#\#CIF\_2.0

################################################################################

# #

# Topology CIF dictionary #

# #

################################################################################

data\_TOPOLOGY\_CIF

\_dictionary.title TOPOLOGY\_CIF

\_dictionary.class Instance

\_dictionary.version 0.9.2

\_dictionary.ddl\_conformance 3.13.1

\_dictionary.date 2021-05-04

\_description.text

;

The Topology CIF dictionary provides datanames for describing crystal

structure topology. This is a DRAFT version and datanames in this

dictionary should not be used until final approval by COMCIFS.

;

save\_TOPOLOGY

\_definition.id TOPOLOGY

\_definition.scope Category

\_definition.class Head

\_description.text

;

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

;

\_name.object\_id TOPOLOGY

\_name.category\_id TOPOLOGY\_CIF

\_import.get [{"file":"cif\_core.dic" "save":"CIF\_CORE" "mode":"Full"}]

save\_

save\_topol

\_definition.id topol

\_name.category\_id TOPOLOGY

\_name.object\_id topol

\_definition.update 2018-01-30

\_definition.scope Category

\_definition.class Set

\_description.text

;

The TOPOL category covers data on connectivity

between atoms and structural groups and the

related structural properties as calculated from

the ATOM, CELL and SYMMETRY data.

;

loop\_

\_description\_example.detail

\_description\_example.case

;

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. Thus, no special TOPOL\_NET section is needed.

;

;

loop\_

\_space\_group\_symop.id

\_space\_group\_symop.operation\_xyz

1 x,y,z

2 1/4-x,1/4-y,z

# Other symmetry elements skipped

13 -y,-x,-z

# Other symmetry elements skipped

192 3/4-z,1/2+y,1/4-x

loop\_

\_atom\_site.label

\_atom\_site.type\_symbol

\_atom\_site.symmetry\_multiplicity

\_atom\_site.fract\_x

\_atom\_site.fract\_y

\_atom\_site.fract\_z

\_atom\_site.occupancy

C1 C 8 0.12500 0.12500 0.12500 1.0000

loop\_

\_topol\_node.label

\_topol\_node.atom\_label

C1 C1

loop\_

\_topol\_link.node\_label\_1

\_topol\_link.node\_label\_2

\_topol\_link.site\_symmetry\_symop\_1

\_topol\_link.site\_symmetry\_translation\_1

\_topol\_link.site\_symmetry\_symop\_2

\_topol\_link.site\_symmetry\_translation\_2

\_topol\_link.distance

\_topol\_link.Voronoi\_solidangle

\_topol\_link.type

\_topol\_link.multiplicity

C1 C1 1 [0 0 0] 13 [0 0 0] 1.5446 22.04 v 16

\_topol\_net.overall\_topology\_RCSR dia

;

;

Example 2 - Connectivity of an underlying net of the calcite

(CaCO3) crystal structure. The nodes of the underlying

net correspond to Ca atoms and carbonate (CO3) groups.

The underlying net has the NaCl (pcu-b in the RCSR

nomenclature) topology. Only the underlying net topology

is described, thus, no special TOPOL\_NET section is needed.

;

;

loop\_

\_space\_group\_symop.id

\_space\_group\_symop.operation\_xyz

1 x,y,z

2 -y,x-y,z

# Other symmetry elements elided

20 1/3+x-y,2/3-y,1/6-z

# Other symmetry elements elided

36 1/3-y,2/3-x,1/6+z

loop\_

\_atom\_site.label

\_atom\_site.type\_symbol

\_atom\_site.site\_symmetry\_multiplicity

\_atom\_site.fract\_x

\_atom\_site.fract\_y

\_atom\_site.fract\_z

\_atom\_site.occupancy

C1 C 6 0.00000 0.00000 0.25000 1.0000

O1 O 18 0.25930 0.00000 0.25000 1.0000

Ca1 Ca 6 0.00000 0.00000 0.00000 1.0000

loop\_

\_topol\_node.label

\_topol\_node.chemical\_formula\_sum

\_topol\_node.fract\_x

\_topol\_node.fract\_y

\_topol\_node.fract\_z

ZA1 CO3 0.00000 0.00000 0.25000

ZB1 Ca 0.00000 0.00000 0.00000

loop\_

\_topol\_link.node\_label\_1

\_topol\_link.node\_label\_2

\_topol\_link.site\_symmetry\_symop\_1

\_topol\_link.site\_symmetry\_translation\_1

\_topol\_link.site\_symmetry\_symop\_2

\_topol\_link.site\_symmetry\_translation\_2

\_topol\_link.distance

\_topol\_link.type

\_topol\_link.multiplicity

ZA1 ZB1 1 [0 0 0] 20 [-1 -1 0] 3.2122 v 36

\_topol\_net.overall\_topology\_RCSR pcu-b

;

;

Example 3 - Connectivity of an underlying net of the cuprite (Cu2O)

crystal structure. Oxygen atoms coincide with the nodes,

while copper atoms represent the edges. There are two

interpenetrating networks of the diamond topology. Only the underlying

net topology is described, thus, no special TOPOL\_NET section is needed.

