Carbon

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http://homepage.mac.com/whitby/

http://web.me.com/whitby/Octahedron/Welcome.html

Reference

Octahedron1stEd.pdf–bookmark CARBON–pages 187-212

Introduction

This material is excerpted from *Octahedron*. It shows how carbon atoms can join to form chains, helixes, rings, and crystals.

CARBON

Diamond

Join directions are tetrahedral

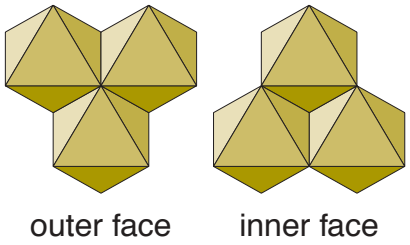
The Bragg representation of the structure of diamond requires join directions which are perpendicular to the faces of a regular tetrahedron. It further requires that each center of such join directions be equivalent except for an inversion between adjoining units. The C-atom alone does not have such join possibilities.

Specific heat requires four atom cfu

The specific heat (C_v) of diamond is 0.124 cal/g[1]. Using 12.0111 as the atomic weight of Carbon and four C-atoms as the cfu produces a value that conforms to the relationship established by DuLong and Petit for solids.

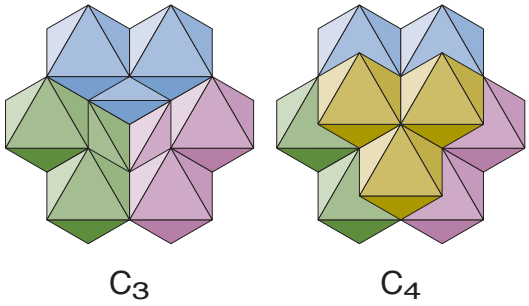
$$(4 \times AtWt \times C_v) = 5.957$$

The diamond cfu



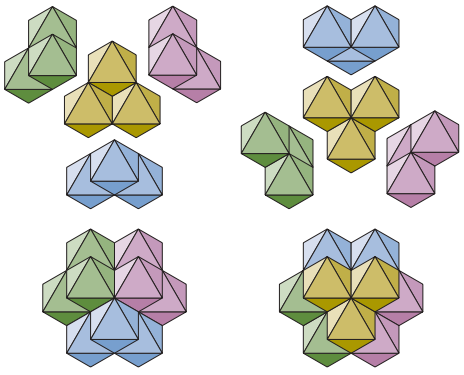
Two views of a C-atom panel for the diamond cfu.

A tetrahedral assembly in which each of the four faces of the tetrahedron is provided by a C-atom provides the cfu for the diamond crystal. The figure shows two views of the C-atom. The inner face is turned toward the centroid of the tetrahedral assembly. The outer face is directed oppositely. The outer face is the inter cfu join face.



The diamond cfu.

The arrangement of the C-atoms is shown in the above figure. The view on the left shows three C-atoms joined so that each shares an edge with the other two C-atoms to form a structurally stable assembly. The view on the right shows the placement of the fourth C-atom of the assembly. Its outer face is towards the viewer.



Assembly of the diamond cfu

The figure to the right shows the assembly of the diamond cfu from opposite viewing directions. The C-atoms which form the cfu are grouped above the assembly.

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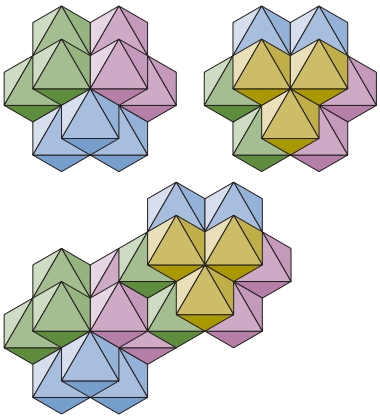
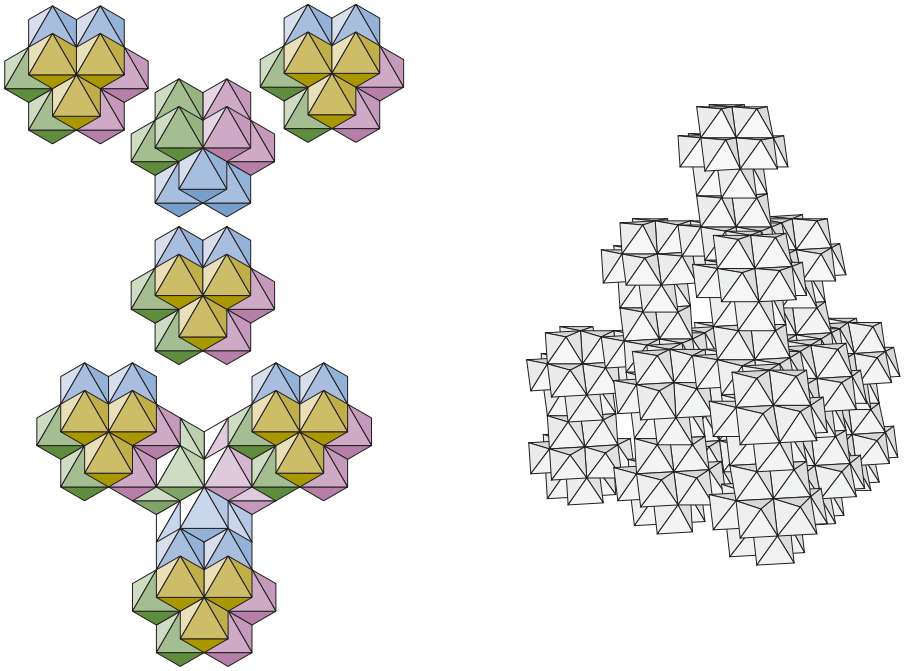
1. *Handbook of Chemistry and Physics* 48th ed., The Chemical Rubber Co., Cleveland 1967

The join between diamond cfus



Diamond cfus joined

The join between the tetrahedra can be seen as a pairing of C-atoms so that the pair appears as a Mg-atom. For identical cfus to join in this manner, one must be inverted relative to the other. The above figure is a view of a diamond cfu which is inverted relative to the view of the previous cfu. The next figure shows the two cfus joined. The two orientations depicted in the above view of the joined pair are the only orientations in the diamond crystal. A cfu of one orientation is joined to as many as four cfus of the other orientation.



Diamond crystal

The arrangement of the cfus in the diamond crystal is shown in two views. The first view is an orthographic projection of the crystalline assembly. The gray colored cfus are identically oriented. The yellow cfus are inverted with respect to the gray. The next view is a perspective view which is nearly at right angles to the first view.

Graphite

Graphite crystal structure

The graphite crystal has cfus which lie in a plane. Each cfu is joined to three others and the angle between the joins is $120°$. The joins of adjacent cfus are inverted. A lone C-atom as cfu cannot produce this crystal.

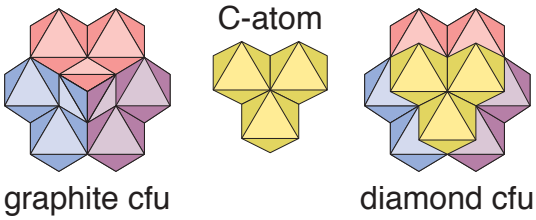
Specific heat requires three atom cfu

The specific heat (C_v) of graphite is 0.170 cal/g. The atomic weight of Carbon is 12.0111. Using three C-atoms for the cfu produces a value which conforms to the relationship established by DuLong and Petit.

$$3 \times AtWt \times C_v = 6.125$$

Comparison of diamond and graphite crystals

Using a three C-atom tetrahedral assembly as the CFU for graphite satisfies the DuLong and Petit relationship and permits the joins required of the cfu to produce the crystalline assembly. The graphite cfu is an open faced

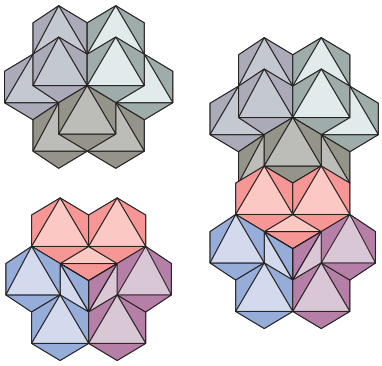


Graphite and diamond cfus.

tetrahedron in which each of the three C-atoms provides a face of the assembly. The graphite cfu differs from the diamond cfu by one C-atom. This relationship is seen in the above figure.

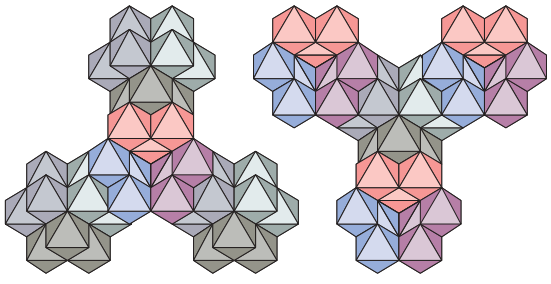
Joining graphite cfus

The join between the graphite cfus is the same as the join between diamond cfus. The



Joining graphite cfus

join is shown in the above figure. The joins between a given cfu and the three adjoining cfus can be seen in the next figure. The cfus are



Two graphite cfu hubs.
The two orientations of the graphite cfu which are required for their joining create two types of hubs within the planar crystalline assembly.

in one of two orientations and the joins are

between cfus which are not in the same orientation. Six cfus can form a ring which is hexagonal. Three of these rings can be joined so that they produce a fourth ring. From this assembly, the hexagonal ring structure attributed to graphite can be seen.

