Crystal Nets as Graphs

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**Introduction to graph theory
and its application to crystal nets**

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Questions, problems, feedback

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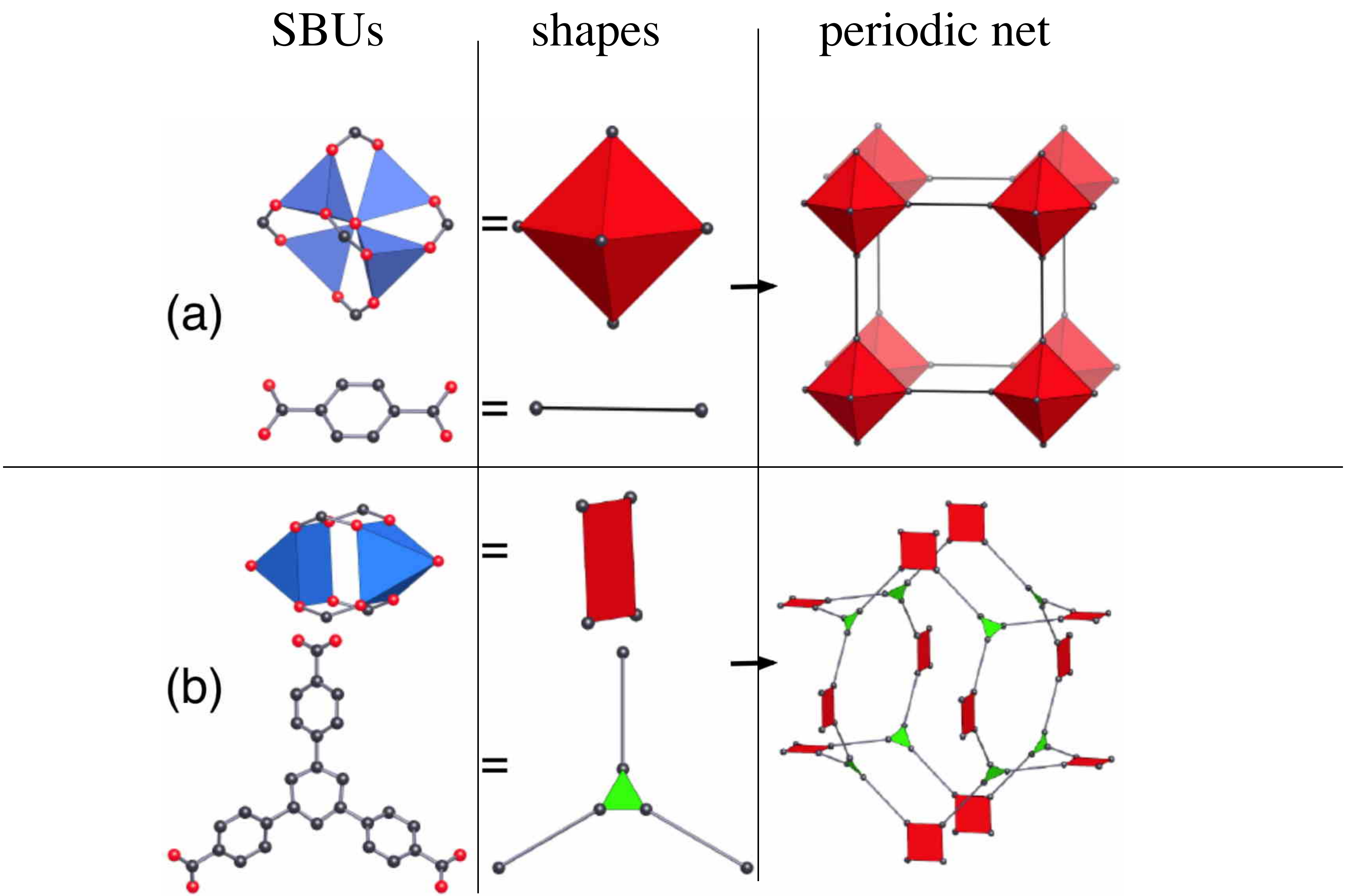
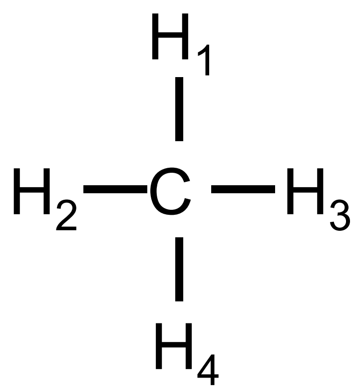


SBUs
shapes
periodic net
(a)
(b)

Now an introduction to graph theory

Molecular topology is a graph



edges:

C H_1

C H_2

C H_3

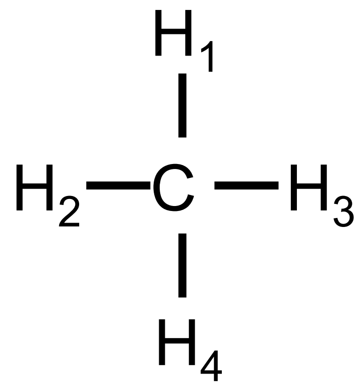
C H_4

atoms (vertices) joined by bonds (edges)
mathematical graph theory is highly developed

Crystals e.g. diamond have topology specified by an **infinite periodic** graph
The mathematics of periodic structures is highly **un**developed.

atoms <-> vertices
SBUs

bonds <-> edges
links



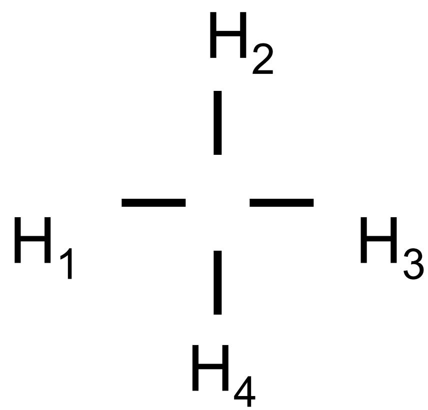
edges:

C H_1

C H_2

C H_3

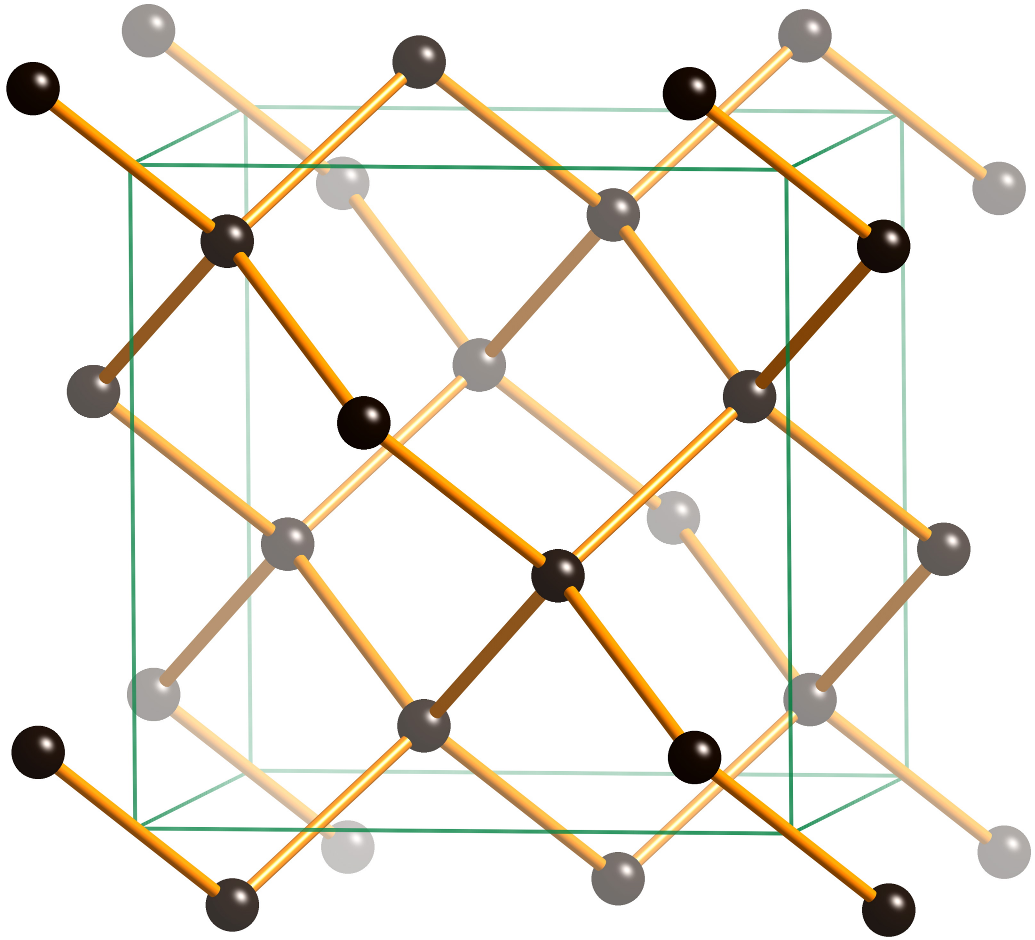
C H_4



same edges

interchanging H_1 and H_2 is an *automorhism* of the graph

→ automorphism group

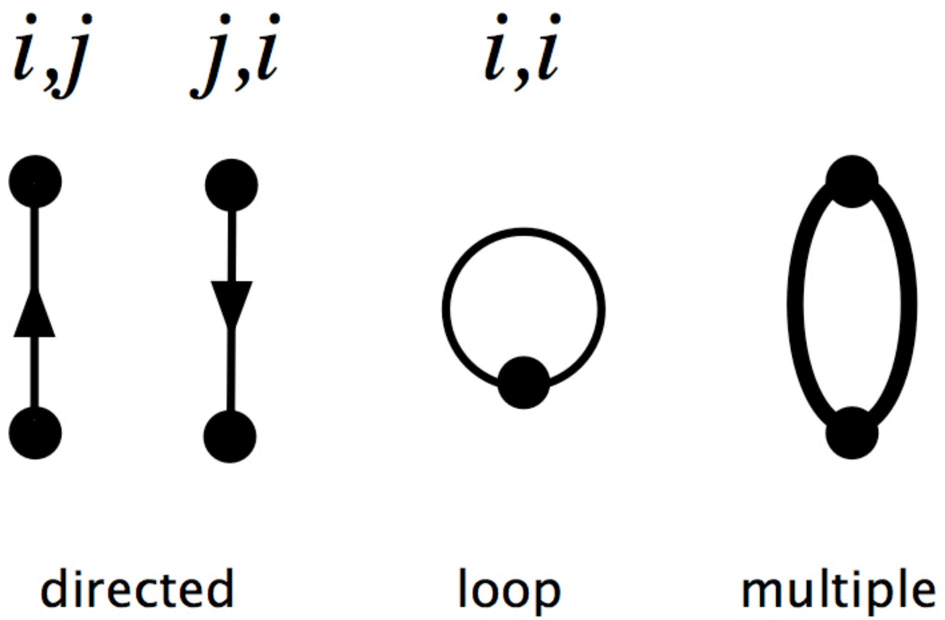


part of the diamond met - a periodic infinite graph

Graph consists of **vertices** ... v_i, v_j ,...

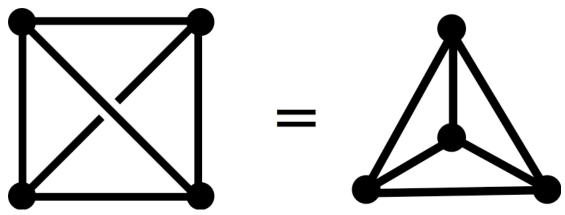
edges (i, j) connect two vertices

special kinds of edge

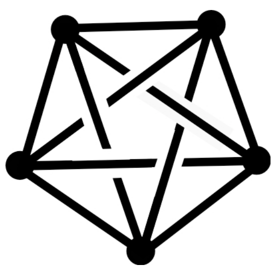


A **faithful embedding** is a realization (e.g. coordinates for vertices) in which edges are finite and do not intersect. Graphs which admit a 2-dimensional faithful embedding are **planar**

The graphs of all convex polyhedra are planar.



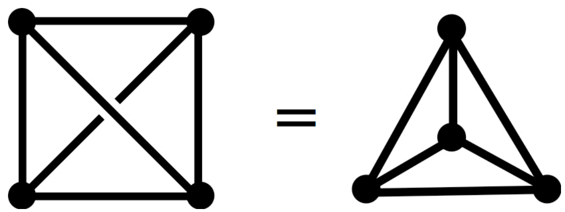
planar



nonplanar

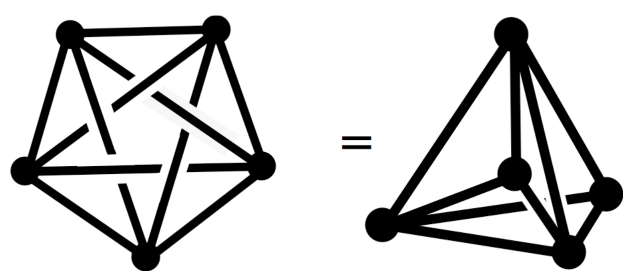
complete graphs –
every vertex linked to every other vertex):

K_4



planar

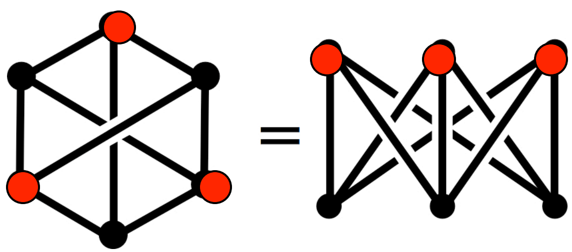
K_5



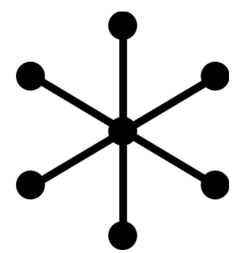
non-planar

Complete bipartite graph $K_{m\,n}$
Two sets of vertices *m* in one set and *n* in the other
all *m* linked only to all *n*

The graph K_{1n} is the same as the star graph S_{n+1}
(an example of a tree)

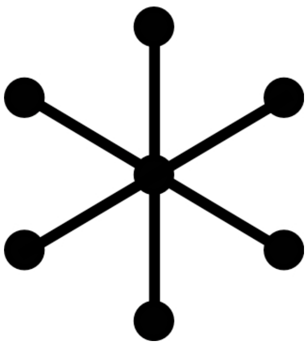


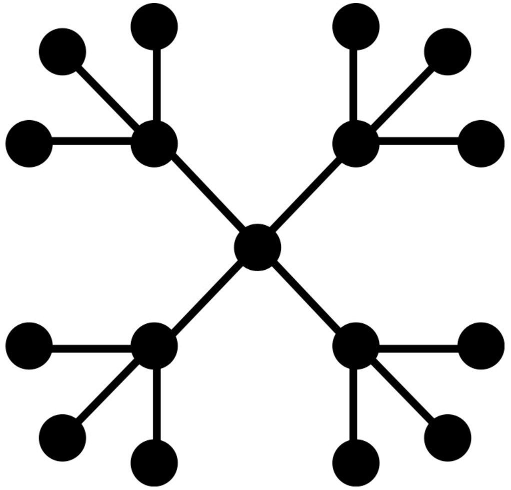
$K_{3\,3}$ (nonplanar)



$K_{1\,6} = S_7$

Tree has no cycles (closed paths)



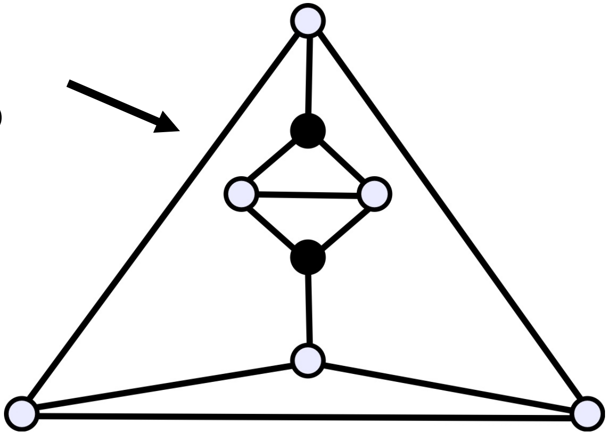


A connected graph
has a continuous path between every pair of vertices

A *k*-connected graph is one in which at least *k* vertices (and their incident edges) have to be deleted to separate the graph into two disjoint pieces.

