Topology CIF dictionary

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The topology CIF dictionary provides data names for describing crystal structure topology.

TOPOLOGY

This category is the parent of all categories in the dictionary.

Example 1 – Connectivity of the diamond crystal structure. All atoms coincide with the nodes and all bonds coincide with the edges, so the atomic network coincides with the underlying net.

```
loop_
_space_group_symop.id
_space_group_symop.operation_xyz
1 x,y,z
2 1/4-x,1/4-y,z
# - - - - data truncated for brevity - - - -
13 -y,-x,-z
# - - - - data truncated for brevity - - - -
192 3/4-z,1/2+y,1/4-x

loop_
_atom_site.label
_atom_site.fract_x
_atom_site.fract_y
_atom_site.fract_z
C1 0.12500 0.12500 0.12500

loop_
_topol_net.id
_topol_net.overall_topology_RCSR
1 dia

loop_
_topol_node.id
_topol_node.net_id
1 1

loop_
_topol_link.id
_topol_link.node_id_1
_topol_link.node_id_2
_topol_link.symop_id_1
_topol_link.translation_1
_topol_link.symop_id_2
_topol_link.translation_2
_topol_link.distance
_topol_link.Voronoi_solid_angle
_topol_link.type
_topol_link.order
_topol_link.multiplicity
1 1 1 1 [0 0 0] 13 [0 0 0] 1.5446 22.04 v 1 16

loop_
_topol_atom.id
_topol_atom.node_id
_topol_atom.atom_label
_topol_atom.element_symbol
1 1 C1 C
```

Example 2 – Connectivity of atomic and underlying nets for an interpenetrating array of two $LiCo(CO)_4$ networks. The atomic net consists of Li, C, O and Co atoms, while the underlying net is built from three kinds of nodes: Li and Co atoms and carbonyl (CO) ligand, labeled as ZA1, ZC1, and ZB1, respectively. Two possible variants are shown: the coordinates of ZA1 are specified by a reference to the Li1 atom, while the coordinates of ZC1 are specified explicitly. Both atomic and underlying nets are described in the TOPOL_NET section.

```
loop_
_space_group_symop.id
_space_group_symop.operation_xyz
1 x,y,z
2 -x,-y,z
3 x,-y,-z
# - - - - data truncated for brevity - - - -
24 -z,y,-x

loop_
_atom_site.label
_atom_site.fract_x
_atom_site.fract_y
_atom_site.fract_z
Li1 0.00000 0.00000 0.00000
C1  0.31850 0.31850 0.31850
O1  0.19920 0.19920 0.19920
Co1 0.50000 0.50000 0.50000

loop_
_topol_net.id
_topol_net.label
_topol_net.z_number
_topol_net.special_details
_topol_net.overall_topology_TOPOS
1 Net_1 2 'Atomic network' 'Unknown'
2 Net_2 2 'Underlying net with carbonyl ligands as nodes'
'2,4T3'

loop_
_topol_node.id
_topol_node.label
_topol_node.net_id
_topol_node.fract_x
_topol_node.fract_y
_topol_node.fract_z
1 Li1 1  .       .       .      # Li
2 C1  1  .       .       .      # C
3 O1  1  .       .       .      # O
4 Co1 1  .       .       .      # Co
5 ZA1 2  .       .       .      # Li
6 ZB1 2 0.25036 0.25036 0.25036 # (CO)
7 ZC1 2  .       .       .      # Co

loop_
_topol_link.id
_topol_link.node_id_1
_topol_link.node_id_2
_topol_link.distance
_topol_link.type
1 1 3 1.9121 v  # Li1-O1
2 2 3 1.1452 v  # C1-O1
3 2 4 1.7422 v  # C1-Co1
4 5 6 2.4032 gl # Li1-(CO)
5 6 7 2.3963 gl # (CO)-Co
```

(Example continued on next page.)

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(Example 2 continued.)

```
loop_
_topol_atom.id
_topol_atom.node_id
_topol_atom.atom_label
_topol_atom.element_symbol
1 1 Li1 Li
2 2 C1  C
3 3 O1  O
4 4 Co1 Co
5 5 Li1 Li
6 6 C1  C
7 6 O1  O
8 7 Co1 Co
```

Example 3 – Connectivity of an underlying net of the calcite ($CaCO_3$) crystal structure. The nodes of the underlying net correspond to Ca atoms and carbonate (CO_3) groups.

```
loop_
_space_group_symop.id
_space_group_symop.operation_xyz
1 x,y,z
2 -y,x-y,z
# - - - - data truncated for brevity - - - -
13 2/3+x,1/3+y,1/3+z
# - - - - data truncated for brevity - - - -
36 1/3-y,2/3-x,1/6+z

loop_
_atom_site.label
_atom_site.fract_x
_atom_site.fract_y
_atom_site.fract_z
C1  0.00000 0.00000 0.25000
O1  0.25930 0.00000 0.25000
Ca1 0.00000 0.00000 0.00000

loop_
_topol_net.id
_topol_net.overall_topology_RCSR
1 pcu-b

loop_
_topol_node.id
_topol_node.label
1 ZA1 # CO3
2 ZB1 # Ca

loop_
_topol_link.id
_topol_link.node_id_1
_topol_link.node_id_2
_topol_link.symop_id_2
_topol_link.translation_2
_topol_link.distance
_topol_link.type
1 1 2 20 [-1 -1 0] 3.2122 gl # (CO3)-Ca

loop_
_topol_atom.id
_topol_atom.node_id
_topol_atom.atom_label
_topol_atom.element_symbol
_topol_atom.symop_id
1 1 C1 C 1
2 1 O1 O 2
3 1 O1 O 2
4 1 O1 O 3
5 2 Ca1 Ca 1
```