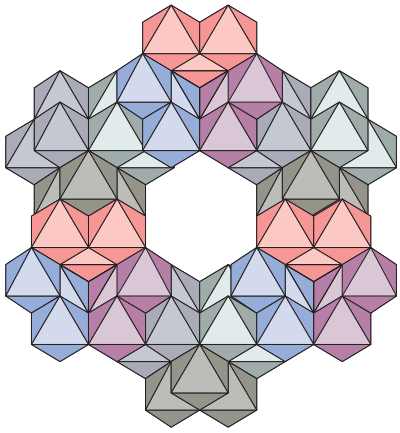
The thickness of the layer is two He-octa facial diameters. The open-faced tetrahedra are in the same plane.

Diamond cfus can form hexagonal layer

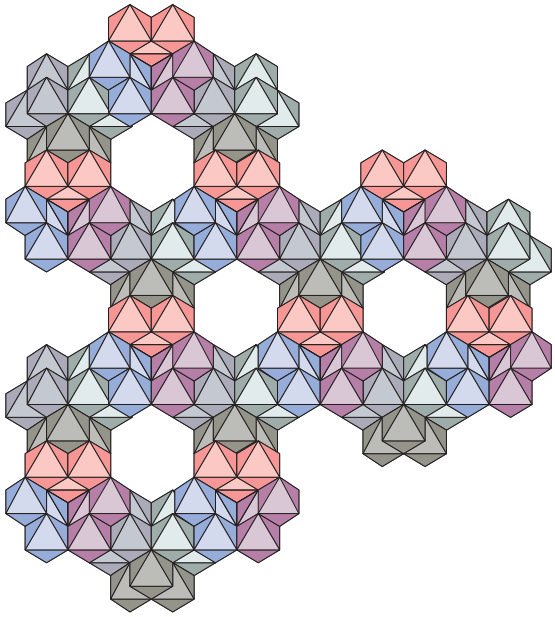
Consideration of the drawings will show that each of the graphite cfus can be replaced with a diamond cfu without disturbing the planar structure. The effect would be the same as adding a C-atom to the open-face of each of the tetrahedral groups. The C-atoms would add a He-octa facial diameter to the width of the planar assembly on each of its sides.

Layer to layer relationship in graphite

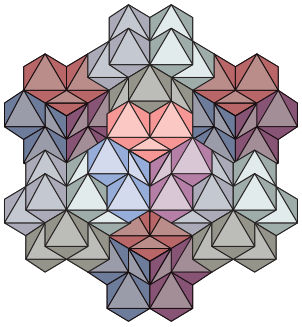
The octahedra in a crystalline structure have the same orientation. The octahedra in adjoining layers of graphite are in the same orientation. There are edge-to-edge joins between octahedra at the layer-to-layer join. The layers could be stacked in a regular way if the hubs were stacked so that their threefold axes were colinear.



Ring of graphite cfus.
The cfus of graphite can form a ring in which alternate units are in the two orientations. There are six positions to which an additional cfu can be joined.

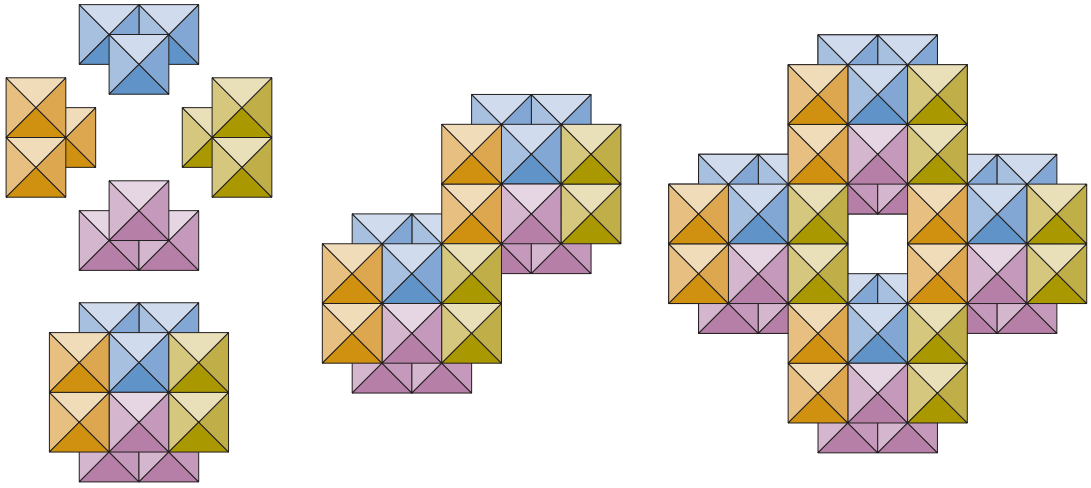


Three graphite cfu rings joined to form a fourth ring.
The crystalline assembly of graphite cfus produces a multiringed plane.



Graphite hub stack.
The two hubs of graphite are shown stacked so that their threefold axes are colinear.

C_4 ring

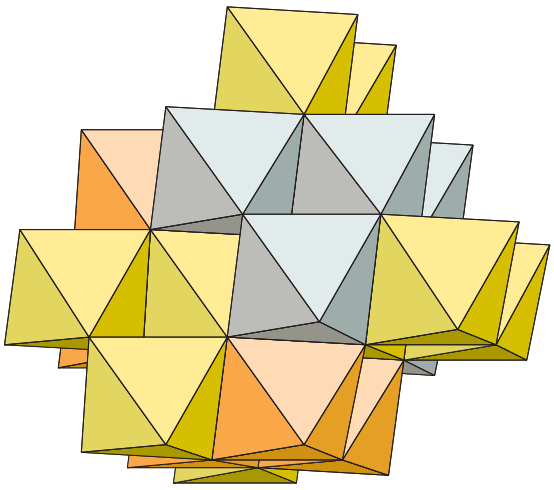


Ring of four C-atoms

On the left, four C-atoms form a ring each of which is cleftly joined to each of two C-atoms and has He-octa edge contact with a third. Each C-atom of the ring has a cleft free for joining.

In the middle, a pair of C_4 rings join in a plane perpendicular to their axes of symmetry. This is a cleft join in which four atoms provide one face each. Two C-atoms from each of two C_4 rings are joined

On the right, four rings join to form a larger ring which can be extended to form a crystalline layer.



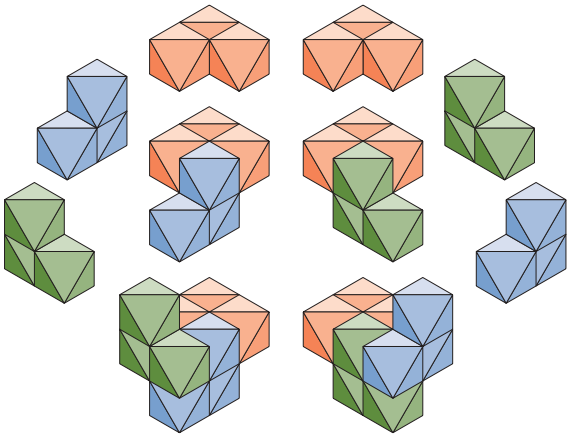
Stack of two C_4 rings viewed in perspective.

Two C_4 rings can be stacked parallel to the axis of symmetry. There are no cleft joins between the paired rings. Each C-atom is joined to the C-atom axially adjacent to it by a pair of He-octa edges. It also shares an edge with each of the C-atoms which are adjacent to this axial neighbor.

The eight C-atoms of the stack are in a cube-like array suggestive of cubane. For this stack to hold the NO_2 groups of octanitrocubane at the corners, each N-atom would have to have a cleft joined to the cleft formed by adjacent C-atoms of one of the rings. Four of the C-atoms have their third clefts blocked by the stacking.