WARNING! Chemists use *k*-connected to mean *k*-coordinated

A 3-valent (3-coordinated) graph that is not 3-connected. Removal of the two vertices shown as filled circles will separate the graph into two pieces.



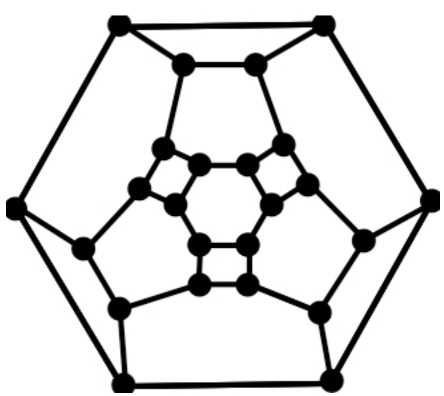
Note: a k+1-connected graph is necessarily *k*-connected

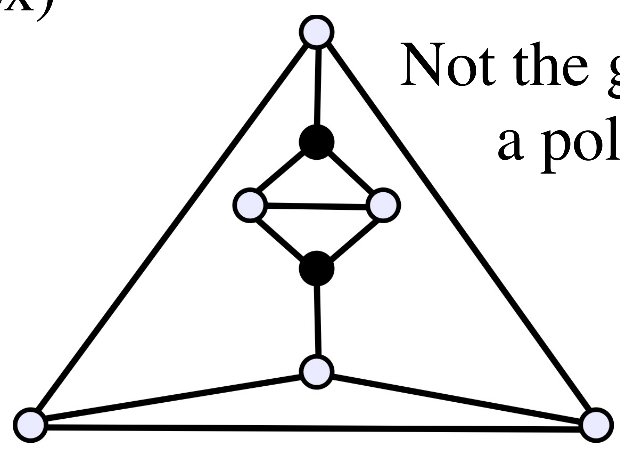
Every 3-connected planar graph can be realized as a convex polyhedron. Steinitz theorem.

A convex polyhedron has planar faces and the line joining any two points on different faces is entirely inside the polyhedron.

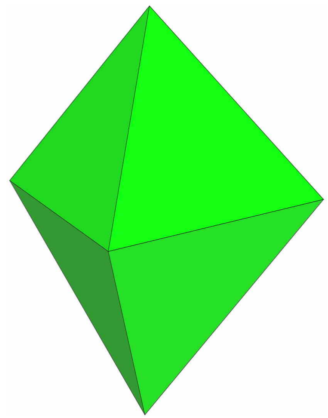
A simple polyhedron has a 3-connected 3-valent graph (three edges meet at each vertex)

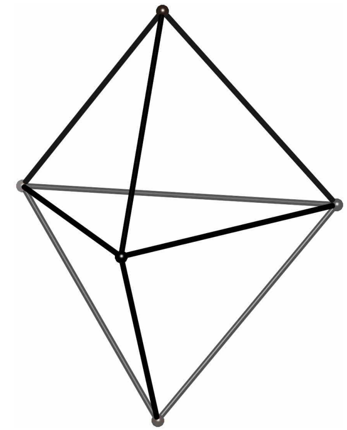
Graph of truncated octahedon (simple)

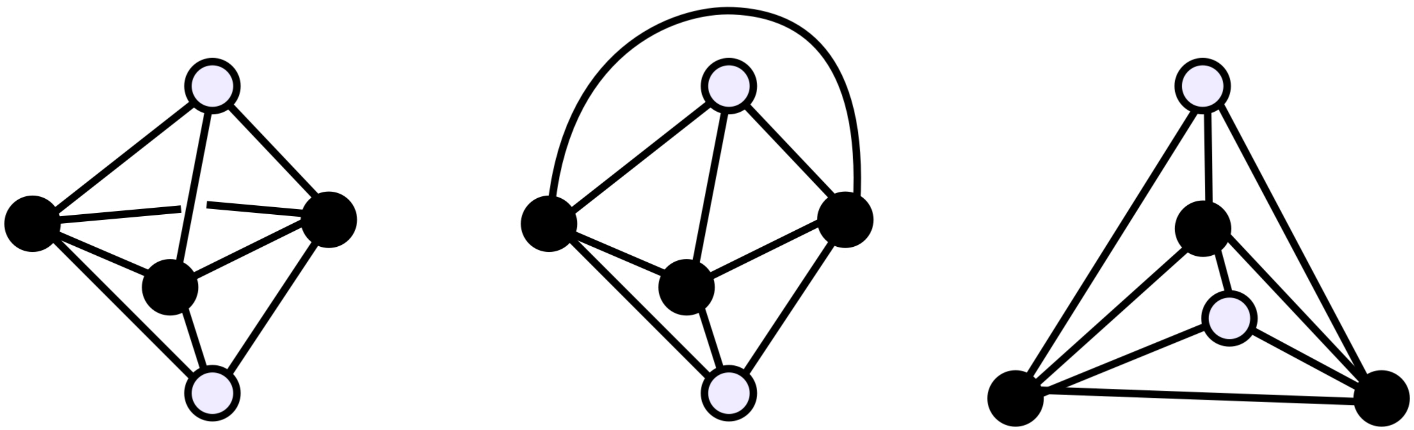




Not the graph of a polyhedron

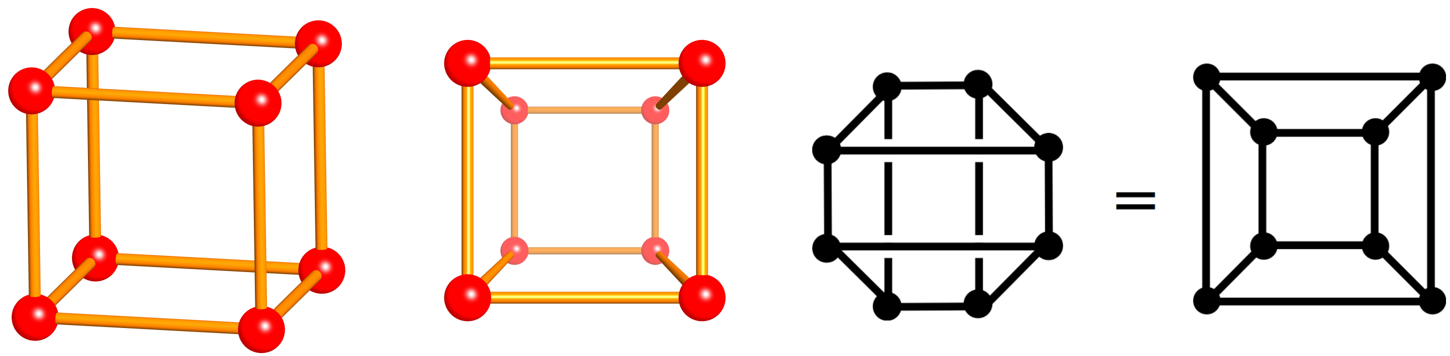




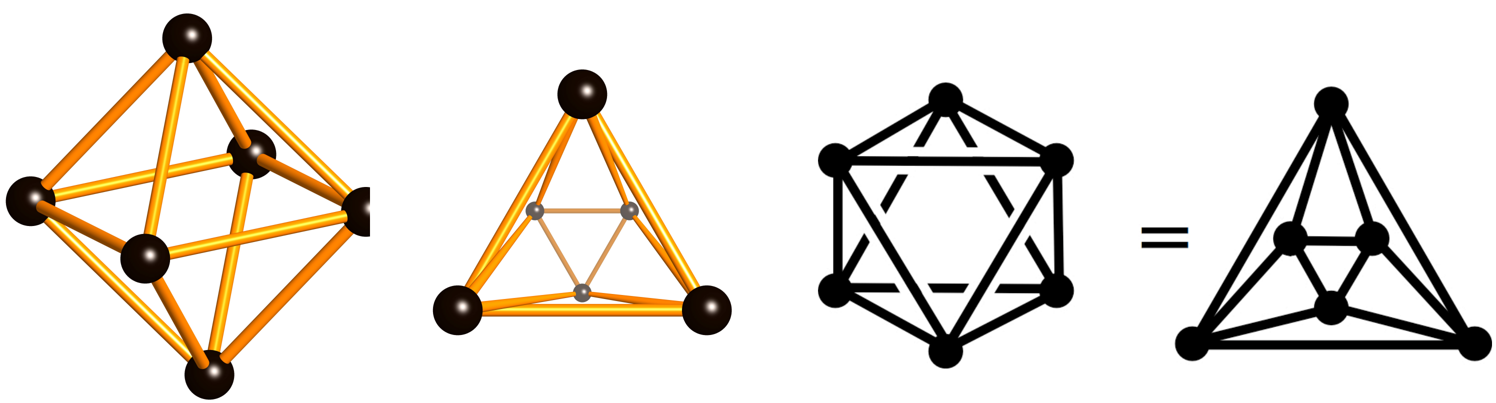


three ways of drawing rge graph of a trigonal bipyramid

More examples of graphs of polyhedra



cube

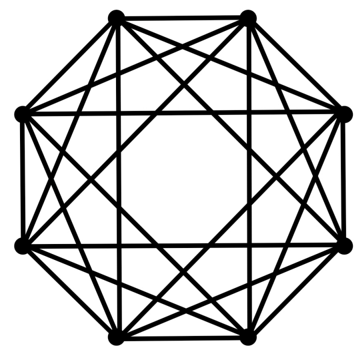


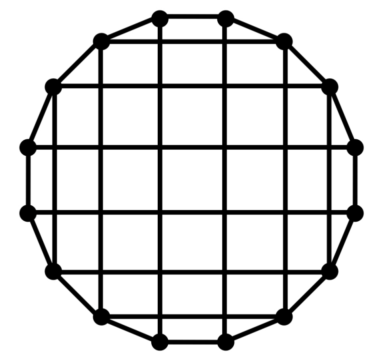
octahedron

Drawings on the right with linear non-intersecting edges are *Schlegel diagrams*.

Some more symmetric (vertex and edge transitive) graphs

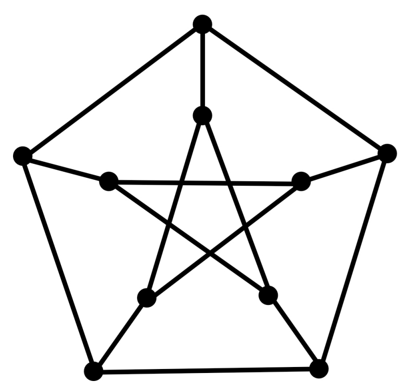
4-D cross polytope
(4-D "octahedron")





tesseract
(4-D "cube")

Petersen graph



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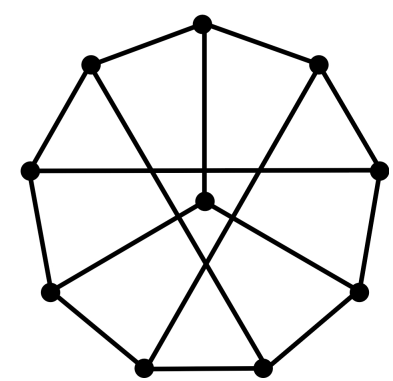
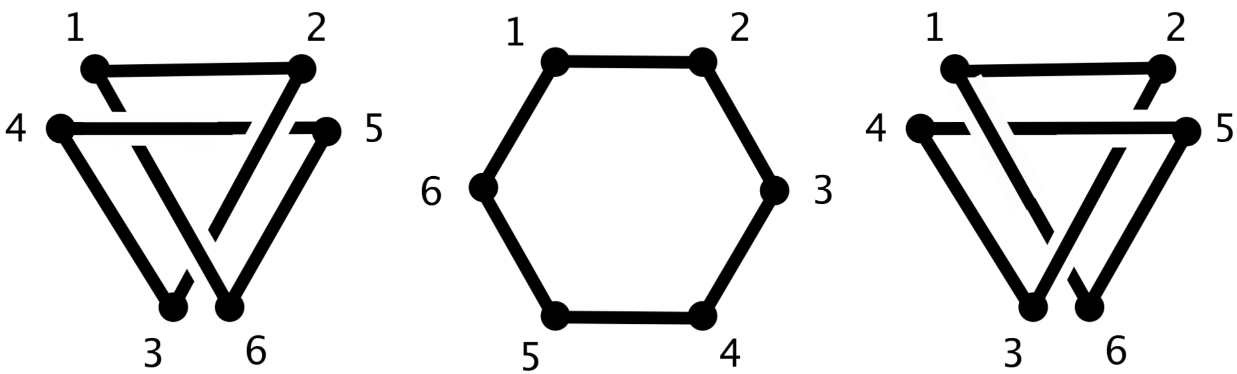
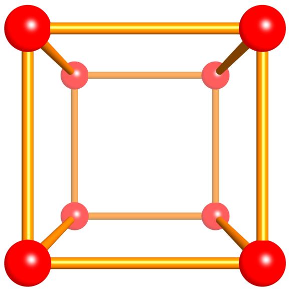
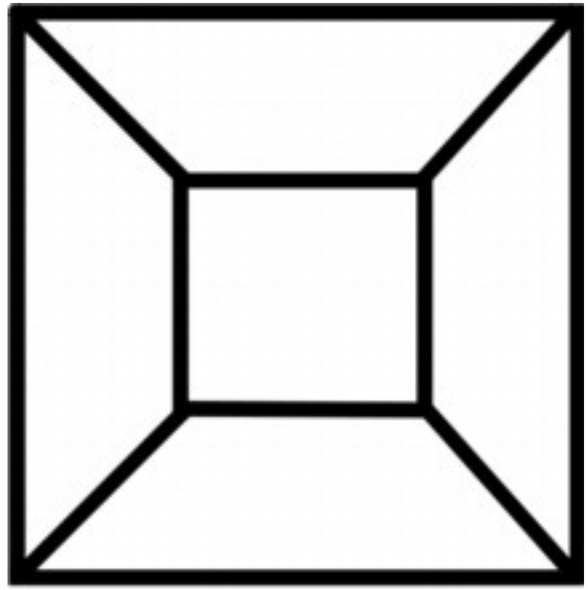


The graphs below are **isomorphic** – there is a one-to-one correspondence between vertices that induces a one-to-one correspondence between edges (vertex 1 is bonded to 2 and 6 in every case, etc.).
The embeddings are not **ambient isotopic** – they cannot be deformed one into another without bonds intersecting. (or going into higher dimensions)

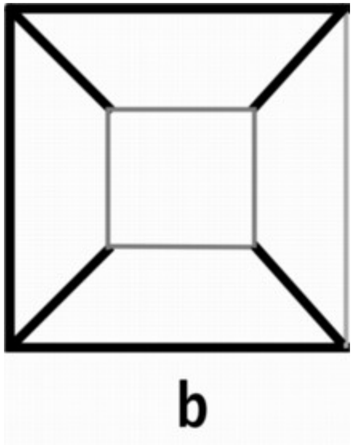






a

This is the graph of a cube (Schlegel diagram)
Note that it is planar



The heavy lines are a connected subgraph without circuits that connects all vertices.