;

;

loop\_

\_space\_group\_symop.id

\_space\_group\_symop.operation\_xyz

1 x,y,z

2 1/2-x,1/2-y,z

# Symmetry elements elided

13 -y,-x,-z

# Symmetry elements elided

48 1/2-z,y,1/2-x

loop\_

\_atom\_site.label

\_atom\_site.type\_symbol

\_atom\_site.site\_symmetry\_multiplicity

\_atom\_site.fract\_x

\_atom\_site.fract\_y

\_atom\_site.fract\_z

\_atom\_site.occupancy

O1 O 2 0.25000 0.25000 0.25000 1.0000

Cu1 Cu 4 0.00000 0.00000 0.00000 1.0000

loop\_

\_topol\_node.label

\_topol\_node.atom\_label

Node1 O1

loop\_

\_topol\_link.id

\_topol\_link.node\_label\_1

\_topol\_link.node\_label\_2

\_topol\_link.site\_symmetry\_symop\_1

\_topol\_link.site\_symmetry\_translation\_1

\_topol\_link.site\_symmetry\_symop\_2

\_topol\_link.site\_symmetry\_translation\_2

\_topol\_link.type

\_topol\_link.multiplicity

1 Node1 Node1 1 [0 0 0] 13 [0 0 0] v 4

loop\_

\_topol\_edge.id

\_topol\_edge.chemical\_formula\_sum

1 Cu

\_topol\_net.overall\_topology\_RCSR dia

;

;

Example 4 - 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; the nodes are labeled as ZA1, ZC1, and

ZB1, respectively. The \_topol\_node\_\* items include references

to atom labels for the atoms and coordinates for the nodes.

Some fields, which values are not required or should be taken

from the ATOM\_SITE block, are specified with the '.' symbol.

Two possible variants are shown: the coordinates of ZA1 are

specified by a reference to 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

# Symmetry elements elided

24 -z,y,-x

loop\_

\_atom\_site.label

\_atom\_site.type\_symbol

\_atom\_site.site\_symmetry\_multiplicity

\_atom\_site.fract\_x

\_atom\_site.fract\_y

\_atom\_site.fract\_z

\_atom\_site.occupancy

Li1 Li 1 0.00000 0.00000 0.00000 1.0000

C1 C 4 0.31850 0.31850 0.31850 1.0000

O1 O 4 0.19920 0.19920 0.19920 1.0000

Co1 Co 1 0.50000 0.50000 0.50000 1.0000

loop\_

\_topol\_net\_id

\_topol\_net.special\_details

\_topol\_net.overall\_topology\_TOPOS

Net\_1 'Atomic net' 'Unknown'

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

loop\_

\_topol\_node.label

\_topol\_node.net\_id

\_topol\_node.chemical\_formula\_sum

\_topol\_node.atom\_label

\_topol\_node.fract\_x

\_topol\_node.fract\_y

\_topol\_node.fract\_z

Li1 Net\_1 . Li1 . . .

C1 Net\_1 . C1 . . .

O1 Net\_1 . O1 . . .

Co1 Net\_1 . Co1 . . .

ZA1 Net\_2 . Li1 . . .

ZB1 Net\_2 CO . 0.25036 0.25036 0.25036

ZC1 Net\_2 . Co1 . . .

loop\_

\_topol\_link.node\_label\_1

\_topol\_link.node\_label\_2

\_topol\_link.distance

\_topol\_link.site\_symmetry\_symop\_1

\_topol\_link.site\_symmetry\_translation\_1

\_topol\_link.site\_symmetry\_symop\_2

\_topol\_link.site\_symmetry\_translation\_2

\_topol\_link.type

\_topol\_link.multiplicity

Li1 O1 1.9121 1 [0 0 0] 3 [0 0 0] v 4

C1 O1 1.1452 1 [0 0 0] 1 [0 0 0] v 4

C1 Co1 1.7422 1 [0 0 0] 1 [0 0 0] v 4

ZA1 ZB1 2.4032 1 [0 0 0] 3 [0 0 0] v 4

ZB1 ZC1 2.3963 1 [0 0 0] 1 [0 0 0] v 4

;

save\_

save\_topol.special\_details

\_definition.id '\_topol.special\_details'

\_name.category\_id topol

\_name.object\_id special\_details

\_definition.update 2018-01-30

\_description.text

;

A description of topological information not covered by the

existing data names in the topology categories.

;

\_type.contents Text

\_type.purpose Describe

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_edge

\_definition.id topol\_edge

\_name.category\_id TOPOLOGY

\_name.object\_id topol\_edge

\_definition.update 2018-01-30

\_definition.scope Category

\_definition.class Loop

\_description.text

;

The TOPOL\_EDGE category describes the chemical composition of

the edges of the underlying net.

;

\_category\_key.name '\_topol\_edge.id'

save\_

save\_topol\_edge.chemical\_formula\_iupac

\_definition.id '\_topol\_edge.chemical\_formula\_iupac'

\_name.category\_id topol\_edge

\_name.object\_id chemical\_formula\_iupac

\_definition.update 2018-01-30

\_description.text

;

Formula of the residue or ion which corresponds to the edge,

expressed in conformance with IUPAC rules.

;

\_type.contents Text

\_type.purpose Encode

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_edge.chemical\_formula\_moiety

\_definition.id '\_topol\_edge.chemical\_formula\_moiety'

\_name.category\_id topol\_edge

\_name.object\_id chemical\_formula\_moiety

\_definition.update 2018-01-30

\_description.text

;

Formula of the residue or ion which corresponds to the edge.

The formula is written in accordance with the rules of the

\_chemical\_formula.moiety tag.

;

\_type.contents Text

\_type.purpose Encode

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_edge.chemical\_formula\_sum

\_definition.id '\_topol\_edge.chemical\_formula\_sum'

\_name.category\_id topol\_edge

\_name.object\_id chemical\_formula\_sum

\_definition.update 2018-01-30

\_description.text

;

Formula of the residue or ion which corresponds to the edge.

The formula is written in accordance with the rules of the

\_chemical\_formula.sum tag.

;

\_type.contents Text

\_type.purpose Encode

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_edge.id

\_definition.id '\_topol\_edge.id'

\_name.category\_id topol\_edge

\_name.object\_id id

\_definition.update 2018-01-30

\_description.text

;

The label of the edge. These must match labels

specified as \_topol\_link.id in the TOPOL\_LINK list.

;

\_name.linked\_item\_id '\_topol\_link.id'

\_type.contents Code

\_type.purpose Link

\_type.source Related

\_type.container Single

save\_

save\_topol\_entangl

\_definition.id topol\_entangl

\_name.category\_id TOPOLOGY

\_name.object\_id topol\_entangl

\_definition.update 2018-01-30

\_definition.scope Category

\_definition.class Set

\_description.text

;

The TOPOL\_ENTANGL category describes entanglements in the

underlying net. This category is a placeholder for future development

of descriptions of entanglement.