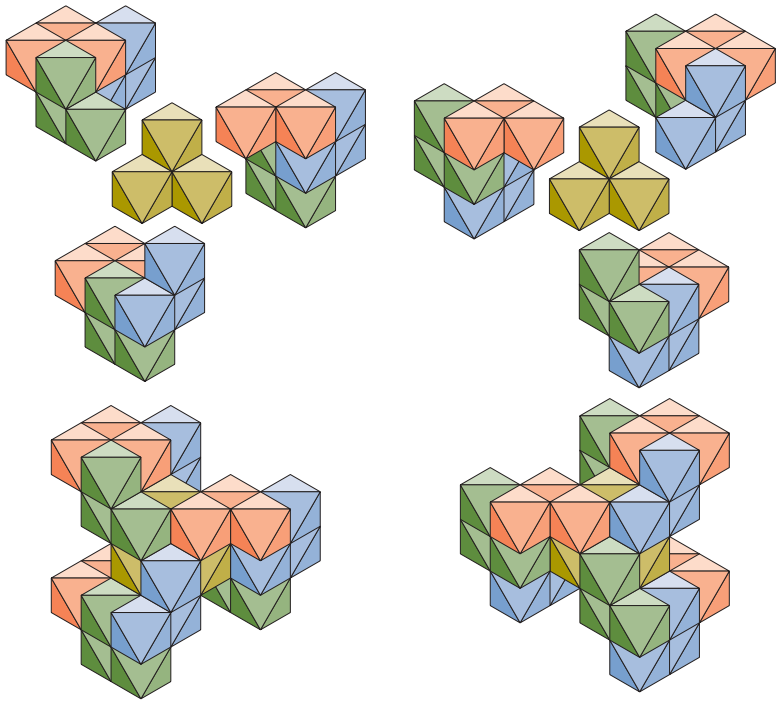
The stack axis runs from lower left to upper right

Carbon helixes



One C-atom, 1/3 turn

The C-atom can form a helix with other C-atoms as shown in the next figure. The C-atoms are cleftly joined. Each C-atom is 1/3 turn different from its two adjoining C-atoms. The figure shows the atom by atom assembly of one turn of two helixes. The helix on the left of the figure is growing clockwise toward the viewer. The helix on the right of the figure is growing counter-clockwise toward the viewer. The C-atoms of each helix have three orientations per turn. One of those orientations is common to a C-atom of each helical turn.



Linking three helixes with a C-atom

Three of turns of the previously described helix can be linked by a C-atom to form an axially extensible unit. The figure shows three turns which are clockwise-toward helical turns. Identical units can be added in either of the axial directions so that a C-atom of each of the helical turns is cleftly joined to a C-atom of a helical turn of the added unit to continue the helix.

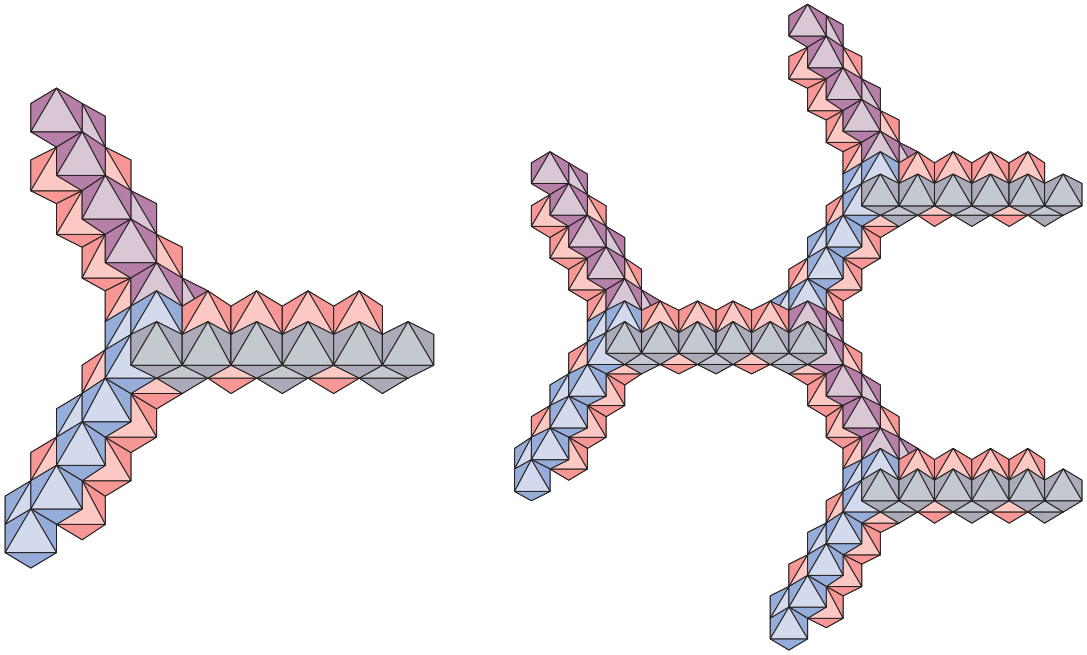
A similar assembly using helixes of the opposite hand is shown in the next figure.

C-atom chain helix

C-atom chains with an odd number of atoms can form a threefold helix. The next figure shows a helix in which each of the units is a straight chain of five C-atoms. This is a counter-clockwise towards helix. Each chain is rotated 1/3 turn relative to each of the two adjoining chains. Each chain is separated from the axially nearest identically oriented chains by a He-octa facial diameter.

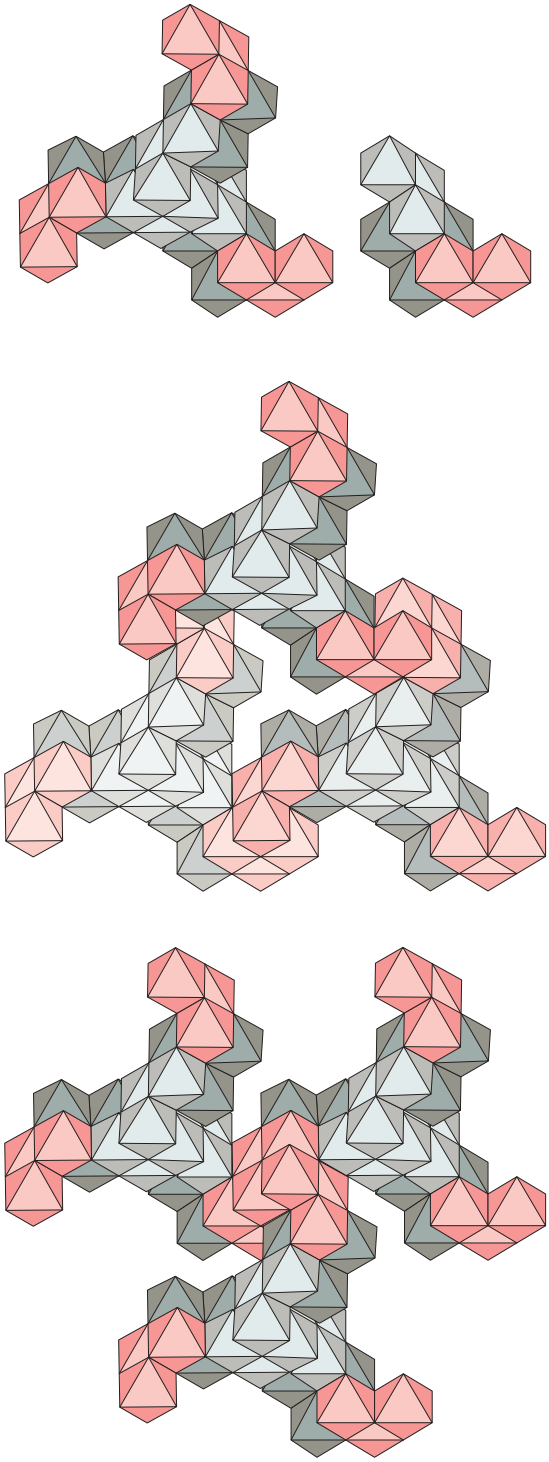
Joining of helixes

The five C-atom unit helixes can join with identical helixes to form a crystalline structure. The C-atoms furthest removed from the helix axis cleftly join with C-atoms of identical helixes to produce a helical join which is opposite in sense to the helixes of the joining units. It can be seen from this happenstance that the chains could form helixes of the opposite sense and form a similar crystalline structure.



Helix formed of chains of C-atoms
On the left is a single turn of carbon chain helix.
On the right, three carbon helixes are linked so as to form a helix of opposite sense.

CCC helix



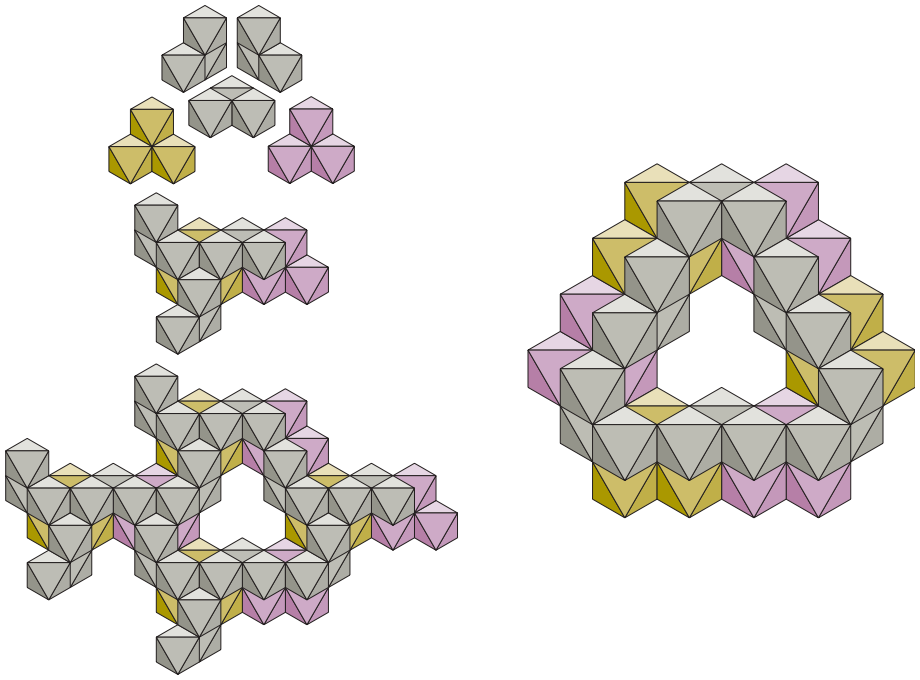
CCC helix.