It is a **spanning tree**.

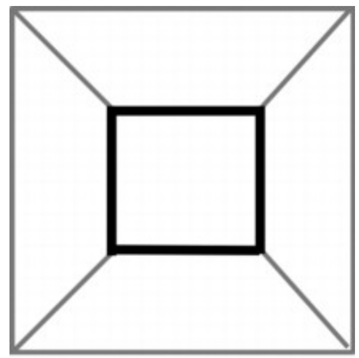
The number of edges necessary to complete the graph is the **cyclomatic number**, g, of the graph (= 5 in this case)

In molecular chemistry this is the number of rings

If there are v vertices and e edges

$$g = 1 - v + e$$

(cubane is pentacyclo-octane)



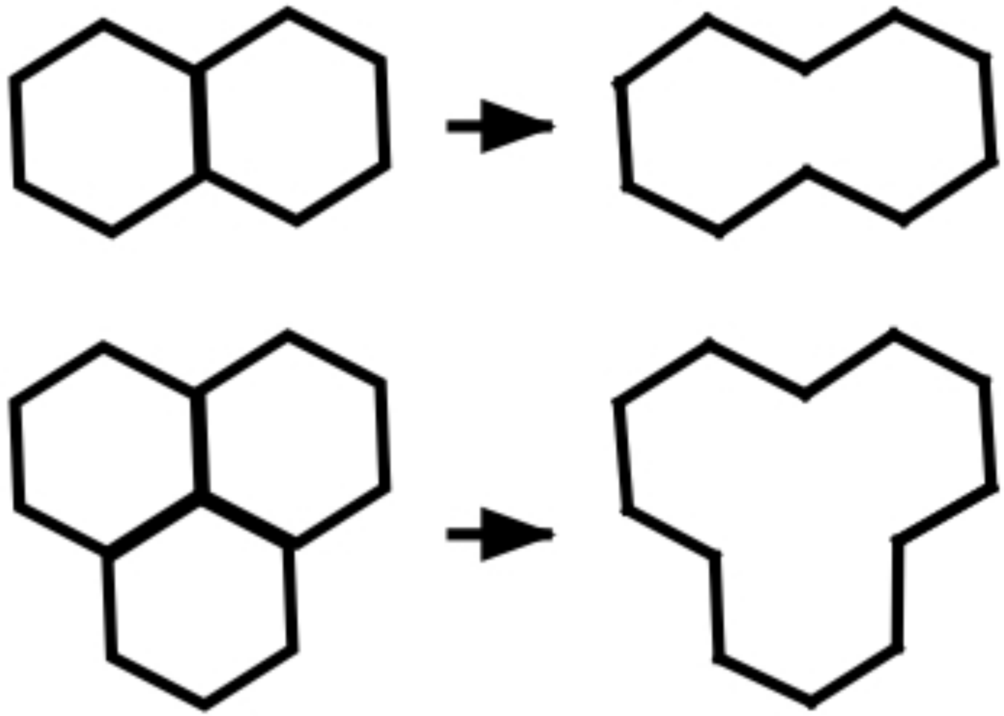
The heavy lines outline a **cycle**
In this case it is also a **strong ring**
as it is not the sum of smaller cycles

Ring (cycle) sum

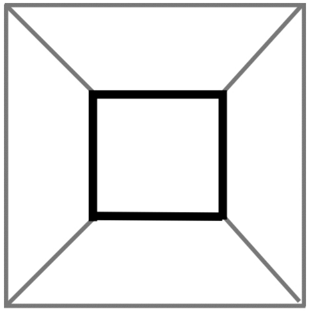
The sum of two rings (cycles) is the set of edges that occur exactly once.

The sum of *n* rings (cycles) is the set of edges that occur an odd number of times.

In solid state chemistry (not molecular chemistry!)
A **ring** is a cycle that is not the sum of two smaller cycles

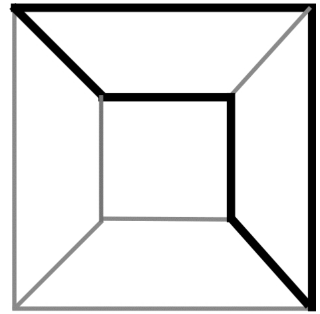


rings sum



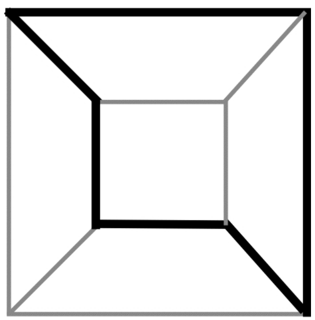
c

A cycle that is a **strong ring** (not the sum of smaller cycles).



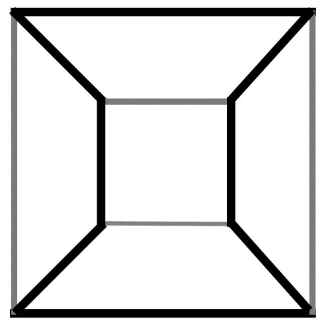
d

A cycle that is not a ring. (It is the sum of two smaller cycles.)



e

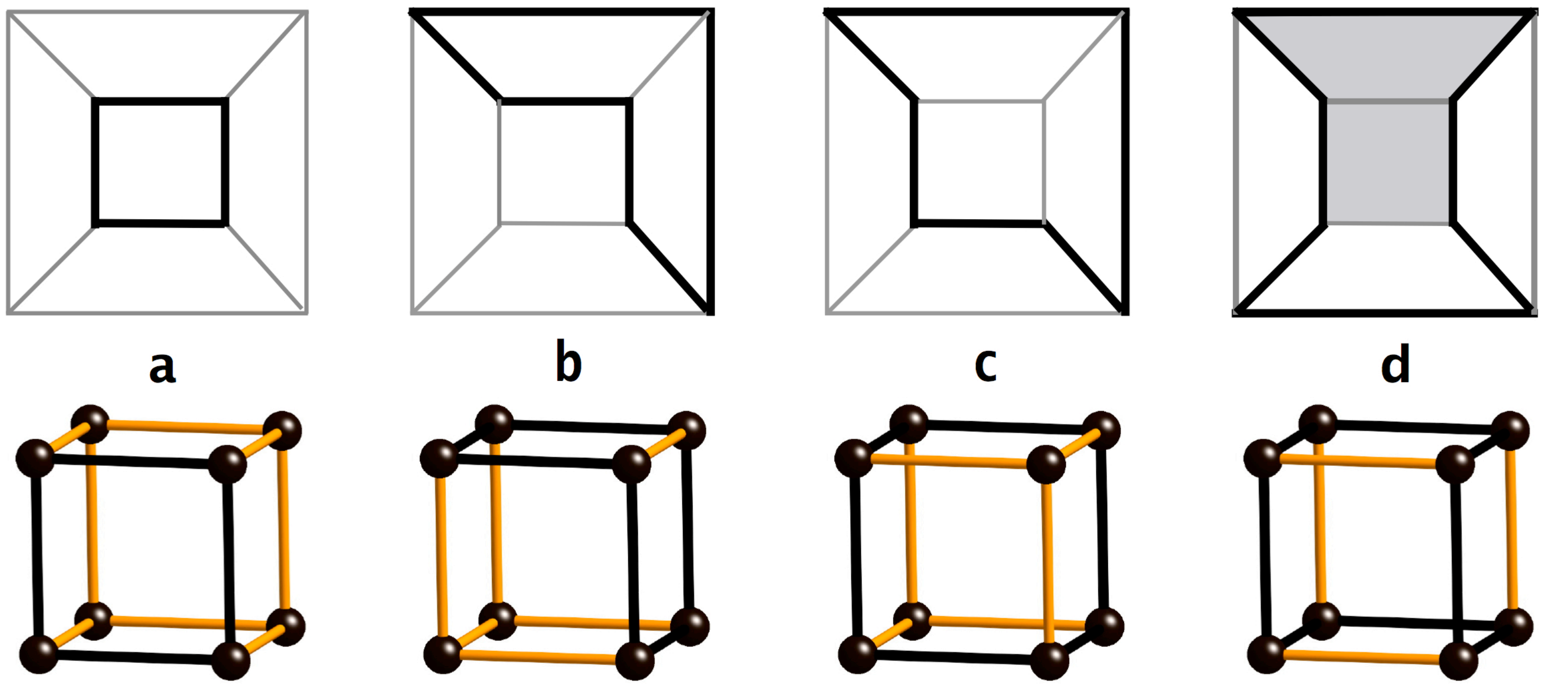
A cycle that is a **ring** (not the sum of two smaller cycles) But **not** a strong ring (it is the sum of three smaller cycles).



f

A cycle that is **not** a ring. It is the sum of two *smaller* cycles: a 6-cycle and a 4-cycle. (Contrast **e** on left.)

Repeated…



strong ring

6-cycle not a ring

(sum of two 4-rings)

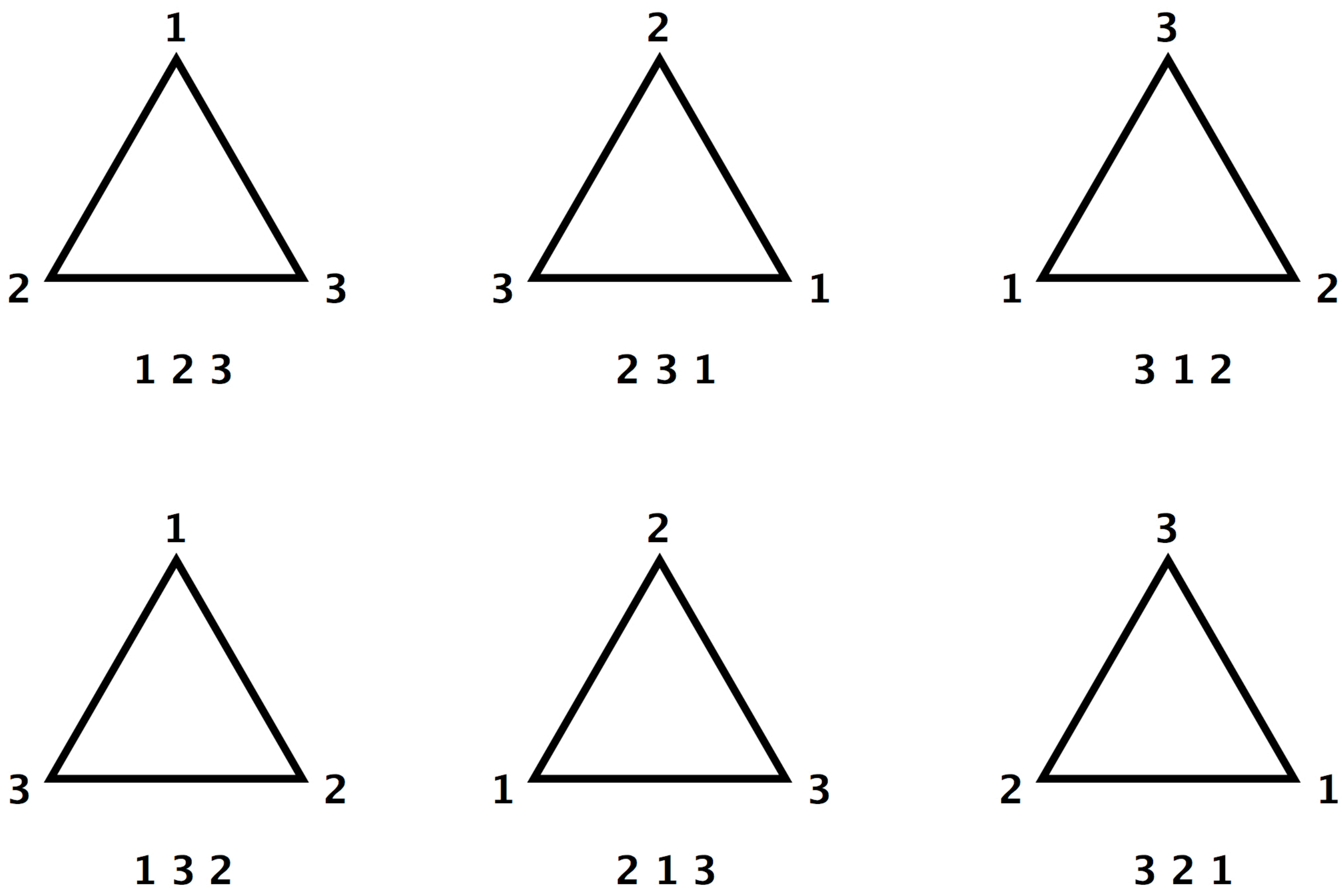
6-ring not a strong ring

(sum of three 4-rings

8-cycle not a ring

(sum of a 4-ring and a 6-ring)

Symmetries of graphs: the automorphism group
An automorphism is a permutation of vertices that preserves the edges.

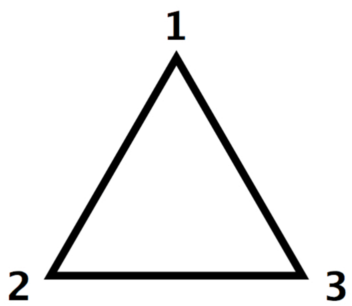


Note 1 2 3 -> 2 3 1

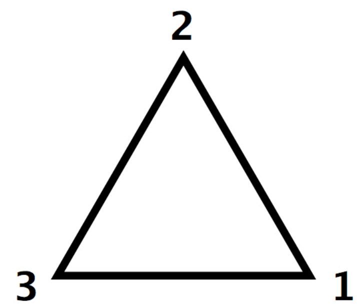
means

put vertex 2 where vertex 1 was
put vertex 3 where vertex 2 was
put vertex 1 where vertex 3 was

Symmetries of graphs: the automorphism group of a planar 3-connected graph is isomorphic to a rigid body symmetry