;

save\_

save\_topol\_link

\_definition.id topol\_link

\_name.category\_id TOPOLOGY

\_name.object\_id topol\_link

\_definition.update 2018-01-30

\_definition.scope Category

\_definition.class Loop

\_description.text

;

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

nodes that are linked are listed in TOPOL\_NODE. In

order to properly describe the connectivity,

\_topol\_link.node\_label\_1,

\_topol\_link.node\_label\_2,

\_topol\_link.site\_symmetry\_symop\_1,

\_topol\_link.site\_symmetry\_translation\_1,

\_topol\_link.site\_symmetry\_symop\_2,

and \_topol\_link.site\_symmetry\_translation\_2 must be given

for each link, which is identified by \_topol\_link.id. Other

items in this category are optional.

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. A62, 356-364.

;

loop\_

\_category\_key.name '\_topol\_link.id'

save\_

save\_topol\_link.node\_label\_1

\_definition.id '\_topol\_link.node\_label\_1'

\_name.category\_id topol\_link

\_name.object\_id node\_label\_1

\_definition.update 2018-01-30

\_type.contents Code

\_description.text

;

The label of the first node of a link. This must match a TOPOL\_NODE.LABEL.

;

\_type.purpose Link

\_type.source Related

\_type.container Single

\_name.linked\_item\_id '\_topol\_node.label'

save\_

save\_topol\_link.node\_label\_2

\_definition.id '\_topol\_link.node\_label\_2'

\_name.category\_id topol\_link

\_name.object\_id node\_label\_2

\_definition.update 2018-01-30

\_type.contents Code

\_description.text

;

The label of the second node of a link. This must match

a TOPOL\_NODE.LABEL.

;

\_type.purpose Link

\_type.source Related

\_type.container Single

\_name.linked\_item\_id '\_topol\_node.label'

save\_

save\_topol\_link.distance

\_definition.id '\_topol\_link.distance'

\_name.category\_id topol\_link

\_name.object\_id distance

\_definition.update 2018-01-30

\_description.text

;

The link length in angstroms.

;

\_enumeration.range 0.:

\_type.contents Real

\_type.purpose Measurand

\_type.source Derived

\_type.container Single

\_units.code angstroms

save\_

save\_topol\_link.id

\_definition.id '\_topol\_link.id'

\_name.category\_id topol\_link

\_name.object\_id id

\_definition.update 2018-01-30

\_description.text

;

The identifier of the link.

;

\_type.contents Code

\_type.purpose Key

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_link.multiplicity

\_definition.id '\_topol\_link.multiplicity'

\_name.category\_id topol\_link

\_name.object\_id multiplicity

\_definition.update 2018-01-30

\_description.text

;

The number of these links in the unit cell.

;

\_enumeration.range 1:

\_type.contents Integer

\_type.purpose Number

\_type.source Derived

\_type.container Single

save\_

save\_topol\_link.order

\_definition.id '\_topol\_link.order'

\_name.category\_id topol\_link

\_name.object\_id order

\_definition.update 2018-05-16

\_description.text

;

The number of electron pairs participating in the bond

described by \_topol\_link.type.

;

\_type.purpose Number

\_type.source Assigned

\_type.container Single

\_type.contents Real

save\_

save\_topol\_link.site\_symmetry\_symop\_1

\_definition.id '\_topol\_link.site\_symmetry\_symop\_1'

\_name.category\_id topol\_link

\_name.object\_id site\_symmetry\_symop\_1

\_definition.update 2018-04-05

\_type.contents Code

\_description.text

;

The symmetry operation that is applied to the coordinates of

the node given by \_topol\_link.node\_label\_1 before addition of

the translations in

\_topol\_link.site\_symmetry\_translation\_1. The value must match

a value of \_space\_group\_symop.id. No normalization of the

resulting coordinates into the interval [0,1) is carried

out. For example, (x+1/2, y+1/2,z) is not the same as (x-1/2,

y+1/2,z) for these purposes.

;

\_type.purpose Link

\_type.source Derived

\_name.linked\_item\_id '\_space\_group\_symop.id'

save\_

save\_topol\_link.site\_symmetry\_symop\_2

\_definition.id '\_topol\_link.site\_symmetry\_symop\_2'

\_name.category\_id topol\_link

\_name.object\_id site\_symmetry\_symop\_2

\_definition.update 2018-04-05

\_type.contents Code

\_description.text

;

The symmetry operation that is applied to the coordinates of

the node given by \_topol\_link.node\_label\_2 before addition of

the translations in

\_topol\_link.site\_symmetry\_translation\_2. The value must match

a value of \_space\_group\_symop.id. No normalization of the

resulting coordinates into the interval [0,1) is carried

out. For example, (x+1/2, y+1/2,z) is not the same as (x-1/2,

y+1/2,z) for these purposes.

;

\_type.purpose Link

\_type.source Derived

\_name.linked\_item\_id '\_space\_group\_symop.id'

save\_

save\_topol\_link.site\_symmetry\_translation\_1

\_definition.id '\_topol\_link.site\_symmetry\_translation\_1'

\_name.category\_id topol\_link

\_name.object\_id site\_symmetry\_translation\_1

\_definition.update 2018-04-05

\_type.contents Integer

\_description.text

;

A vector of lattice translations that are added to the

coordinates after application of the symmetry operation given by

\_topol\_link.site\_symmetry\_symop\_1 to generate the node used in

calculating the link. For example, if the symmetry operation

referred to by \_topol\_link.site\_symmetry\_symop\_id is

(x-1/2,y+1/2,z), the translation vector 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).