Example 4 – Connectivity of an underlying net of the cuprite (Cu_2O) crystal structure. Oxygen atoms coincide with the nodes, while copper atoms represent the edges. There are two interpenetrating networks of the diamond topology.

```
loop_
_space_group_symop.id
_space_group_symop.operation_xyz
1 x,y,z
2 1/2-x,1/2-y,z
# - - - - data truncated for brevity - - - -
20 -z,1/2+y,1/2+x
# - - - - data truncated for brevity - - - -
48 1/2-z,y,1/2-x

loop_
_atom_site.label
_atom_site.fract_x
_atom_site.fract_y
_atom_site.fract_z
O1  0.25000 0.25000 0.25000
Cu1 0.00000 0.00000 0.00000

loop_
_topol_net.id
_topol_net.z_number
_topol_net.overall_topology_RCSR
1 2 'dia'

loop_
_topol_node.id
_topol_node.net_id
1 1

loop_
_topol_link.id
_topol_link.node_id_1
_topol_link.node_id_2
_topol_link.symop_id_2
_topol_link.type
1 1 1 13 gl

loop_
_topol_atom.id
_topol_atom.node_id
_topol_atom.link_id
_topol_atom.atom_label
_topol_atom.element_symbol
1 1 . O1  O
2 . 1 Cu1 Cu
```

Example 5 – MOF-5 (multiple nets; two polyatomic nodes and a molecular linker).

```
loop_
_space_group_symop.id
_space_group_symop.operation_xyz
1 x,y,z
2 -x,-y,z
# - - - - data truncated for brevity - - - -
5 z,x,y
# - - - - data truncated for brevity - - - -
26 x,y,-z
# - - - - data truncated for brevity - - - -
37 y,x,z
# - - - - data truncated for brevity - - - -
192 1/2-z,1/2+y,-x

loop_
_atom_site.label
_atom_site.fract_x
_atom_site.fract_y
_atom_site.fract_z
H1  0.30590 0.19410 0.04520
C1  0.25000 0.25000 0.11050
C2  0.28310 0.21690 0.02630
C3  0.25000 0.25000 0.05380
O1  .25000 0.25000 0.25000
O2  0.28180 0.21820 0.13390
Zn1 0.29350 0.20650 0.20650

loop_
_topol_net.id
_topol_net.label
_topol_net.special_details
_topol_net.overall_topology_TOPOS
1 Net_1 'Atomic network' 'Unknown'
2 Net_2 'Underlying net with zinc tetranuclear complex groups
as nodes and benzene rings as links (cluster representation)'
'pcu'
3 Net_3 'Underlying net with zinc, oxygen and
benzenedicarboxylato ligands as 4-coordinate nodes (standard
representation)' 'fff'
```

(Example continued on next page.)

(Example 5 continued.)

```
loop_
_topol_node.id
_topol_node.net_id
1  1  # H1
2  1  # C1
3  1  # C2
4  1  # C3
5  1  # O1
6  1  # O2
7  1  # Zn1
8  2  # C6O13Zn4
9  3  # C8H4O4
10 3  # O1
11 3  # Zn1

loop_
_topol_link.id
_topol_link.node_id_1
_topol_link.node_id_2
_topol_link.symop_id_2
_topol_link.distance
_topol_link.type
1   1  3  .   0.9594 v  # H1-C2
2   2  6  37  1.3013 v  # C1-O2
3   2  4  .   1.4554 ar # C1-C3
4   3  3  26  1.3502 ar # C2-C2
5   3  4  .   1.3936 ar # C2-C3
6   5  7  .   1.9340 v  # O1-Zn1
7   6  7  .   1.9114 v  # O2-Zn1
8   8  8  26 12.8345 gl # (C6O13Zn4)-(C6H4)-(C6O13Zn4)
9   9 11  5   5.5309 gl # (C8H4O4)-Zn1
10 10 11  .   1.9340 v  # O1-Zn1

loop_
_topol_atom.id
_topol_atom.atom_label
_topol_atom.node_id
_topol_atom.link_id
_topol_atom.symop_id
_topol_atom.element_symbol
1   H1   1   .   1 H
2   C1   2   .   1 C
3   C2   3   .   1 C
4   C3   4   .   1 C
5   O1   5   .   1 O
6   O2   6   .   1 O
7   Zn1  7   .   1 Zn
10  C1   8   .   1 C
11  C1   8   .  55 C
12  O2   8   .  55 O
13  O2   8   .  80 O
14  O2   8   .   6 O
15  O2   8   .  59 O
16  O2   8   .  42 O
17  O2   8   .  78 O
18  C1   8   .  78 C
19  C1   8   .   5 C
20  Zn1  8   .   6 Zn
21  Zn1  8   .  55 Zn
22  C1   8   .  69 C
# - - - - data truncated for brevity - - - -
31  O2   8   .   1 O
32  O2   8   .  37 O
33  O2   9   .  14 O
34  O2   9   .  26 O
35  O2   9   .   1 O
36  O2   9   .  37 O
37  C1   9   .  14 C
38  C3   9   8  14 C
39  C2   9   8  14 C
40  H1   9   8  14 H
41  C2   9   8  37 C
42  H1   9   8  37 H
43  C2   9   8  26 C
44  H1   9   8  26 H
45  C2   9   8   1 C
46  H1   9   8   1 H
47  C3   9   8   1 C
48  C1   9   .   1 C
49  O1  10   .   1 O
50  Zn1 11   .   1 Zn
```