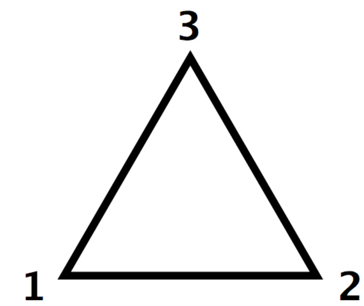


1 2 3



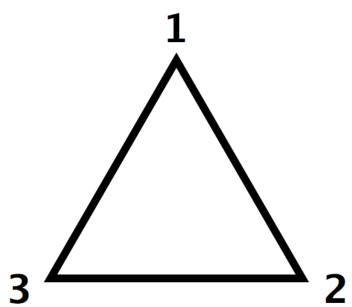
2 3 1

rotate clockwise



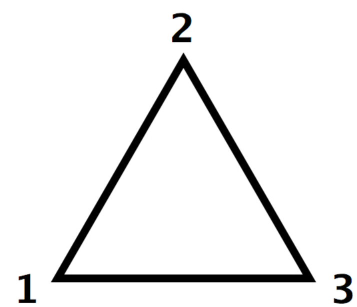
3 1 2

rotate anticlockwise



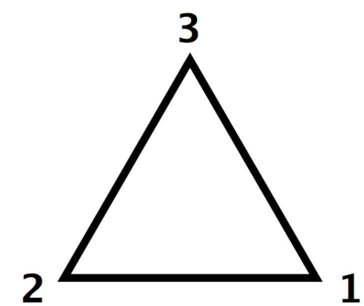
1 3 2

reflect



2 1 3

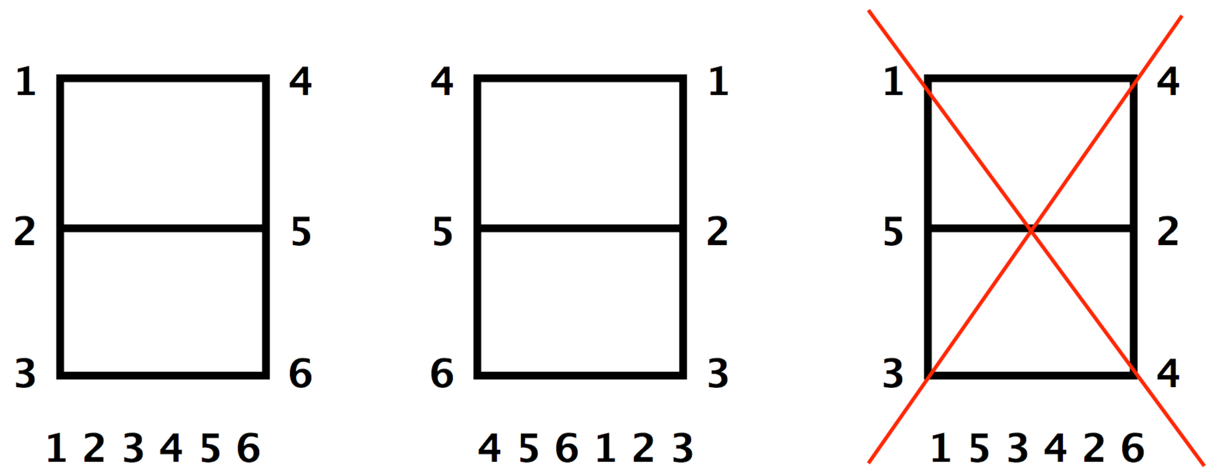
reflect



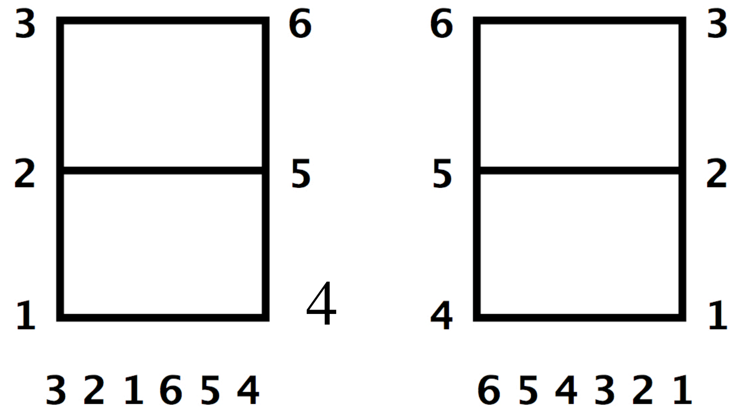
3 2 1

reflect

isomorphic to $3m$

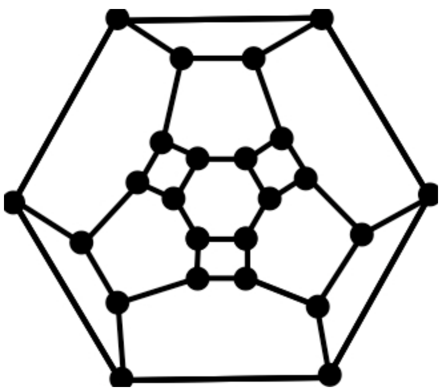


there is no edge 15 in the graph

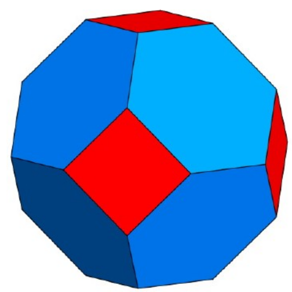


isomorphic to 2*mm*

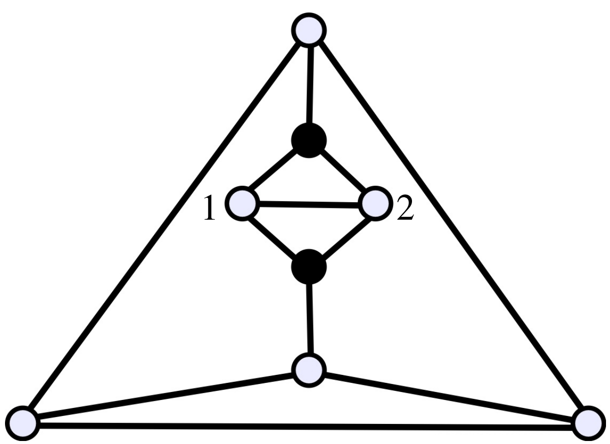
A planar 3-connected graph has combinatorial symmetry isomorphic to the symmetry group of the most-symmetric embedding.



graph of truncated octahedron

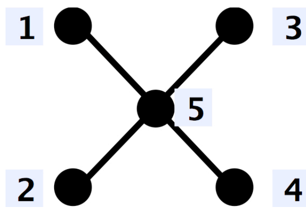


symmetry $m\text{-}3m$. Order 48



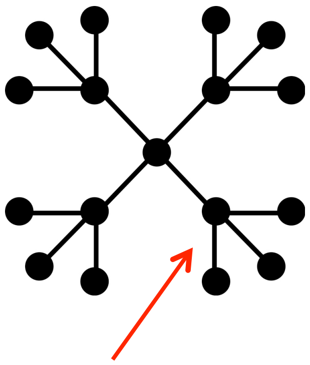
A graph that is not 3-connected can have symmetries that do not correspond to rigid-body symmetries. Interchange of vertices 1 and 2 leaving the rest fixed is a graph automorphism symmetries of molecular graphs

methane CH_4



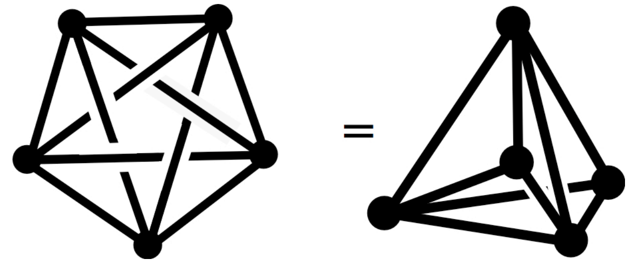
any permutation of vertices 1,2,3,4 is an automorphism of the graph. The automorphism group has order 4! = 24 and is isomorphic to -43*m* (T_d).

neopentane $C(CH_3)_4$
The symmetry of the graph has order 3x3x3x3x24 = 1944
symmetry of flexible molecule



it's not 3-connected! if I delete this vertex, three vertices are isolated

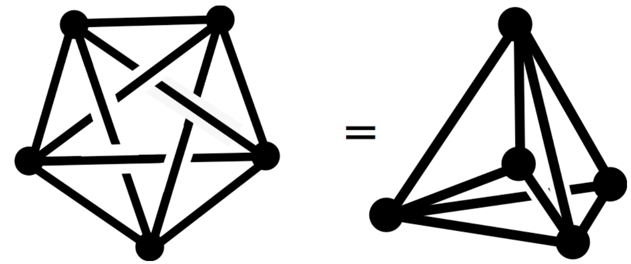
Remember K_5?
In four dimensions it has a symmetrical embedding a simplex (generalization of tetrahedron). Order of symmetry = 5! = 120

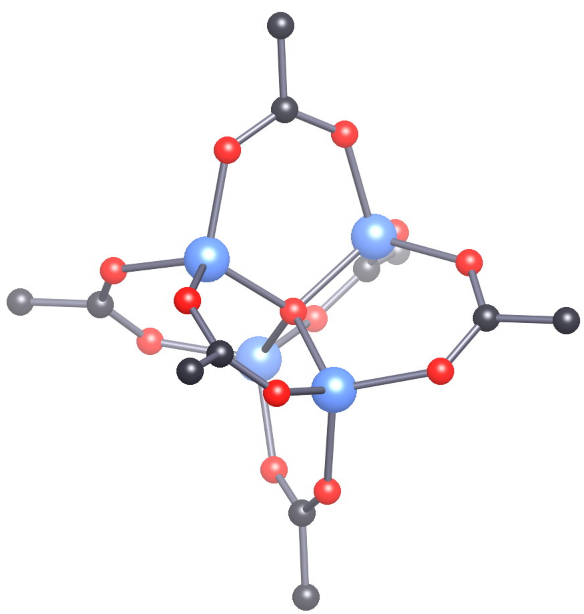


The graph automorhism ("symmetry") group is isomorphic to the symmetric group S_5 corresponding to the group of permutations of 5 things.

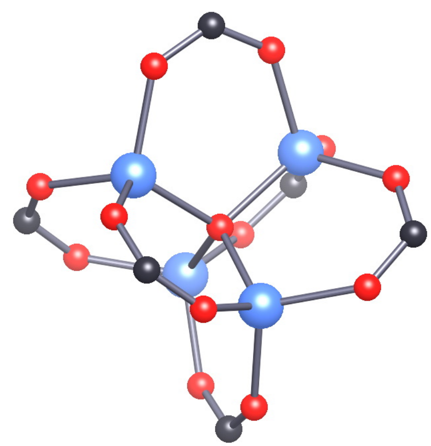
It is also isomorphic to I_h, the group of symmetries of a regular icosahahedron.

K_5

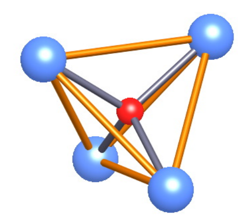




basic Zn acetate (no H)



methyl carbon deleted

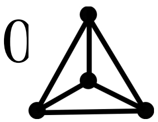


underlying graph is K_5

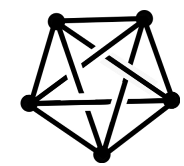
An ***n*-periodic** graph has a realization (not necessarily an embedding) with translational symmetry in exactly *n* independent directions.

Distinguish *n*-periodic from *n*-dimensional

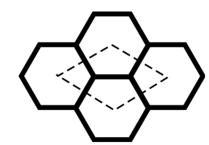
K_4 (graph of tetrahedron) is 2-dimensional but 0 periodic



K_5 is 3-dimensional but 0-periodic



net of graphite layer (honeycomb) is 2-dimensional and 2-periodic.



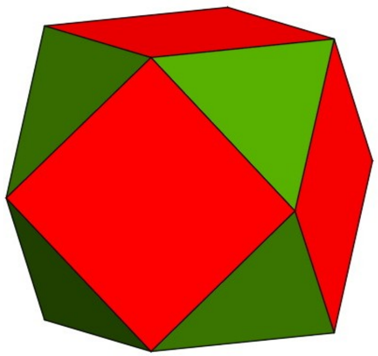
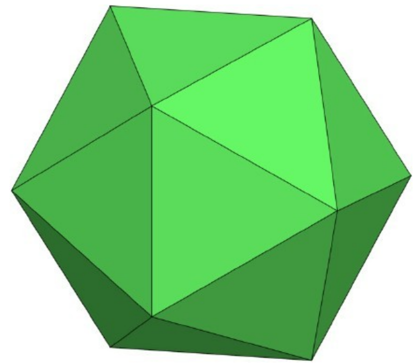
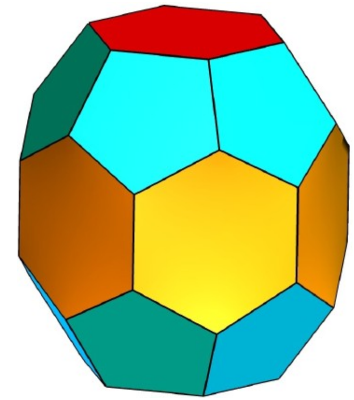
A **net**, as used in solid state chemistry, is a periodic connected simple graph.
(*connected* = there is a continuous path between every pair of vertices)
(*simple* = at most one undirected edge for a pair of vertices)

Vertex and facesymbols for polyhedra and plane nets

(both of these are tilings of two-dimensional surfaces - the surface of a sphere and the euclidean plane respectively).

Vertex Symbol. Give the size of faces in cyclic order around each kind of vertex.

Face symbol. Only for polyhedra (and 3-D cages) Guve the size and total number of faces

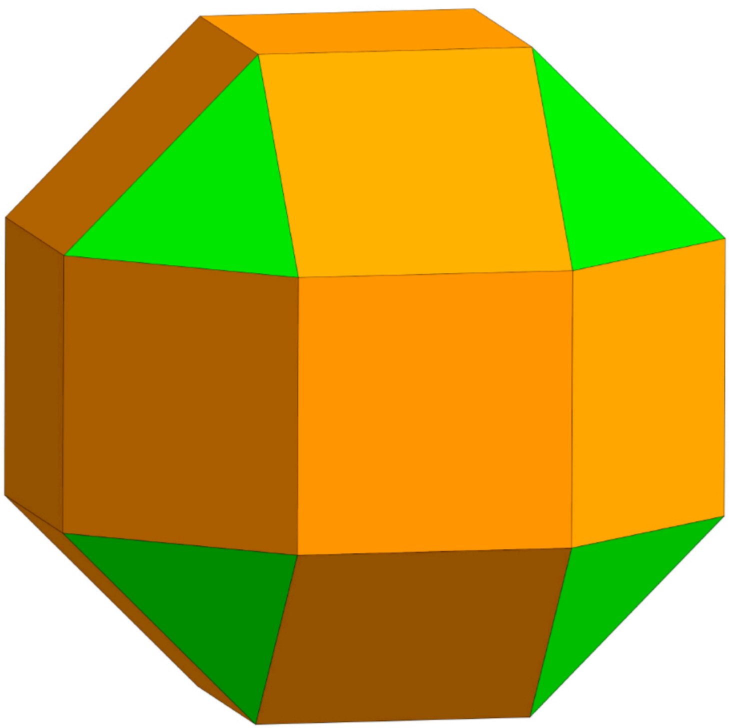
vertex symbol (used mainly when one kind of vertex)

3.4.3.4	3^5	$(5^2.6)_2(5.6^2)$
(not 4.3.4.3)	(short for 3.3.3.3.3)	

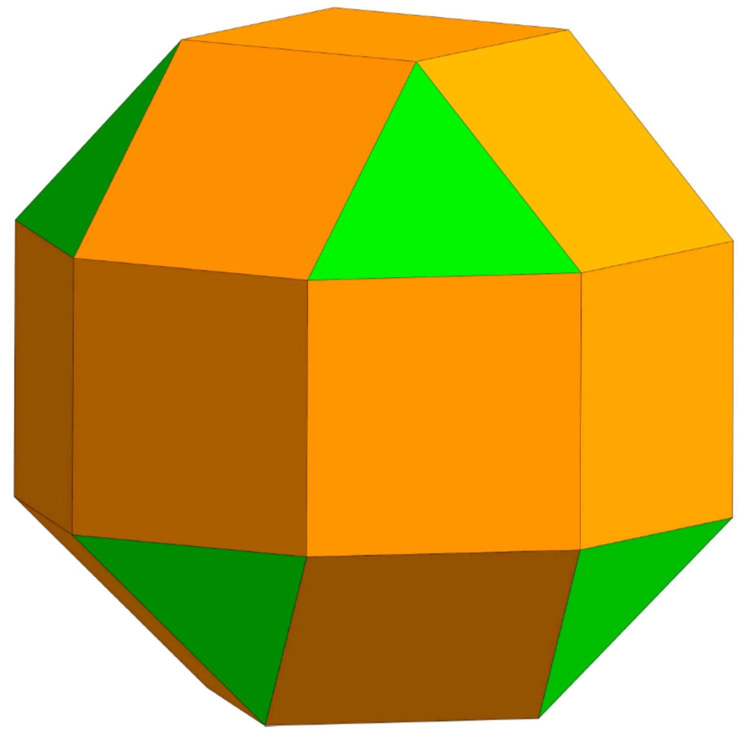
face symbol

$[3^8.4^6]$	$[3^{20}]$	$[5^{12}.6^8]$

Two distinct polyhedra with the same
vertex symbol 3.4^3
face symbol $[3^8.4^{18}]$