;

\_type.purpose Number

\_type.dimension '[3]'

\_type.source Derived

\_type.container Matrix

save\_

save\_topol\_link.site\_symmetry\_translation\_2

\_definition.id '\_topol\_link.site\_symmetry\_translation\_2'

\_name.category\_id topol\_link

\_name.object\_id site\_symmetry\_translation\_2

\_definition.update 2018-04-05

\_type.contents Integer

\_description.text

;

A vector of lattice translations that are added to the

coordinates after application of the symmetry operation given by

\_topol\_link.site\_symmetry\_symop\_2 to generate the node used in

calculating the link. For example, if the symmetry operation

referred to by \_topol\_link.site\_symmetry\_symop\_2 is

(x-1/2,y+1/2,z), the translation vector 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).

;

\_type.purpose Number

\_type.dimension '[3]'

\_type.source Derived

\_type.container Matrix

save\_

save\_topol\_link.special\_details

\_definition.id '\_topol\_link.special\_details'

\_name.category\_id topol\_link

\_name.object\_id special\_details

\_definition.update 2018-05-24

\_description.text

;

Information about the link that is not expressed using other

data names, for example, bond subtypes and explanations

of links with \_topol\_link.type of 'sb'.

;

\_type.contents Text

\_type.purpose Describe

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_link.type

\_definition.id '\_topol\_link.type'

\_name.category\_id topol\_link

\_name.object\_id type

\_definition.update 2018-02-06

\_type.container Single

\_type.purpose State

\_description.text

;

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 name. The

number of electron pairs participating in the bond can be indicated

using \_topol\_link.order.

;

\_type.contents Code

loop\_

\_enumeration\_set.state

\_enumeration\_set.detail

ar 'aromatic bond'

v 'valence bond'

pi 'pi bond'

hb 'hydrogen bond'

vw 'van der Waals contact'

sb 'special bond type described in \_topol\_link.special\_details'

. 'no bond'

\_type.source Assigned

save\_

save\_topol\_link.Voronoi\_solidangle

\_definition.id '\_topol\_link.Voronoi\_solidangle'

\_name.category\_id topol\_link

\_name.object\_id voronoi\_solidangle

\_definition.update 2018-02-06

\_enumeration.range 1:50

\_description.text

;

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.

;

\_type.contents Real

\_type.purpose Measurand

\_type.source Derived

\_type.container Single

\_units.code none

save\_

save\_topol\_net

\_definition.id topol\_net

\_name.category\_id TOPOLOGY

\_name.object\_id topol\_node

\_definition.update 2021-05-03

\_definition.scope Category

\_definition.class Loop

\_description.text

;

The TOPOL\_NET category describes an underlying net, its

topological properties and occurrence in other structures.

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

;

\_category\_key.name '\_topol\_net.id'

save\_

save\_topol\_net.genus

\_definition.id '\_topol\_net.genus'

\_name.category\_id topol\_net

\_name.object\_id genus

\_definition.update 2018-02-06

\_description.text

;

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.

;

\_type.contents Index

\_type.purpose Number

\_type.source Derived

\_type.container Single

save\_

save\_topol\_net.occurrence\_total

\_definition.id '\_topol\_net.occurrence\_total'

\_name.category\_id topol\_net

\_name.object\_id occurrence\_total

\_definition.update 2018-02-13

\_description.text

;

The total number of occurrences in literature and databases of the

underlying net topology at the time the data file was prepared.

;

\_type.contents Count

\_type.purpose Number

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_net.overall\_topology

\_definition.id '\_topol\_net.overall\_topology'

\_name.category\_id topol\_net

\_name.object\_id overall\_topology

\_definition.update 2018-01-30

\_description.text

;

The overall topology symbol in an arbitrary form.

;

\_type.contents Text

\_description\_example.case 'face-centered cubic topology'

\_type.purpose Describe

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_net.overall\_topology\_EPINET

\_definition.id '\_topol\_net.overall\_topology\_EPINET'

\_name.category\_id topol\_net

\_name.object\_id overall\_topology\_EPINET

\_definition.update 2018-01-30

\_description.text

;

The identifier for the overall topology as listed

in the EPINET database at http://epinet.anu.edu.au.

;

\_type.contents Text

\_description\_example.cas sqc6

\_type.purpose Encode

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_net.overall\_topology\_RCSR

\_definition.id '\_topol\_net.overall\_topology\_RCSR'

\_name.category\_id topol\_net

\_name.object\_id overall\_topology\_RCSR

\_definition.update 2018-01-30

\_description.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.

;

\_type.contents Text

\_description\_example.case dia

\_type.purpose Encode

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_net.overall\_topology\_SP

\_definition.id '\_topol\_net.overall\_topology\_SP'

\_name.category\_id topol\_net

\_name.object\_id overall\_topology\_SP

\_definition.update 2018-01-30

\_description.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.

A62, 152-167.

;

\_type.contents Text

\_description\_example.case 4/6/c1

\_type.purpose Encode

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_net.overall\_topology\_TOPOS

\_definition.id '\_topol\_net.overall\_topology\_TOPOS'

\_name.category\_id topol\_net

\_name.object\_id overall\_topology\_TOPOS

\_definition.update 2018-02-06

\_description.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.

;

\_type.contents Text

loop\_

\_description\_example.case

\_description\_example.detail

'3,3,4T3'

;

The third three-periodic trinodal net with two 3-coordinated and one

4-coordinated independent nodes

;

\_type.purpose Encode

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_net.period

\_definition.id '\_topol\_net.period'

\_name.category\_id topol\_net

\_name.object\_id period

\_definition.update 2018-01-30

\_type.container Single

\_type.purpose State

\_description.text

;

Periodicity of the underlying net. The allowed data values

have the following meaning:

0 0-periodic (finite)

1 1-periodic (chain)

2 2-periodic (layer)

3 3-periodic (framework)

;

\_type.contents Count

\_enumeration.range 0:3

\_type.source Derived

save\_

save\_topol\_net.special\_details

\_definition.id '\_topol\_net.special\_details'

\_name.category\_id topol\_net

\_name.object\_id special\_details

\_definition.update 2021-05-03

\_description.text

;

An arbitrary description of the net.