The top figure on the left shows a group consisting of three C-atoms. The join between the center C-atom and either of the other two is left handed. Three identical groups form a helix in which the light gray C-atom of one group is cleftly joined to the light gray C-atom of each adjoining group.

The middle figure on the left shows a ring of CCC helixes. Each helix joins to the other two helixes by cleft joins between the red colored C-atoms.

The bottom figure shows three CCC helixes each of which contributes a red colored C-atom to form a helix.

CC_3C group

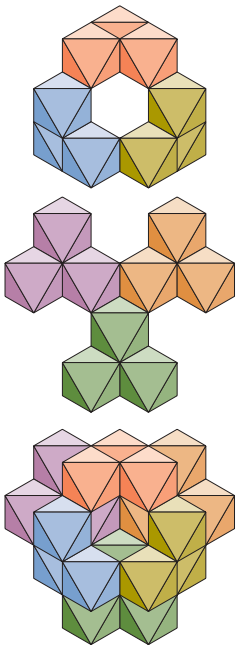


Ring of four CC_3C-groups

At the top of he figure on the left are the five C-atoms which form the CC_3C group which is shown below them. Four of the groups combine to form the ring on the bottom left. The group acts here as the cfu for a planar crystal. Each of the groups contributes three of its C-atoms to the formation of C_{12} ring shown on the right.

C_6 ring

Six C-atoms can join in a compact ring which has threefold symmetry. Each C-atom is cleftly joined to each of the neighboring C-atoms of the ring. Each also shares a He-octa edge with each of the C-atoms next to the nearest neighbors. These joins are shown by isolating these near neighbors which then appear as rings of three C-atoms each. The C-atoms are



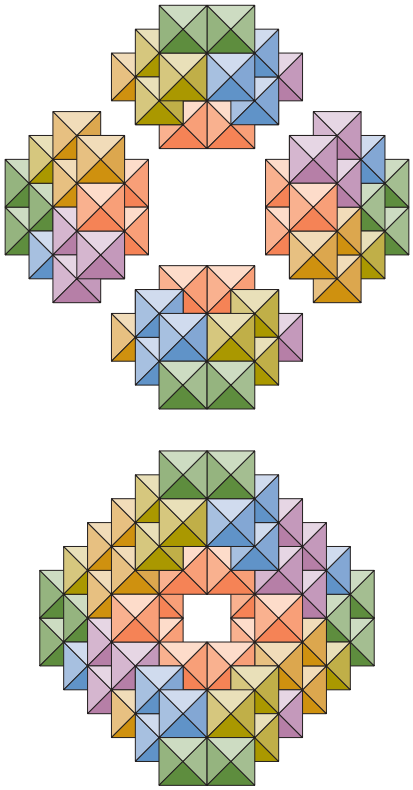
C_6-ring
The two groups of three C-atoms each above at the top of the figure are combined in the C_6-ring at the bottom.

triplets of He-octas which are planar. Three C-atoms whose planes are parallel to the plane of the ring are shown here and the edgial joins between them are such that they share a common vertex at the center of symmetry. The plane of each of the C-atoms of the second group make an angle of $2 \times \operatorname{atan} \sqrt{\frac{1}{2}}$ with the plane of the ring.

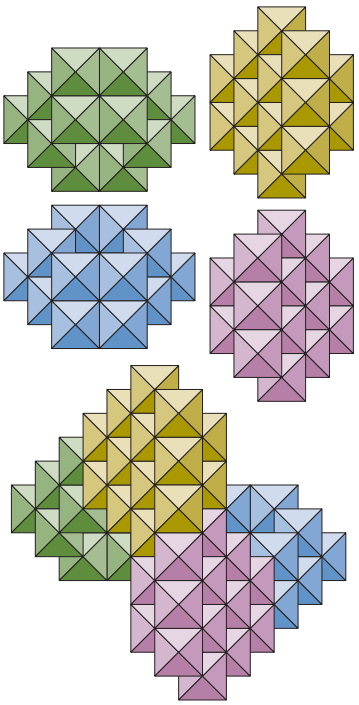
Ring of four C_6 rings

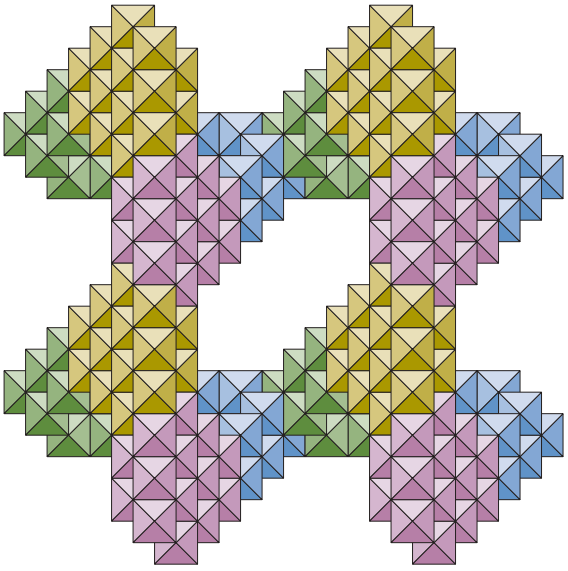
This group is equivalent to the four C-atom ring except that each C-atom is replaced with a ring of six C-atoms. Each ring adjoins two other rings and the connection is through a cleft join between a C-atom of each ring.

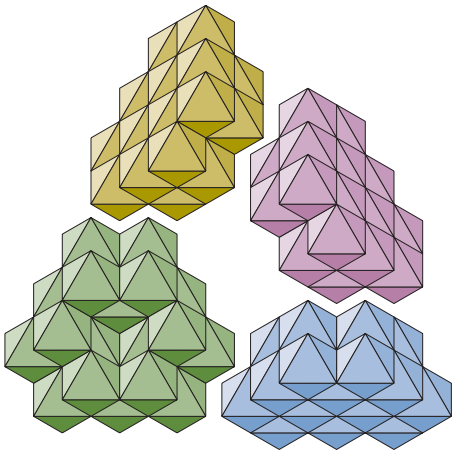
The following figure is a a view normal to the plane of the ring.

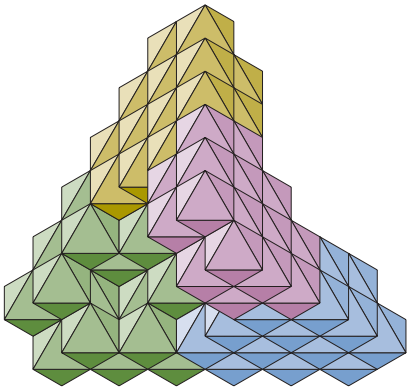


Ring of four C_6-rings, view A







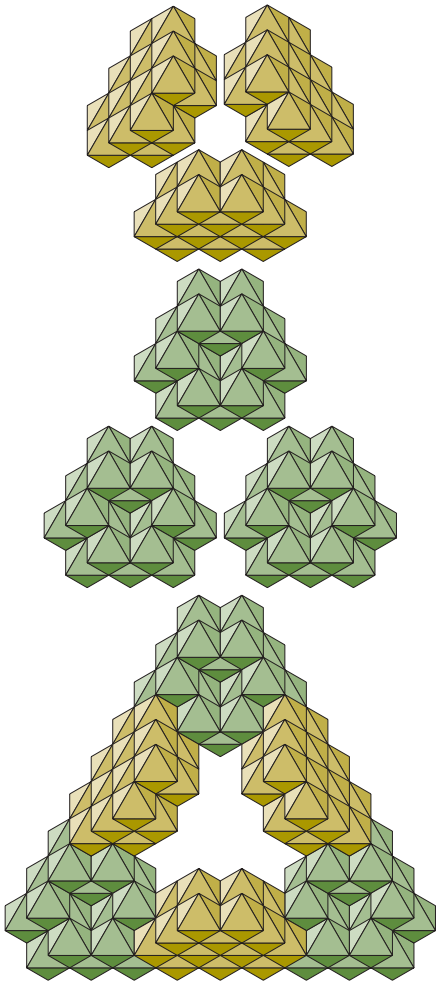


Ring of four $4C_6$ rings

The figure on the top right shows four C_6 rings which cleftly join to form the ring just below them. This ring is identical to the one shown in the previous figure but is viewed from another direction. Four of the $4C_6$ rings cleftly join to form the ring at the bottom left.