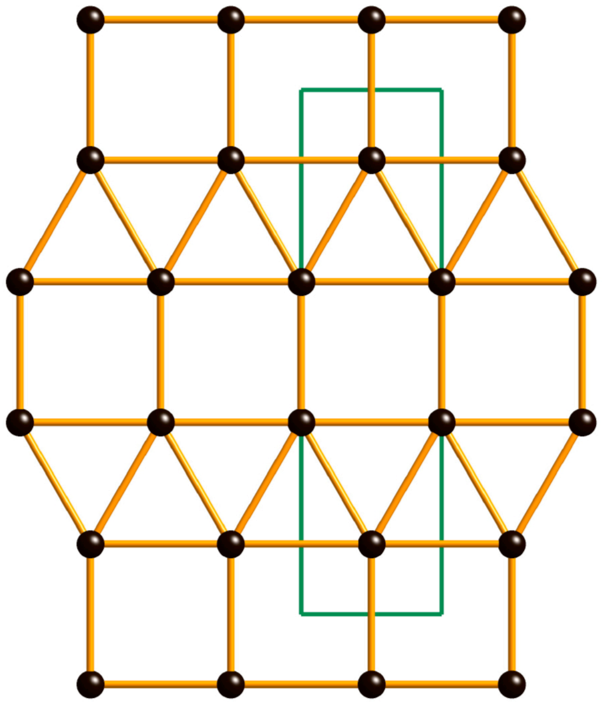


symmetry O_h

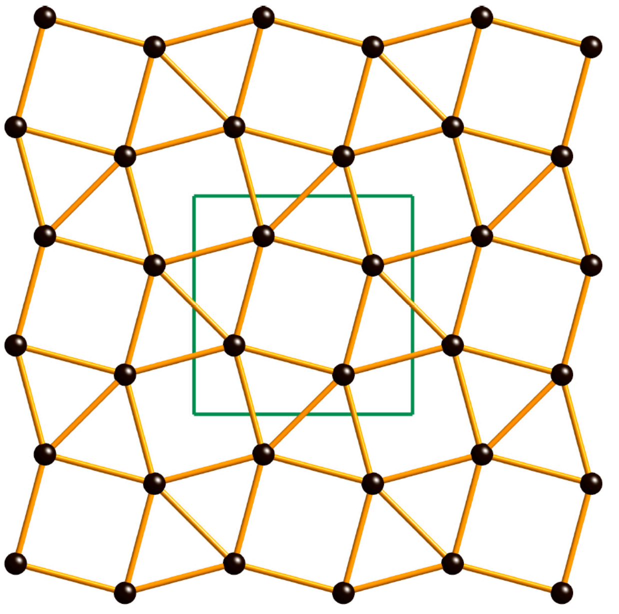


symmetry D_{4d}

plane nets

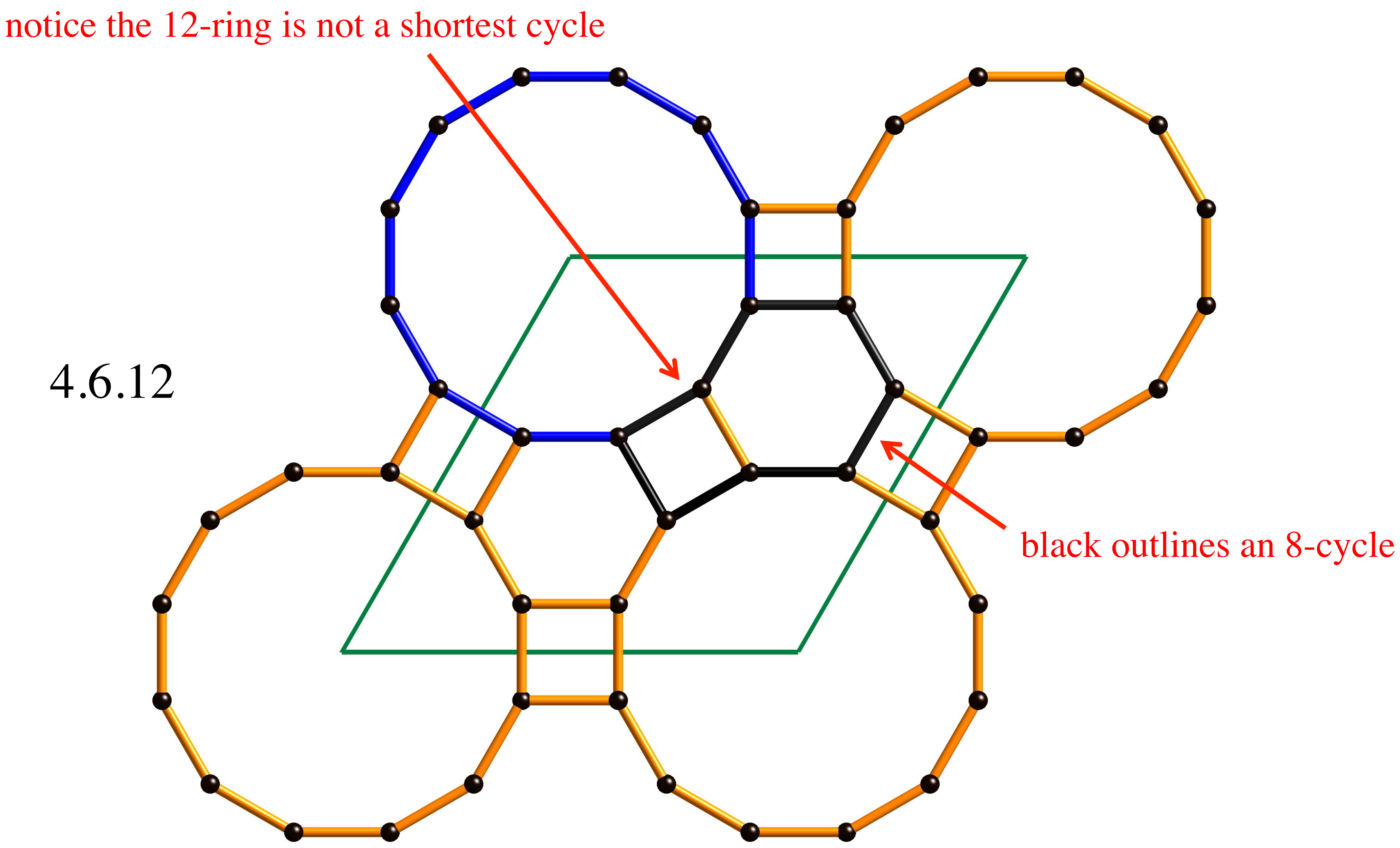


$3^3.4^2$



$3^2.4.3.4$

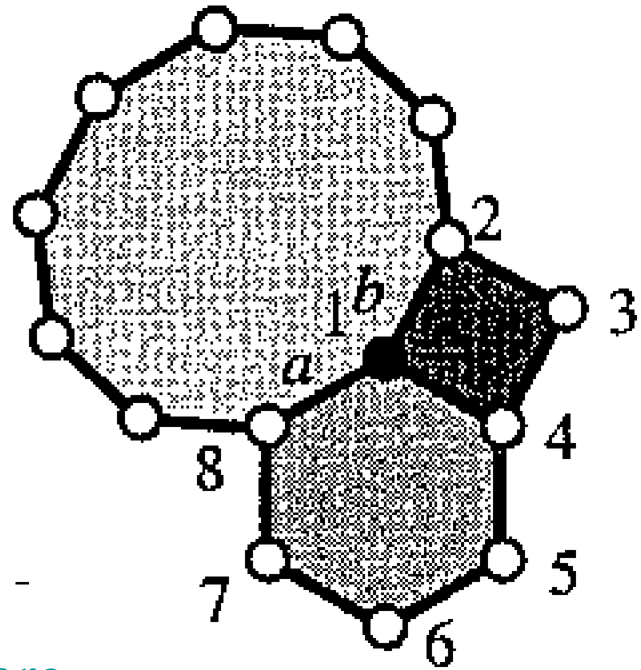
not that giving rings in cyclic order distinguishes these two


notice the 12-ring is not a shortest cycle
4.6.12
black outlines an 8-cycle

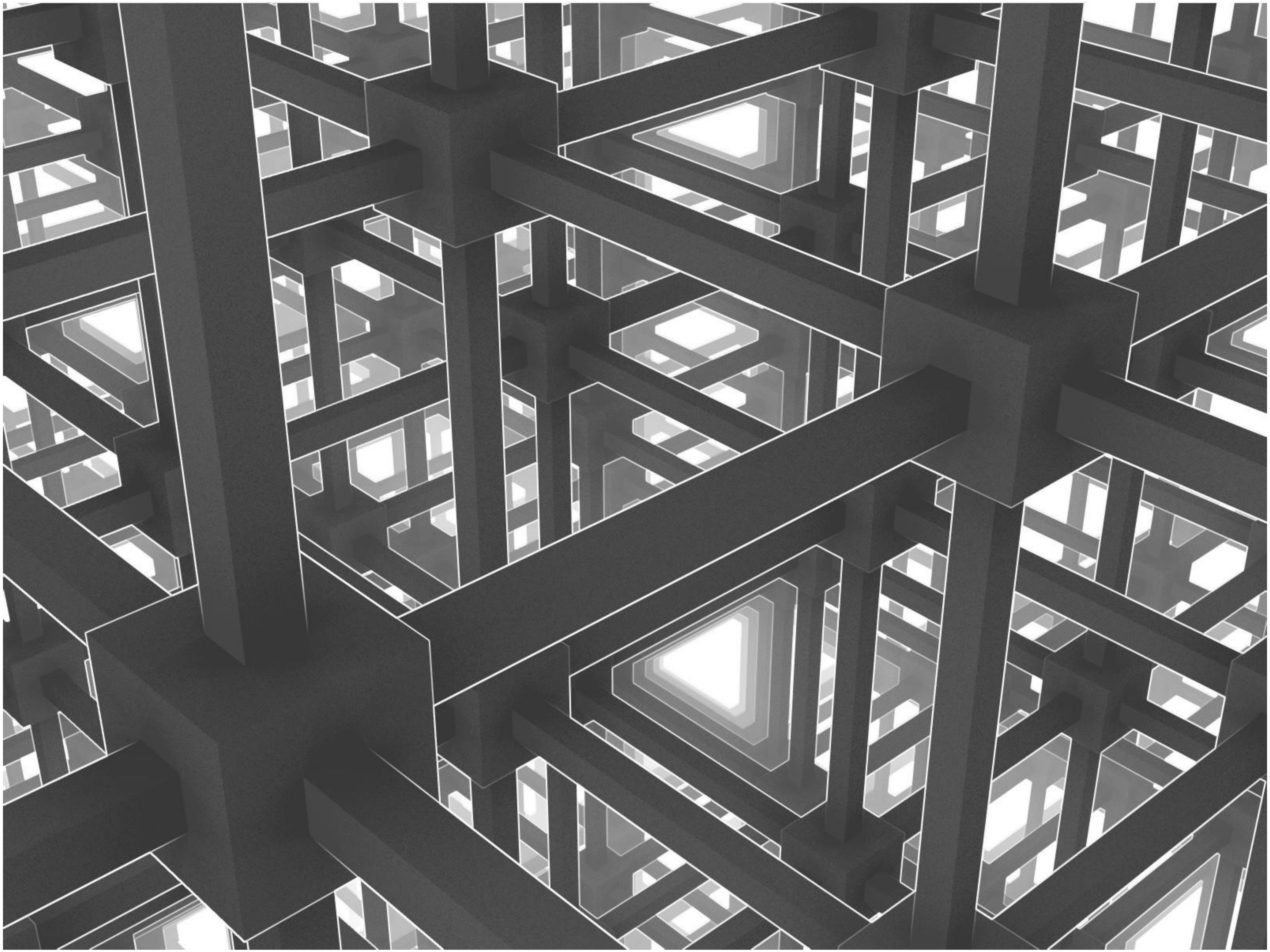
Fragment of the polyhedron
vertex symbol 4.6.10

Note we use rings not cycles.
In the angle with edges *ab* there
ia an 8-cycle.

So in the vertex symbols for nets
we use rings



(notice that the faces of polyhedra are rings but may not be strong rings. Think of a pyramid)

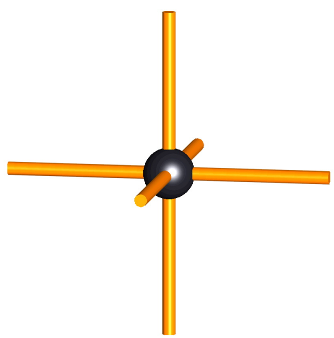


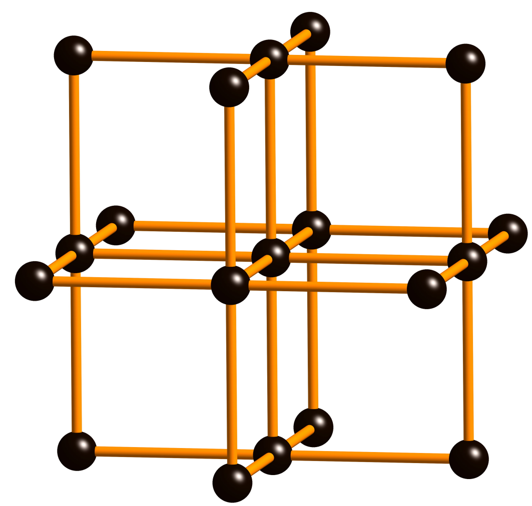
3-periodic nets (graphs)

Point symbols for 3-periodic nets

At each n-corrdinated vertex there are $N = n(n\text{-}1)/2$ angles "Point symbol" $A^aB^bC^c$... gives the size (A, B, C...) of the shortest cycle at each angle and the numbers of shortest cycles of each size so that $a + b + c + ... = N$.

Diamond (**dia**) 4-coordinated; shortest cycle at each angle is 6-cycle. The point symbol is 6^6.
Primitive cubic lattice (**pcu**) $4^{12}6^3$.