;

\_type.contents Text

\_type.purpose Describe

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_net.td10

\_definition.id '\_topol\_net.td10'

\_name.category\_id topol\_net

\_name.object\_id td10

\_definition.update 2018-01-30

\_description.text

;

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.

;

\_type.contents Index

\_type.purpose Number

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_net.total\_point\_symbol

\_definition.id '\_topol\_net.total\_point\_symbol'

\_name.category\_id topol\_net

\_name.object\_id total\_point\_symbol

\_definition.update 2018-01-30

\_description.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.

;

\_type.contents Text

loop\_

\_description\_example.case

\_description\_example.detail

'{6^6}' 'Point symbol for diamond'

'{4.6^2}\_2{4^2.6^10.8^3}' '3,6-coordinated underlying net of TiO2'

\_type.purpose Encode

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_net

\_definition.id topol\_net

\_name.category\_id TOPOLOGY

\_name.object\_id topol\_node

\_definition.update 2021-05-03

\_definition.scope Category

\_definition.class Loop

\_description.text

;

The TOPOL\_NET category describes an underlying net, its

topological properties and occurrence in other structures.

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

;

loop\_

\_category\_key.name

'\_topol\_net.id'

save\_

save\_topol\_net.genus

\_definition.id '\_topol\_net.genus'

\_name.category\_id topol\_net

\_name.object\_id genus

\_definition.update 2018-02-06

\_description.text

;

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.

;

\_type.contents Index

\_type.purpose Number

\_type.source Derived

\_type.container Single

save\_

save\_topol\_net.id

\_definition.id '\_topol\_net.id'

\_name.category\_id topol\_net

\_name.object\_id id

\_definition.update 2021-05-05

\_description.text

;

The identifier of the underlying net.

;

\_type.contents Text

\_type.purpose Key

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_net.occurrence\_total

\_definition.id '\_topol\_net.occurrence\_total'

\_name.category\_id topol\_net

\_name.object\_id occurrence\_total

\_definition.update 2018-02-13

\_description.text

;

The total number of occurrences in literature and databases of the

underlying net topology at the time the data file was prepared.

;

\_type.contents Count

\_type.purpose Number

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_net.overall\_topology

\_definition.id '\_topol\_net.overall\_topology'

\_name.category\_id topol\_net

\_name.object\_id overall\_topology

\_definition.update 2018-01-30

\_description.text

;

The overall topology symbol in an arbitrary form.

;

\_type.contents Text

loop\_

\_description\_example.case

'face-centered cubic topology'

\_type.purpose Describe

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_net.overall\_topology\_EPINET

\_definition.id '\_topol\_net.overall\_topology\_EPINET'

\_name.category\_id topol\_net

\_name.object\_id overall\_topology\_EPINET

\_definition.update 2018-01-30

\_description.text

;

The identifier for the overall topology as listed

in the EPINET database at http://epinet.anu.edu.au.

;

\_type.contents Text

loop\_

\_description\_example.case

sqc6

\_type.purpose Encode

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_net.overall\_topology\_RCSR

\_definition.id '\_topol\_net.overall\_topology\_RCSR'

\_name.category\_id topol\_net

\_name.object\_id overall\_topology\_RCSR

\_definition.update 2018-01-30

\_description.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.

;

\_type.contents Text

loop\_

\_description\_example.case

dia

\_type.purpose Encode

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_net.overall\_topology\_SP

\_definition.id '\_topol\_net.overall\_topology\_SP'

\_name.category\_id topol\_net

\_name.object\_id overall\_topology\_SP

\_definition.update 2018-01-30

\_description.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.

A62, 152-167.

;

\_type.contents Text

loop\_

\_description\_example.case

4/6/c1

\_type.purpose Encode

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_net.overall\_topology\_TOPOS

\_definition.id '\_topol\_net.overall\_topology\_TOPOS'

\_name.category\_id topol\_net

\_name.object\_id overall\_topology\_TOPOS

\_definition.update 2018-02-06

\_description.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.

;

\_type.contents Text

loop\_

\_description\_example.case

\_description\_example.detail

'3,3,4T3'

;

The third three-periodic trinodal net with two 3-coordinated and one

4-coordinated independent nodes

;

\_type.purpose Encode

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_net.period

\_definition.id '\_topol\_net.period'

\_name.category\_id topol\_net

\_name.object\_id period

\_definition.update 2018-01-30

\_type.container Single

\_type.purpose State

\_description.text

;

Periodicity of the underlying net. The allowed data values

have the following meaning:

0 0-periodic (finite)

1 1-periodic (chain)

2 2-periodic (layer)

3 3-periodic (framework)

;

\_type.contents Count

\_enumeration.range 0:3

\_type.source Derived

save\_

save\_topol\_net.special\_details

\_definition.id '\_topol\_net.special\_details'

\_name.category\_id topol\_net

\_name.object\_id special\_details

\_definition.update 2021-05-03

\_description.text

;

An arbitrary description of the net.

;

\_type.contents Text

\_type.purpose Describe

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_net.td10

\_definition.id '\_topol\_net.td10'

\_name.category\_id topol\_net

\_name.object\_id td10

\_definition.update 2018-01-30

\_description.text

;

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.

;

\_type.contents Index

\_type.purpose Number

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_net.total\_point\_symbol

\_definition.id '\_topol\_net.total\_point\_symbol'

\_name.category\_id topol\_net

\_name.object\_id total\_point\_symbol

\_definition.update 2018-01-30

\_description.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.