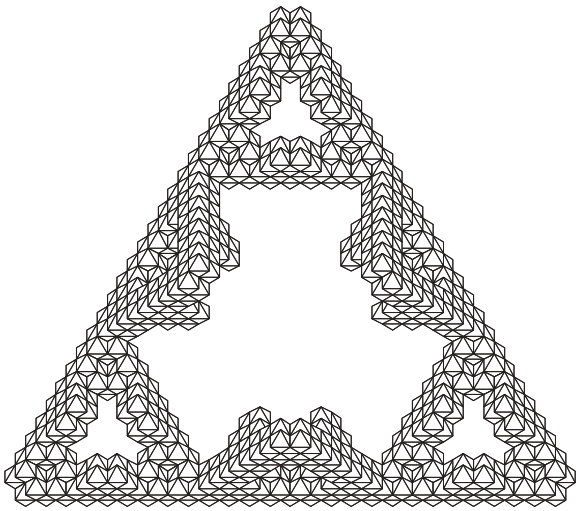
The figure directly above shows the assembly of the $4C_6$ ring from a third viewing direction.

Ring of six C_6 rings



Ring of six C_6-rings

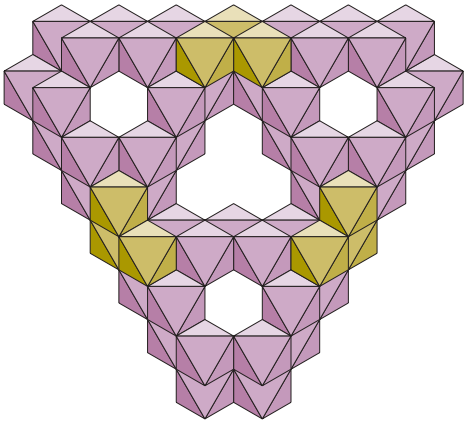
Two groups of three C_6 rings are shown at the top of the figure on the left. Together, they form the ring at the bottom of the left figure. The structure of this ring of rings is analogous in structure to the rings which make it—each of the C-atoms of the first is replaced with a ring of six C-atoms and the joins between the rings is the same as that between the C-atoms



Ring of six $6C_6$-rings

A ring of six $6C_6$ rings is formed in the same way as the rings of which it is made.

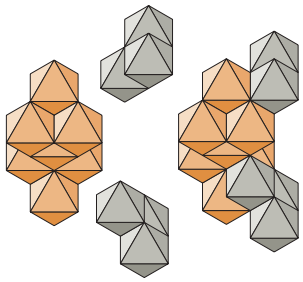
CC_6 group



Ring of three C_6-rings with C-atom links.

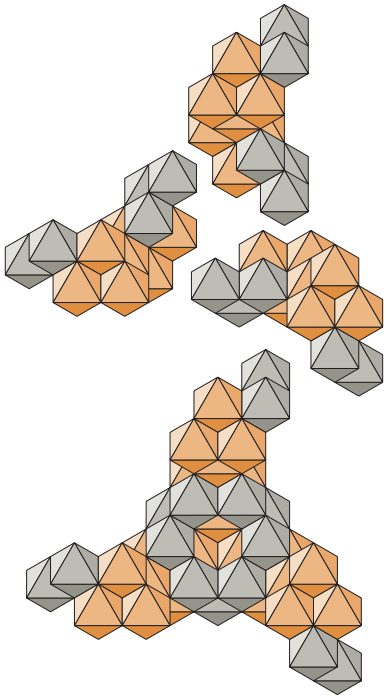
The addition of a C-atom to a C_6 ring permits the formation of a ring of three CC_6 groups.

CN



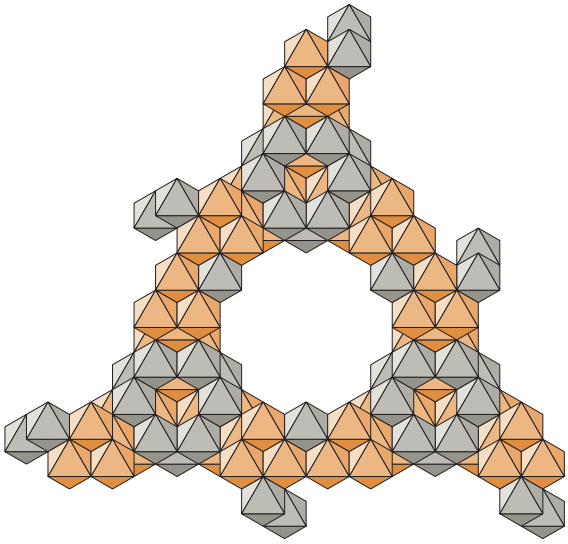
CN_2C unit

The plane-forming unit to the left is composed of a triplet-paired N_2 group to each N-atom of which a C-atom is cleft joined right-handedly.



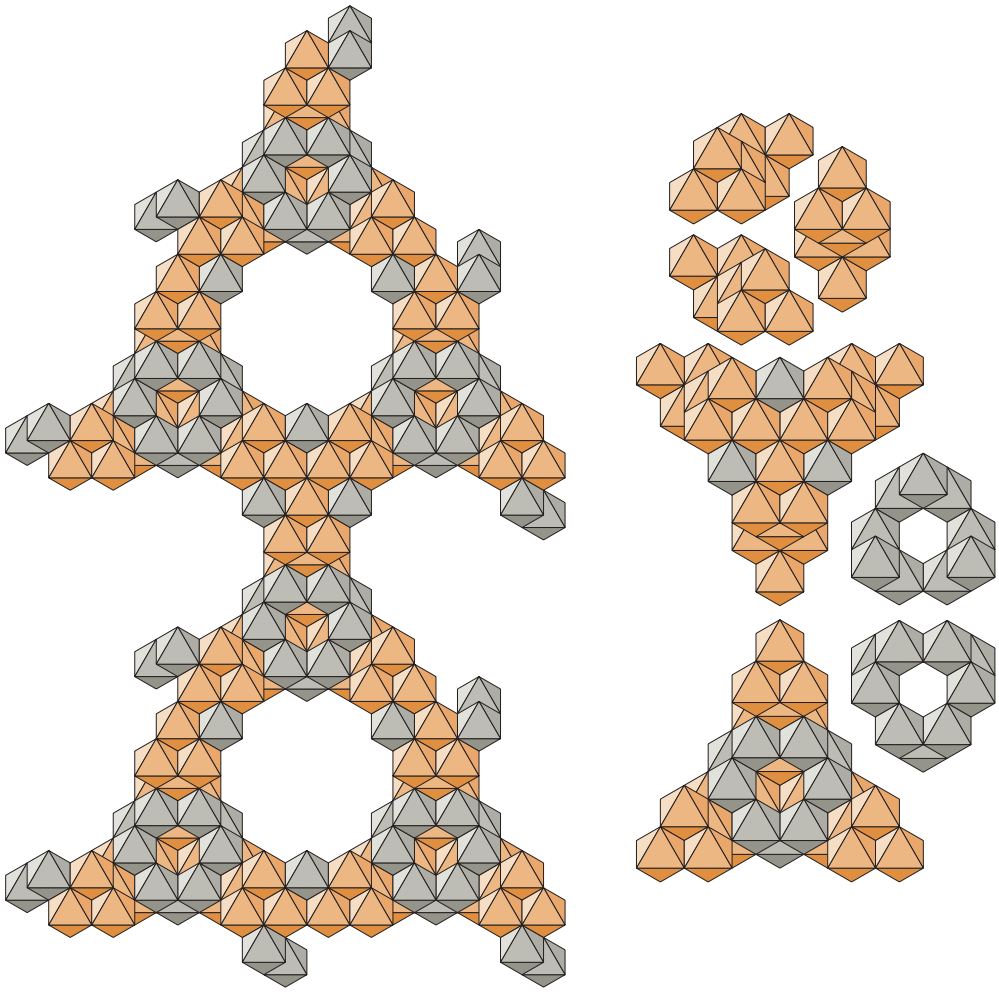
Three CN_2C ring.

The three CN2C units grouped at the top of the figure are identical except for a rotation of one-third of a revolution. A C-atom of one unit cleftly joins to an N-atom of a second unit. A third unit joins to each of the first two completing the ring which is at the bottom of the figure.



Ring of three $3CN_2C$ rings

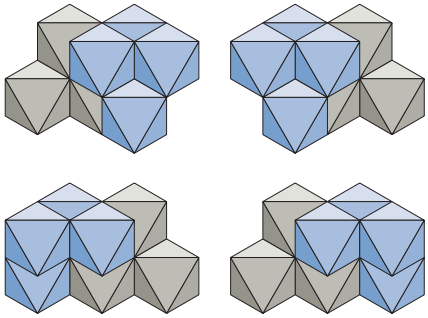
This ring of rings is held together by cleft joins between C-atoms and N-atoms.