Point symbol is often called "Schläfli symbol"*

This is unfortunate because in mathematics "Schläfli symbol" refers to a symbol for a tiling

*including in some of my older papers! Mea culpa

Please

DO NOT USE "SCHLÄFLI SYMBOL" FOR POINT SYMBOL OR VERTEX SYMBOL

A POINT SYMBOL IS NOT A "TOPOLOGY"

V. A. Blatov. M.O'Keeffe, D. M. Proserpio
CrystEngComm **2010**, *12*, 44

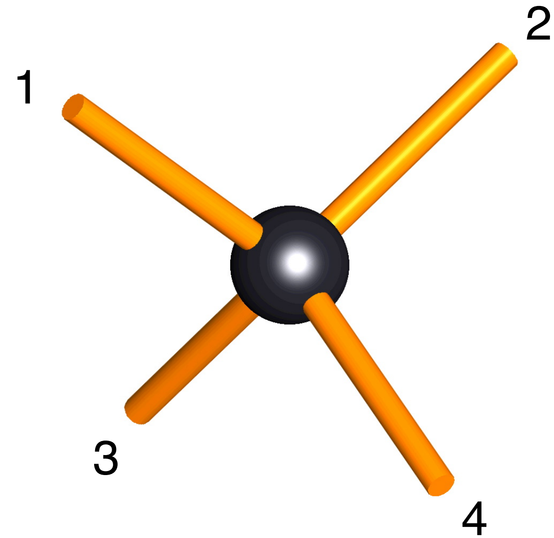
Vertex symbols for 3-periodic nets

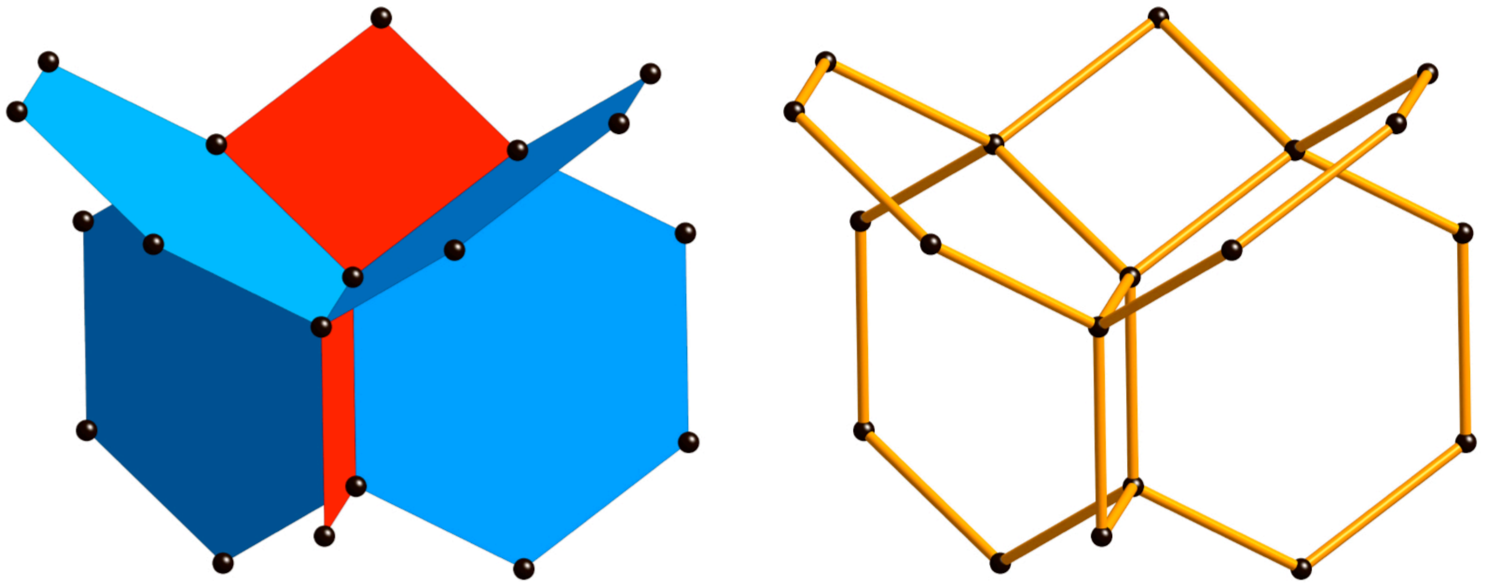
(used mainly for 3- or 4-coordinated vertices)

$A_a \cdot B_b \cdot C_c$.... with $n(n$-1)/2 entries for n-coordination

A, B, C ... are the sizes of the smallest *ring* at an angle and a, b, c ... are the numbers of those rings.

For 4-coordinated only angles are grouped in opposite pairs; 12,34 and 13,24 and 14,23



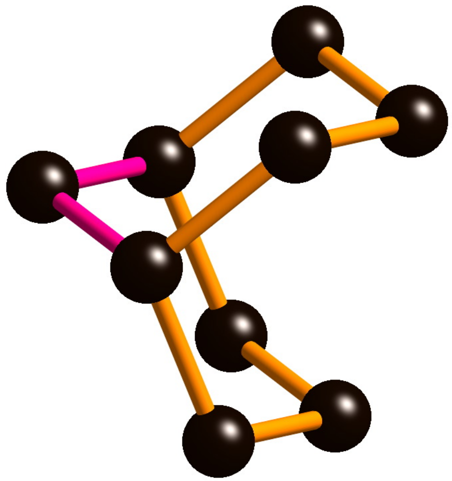


Environment of a vertex of the sodalite net (**sod**)

point symbol $4^2.6^4$

vertex symbol 4.4.6.6.6.6 this tells us the 4-rings don't share n edge

In diamond (**dia**) there are two 6- rings at each angle



vertex symbol $6_2.6_2.6_2.6_2.6_2$

If rings are planar (flat) only one per angle

For feldspar (**fel**) with two kind of vertex, both with point symbol $4^2.6^3.8$, the vertex symbols are $4{\cdot}6{\cdot}4{\cdot}6{\cdot}8_2{\cdot}10_{10}$ and $4{\cdot}6_2{\cdot}4{\cdot}8{\cdot}6{\cdot}6_2$. Notice that, subsequent to the constraint that opposite angles are paired, the numbers are written in lexicographic order (smallest numbers first).

Can be many shortest rings:

uml $4.6_{2.}4.6_3.6.18_{1422}$

For coordination > 4 the symbol is sorted so smallest rings come first. For a 6-coordinated net known as **pcu-m** it is

$$3.3.3.3.4.4.4.8_2.8_2.8_3.9_2.9_3.9_4.9_5.9_6$$

Sometimes an angle does not contain a ring
Vertex symbol for 4-coordinated **cds** net is

$$6.6.6.6.6_2.*$$

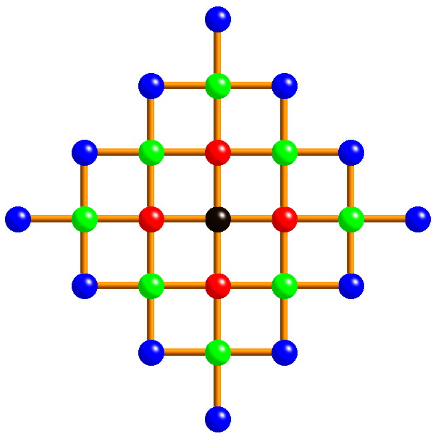
For the 6-coordinated **pcu** net it is:

$$4.4.4.4.4.4.4.4.4.4.4.4.*.*.*$$

Coordination sequence for a vertex

$n_1, n_2, n_3, n_k, \ldots$

n_k is the number of vertices linked to the reference vertex by a path of exactly k steps



square lattice coordination sequence is 4, 8, 12,…

cumulative sequence

$c_k = \Sigma_{1 \text{ to } k}\, n_k$

$\text{TD}_{10} = 1 + c_{10}$

If there is more than one kind of vertex, then for TD_{10} use weighted average of c_{10}

used as a search tool for zeolite-like nets

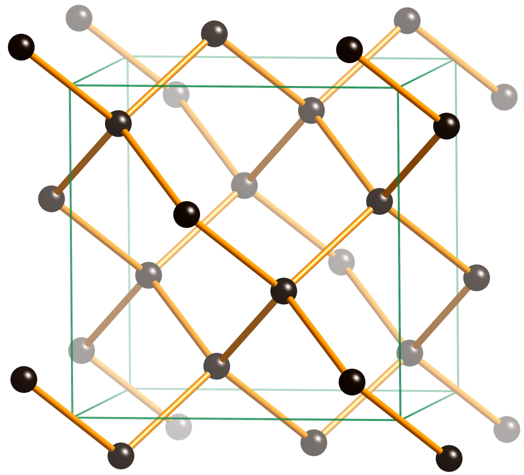
topological density:
2-periodic limit $k \to \infty,\ c_k/2k^2$
3-periodic limit $k \to \infty,\ c_k/3k^3$

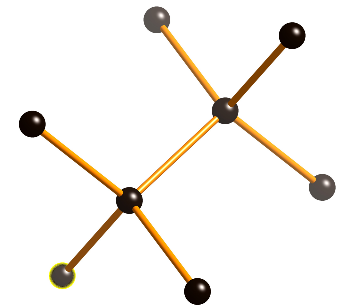
next nets as periodic graphs

Crystal nets as periodic simple connected graphs

periodic
simple - no loops or mutiple edges
connected - a path from every vertex to every other

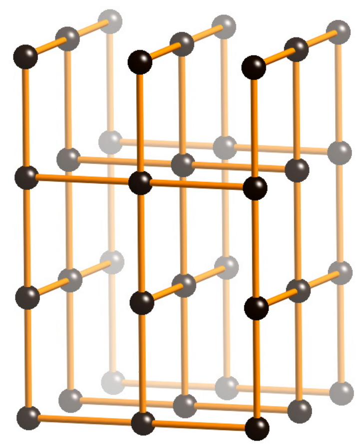
diamond
net (**dia**)

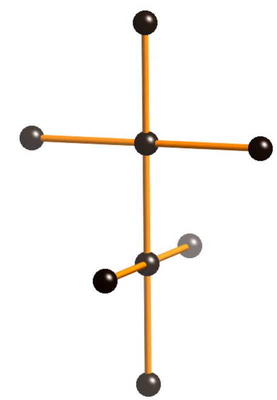




minimum repeat unit
2 vertices, 4 bonds

$CdSO_4$ net
(**cds**)

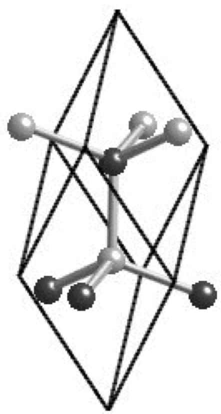


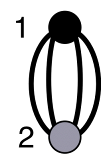


Quotient graph* and vector representation

net | unit cell | quotient graph | vector representation

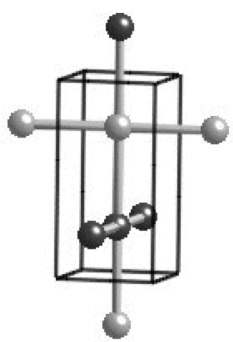
dia

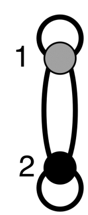




from	to	in unit cell
1	2	0 0 0
1	2	1 0 0
1	2	0 1 0
1	2	0 0 1

cds





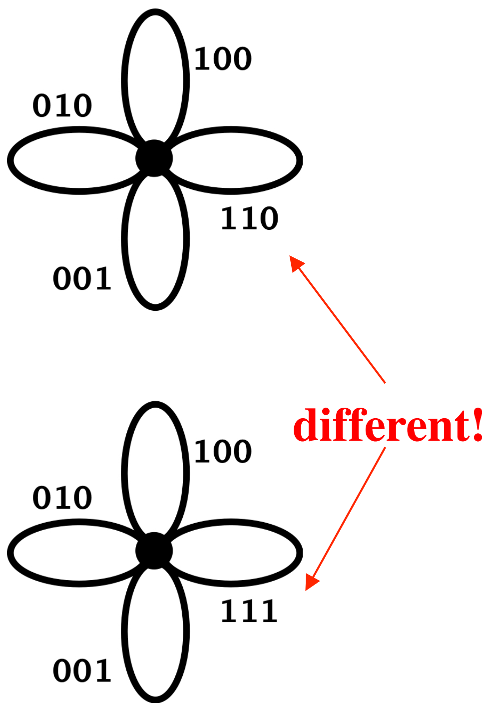
from	to	in unit cell
1	2	0 0 0
1	1	1 0 0
2	2	0 1 0
1	2	0 0 1

*Chung, Hahn & Klee, 1984

The same unlabeled quotient graph may be the graph of different nets. E.g.:

hex
(hexagonal lattice)

bcu
(body-centered cubic lattice)



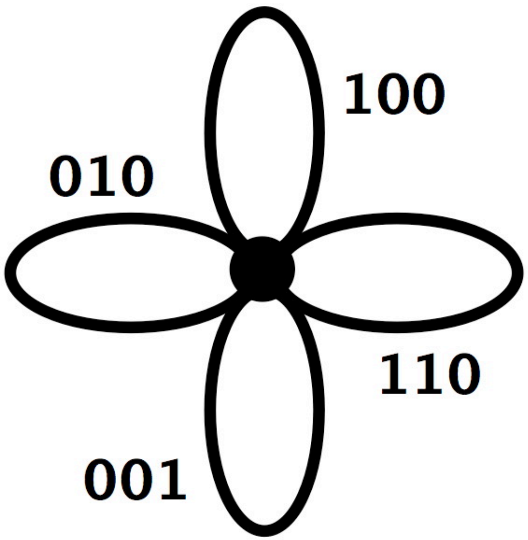
hex:

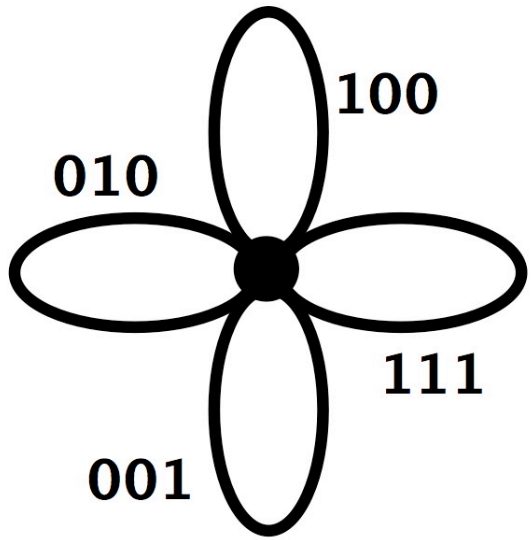
1 1 100
1 1 010
1 1 001
1 1 110

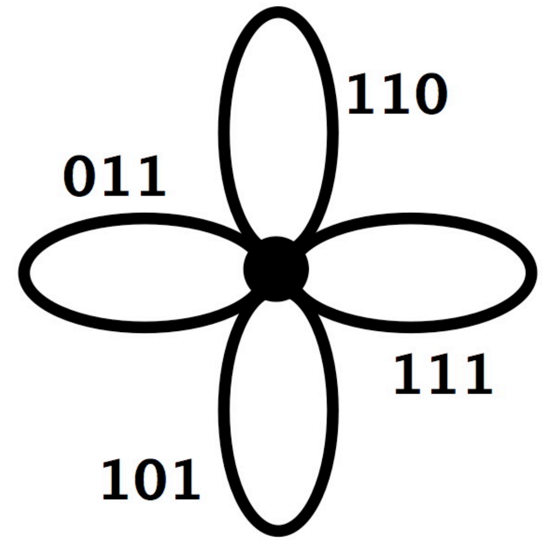
bcu:

1 1 100
1 1 010
1 1 001
1 1 111

Examples of nets with the same unlabelled quotient graph
(these examples are *lattice nets* - one vertex in the repeat unit)



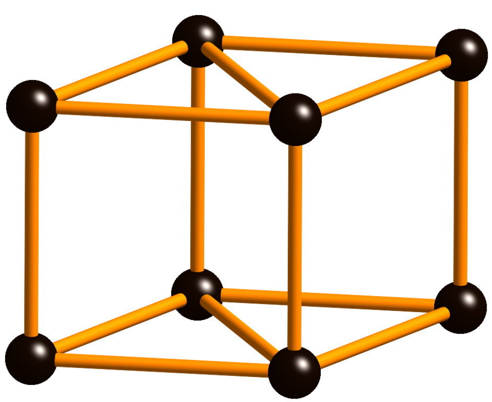


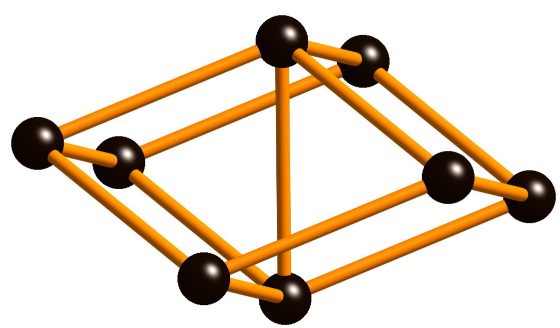


hex

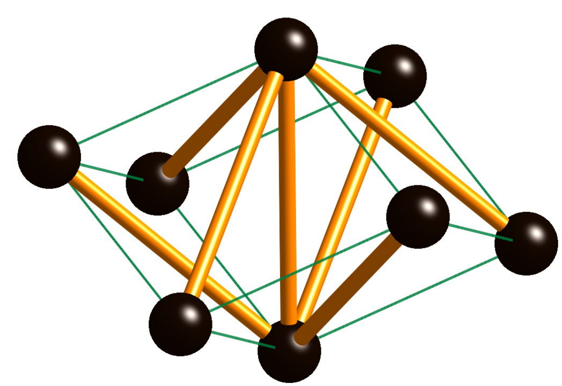
bcu

ilc



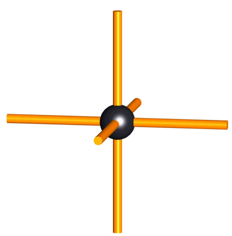


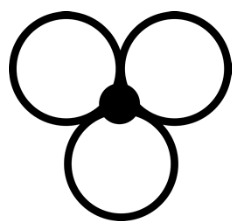
primitive sell of body-centered cubic



Notice that the quotient graph has the same number of vertices, v and edges, e, as the repeat unit (primitive cell) of the net.
The cyclomatic number of the quotient graph is $g = 1 - v + e$
We call this the **genus** of the net.