Example 6 – Cyanamide (simple atomic network example with hydrogen bonding).

```
loop_
_space_group_symop.id
_space_group_symop.operation_xyz
1 x,y,z
2 1/2-x,-y,1/2+z
3 1/2+x,1/2-y,-z
4 -x,1/2+y,1/2-z
5 -x,-y,-z
6 1/2+x,y,1/2-z
7 1/2-x,1/2+y,z
8 x,1/2-y,1/2+z

loop_
_atom_site.label
_atom_site.fract_x
_atom_site.fract_y
_atom_site.fract_z
H1 0.19700 0.11100 0.02200
H2 0.05900 0.26600 0.08700
C1 0.14120 0.08370 0.23120
N1 0.14590 0.16990 0.10179
N2 0.14010 0.01250 0.34609

loop_
_topol_node.id
1 2 3 4 5

loop_
_topol_link.id
_topol_link.node_id_1
_topol_link.node_id_2
_topol_link.distance
_topol_link.symop_id_2
_topol_link.translation_2_x
_topol_link.translation_2_y
_topol_link.translation_2_z
_topol_link.type
_topol_link.order
1 1 4 0.8988 1 0 0  0 v  1 # H1-N1
2 1 5 2.1228 2 0 0 -1 hb ? # H1-N2
3 2 4 0.8826 1 0 0  0 v  1 # H2-N1
4 2 5 2.2152 4 0 0  0 hb ? # H2-N2
5 3 5 1.1520 1 0 0  0 v  3 # C1-N2
6 3 4 1.3148 1 0 0  0 v  1 # C1-N1

loop_
_topol_atom.id
_topol_atom.atom_label
_topol_atom.node_id
_topol_atom.element_symbol
1 H1 1 H
2 H2 2 H
3 C1 3 C
4 N1 4 N
5 N2 5 N
```

Example 7 – FAU zeolite tiling example.

```
loop_
_space_group_symop.id
_space_group_symop.operation_xyz
1 x,y,z
2 1/4-x,1/4-y,z
# - - - - data truncated for brevity - - - -
13 -y,-x,-z
# - - - - data truncated for brevity - - - -
41 x,z,y
42 z,y,x
# - - - - data truncated for brevity - - - -
47 x,1/4-z,1/4-y
# - - - - data truncated for brevity - - - -
192 3/4-z,1/2+y,1/4-x

loop_
_atom_site.label
_atom_site.fract_x
_atom_site.fract_y
_atom_site.fract_z
Si1 0.94690 0.12510 0.03640
```

(Example continued on next page.)

(Example 7 continued.)

```
loop_
_topol_net.id
_topol_net.overall_topology_iza
1 FAU

loop_
_topol_node.id
_topol_node.net_id
_topol_node.label
1 1 Si

loop_
_topol_link.id
_topol_link.node_id_1
_topol_link.node_id_2
_topol_link.distance
_topol_link.symop_id_2
_topol_link.translation_2
_topol_link.type
1 1 1 3.0470 47 [0 0 0] gl
2 1 1 3.0473 13 [1 1 0] gl
3 1 1 3.0539 41 [0 0 0] gl
4 1 1 3.0814 42 [1 0 -1] gl

loop_
_topol_atom.id
_topol_atom.node_id
_topol_atom.atom_label
_topol_atom.element_symbol
1 1 Si1 Si

loop_
_topol_tiling.id
_topol_tiling.net_id
_topol_tiling.signature
_topol_tiling.vertices
_topol_tiling.edges
_topol_tiling.faces
_topol_tiling.tiles
_topol_tiling.d_size
1 1 '2[4^6.6^2]+[4^6.6^8]+[4^18.6^4.12^4]' 1 4 5 3 24
```

TOPOL

The TOPOL category covers data on connectivity between atoms and structural groups and the related structural properties as calculated from the ATOM, CELL and SPACE_GROUP data.

_topol.special_details (*Text*)
A description of topological information not covered by the existing data items in the topology categories.

TOPOL_ATOM

The TOPOL_ATOM category provides information on the atoms of the initial structure that compose links or nodes of a net. The **_topol_atom.atom_label** value must match a value for **_atom_site.label**.