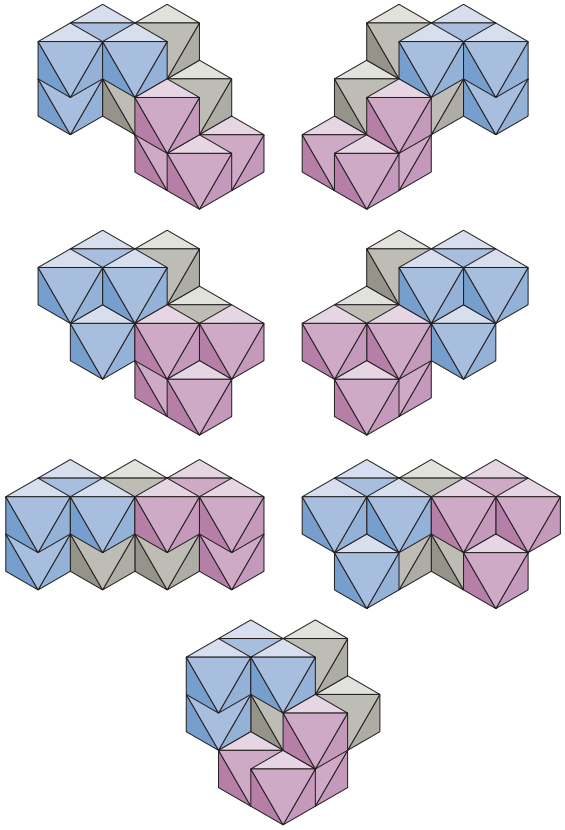
Pair of rings each composed of three $3CN_2C$ rings.

The figure on the left shows a pair of three $3CN_2C$ rings joined cleftly by two C-atom to N-atom joins. The figure on the right shows a ring of three CN2 units which occurs throughout the assembly on the left.

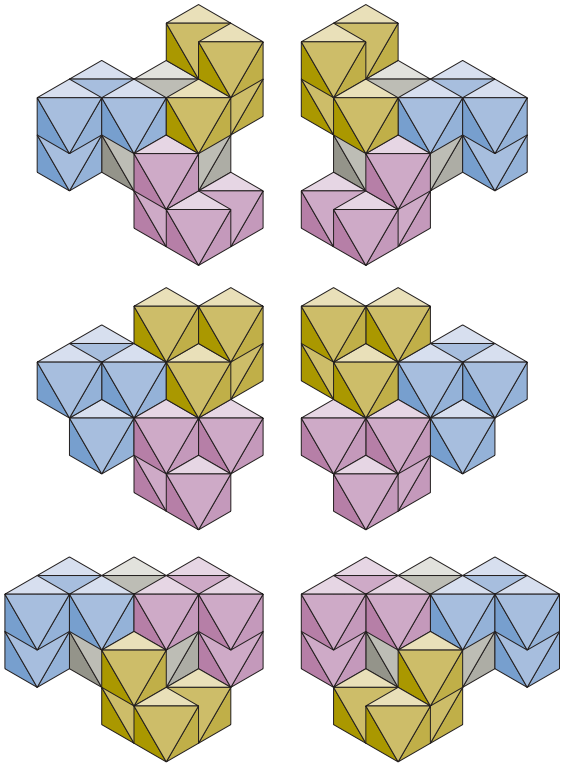
CO, CO_2, and CO_3



CO groups

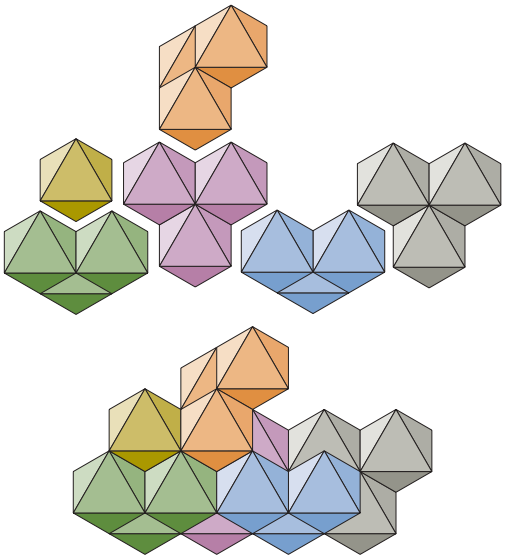


CO_2 groups



CO_3 groups

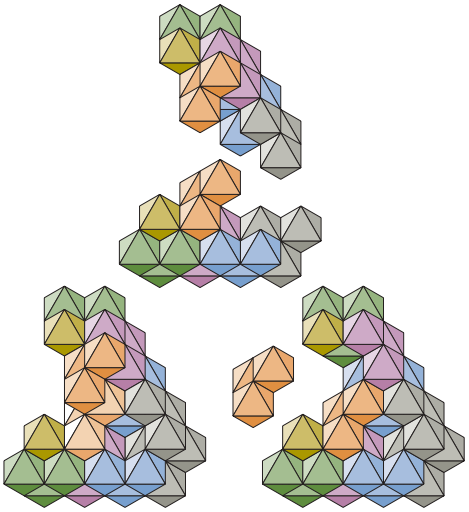
Isoprene



Isoprene

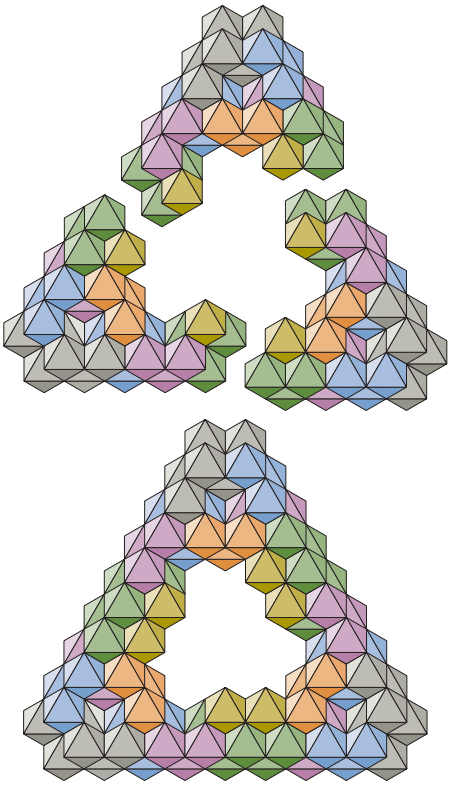
The isoprene unit consists of a chain of four C-atoms to which a C-atom is attached. The figure shows the atoms which combine to form the isoprene unit at the top and the assembled unit below. The chain is formed by the gray, blue, violet, and green C-atoms. The orange C-atom is the branch atom. The yellow octahedron is an H_3-group.

Limonene



Limonene

Two isoprene units can join so that three of chain atoms and the branch atom of one unit combine with two chain atoms of the second unit to form a C_6-ring. The gray, blue, violet, and orange C-atoms of the lower unit combine with the gray and blue C-atoms of the upper unit to form the ring. The two isoprene units are shown at the top. At the bottom left is the completed assembly. At the bottom right, the branch atom of the upper unit has been displaced so that the connection between the units can be shown.

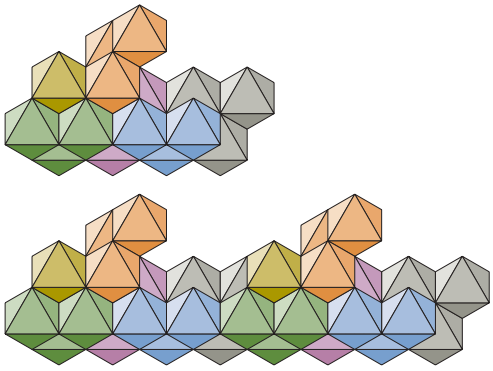


Limonene ring.

Three limonene units can form a threefold ring. The units which from the ring are shown at the top of the figure, the completed ring is at the bottom. The units are shown without the displaced orange C-atom.

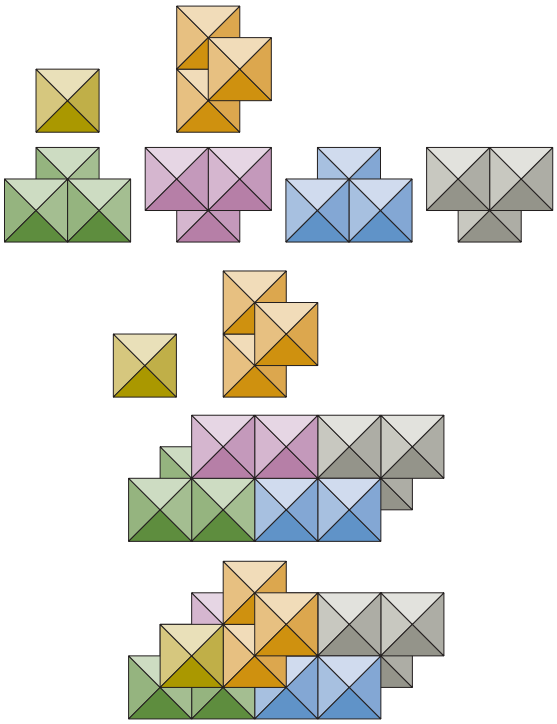
The three limonene units are rotated 120° relative to adjacent units. The join is effected with C-atom to C-atom cleft joins. The unit includes six isoprene units of five C-atoms each for thirty C-atoms. Cf. cholesterol.