(The reason is this. Imagine the repeat unit of the net there will be pairs of bonds going to the *uvw* cell and the *-u-v-w* cell. Join these. Now inflate the bonds to get a *handlebody* of g holes.)



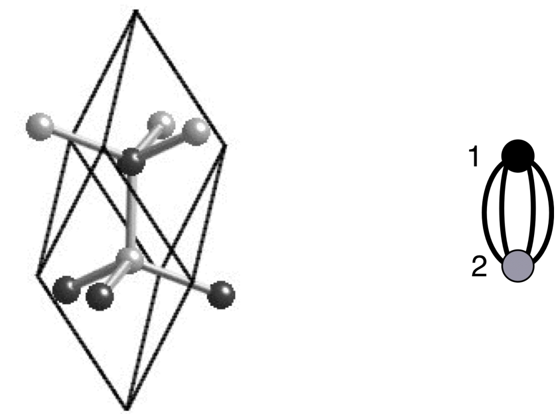


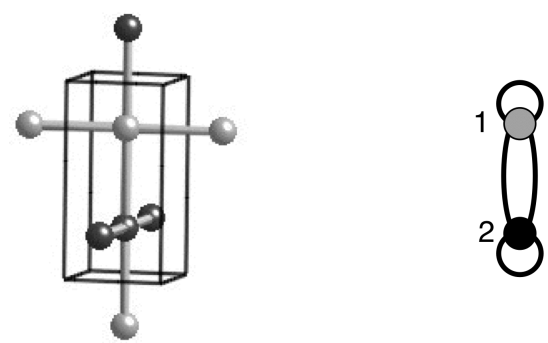
pcu has $v = 1$, $e = 3$ (six half edges)
$g = 1 - v + e = 3$ = cyclomatic number of quotient graph.

An N-periodic net must have $g \geq N$. Nets with $g = N$ are **minimal nets** (Beukemann & Klee)

Minimal net. For 3 dimensions there are 15 minimal nets (there are 15 connected graphs with cyclomatic number 3 Beukemann & Klee, *Z. Krist* 1992.

the **dia** and **cds** nets are the only 4-c minimal nets. (2 vertices in the primitive cell)





Systre (O. Delgado-Friedrichs)

vector representation

↓

Barycentric (center of mass) coordinates

↓

symmetry

↓

canonical form

↓

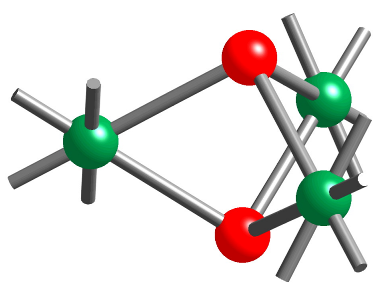
equal edge, minimal density embedding

O. Delgado-friedrichs & M. O'Keeffe, *Acta Crystallogr.* **A59**, 351 (2003)

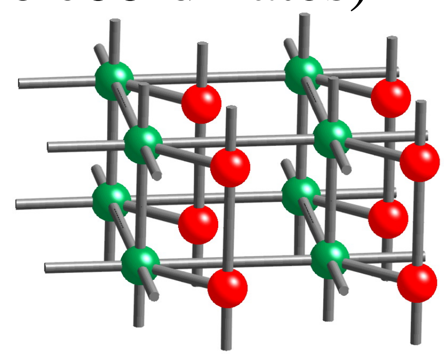
barycentric coordinates (equilibrium placement, Olaf Delgado-Friedrichs 2005 after Tutte 1960)

once one vertex fixed, rest unique
rational, hence exact, using integer arithmetic

problem: there may be collisions (two or more vertices with the same coordinates)



vertices with
common neighbors



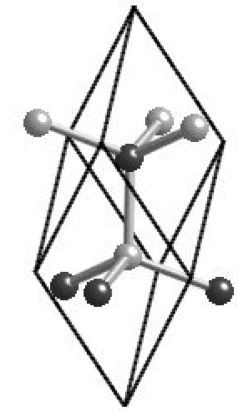
“dangling” vertices & ladders

collisions rare in crystal nets!

barycentric coordinates, example of diamond

dia

from	to	in unit cell
1	2	0 0 0
1	2	1 0 0
1	2	0 1 0
1	2	0 0 1



let vertex 2 be at 0,0,0 and vertex 1 at x, y, z then coordinates of neighbors of 1 are

0 0 0
1 0 0
0 1 0
0 0 1

average 1/4, 1/4, 1/4

thus $x = 1/4$, $y = 1/4$, $z = 1/4$

Systre

Olaf Delgado-Friedrichs

Symmetry

Once Systre has determined a placement (barycentric coordinates) the automorphisms of the net (including translations) can be found. For nets without collisions these correspond to operations of a space group which is identified.

Systre first looks for translations. If any found a reduced cell is determined.

Then find matrices **A** and translations **t** such that

$\mathbf{A}\mathbf{x}_1 + \mathbf{t} = \mathbf{x}_2$ where $\mathbf{x}_1$ and $\mathbf{x}_2$ are coordinate triples.

A,**t** can be identified with a symmetry operation.

Symmetry operations must map vertices and edges.

Two important results (Olaf Delgado-Friedrichs)

1. 3-periodic nets without collisions have an isomorphism group isomorphic with a space group.

If this group is chiral, the net is chiral
If not, not.

2. The graph-isomorphism problem is solved for nets without collisions.

Systre finds the symmetry and "Systre key" (unique signature)

Canonical form of vector representation

Olaf Delgado-Friedrichs

The vector representation of a net is a string of digits that codes exclusively for that net. But:

(a) there are $n!$ ways of numbering the vertices in the unit cell (n can easily be > 100)
(b) there is an essentially infinite number of choices of basis vectors

Systre solves these problems to find a unique canonical form for each topology.

Number vertices in order of barycentric coordinates
$x_i < x_j$; if $x_i = x_j$ then $y_i < y_j$; if $y_i = y_j$ then $z_i < z_j$

We have gone from n! to n possible numbering schemes

Basis vectors must be 100 010 001

Write out all possible representations (not so many) as a string of digits
e.g. (1 2 0 0 0   1 2 0 0 1   1 2 0 1 0   1 2 1 0 0)

Keep the lexicographically smallest as canonical form

It has been proved that this is unique and can be done in polynomial time

Systre

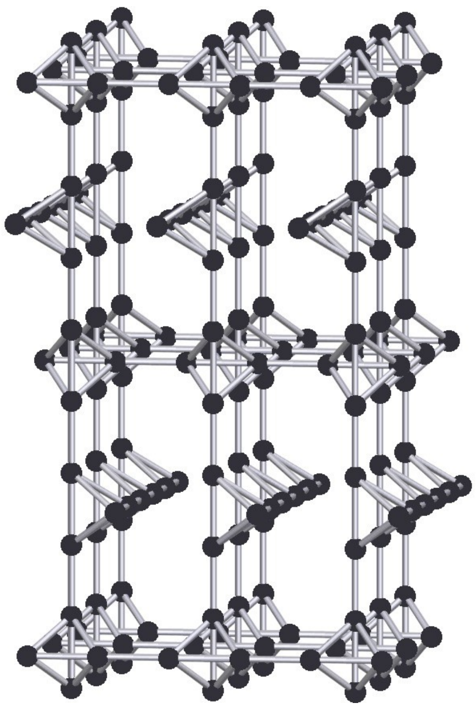
structure

Once we have the canonical form for a new net, we can compare it to those of known structures. If it matches one, we know that the new net is isomorphic with that one. If there are no matches, the net is different from those known structures. Thus, for the first time, one can determine without ambiguity whether two nets are isomorphic or not!

Systre
realization

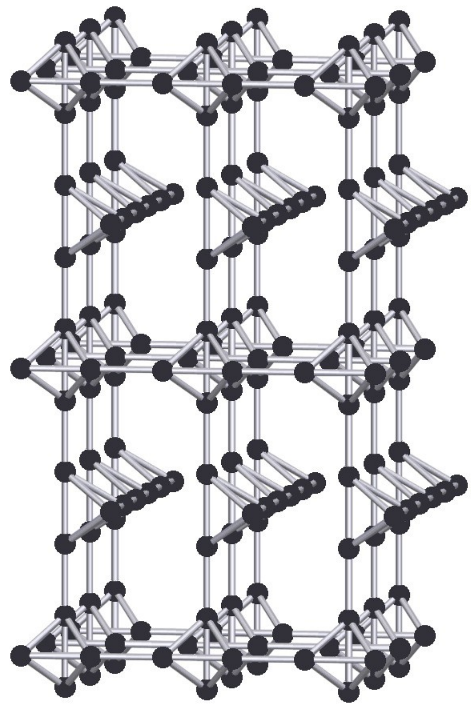
The final step in Systre is finding a maximum symmetry realization, which may, or may not, be an embedding.
If possible all edges are constrained to be equal (e.g. to 1.0)
The, subject to that constraint, the volume is maximized (density minimized).

For a periodic net without collisions, the combinatorial symmetry including translations is isomorphic to the maximum achievable symmetry (space group) of a realization (which may not be a good embedding). Here are three realizations – not ambient isotopic – of a net with combinatorial symmetry $I4_1/amd$



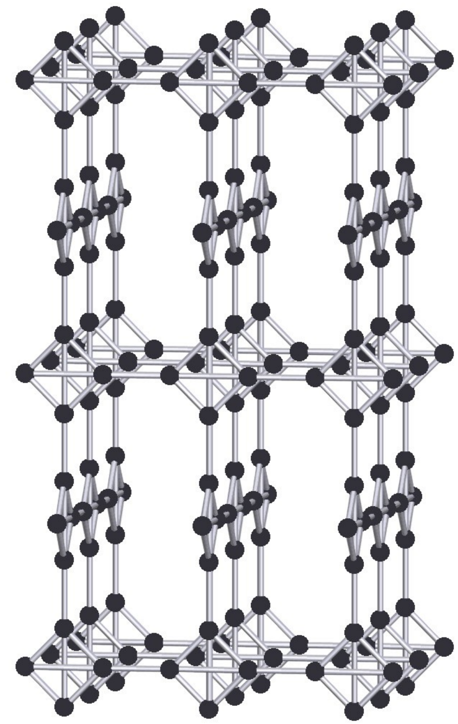
good $P4_122$

chiral



good $Ama2$

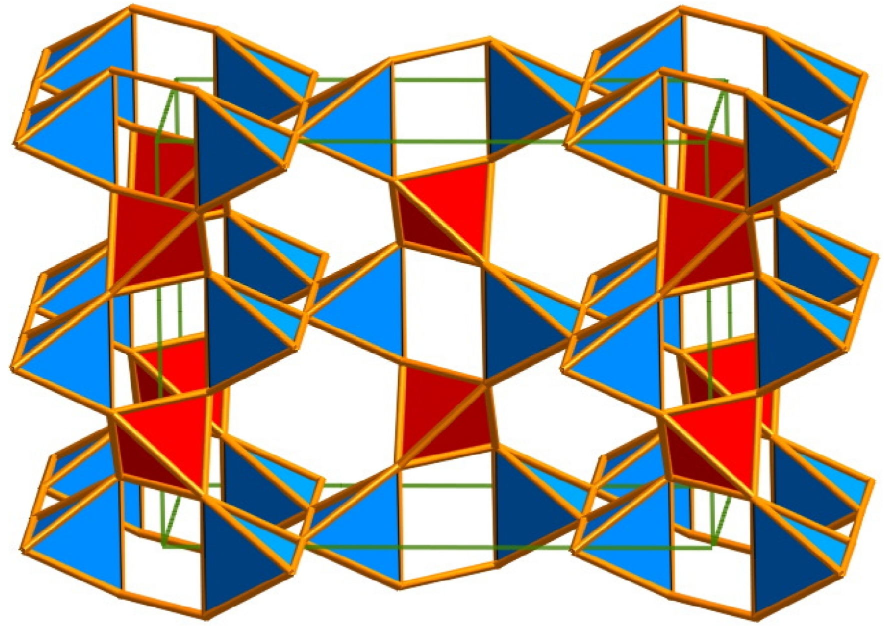
polar



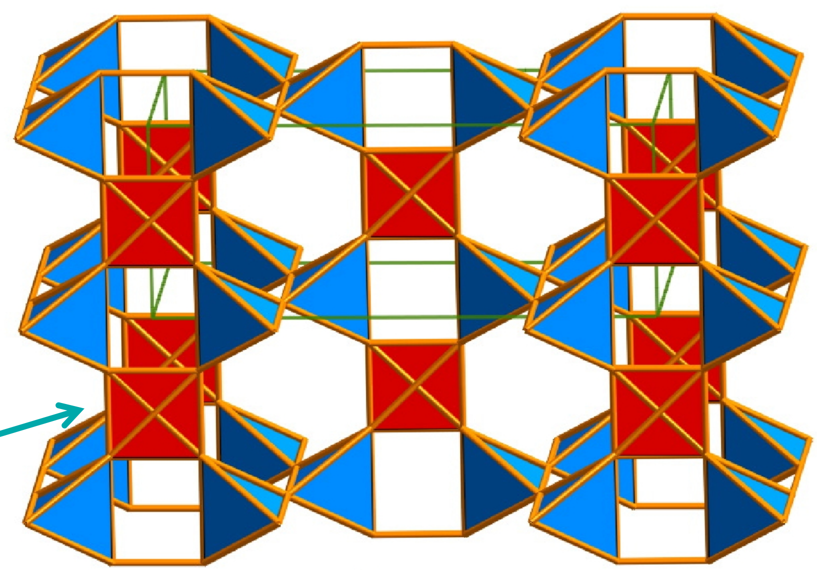
bad (edges intersect)

$I4_1/amd$

anion net of moganite (a form of SiO_2 - also structure of BeH_2)



symmetry for tetrahedral coordination → Ibam



maximum symmetry (the net of zeolite ASV behaves similarly) → Cmmm

square, edges intersect

Get Systre at **www.gavrog.org**

requires Java (on Apple Macintosh and many others or free donload, if not already installed)

Systre input for periodic graph:

```
PERIODIC_GRAPH
ID "diamond"
EDGES
1 2 0 0 0
1 2 1 0 0
1 2 0 1 0
1 2 0 0 1
END
```

Examples of Systre input

```
CRYSTAL
GROUP P6122
ATOM 1 4  0.28727 0.59679 0.02762
EDGE 1 0.69048 1.40321 -0.02762
EDGE 1 0.40321 0.71273 -0.19429
EDGE 1 0.59679 0.30952 -0.13905
END
```

give symmetry
and one of each kind
of vertex ("atom") and
edge

```
CRYSTAL
ID 'banalsite'
GROUP Ibam
CELL 8.496 9.983 16.775 90.0 90.0 90.0
ATOM 1 4 0.2283 0.4429 0.4067
ATOM 2 4 0.0754 0.3095 0.1586
END
```

If no edges given
Systre will take the n
nearest nighbors of each
atom of coordination
number n. Now unit cell
is necessary

Systre output

Structure #1 - "diamond".