Category key(s): **_topol_atom.id**

_topol_atom.atom_label (*Word*)
A pointer to an atom that is associated with a link or a node (not including link end-point atoms). It must coincide with a value given for **_atom_site.label**.

Values must match those for the following item(s):
_atom_site.label

_topol_atom.element_symbol (*Text*)
The element symbol for this atom, written in accordance with the IUPAC systematic nomenclature for periodic elements. This should be a single element symbol found on the official IUPAC Periodic Table. For example: 'C', 'H', or 'Co', without isotope or charge. Data items in the ATOM_SITE category that do not correspond to elements of the periodic table should be represented here as '.'.

_topol_atom.id (*Integer*; none)
The unique identifier of a topological 'atom' that is associated with a link or node.

The permitted range is $1 \rightarrow \infty$.

_topol_atom.link_id (*Integer*; none)
The link associated with this atom, if applicable. It must match a value provided for **_topol_link.id**. Note that this association is in a bridging or molecular linker sense, not the end points of the link. For example, a net may specify a link that is composed of a carbonyl CO group or an aromatic ring, representing those groups for the purposes of the net.

Values must match those for the following item(s):
_topol_link.id.
The permitted range is $1 \rightarrow \infty$.

_topol_atom.node_id (*Integer*; none)
The node associated with this atom, if applicable. It must match a value provided for **_topol_node.id**.

Values must match those for the following item(s):
_topol_node.id.
The permitted range is $1 \rightarrow \infty$.

_topol_atom.symop_id (*Integer*; none)
The identifier of the symmetry operation that is to be applied to the coordinates of the atom given by **_topol_atom.atom_label** before addition of the translations given by **_topol_atom.translation**. The value must match a value of **_space_group_symop.id**. If this item is omitted or assigned to '.', the identity operation is assumed.

Values must match those for the following item(s):
_space_group_symop.id.
The permitted range is $1 \rightarrow 192$. Where no value is given, the assumed value is '1'.

_topol_atom.translation (*Integer*[3]; none)
The lattice translation vector that must be added to the coordinates after application of the symmetry operation specified by **_topol_atom.symop_id** to generate the atom belonging to a link or a node. For example, if the symmetry operation referred to by **_topol_atom.symop_id** is $(x - \frac{1}{2}, y + \frac{1}{2}, z)$, **_topol_atom.translation** is $[0, -1, 0]$ and the original position is $(0.2, 0.7, 1.0)$ in fractional coordinates, then the resultant position is $(-0.3, 0.2, 1.0)$. Alternatively, **_topol_atom.translation_x**, **_topol_atom.translation_y**, and **_topol_atom.translation_z** data items may be used to describe separate components of the vector for CIF1 compatibility. If this item is omitted or assigned to '.' it is assumed to be equal to $[0, 0, 0]$.

Where no value is given, the assumed value is '[0'.

_topol_atom.translation_x (*Integer*; none)
The x component of the vector of lattice translations that is added to the coordinates after application of the symmetry operation given by **_topol_atom.symop_id** to generate an atom belonging to a link or a node. Default value is 0.

Where no value is given, the assumed value is '0'.

_topol_atom.translation_y (*Integer*; none)
The *y* component of the vector of lattice translations that is added to the coordinates after application of the symmetry operation given by **_topol_atom.symop_id** to generate an atom belonging to a link or a node. Default value is 0.

Where no value is given, the assumed value is '0'.

_topol_atom.translation_z (*Integer*; none)
The *z* component of the vector of lattice translations that is added to the coordinates after application of the symmetry operation given by **_topol_atom.symop_id** to generate an atom belonging to a link or a node. Default value is 0.

Where no value is given, the assumed value is '0'.

TOPOL_ENTANGL

The TOPOL_ENTANGL category describes entanglements in the underlying net. This category is a placeholder for future development of descriptions of entanglement.

TOPOL_LINK

The TOPOL_LINK category describes the crystal structure connectivity and encodes the weighted colored symmetry-labeled quotient graph, from which the whole periodic net describing the overall topology of the crystal structure can be restored. The definition of symmetry-labeled quotient graph was given by Klein (1996) and examples of weights and colors for the graph edges and vertices are provided by Blatov (2006). The connections described in TOPOL_LINK may correspond to any vectors in the structure, not just bonds or contacts. The two end-point references are to nodes listed in TOPOL_NODE using **_topol_link.node_id_1** and **_topol_link.node_id_2**. In the case of multiple nets, **_topol_link.net_id** is required. Other items in this category are optional. If the link itself represents atoms (as in the case of a molecular linker), the atoms comprising the link must be referenced by **_topol_atom.link_id**.

References: Klein, H.-J. (1996). Systematic generation of models for crystal structures. *Math. Model. Sci. Comput.* **6**, 325–330; Blatov, V. A. (2006). A method for hierarchical comparative analysis of crystal structures. *Acta Cryst.* A**62**, 356–364, DOI:10.1107/S0108767306025591.

Category key(s): **_topol_link.id**

_topol_link.distance (*Real*; Å)
The link length in ångströms.

