrees (coordination numbers) of all independent nodes; *D* is one of the letters *C*, *L*, or *T* designating the dimensionality of the net (*C* – chain, *L* – layer, *T* – three-periodic); n enumerates non-isomorphic nets with a given N*D* sequence. For instance, the symbol 3,3,4*T*3 denotes the 3rd (by the order) three-periodic trinodal net with two 3-coordinated and one 4-coordinated independent nodes. For finite (molecular) graphs the symbols N*M*k-n are used, where k is the number of vertices (atoms) in the graph.
* Zeolite capital three-letter symbols, see http://www.iza-structure.org/databases/ for details.
* Subnet **s**-d-*G*-n symbols (Blatov, 2007; Blatov & Proserpio 2009), where **s** is a conventional name of the initial net, d is a set of ascending integers equal to degrees of all inequivalent nodes in the subnet, *G* is the space group for the most symmetrical embedding of the subnet, n is optional and enumerates non-isomorphic subnets with a given **s**-d-*G* sequence. Examples: **scu**-3,6-*P*42/*mnm*-2 (is a 3,6-c net derived from 4,8-c **scu**); **acs**-4-*Pbcn* (is a 4-c net derived from 6-c **acs**)
* Subnet transformation symbols **s**/*G*→*S*1→…→*S*n;BS (Blatov, 2007), where **s** is a conventional name of the initial net, *G* is the space group of the initial net, *S*1, …, *S*n is the sequence of group-subgroup transformations to obtain the symmetry of the resulting subnet, *S*n, BS is the set of numbers of non-equivalent edges to be retained in the subnet. For instance, the notation fny/P 63/m c m->P 63 2 2 (0,0,1/4);Bond sets: 2,3,4,5 means that the subnet is derived from the RCSR net **fny** by decreasing its space-group symmetry from *P*63/*mcm* to *P*6322 with shifting the origin by (0, 0, 1/4) vector and breaking all non-equivalent edges in the resulting net except the edges No 2, 3, 4 and 5.

The \_topol\_net.occurrence\_total item specifies the total occurrence of the net topology in crystal structures. An arbitrarily detailed description of the net can be provided in the \_topol\_net.special\_details item.

TOPOL\_ENTANGL

This category contains no items, because the descriptors of entanglements in crystal structures have not been standardized yet. However, the importance of entanglements in the topological description is acknowledged , and this category is expected to be developed in future versions of the dictionary.

TOPOL\_TILING, TOPOL\_TILING\_FACES, and TOPOL\_TILING\_TILE

These three categories describe a tiling, which is carried by the underlying net. Since only a single unentangled net can carry tilings, these data can be included only if a single net is described in the TOPOL\_NET section. As a rule, natural tiling (Blatov *et al*., 2007) is described, since it contains minimal cages, which can be combined to provide all other larger cages, including infinite channels.

Items in these categories include:

\_topol\_tiling.vertices

\_topol\_tiling.edges

\_topol\_tiling.faces

\_topol\_tiling.tiles

\_topol\_tiling.signature

\_topol\_tiling.Dsize

\_topol\_tiling.dual

\_topol\_tiling\_faces.tile\_id

\_topol\_tiling\_faces.size

\_topol\_tiling\_tile.count

\_topol\_tiling\_tile.id

TOPOL\_OCCURRENCE

The TOPOL\_OCCURRENCE category stores information on the occurrences of a particular net topology in other crystal structures and can be used together with the \_topol\_net.overall\_topology\_\* items for developing topological databases. Items include:

* \_topol\_occurrence.id

\_topol\_occurrence.net\_id → \_topol\_net.id

\_topol\_occurrence.citation\_id → \_citation.id

Reference or collection codes of crystal structure determinations can be used as \_topol\_occurrence.id values, for example, reference codes from the Cambridge Structural Database or collection codes from the Inorganic Crystal Structure Database.

**3.3. Development of the supporting software and databases**

The CIF topological data can be read and generated by the *ToposPro* program package (Blatov *et al*., 2014) and online service *TopCryst* (https://topcryst.com). Jmol/JSmol software (https://jmol.sourceforge.net) can also read and visualize the nets specified in the topoCIF format. The topological databases Reticular Chemistry Structure Resource (RCSR, http://rcsr.net/) and ToposPro Collections (TTD and TTO, https://topospro.com) use the topoCIF topological descriptors and, hence, one can use the topoCIF format for exporting or importing information to or from these databases. Thus, the crystallographic information on old and new structure determinations can be supplemented with the connectivity data, stored and shared.

**4. Net Reconstruction from CIF Data**

The periodic net described by a topoCIF file is fully defined by its set of TOPOL\_ATOM, TOPOL\_NODE, and TOPOL\_LINK data. The method of constructing a net for visualization or analysis from this data is not trivial, since generally a CIF file only provides locations for the asymmetric unit. Below we describe a sketch of the corresponding algorithm as implemented in Jmol. This algorithm presumes that we first want to start with a set of nodes based on some sort of finite spatial boundaries (one or more unit cells, for example), and then add to that the relevant links. Net construction proceeds in the following order:

* Reading relevant \_cell, \_symmetry, \_symmetry\_equiv\_pos, \_atom\_site, \_topol\_net, \_topol\_link, \_topol\_node, and \_topol\_atom data (which could come in any order within a CIF file).
* Processing the \_topol\_atom associations by
  + applying indicated symmetry operations and translations, and
  + associating each atom with its designated link or node.
* Creating any nodes needed for links that have not been already defined from \_topol\_atom
* Processing all additional node symmetry operations and translations.
* Processing all additional link symmetry operations and translations.
* Applying all space group symmetry operations for all identified points, whether atoms, nodes, or link end-points.
* Removing any unconnected atoms, nodes, or links.

A reference dual Java/JavaScript implementation can be found at SourceForge (<https://sourceforge.net/p/jmol/code/HEAD/tree/trunk/Jmol/src/org/jmol/adapter/readers/cif/TopoCifParser.java>) or GitHub (<https://github.com/BobHanson/Jmol-SwingJS/blob/master/src/org/jmol/adapter/readers/cif/TopoCifParser.java>).

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