β-Carotene



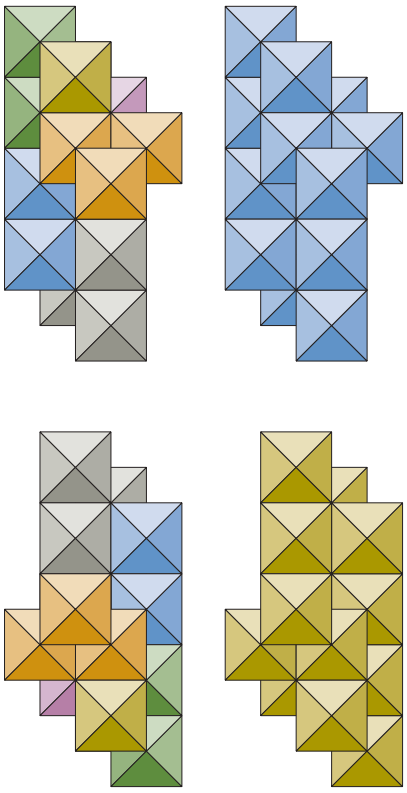
Isoprene chaining

The chain portion of the isoprene unit is extended by the chain portion of a second isoprene unit in the next figure. A single unit is shown at the top and a pair of joined units is below it.



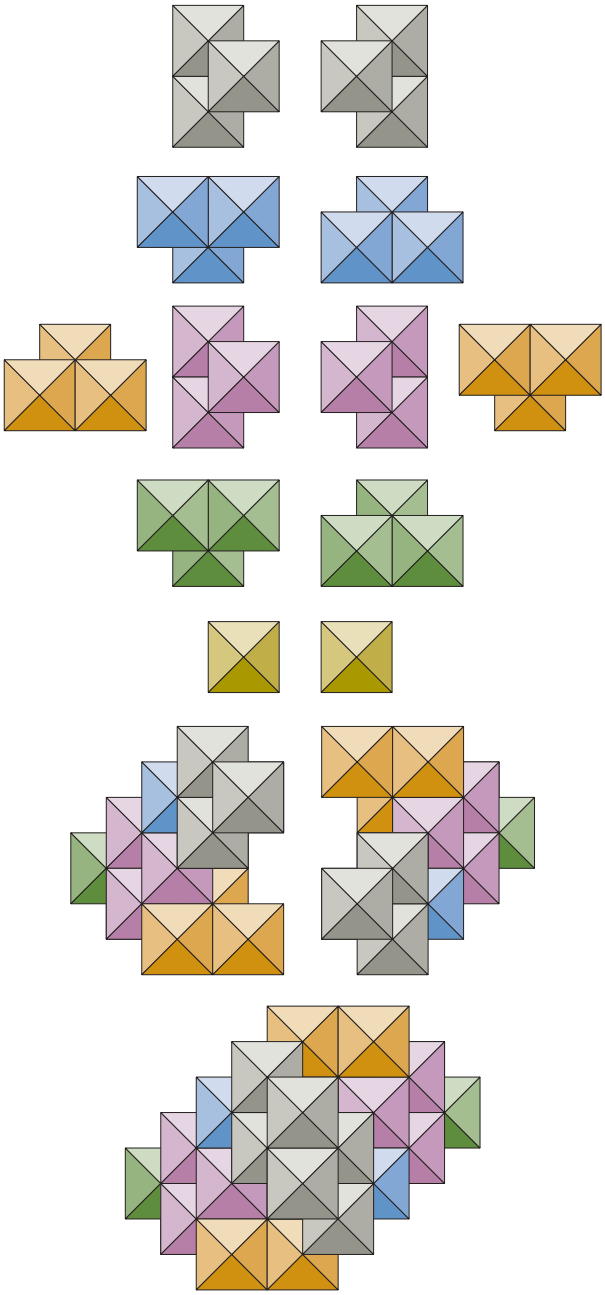
Assembly of isoprene unit, vertexial view

The isoprene unit is shown in a vertexial view normal to the chain in the next figure. The atoms which form the unit are at the top and the assembled unit is at the bottom. Between them, the chain is shown separately from the branch atom and the H_3-group.



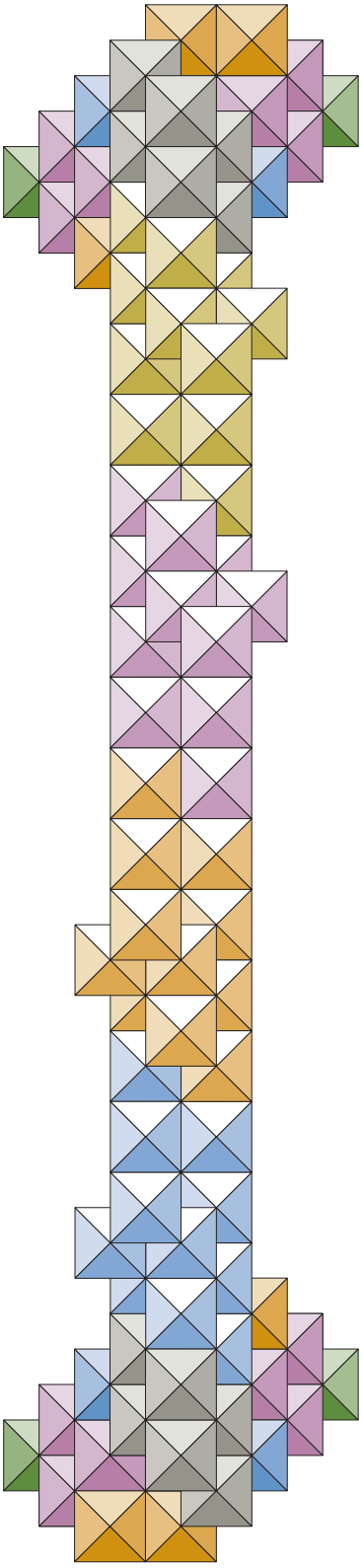
Isoprene units oriented for chaining

Two vertexial views of the chain are shown in the next figure. The atoms maintain their coloring in the left column. In the right, the He-octas of each unit have the same color. The bottom units are rotated one half turn about the viewing axis relative to the top units.



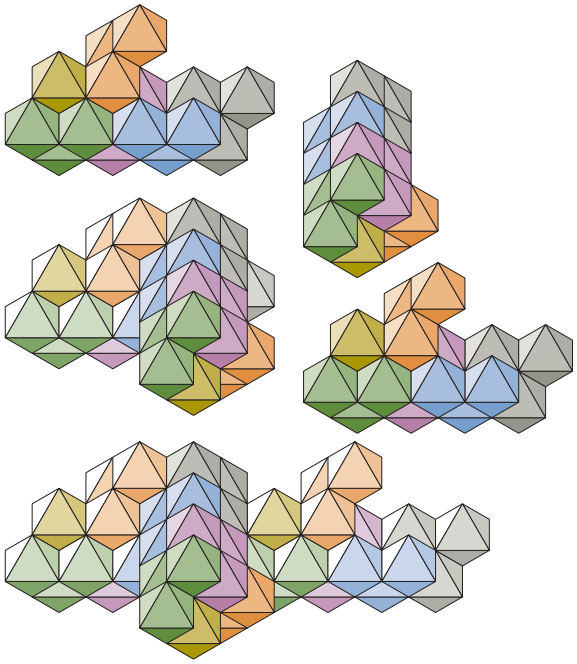
Isoprene cyclization

The cyclization of two isoprene units is shown here. The atoms are shown above the units they form in the left and right columns. The paired units are shown at the bottom.



β-Carotene

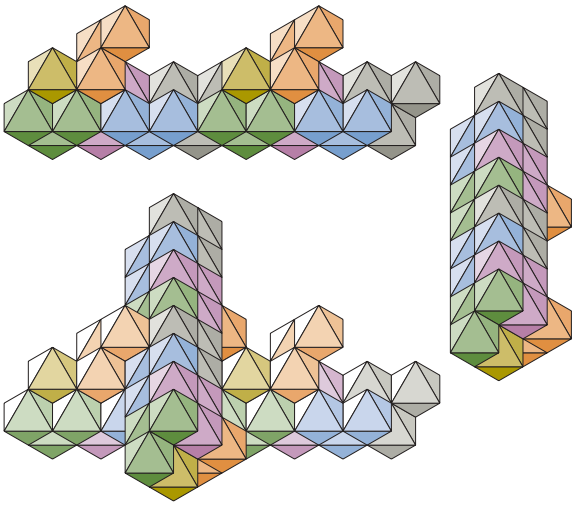
Two cyclicized units are connected by four isoprene units which consist of two pairs of units which are antiparallel components of a single chain. This is a β-carotene unit.