The permitted range is 0. → ∞.

_topol_link.distance_su (*Real*; Å)
Standard uncertainty of **_topol_link.distance**.

Values must match those for the following item(s):
_topol_link.distance

_topol_link.id (*Integer*; none)
The identifier of the link.

The permitted range is 1 → ∞.

_topol_link.label (*Text*)
An optional not necessarily unique label for this link.

_topol_link.multiplicity (*Integer*; none)
The number of these links in the unit cell.

The permitted range is 1 → ∞.

_topol_link.net_id (*Integer*; none)
The identifier of the net, to which this node belongs.

Values must match those for the following item(s):
_topol_net.id.
The permitted range is 1 → ∞.

_topol_link.node_id_1 (*Integer*; none)
The identifier of the first node associated with a link This must match a **_topol_node.id** value.

Values must match those for the following item(s):
_topol_node.id.
The permitted range is 1 → ∞.

_topol_link.node_id_2 (*Integer*; none)
The identifier of the second node associated with a link This must match a **_topol_node.id** value.

Values must match those for the following item(s):
_topol_node.id.
The permitted range is 1 → ∞.

_topol_link.order (*Real*; none)
The number of electron pairs participating in the bond described by **_topol_link.type**.

_topol_link.special_details (*Text*)
Information about the link that is not expressed using other data items, for example, bond subtypes and explanations of links with **_topol_link.type** of 'sb'.

_topol_link.symop_id_1 (*Integer*; none)
The identifier of the symmetry operation that is to be applied to the coordinates of the node given by **_topol_link.node_id_1** before addition of the translations given by **_topol_link.translation_1**. The value must match a value of **_space_group_symop.id**. If this item is omitted or assigned to '.', the identity operation is assumed.

Values must match those for the following item(s):
_space_group_symop.id.
The permitted range is 1 → 192. Where no value is given, the assumed value is '1'.

_topol_link.symop_id_2 (*Integer*; none)
The identifier of the symmetry operation that is to be applied to the coordinates of the node given by **_topol_link.node_id_2** before addition of the translations given by **_topol_link.translation_2**. The value must match a value of **_space_group_symop.id**. If this item is omitted or assigned to '.', the identity operation is assumed.

Values must match those for the following item(s):
_space_group_symop.id.
The permitted range is 1 → 192. Where no value is given, the assumed value is '1'.

_topol_link.translation_1 (*Integer*[3]; none)
The lattice translation vector that must be added to the coordinates after application of the symmetry operation given by **_topol_link.symop_id_1** to generate the node used in calculating the link. For example, if the symmetry operation referred to by **_topol_link.symop_id_1** is $(x-\frac{1}{2}, y+\frac{1}{2}, z)$, **_topol_link.translation_1** is $[0,-1,0]$ and the original position is $(0.2, 0.7, 1.0)$ in fractional coordinates, then the resultant position is $(-0.3, 0.2, 1.0)$. Alternatively, **_topol_link.translation_1_x**, **_topol_link.translation_1_y** and **_topol_link.translation_1_z** data items may be used to describe separate components of the vector.

Where no value is given, the assumed value is '[0'.

_topol_link.translation_1_x (*Integer*; none)
The *x* component of the vector of lattice translations that is added to the coordinates after application of the symmetry operation given by **_topol_link.symop_id_1** to generate the node used in calculating the link.

Where no value is given, the assumed value is '0'.

_topol_link.translation_1_y (*Integer*; none)
The y component of the vector of lattice translations that is added to the coordinates after application of the symmetry operation given by **_topol_link.symop_id_1** to generate the node used in calculating the link.

Where no value is given, the assumed value is '0'.

_topol_link.translation_1_z (*Integer*; none)
The z component of the vector of lattice translations that is added to the coordinates after application of the symmetry operation given by **_topol_link.symop_id_1** to generate the node used in calculating the link.

Where no value is given, the assumed value is '0'.

_topol_link.translation_2 (*Integer*[3]; none)
The lattice translation vector that must be added to the coordinates after application of the symmetry operation given by **_topol_link.symop_id_2** to generate the node used in calculating the link. For example, if the symmetry operation referred to by **_topol_link.symop_id_2** is $(x - \frac{1}{2}, y + \frac{1}{2}, z)$, **_topol_link.translation_2** is $[0, -1, 0]$ and the original position is $(0.2, 0.7, 1.0)$ in fractional coordinates, then the resultant position is $(-0.3, 0.2, 1.0)$. Alternatively, **_topol_link.translation_2_x**, **_topol_link.translation_2_y** and **_topol_link.translation_2_z** data items may be used to describe separate components of the vector.

Where no value is given, the assumed value is '[0'.

_topol_link.translation_2_x (*Integer*; none)
The x component of the vector of lattice translations that is added to the coordinates after application of the symmetry operation given by **_topol_link.symop_id_2** to generate the node used in calculating the link.

Where no value is given, the assumed value is '0'.

_topol_link.translation_2_y (*Integer*; none)
The y component of the vector of lattice translations that is added to the coordinates after application of the symmetry operation given by **_topol_link.symop_id_2** to generate the node used in calculating the link.