;

\_type.contents Text

loop\_

\_description\_example.case

\_description\_example.detail

'{6^6}' 'Point symbol for diamond'

'{4.6^2}\_2{4^2.6^10.8^3}' '3,6-coordinated underlying net of TiO2'

\_type.purpose Encode

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_node

\_definition.id topol\_node

\_name.category\_id TOPOLOGY

\_name.object\_id topol\_node

\_definition.update 2018-02-06

\_definition.scope Category

\_definition.class Loop

\_description.text

;

The TOPOL\_NODE category describes the chemical composition,

structure and topological properties of the nodes of the underlying

net. Nodes may be specified by reference to atom sites, or by

explicitly giving their coordinates.

Reference: Blatov, V. A., O'Keeffe, M. & Proserpio, D. M. (2010).

Cryst. Eng. Comm. 12, 44-48.

;

\_category\_key.name '\_topol\_node.label'

save\_

save\_topol\_node.atom\_label

\_definition.id '\_topol\_node.atom\_label'

\_name.object\_id atom\_label

\_name.category\_id topol\_node

\_definition.class Datum

\_description.text

;

The atom label corresponding to this node. Not all nodes have

to coincide with atom sites. If a node does not correspond to an atom,

then this item, if present, should be represented by '.'.

;

\_type.purpose Link

\_type.source Related

\_type.container Single

\_type.contents Code

\_name.linked\_item\_id '\_atom\_site.label'

save\_

save\_topol\_node.chemical\_formula\_iupac

\_definition.id '\_topol\_node.chemical\_formula\_iupac'

\_name.category\_id topol\_node

\_name.object\_id chemical\_formula\_iupac

\_definition.update 2018-01-30

\_description.text

;

Formula of the residue or ion which corresponds to the node,

expressed in conformance with IUPAC rules.

;

\_type.contents Text

\_type.purpose Encode

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_node.chemical\_formula\_moiety

\_definition.id '\_topol\_node.chemical\_formula\_moiety'

\_name.category\_id topol\_node

\_name.object\_id chemical\_formula\_moiety

\_definition.update 2018-01-30

\_description.text

;

Formula of the residue or ion which corresponds to the node.

The formula is written in accordance with the rules of the

\_chemical\_formula.moiety tag.

;

\_type.contents Text

\_type.purpose Encode

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_node.chemical\_formula\_sum

\_definition.id '\_topol\_node.chemical\_formula\_sum'

\_name.category\_id topol\_node

\_name.object\_id chemical\_formula\_sum

\_definition.update 2018-01-30

\_description.text

;

Formula of the residue or ion which corresponds to the node.

The formula is written in accordance with the rules of the

\_chemical\_formula.sum tag.

;

\_type.contents Text

\_type.purpose Encode

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_node.structural\_formula\_InChI

\_definition.id '\_topol\_node.structural\_formula\_InChI'

\_name.category\_id topol\_node

\_name.object\_id structural\_formula\_inchi

\_definition.update 2018-04-05

\_description.text

;

Formula of the residue or ion which corresponds to the node.

The formula is written in accordance with the rules for IUPAC

international chemical identifiers (InChI) as described

by Heller et al. (2015).

Reference: Heller, S. R., McNaught, A., Pletnev, I. &

Tchekhovskoi, D. (2015). J. Cheminformat. 7:23,

DOI:10.1186/s13321-015-0068-4.

;

\_type.contents Text

\_type.purpose Encode

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_node.structural\_formula\_SMILES

\_definition.id '\_topol\_node.structural\_formula\_SMILES'

\_name.category\_id topol\_node

\_name.object\_id structural\_formula\_smiles

\_definition.update 2018-04-05

\_description.text

;

Formula of the residue or ion which corresponds to the node.

The formula is written in SMILES notation for describing

chemical structure as formalised by the OpenSMILES group

(https://www.opensmiles.org).

;

\_type.contents Text

\_type.purpose Encode

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_node.coordination\_sequence

\_definition.id '\_topol\_node.coordination\_sequence'

\_name.category\_id topol\_node

\_name.object\_id coordination\_sequence

\_definition.update 2018-02-06

\_description.text

;

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 kth 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.

;

\_type.contents Integer

\_type.container List

loop\_

\_description\_example.case

\_description\_example.detail

[4 12 24 42 64 92 124 162 204 252]

'The diamond coordination sequence'

\_type.purpose Number

\_type.source Derived

save\_

save\_topol\_node.extended\_point\_symbol

\_definition.id '\_topol\_node.extended\_point\_symbol'

\_name.category\_id topol\_node

\_name.object\_id extended\_point\_symbol

\_definition.update 2018-02-06

\_description.text

;

The extended point symbol of the node lists all shortest circuits

for each angle for each non-equivalent atom. A(b).B(c)... there

are b A-rings and c B-rings for all the N(N-1) circuits per node.

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).

;

\_type.contents Text

loop\_

\_description\_example.case

\_description\_example.detail

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'

\_type.purpose Encode

\_type.source Derived

\_type.container Single

save\_

save\_topol\_node.fract\_x

\_definition.id '\_topol\_node.fract\_x'

\_name.object\_id fract\_x

\_name.category\_id topol\_node

\_definition.class Datum

\_description.text

;

fractional x coordinate of this node.

;

\_type.purpose Link

\_type.source Related

\_type.container Single

\_type.contents Code

\_name.linked\_item\_id '\_atom\_site.label'

\_method.purpose Definition

\_method.expression

;

\_enumeration.default = atom\_site[topol\_node.atom\_label].fract\_x

;

save\_

save\_topol\_node.fract\_y

\_definition.id '\_topol\_node.fract\_y'

\_name.object\_id fract\_y

\_name.category\_id topol\_node

\_definition.class Datum

\_description.text

;

fractional y coordinate of this node.

;

\_type.purpose Link

\_type.source Related

\_type.container Single

\_type.contents Code

\_name.linked\_item\_id '\_atom\_site.label'

\_method.purpose Definition

\_method.expression

;

\_enumeration.default = atom\_site[topol\_node.atom\_label].fract\_y

;

save\_

save\_topol\_node.fract\_z

\_definition.id '\_topol\_node.fract\_z'

\_name.object\_id fract\_z

\_name.category\_id topol\_node

\_definition.class Datum

\_description.text

;

fractional z coordinate of this node.