Structure of dimension 3.
Given space group is P1.
2 nodes and 4 edges in repeat unit as given.

Given repeat unit is accurate. Point group has 48 elements. 1 kind of node.
Equivalences for non-unique nodes: 2 --> 1
Ideal space group is Fd-3m.
Structure was found in built in archive: Name: dia

Relaxed cell parameters:
a = 2.30940, b = 2.30940, c = 2.30940
alpha = 90.0000, beta = 90.0000, gamma = 90.0000
Cell volume: 12.31681
Relaxed positions:
Node 1: 0.12500 0.12500 0.62500
Edges:
0.12500 0.12500 0.62500 <-> 0.37500 0.37500 0.37500
Edge centers:
0.25000 0.25000 0.50000

Edge statistics: minimum = 1.00000, maximum = 1.00000, average = 1.00000
Angle statistics: minimum = 109.47122, maximum = 109.47122, average = 109.47122
Shortest non-bonded distance = 1.63299

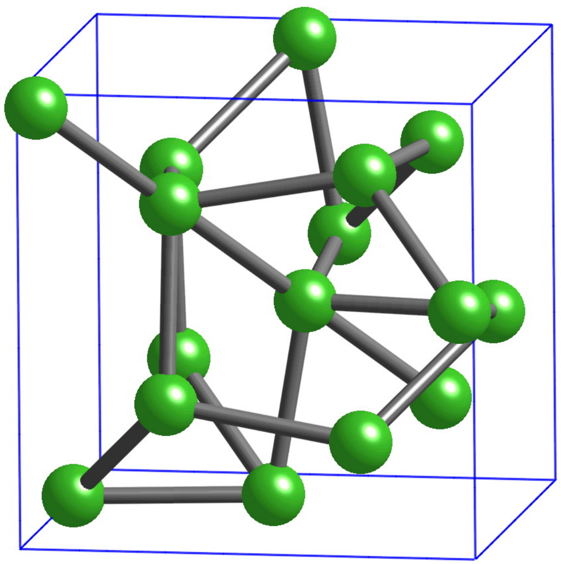
Degrees of freedom: 1

Sphere Packings

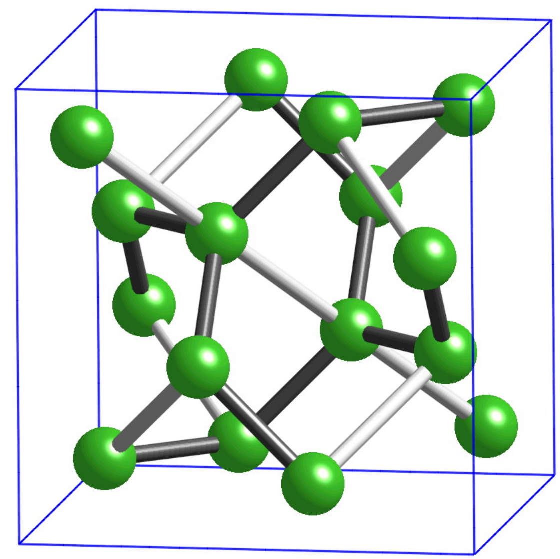
If an embedding of a net has all edges equal and these are the shortest distances between vertices we say that the structure is a sphere packing.
Many (most?) nets of interest in crystal chemistry have embeddings as sphere packings.
A lot is known about sphere-transitive (one kind of sphere) packings **(W. Fischer, E. Koch, H. Sowa)**

Not all sphere packings can be realized as sphere packings at full symmetry. (next slides):

Sphere packing 5/5/c1 (W. Fischer) symbol **fnm**



I-43d 0.0366, x, x
5 equidistant neighbors

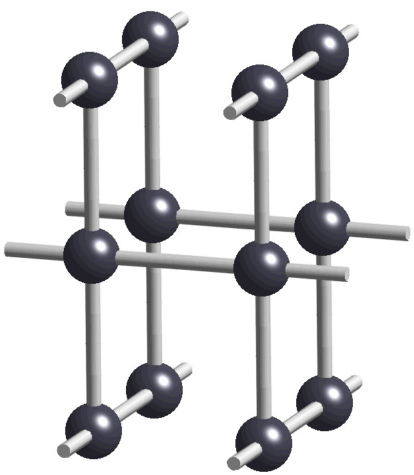


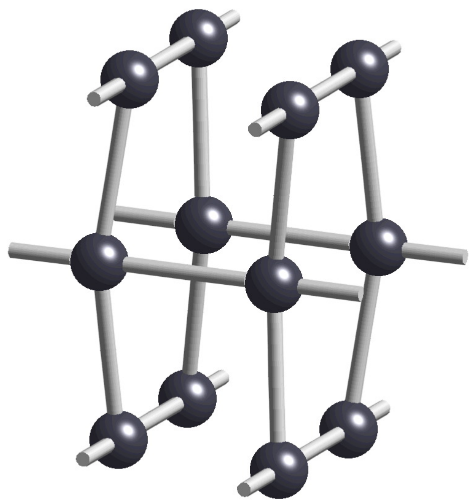
$x = 0.125$. True symmetry
Ia-3d. 3 nearest neighbors

Examples of important 4-coordinated nets that are not 4-coordinated sphere packings in maximum symmetry embeddings

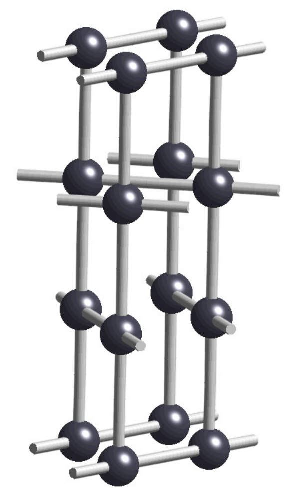
can be realized as 4-coordinated SP:

cannot be realized as 4-coordinated SP





cds



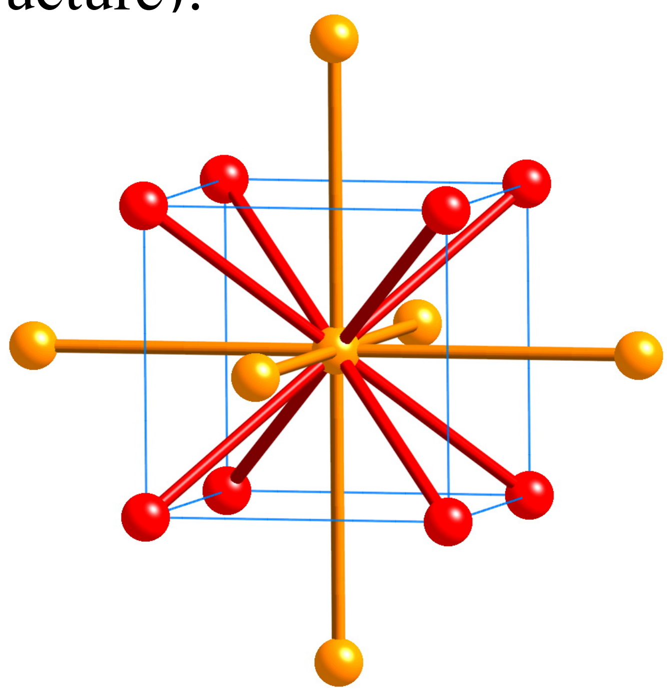
qzd

P4_2/*mmc*
6 equidistant neighbors

P4_2/*mbc* (*a*´=2*a*)
4 equidistant neighbors

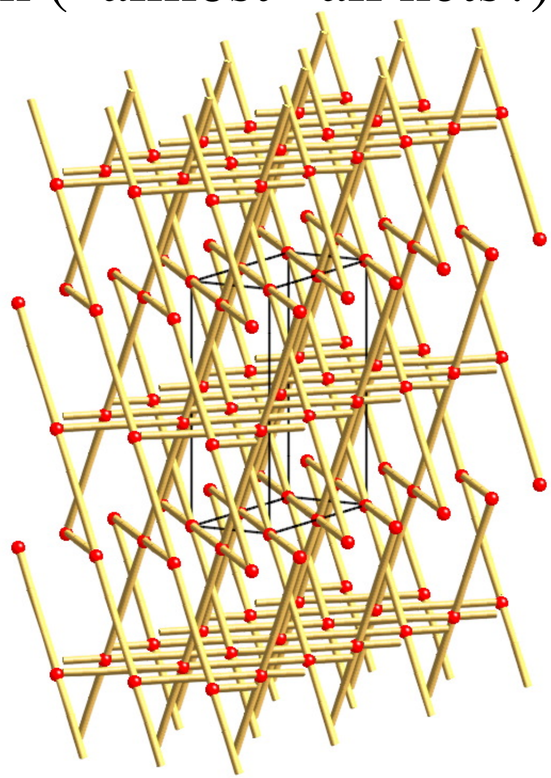
P$6_2$22
8 equidistant neighbors

Example of a structure for which there is no embedding with all edges equal. this is the body-centered cubic lattice with edges linking first- and second geometric neighbors. (for some purposes this is the ‘best’ way to consider this structure).



bcu-x
(the symbol **bcu** refers to 8-coordination)

Example of a net in which intervertex distances are always shorter than edges.
Minimum intervertex distance ~ 0.88 longest edge.
Such nets rare in crystal chemistry, but in principle very common ("almost" all nets?)



tcb a net with vertex symbol $8_2 \cdot 8_2 \cdot 8_5 \cdot 8_5 \cdot 8_5 \cdot 8_5$

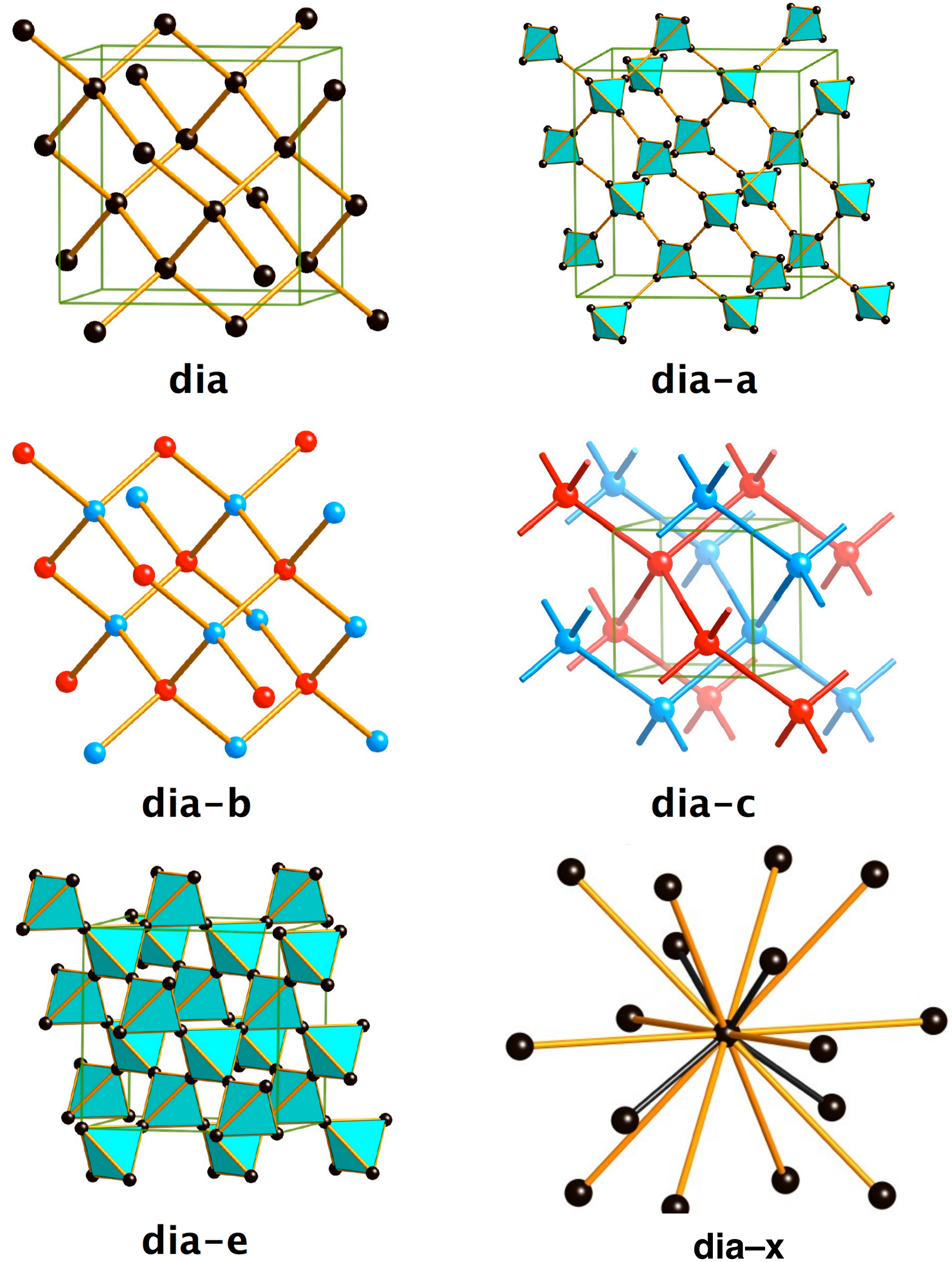
J.-F. Ma et al. 2003; M.-L. Tong et al. 2003

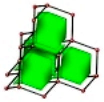
RCSR symbols for nets

dia
typical three letter code
dor the diamond net

derived net

dia-a = **a**ugmented
dia-b = **b**inary version
dia-c = **c**atenated
dia-d = **d**ual
dia-e = **e**dge net
dia-x = e**x**tended coord.





dia

names: diamond, D, 4/6/c1
key words: regular net, uniform net, isohedral tiling, self dual net, quasisimple tiling, good
references: Acta Cryst. A59, 22-27 (2003), Acta Cryst. A60, 517-520 (2004)

embed type	space group	volume	density	genus	td10
1a	Fd-3m	12.3168	0.6495	3	981

unit cell:

a	b	c	alpha	beta	gamma
2.3094	2.3094	2.3094	90.0	90.0	90.0

vertices: 1

vertex	cn	x	y	z	symbolic	Wyckoff	symmetry	order
V1	4	0.125	0.125	0.125	1/8, 1/8, 1/8	8 a	-43m	24

vertex	cs_1	cs_2	cs_3	cs_4	cs_5	cs_6	cs_7	cs_8	cs_9	cs_{10}	cum_{10}	vertex symbol
V1	4	12	24	42	64	92	124	162	204	252	981	6(2).6(2).6(2).6(2).6(2).6(2)

edges: 1

edge	x	y	z	symbolic	Wyckoff	symmetry
E1	0.0	0.0	0.0	0, 0, 0	16 c	-3m

tiling:

tiling	dual	vertices	edges	faces	tiles	D-symbol
[6^4]	dia	1	1	1	1	2

Export 3dt input: dia.cgd

occurrences: [show|hide]

A page from the RCSR

rcsr.anu.edu.au

M. O'Keeffe, M. A. Peskov, S. J. Ramsden, O. M. Yaghi
Accts. Chem. Res. **41**, 1782 (2008)

What nets are there?

It is convenient to discuss tiling first end