Where no value is given, the assumed value is '0'.

_topol_link.translation_2_z (*Integer*; none)
The z component of the vector of lattice translations that is added to the coordinates after application of the symmetry operation given by **_topol_link.symop_id_2** to generate the node used in calculating the link.

Where no value is given, the assumed value is '0'.

_topol_link.type (*Code*)
The chemical bond type associated with the connection between the two sites. If no bond exists, use an undelimited period character. If the bond type is unknown, use ? or leave out the data item. The number of electron pairs participating in the bond can be indicated using **_topol_link.order**. The value 'sb' or 'gl' should be used for any case where the connection is not a bond between two atoms.

The data value must be one of the following:

ar	aromatic bond
v	valence bond
pi	π bond
hb	hydrogen bond
vw	van der Waals contact
sb	special bond type described in **_topol_link.special_details**
gl	generic link

_topol_link.Voronoi_solid_angle (*Real*; none)
The solid angle fraction of the interatomic contact A—X, which is the percentage of the sphere of unit radius cut by the pyramid with the basal face of the Voronoi polyhedron of A or X, the two atoms defining the contact. The total solid angle (the whole sphere) is equal to 100. The face used is that corresponding to the A—X interatomic contact.

The permitted range is $0 \rightarrow 50$.

_topol_link.Voronoi_solid_angle_su (*Real*; none)
Standard uncertainty of **_topol_link.Voronoi_solid_angle**.

Values must match those for the following item(s):
_topol_link.Voronoi_solid_angle

TOPOL_NET

The TOPOL_NET category describes an atomic network or underlying net.

Reference: Delgado-Friedrichs, O., Foster, M. D., O'Keeffe, M., Proserpio, D. M., Treacy, M. M. J. & Yaghi, O. M. (2005). *J. Solid State Chem.* **178**, 2533–2554, DOI:10.1016/j.jssc.2005.06.037.

Category key(s): **_topol_net.id**

_topol_net.genus (*Integer*; none)
The genus of the underlying net, defined as the cyclomatic number of its own quotient graph: $g = 1 + e - v$, where e and v are the number of edges and vertices in the quotient graph. The quotient graph is a finite graph that contains all of the information of the periodic net: the vertices of the graph are the vertices of a translational repeat unit and the edges are all the edges of the repeat unit.

Reference: Delgado-Friedrichs, O. & O'Keeffe, M. (2005). *J. Solid State Chem.* **178**, 2480–2485, DOI:10.1016/j.jssc.2005.06.011.

_topol_net.id (*Integer*; none)
The unique integer identifier for this net, generally a serial number starting with 1.

The permitted range is $1 \rightarrow \infty$.

_topol_net.label (*Text*)
An optional not-necessarily unique label for this net.

_topol_net.overall_topology (*Text*)
The overall topology symbol in an arbitrary form.

Example: 'face-centered cubic topology'

_topol_net.overall_topology_EPINET (*Text*)
The identifier for the overall topology as listed in the EPINET database at http://epinet.anu.edu.au.

Example: 'sqc6'

_topol_net.overall_topology_IZA (*Text*)
The three-letters symbol for a Zeolite Framework Types that has been approved by the Structure Commission of the International Zeolite Association (IZA-SC).

Reference: Database for Zeolite Structures http://www.iza-structure.org/databases/

Example: 'FAU'

_topol_net.overall_topology_RCSR (*Text*)
The overall topology symbol according to the RCSR nomenclature described by O'Keeffe et al. (2008).

Reference: O'Keeffe, M., Peskov, M. A., Ramsden, S. J. & Yaghi, O. M. (2008). *Acc. Chem. Res.* **41**, 1782–1789, DOI:10.1021/ar800124u.

Example: 'dia'

_topol_net.overall_topology_SP (*Text*)
The overall topology symbol according to the nomenclature of Fischer for sphere packings described by Koch et al. (2006).

Reference: Koch, E., Fischer, W. & Sowa, H. (2006). *Acta Cryst.* A**62**, 152–167, DOI:10.1107/S010876730600362X.

Example: '4/6/c1'

_topol_net.overall_topology_TOPOS (*Text*)
The overall topology symbol according to the *TOPOS* nomenclature. *TOPOS* symbols *NDn* are interpreted as follows: *N* is a sequence of degrees (coordination numbers) of all independent nodes; *D* is one of the letters C (chain), L (layer) or T (three-periodic) designating the dimensionality of the net; and *n* enumerates non-isomorphic nets with a given *ND* sequence. For finite (molecular) graphs the symbols *NMK-n* are used, where *k* is the number of vertices (atoms) in the graph.

Reference: Aman, F., Asiri, A. M., Siddiqui, W. A., Arshad, M. N., Ashraf, A., Zakharov, N. S. & Blatov, V. A. (2014). *Cryst. Eng. Comm.* **16**, 1963–1970, DOI:10.1039/C3CE42218F.

Example: '3,3,4T3' (The third non-isomorphic three-periodic trinodal net with two 3-coordinated and one 4-coordinated independent nodes.)

_topol_net.period (*Code*)
The periodicity of the underlying net.