;

\_type.purpose Link

\_type.source Related

\_type.container Single

\_type.contents Code

\_name.linked\_item\_id '\_atom\_site.label'

\_method.purpose Definition

\_method.expression

;

\_enumeration.default = atom\_site[topol\_node.atom\_label].fract\_z

;

save\_

save\_topol\_node.label

\_definition.id '\_topol\_node.label'

\_name.category\_id topol\_node

\_name.object\_id label

\_definition.update 2018-01-30

\_description.text

;

The label of the node, which corresponds to a particular

node of the crystal structure representation.

;

\_type.contents Text

\_type.purpose Key

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_node.point\_symbol

\_definition.id '\_topol\_node.point\_symbol'

\_name.category\_id topol\_node

\_name.object\_id point\_symbol

\_definition.update 2018-02-06

\_description.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) circuits

;

\_type.contents Text

loop\_

\_description\_example.case

\_description\_example.detail

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'

\_type.purpose Encode

\_type.source Derived

\_type.container Single

save\_

save\_topol\_node.symmetry\_multiplicity

\_definition.id '\_topol\_node.symmetry\_multiplicity'

\_name.object\_id symmetry\_multiplicity

\_name.category\_id topol\_node

\_definition.class Datum

\_description.text

;

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).

;

\_type.purpose Number

\_type.source Derived

\_type.container Single

\_type.contents Index

\_enumeration.range 1:192

\_definition.update 2018-02-23

save\_

save\_topol\_node.vertex\_symbol

\_definition.id '\_topol\_node.vertex\_symbol'

\_name.category\_id topol\_node

\_name.object\_id vertex\_symbol

\_definition.update 2018-02-06

\_description.text

;

The vertex symbol of a node provides similar information to the

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.

;

\_type.contents Text

loop\_

\_description\_example.case

\_description\_example.detail

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'

\_type.purpose Encode

\_type.source Derived

\_type.container Single

save\_

save\_topol\_node.Wyckoff\_symbol

\_definition.id '\_topol\_node.Wyckoff\_symbol'

\_name.object\_id Wyckoff\_symbol

\_name.category\_id topol\_node

\_definition.class Datum

\_description.text

;

The Wyckoff symbol (letter) as listed in the space-group section

of International Tables for Crystallography, Vol. A (1987).

;

\_definition.update 2018-02-23

\_type.purpose Encode

\_type.source Assigned

\_type.container Single

\_type.contents Code

save\_

save\_topol\_occurrence

\_definition.id topol\_occurrence

\_name.category\_id TOPOLOGY

\_name.object\_id topol\_occurrence

\_definition.update 2018-01-30

\_definition.scope Category

\_definition.class Loop

\_description.text

;

The TOPOL\_OCCURRENCE category lists the appearances of the

underlying net topology in crystal structures.

;

\_category\_key.name '\_topol\_occurrence.id'

save\_

save\_topol\_occurrence.id

\_definition.id '\_topol\_occurrence.id'

\_name.category\_id topol\_occurrence

\_name.object\_id id

\_definition.update 2018-02-13

\_description.text

;

A unique identifier for the literature or database reference.

;

\_type.contents Text

\_type.purpose Key

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_occurrence.citation\_id

\_definition.id '\_topol\_occurrence.citation\_id'

\_name.category\_id topol\_occurrence

\_name.object\_id citation\_id

\_definition.update 2018-04-17

\_description.text

;

Reference to a publication, where a crystal structure with the

underlying net topology was characterized. This item is a pointer

to an item described in the core CITATION category. If a publication

and database entry are not directly related, they should be listed

in separate rows.

;

\_type.contents Code

\_type.purpose Link

\_type.source Related

\_type.container Single

\_name.linked\_item\_id '\_citation.id'

save\_

save\_topol\_tiling

\_definition.id topol\_tiling

\_name.category\_id TOPOLOGY

\_name.object\_id topol\_tiling

\_definition.update 2018-02-06

\_definition.scope Category

\_definition.class Set

\_description.text

;

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. A63, 418-425.

;

save\_

save\_topol\_tiling.Dsize

\_definition.id '\_topol\_tiling.Dsize'

\_name.category\_id topol\_tiling

\_name.object\_id Dsize

\_definition.update 2018-01-30

\_description.text

;

The number of distinct (not symmetry-related) chambers in the

tiling.

;

\_type.contents Index

\_type.purpose Number

\_type.source Derived

\_type.container Single

save\_

save\_topol\_tiling.dual

\_definition.id '\_topol\_tiling.dual'

\_name.category\_id topol\_tiling

\_name.object\_id dual

\_definition.update 2018-01-30

\_description.text

;

The overall topology symbol of the dual net, which corresponds

to the net of the dual of the natural tiling.

;

\_type.contents Text

\_type.purpose Encode

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_tiling.edges

\_definition.id '\_topol\_tiling.edges'

\_name.category\_id topol\_tiling

\_name.object\_id edges

\_definition.update 2018-01-30

\_description.text

;

Number of independent tile edges in the natural tiling.

;

\_type.contents Index

\_type.purpose Number

\_type.source Recorded

\_type.container Single

save\_

save\_topol\_tiling.faces

\_definition.id '\_topol\_tiling.faces'

\_name.category\_id topol\_tiling

\_name.object\_id faces

\_definition.update 2018-01-30

\_description.text

;

Number of independent tile faces in the natural tiling.

;

\_type.contents Index

\_type.purpose Number

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_tiling.signature

\_definition.id '\_topol\_tiling.signature'

\_name.category\_id topol\_tiling

\_name.object\_id signature

\_definition.update 2018-02-06

\_description.text

;

The tiling signature, written in the form

\a[A^a^ . B^b^ ...]+\b[C^c^ . D^d^ ...]+...,

where square brackets envelop tile symbols, \a,\b,... are stoichiometric

coefficients, A, B, C, D, ... are sizes of tile faces, a,b,c,d, ... are

numbers of the faces of a given size in the tile.