β-Carotene assembly detail

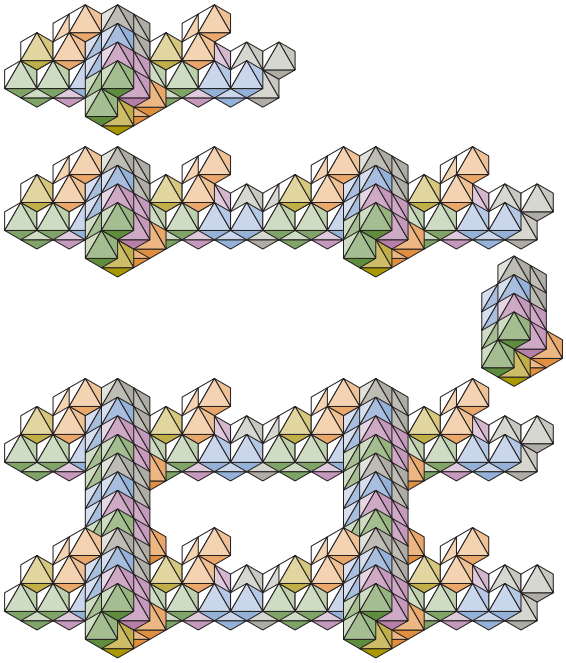
The cyclicized pair of units is shown in another orientation in the figure. The unit in the top left has a chain axis which is parallel to the top edge of the page. An identical unit on the right has an axis which makes an oblique angle with the viewing plane and is perpendicular to the chain axis of the first unit. In the second row of the left column, the two units are paired in the same manner as for the β-carotene assembly. A third isoprene is shown on the right which adds to the pair and extends the chain of the first isoprene unit.

Lattice of isoprene chains



Isoprene chaining—perpendicular junction

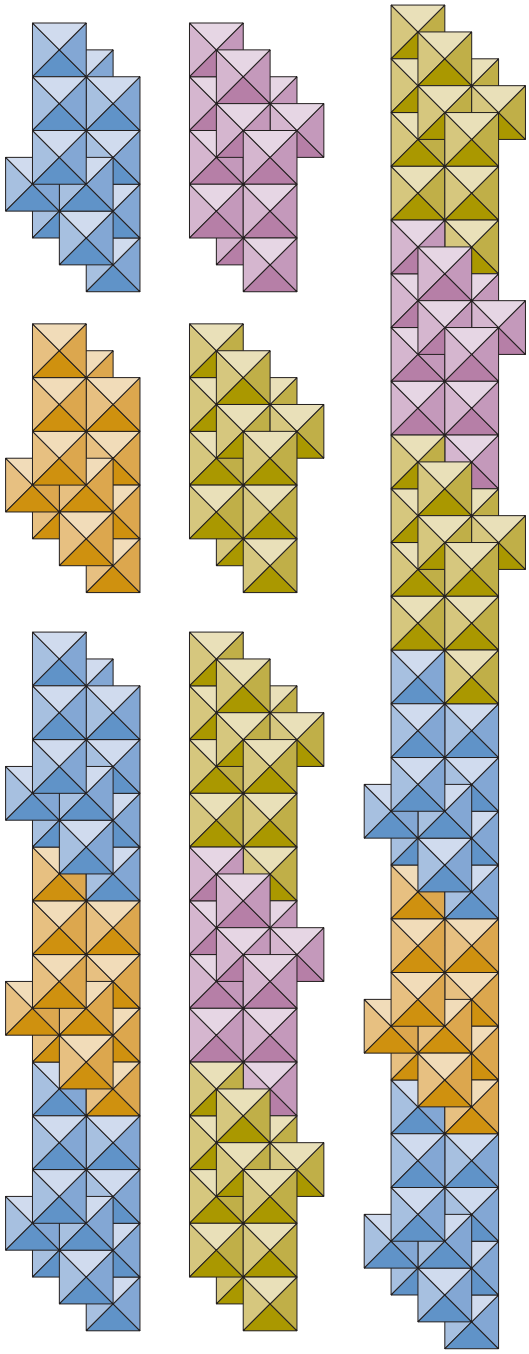
Two isoprene chains of two units each are depicted here. The axes of the two chains are perpendicular. The joined pair is shown at the bottom of the figure.



Square lattice of isoprene chains

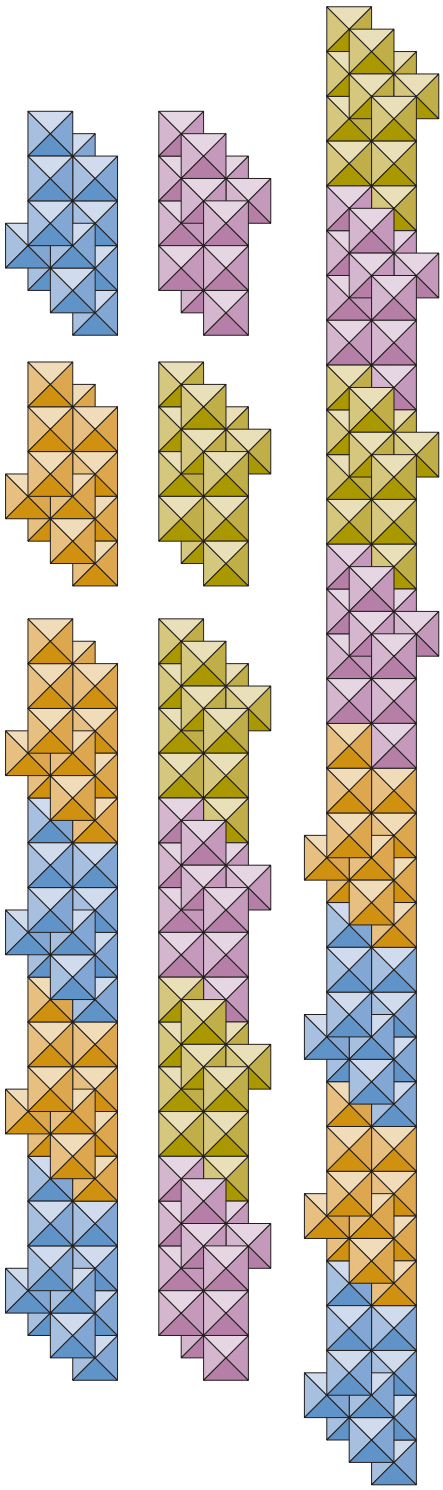
The perpendicular joining of isoprene chains permits the construction of a square lattice which can be extended in the plane. A one unit isoprene chain is joined to a perpendicular two unit isoprene chain at the top of the figure. In the second row, two identical units are joined so as to extend the two unit chain. Two of these chains are joined by a one unit extension between their perpendicular units.

Squalene



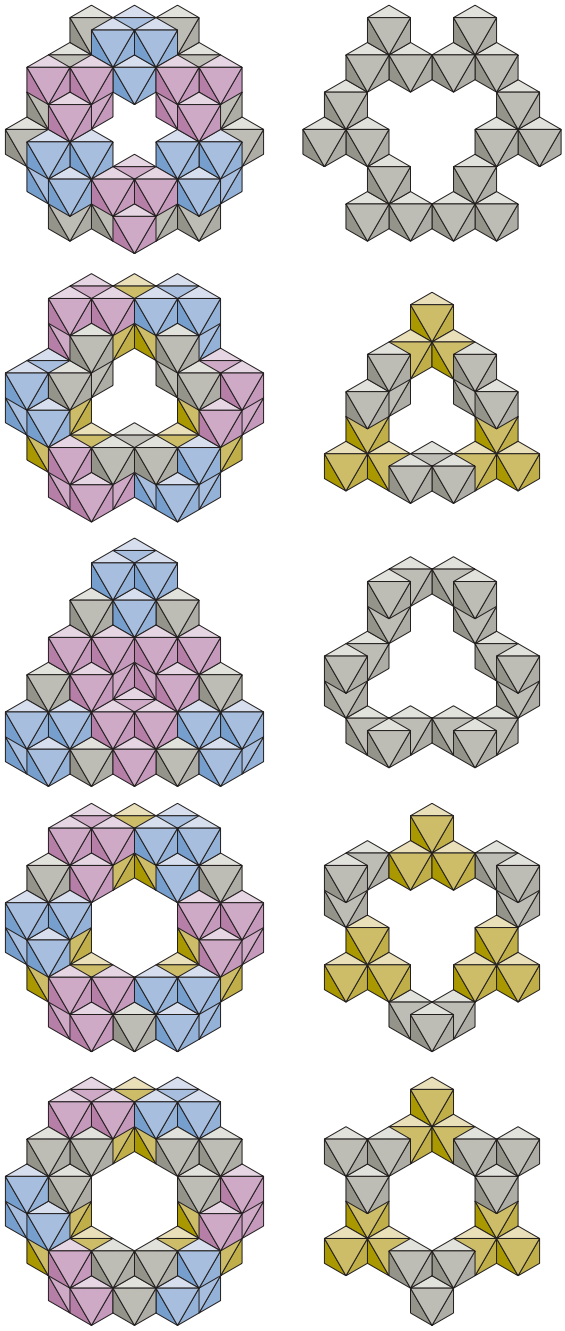
Squalene
The figure shows the assembly of two oppositely directed chains of three isoprene units each to form squalene. The isoprene units are colored according to their orientation.

Phytoene



Phytoene
The figure shows the formation of phytoene from two chains of four isoprene units each.

Inositol



Inositol

There are five different rings of six CO groups each shown here. The complete rings are in the lefthand column. On the right, the arrangement of the C-atoms are shown. Each of the rings is two He-octa facial diameters thick. Each is six He-octa edgial diameters wide. Each is six and two-thirds He-octa facial altitudes deep.