The data value must be one of the following:

0	0-periodic (finite)
1	1-periodic (chain)
2	2-periodic (layer)
3	3-periodic (framework)

_topol_net.special_details (*Text*)
An arbitrary description of the net.

_topol_net.td10 (*Integer*; none)
The topological density TD10 of the underlying net. This is the cumulative sum of the first ten shells of topological neighbours including the central atom. For structures with more than one kind of vertex in the asymmetric unit the value given is a weighted average over the vertices.

_topol_net.total_point_symbol (*Text*)
The total point symbol of the underlying net. This value summarizes all the point symbols for the non-equivalent nodes with their stoichiometric coefficients.

Examples: '{6^6}' (Point symbol for diamond), '{4.6^2}2{4^2.6^10.8^3}' (3,6-coordinated underlying net of TiO2)

_topol_net.z_number (*Integer*; none)
For 3-periodic nets, the number of symmetry-equivalent nets of this kind in the crystal structure.

The permitted range is $1 \rightarrow \infty$.

TOPOL_NODE

The TOPOL_NODE category, along with TOPOL_ATOM, describes the topological properties, position, and chemical composition of the nodes of the underlying net. The TOPOL_NODE category is optional. It is only required for polyatomic nodes or in cases where the label given to the node is different from **_atom_site.label**. Data items **_topol_node.fract_x**, **_topol_node.fract_y**, and **_topol_node.fract_z** must be present only if the node's position cannot be derived from other data items in TOPOL_NODE or TOPOL_ATOM. Fractional coordinates can be given in other cases, but are to be considered secondary to calculations based on explicit or default symmetry transformations, present only for convenience. In the case of multiple nets, **_topol_node.net_id** is also required.

Reference: Blatov, V. A., O'Keeffe, M. & Proserpio, D. M. (2010). *Cryst. Eng. Comm.* **12**, 44–48, DOI:10.1039/B910671E.

Category key(s): **_topol_node.id**

_topol_node.coordination_sequence (*Integer*; none)
The coordination sequence is a sequence of numbers counting the atoms in the 1st, 2nd, 3rd *etc.* coordination shells of any given node in the net. In other words, the *k*th entry in the list is the number of vertices linked to the node by a path of exactly k steps. It is usually listed up to $k = 10$. Alternatively, the **_topol_node.coordination_sequence_plain** data item can be used to represent the coordination sequence as plain text.

Example: '[4' (The diamond coordination sequence)

_topol_node.coordination_sequence_plain (*Text*)
A CIF1-compatible alternative representation of the coordination sequence as plain text, as a quoted string of white-space-separated numbers.

Example: '4 12 24 42 64 92 124 162 204 252' (The diamond coordination sequence)

_topol_node.extended_point_symbol (*Text*)
The extended point symbol of a *N*-coordinated node lists all shortest circuits for each of the $N(N-1)/2$ angles (pairs of edges) incident to the node. It is written as $A(a).B(b)\ldots$ where $A, B, \ldots$ designate sizes of circuits, which meet at angles $A, B, \ldots$, and $a, b, \ldots$ designate numbers of these circuits. It is sorted so shortest circuits come first. For a 4-coordinated node connected to nodes w, x, y, z, the angles are ordered in opposite pairs; wx, yz; wy, xz; wz, xy (written in lexicographic order smallest numbers first).

Examples: '6(2).6(2).6(2).6(2).6(2).6(2)' (ES for a vertex in the diamond structure), '4.6(2).4.8(3).6(2).6(2)' (ES for one vertex of feldspar net), '7(2).9(2).7(3).7(3).7(3).7(3)' (ES for the vertex of qzd net), '4.4.4.4.6(3).6(3).6(5).6(5).6(5).6(5)' (ES for the vertex of 5-c sqp net)

_topol_node.fract_x (*Real*; none)
The fractional x coordinate of this node. If present, this data item indicates the final, symmetry-transformed x coordinate of the node. This data item is only necessary if this node is not referenced by **_topol_atom.node_id**.

_topol_node.fract_x_su (*Real*; none)
Standard uncertainty of **_topol_node.fract_x**.

Values must match those for the following item(s):
_topol_node.fract_x

_topol_node.fract_y (*Real*; none)
The fractional y coordinate of this node. If present, this data item indicates the final, symmetry-transformed y coordinate of the node. This data item is only necessary if this node is not referenced by **_topol_atom.node_id**.

_topol_node.fract_y_su (*Real*; none)
Standard uncertainty of **_topol_node.fract_y**.

Values must match those for the following item(s):
_topol_node.fract_y

_topol_node.fract_z (*Real*; none)
The fractional z coordinate of this node. If present, this data item indicates the final, symmetry-transformed z coordinate of the node. This data item is only necessary if this node is not referenced by **_topol_atom.node_id**.

_topol_node.fract_z_su (*Real*; none)
Standard uncertainty of **_topol_node.fract_z**.
Values must match those for the following item(s):
_topol_node.fract_z

_topol_node.id (*Integer*; none)
The identifier of the node.
The permitted range is $1 \rightarrow \infty$.