;

\_type.contents Text

loop\_

\_description\_example.case

\_description\_example.detail

'[6^4]' 'Natural tiling for diamond'

'3[4^6]+[4^6.6^8]+[4^12.6^8.8^6]' 'Natural tiling for zeolite LTA'

\_type.purpose Encode

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_tiling.tiles

\_definition.id '\_topol\_tiling.tiles'

\_name.category\_id topol\_tiling

\_name.object\_id tiles

\_definition.update 2018-01-30

\_description.text

;

Number of independent tiles in the natural tiling.

;

\_type.contents Index

\_type.purpose Number

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_tiling.vertices

\_definition.id '\_topol\_tiling.vertices'

\_name.category\_id topol\_tiling

\_name.object\_id vertices

\_definition.update 2018-01-30

\_description.text

;

Number of independent tile vertices in the natural tiling.

;

\_type.contents Index

\_type.purpose Number

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_tiling\_faces

\_definition.id topol\_tiling\_faces

\_name.category\_id TOPOLOGY

\_name.object\_id topol\_tiling\_faces

\_definition.update 2018-02-13

\_definition.scope Category

\_definition.class Loop

\_description.text

;

The TOPOL\_TILING\_FACES category tabulates the faces

belonging to each tile in the tiling. Together with the

TOPOL\_TILING\_TILES category it tabulates the information

contained in \_topol\_tiling.signature. See the

TOPOL\_TILING category for further information.

;

loop\_

\_category\_key.name

'\_topol\_tiling\_faces.tile\_id'

'\_topol\_tiling\_faces.size'

loop\_

\_description\_example.detail

\_description\_example.case

'Expanded description of 3[4^6^]+[4^6^.6^8^]+[4^12^.6^8^.8^6^] tiling'

;

loop\_

\_topol\_tiling\_tile.id

\_topol\_tiling\_tile.count

a 3

b 1

c 1

loop\_

\_topol\_tiling\_faces.tile\_id

\_topol\_tiling\_faces.size

\_topol\_tiling\_faces.count

a 4 6

b 4 6

b 6 8

c 4 12

c 6 8

c 8 6

;

save\_

save\_topol\_tiling\_faces.count

\_definition.id '\_topol\_tiling\_faces.count'

\_name.category\_id topol\_tiling\_faces

\_name.object\_id count

\_definition.update 2018-02-13

\_description.text

;

The number of faces of this size in the tile.

;

\_type.contents Index

\_type.purpose Number

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_tiling\_faces.size

\_definition.id '\_topol\_tiling\_faces.size'

\_name.category\_id topol\_tiling\_faces

\_name.object\_id size

\_definition.update 2018-02-13

\_description.text

;

The size of the tile face.

;

\_type.contents Count

\_enumeration.range 3:

\_type.purpose Number

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_tiling\_faces.tile\_id

\_definition.id '\_topol\_tiling\_faces.tile\_id'

\_name.category\_id topol\_tiling\_faces

\_name.object\_id tile\_id

\_definition.update 2018-02-13

\_description.text

;

The tile to which this face belongs. It must be one of the values provided

in \_topol\_tiling\_tile.id.

;

\_type.contents Code

\_name.linked\_item\_id '\_topol\_tiling\_tile.id'

\_type.purpose Link

\_type.source Related

\_type.container Single

save\_

save\_topol\_tiling\_tile

\_definition.id topol\_tiling\_tile

\_name.category\_id TOPOLOGY

\_name.object\_id topol\_tiling\_tile

\_definition.update 2018-02-13

\_definition.scope Category

\_definition.class Loop

\_description.text

;

The TOPOL\_TILING\_TILE category provides information on

each of the tiles in the tiling. Together with the

TOPOL\_TILING\_FACES category it tabulates the information

contained in \_topol\_tiling.signature. See the

TOPOL\_TILING category for further information.

;

\_category\_key.name '\_topol\_tiling\_tile.id'

save\_

save\_topol\_tiling\_tile.count

\_definition.id '\_topol\_tiling\_tile.count'

\_name.category\_id topol\_tiling\_tile

\_name.object\_id count

\_definition.update 2018-02-13

\_description.text

;

The number of this kind of tile in the tiling.

;

\_type.contents Index

\_type.purpose Number

\_type.source Assigned

\_type.container Single

save\_

save\_topol\_tiling\_tile.id

\_definition.id '\_topol\_tiling\_tile.id'

\_name.category\_id topol\_tiling\_tile

\_name.object\_id id

\_definition.update 2018-02-13

\_description.text

;

An arbitrary, unique identifier for this tile type.

;

\_type.contents Code

\_type.purpose Key

\_type.source Assigned

\_type.container Single

save\_

loop\_

\_dictionary\_audit.version

\_dictionary\_audit.date

\_dictionary\_audit.revision

0.3 2018-02-23

;

Changed topol\_bond to topol\_link using node labels instead of atom labels.

Added coordinates, multiplicity and Wyckoff symbol to topol\_node.

Added in type and linking information. (J Hester.)

;

0.4 2018-02-27

;

Added long-form examples provided by V Blatov. Version for review.

;

0.5 2018-04-05

;

Added InChI, SMILES structural formulas and replaced symops with explicit

symmetry operator ids and vector translations. Clarified bond types.

;

0.9 2018-05-28

;

Version for final approval after review. Removed most datanames from

TOPOL\_ENTANGL and subcategories.

;

0.9.1 2019-07-17

;

Fixed a few typos. (B. McMahon)

;

0.9.2 2021-05-04

;

Replaced TOPOL\_REPRES category by TOPOL\_NET; all TOPOL\_REPRES categories are

moved to TOPOL category; Example 4 added

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