_topol_node.label (*Text*)
An optional not-necessarily unique label for this node.

_topol_node.net_id (*Integer*; none)
The unique identifier of the net to which this node belongs.
Values must match those for the following item(s):
_topol_net.id.
The permitted range is $1 \rightarrow \infty$.

_topol_node.point_symbol (*Text*)
The (short) point symbol of the node. This lists the number and size of the shortest closed chains of connected nodes (circuits) starting from any non-equivalent node in the net. For an N-coordinated node there are $N(N-1)/2$ circuits.
Examples: '6^6' (Point symbol for a diamond vertex), '4^2.6^3.8' (Point symbol for a feldspar 4-coordinated vertex), '7^5.9' (Point symbol for the vertex of 4-c qzd net), '4^4.6^6' (Point symbol for the vertex of 5-c sqp net)

_topol_node.symmetry_multiplicity (*Integer*; none)
The number of different sites that are generated by the application of the space-group symmetry to the coordinates given for this site. It is equal to the multiplicity given for this Wyckoff site in *International Tables for Crystallography* Vol. A (2002).
The permitted range is $1 \rightarrow 192$.

_topol_node.vertex_symbol (*Text*)
The vertex symbol of a node provides similar information to the **_topol_node.extended_point_symbol**, but only for rings, which are circuits that contain no shortcuts, that is, are not the sum of two smaller circuits. There may be circuits that cannot be rings. If there are no rings meeting at a particular angle of the node, the symbol '*' is used instead of the $A(a)$ symbol. It is sorted so shortest rings come first. For 4-coordinated nodes only, the angles are grouped in opposite pairs; ab, cd and ac, bd and ad, bc (written in lexicographic order smallest numbers first). In the ordering the symbol '*' is equivalent to zero.
Examples: '6(2).6(2).6(2).6(2).6(2).6(2)' (Vertex symbol for diamond), '4.6(2).4.8.6.6(2)' (VS for one vertex of feldspar net), '7(2).*.7(3).7(3).7(3).7(3)' (VS for the vertex of qzd net), '4.4.4.4.6.6.6(5).6(5).6(5).6(5)' (VS for the vertex of 5-c sqp net)

_topol_node.Wyckoff_symbol (*Text*)
The Wyckoff symbol (letter) as listed in the space-group section of *International Tables for Crystallography*, Vol. A (1987).
The data value must be one of the following:
a b c d e f g h i j k l m n o p q r s t u v w x y z \a

TOPOL_TILING

The TOPOL_TILING category describes the natural tiling corresponding to the underlying net. A tiling is a partition of crystal space using generalised polyhedra, and a natural tiling is one for which tiles are the smallest possible that conserve the full symmetry of the net and for which the faces are all locally strong rings. This means that there is no single largest face (face with the largest number of vertices) as such a face will be the sum of the other smaller faces. The tile signature contains the sizes of the tile faces and the number of faces of a given size in the tile.
Reference: Blatov, V. A., Delgado-Friedrichs, O., O'Keeffe M. & Proserpio D. M. (2007). *Acta Cryst.* A**63**, 418–425, DOI:10.1107/S0108767307038287.
Category key(s): **_topol_tiling.id**

_topol_tiling.d_size (*Integer*; none)
The number of distinct (not symmetry-related) chambers in the tiling as expressed by the Delaney Dress symbol or just D-symbol, as a measure of the complexity of the tiling (D-size).
Reference: Blatov, V. A., O'Keeffe, M. & Proserpio, D. M. (2010). *Cryst. Eng. Comm.* **12**, 44–48, DOI:10.1039/B910671E.
The permitted range is $1 \rightarrow \infty$.

_topol_tiling.dual (*Text*)
The overall topology symbol of the dual net, which corresponds to the net of the dual of the natural tiling.

_topol_tiling.edges (*Integer*; none)
The number of independent tile edges in the natural tiling.

_topol_tiling.faces (*Integer*; none)
The number of independent tile faces in the natural tiling.

_topol_tiling.id (*Integer*; none)
The unique identifier of the tiling.
The permitted range is $1 \rightarrow \infty$.

_topol_tiling.net_id (*Integer*; none)
The identifier of the net that carries this tiling.
Values must match those for the following item(s):
_topol_net.id.
The permitted range is $1 \rightarrow \infty$.

_topol_tiling.signature (*Text*)
The tiling signature, written in the form $n[A\hat{}a.B\hat{}b\ldots] + m[C\hat{}c.D\hat{}d\ldots]+\ldots$, where square brackets envelop tile symbols, $n, m, \ldots$ are stoichiometric coefficients, $A, B, C, D, \ldots$ are sizes of tile faces, and $a, b, c, d, \ldots$ are numbers of the faces of a given size in the tile.
Examples: '[6^4]' (Natural tiling for diamond), '3[4^6]+[4^6.6^8]+[4^12.6^8.8^6]' (Natural tiling for zeolite LTA)

_topol_tiling.tiles (*Integer*; none)
The number of independent tiles in the natural tiling.

_topol_tiling.vertices (*Integer*; none)
The number of independent tile vertices in the natural tiling.