Crystal

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

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

Reference

Octahedron1stEd.pdf–bookmark CRYSTAL–pages 67-84

Introduction

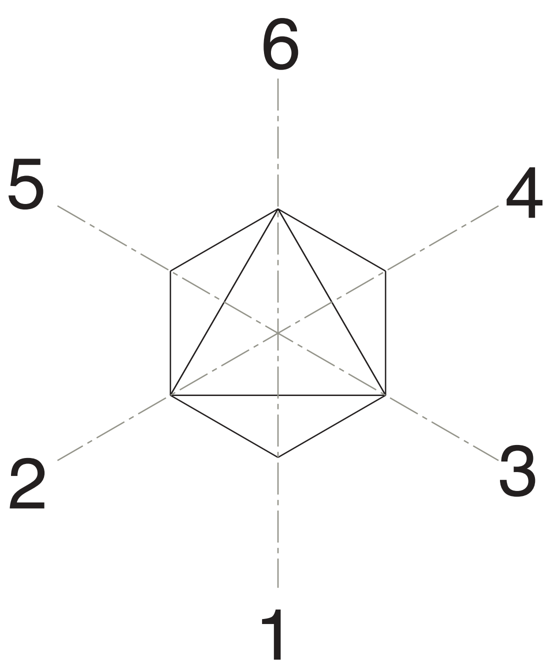
This material is excerpted from *Octahedron*. It shows how crystal forms are defined by the octahedral features of the octahedral particle which joins with identical particles to form the atoms.

CRYSTAL

The periodicity of the elements defines an atomic growth pattern which requires that the atoms be formed of identical regular octahedra in identical orientation. If atoms join so that each octahedron of one atom has an orientation which is identical to that of each octahedron of the other atom, it follows that any crystalline form which results from such joining must be modelable using identical regular octahedra in identical orientation.

Crystalline geometry

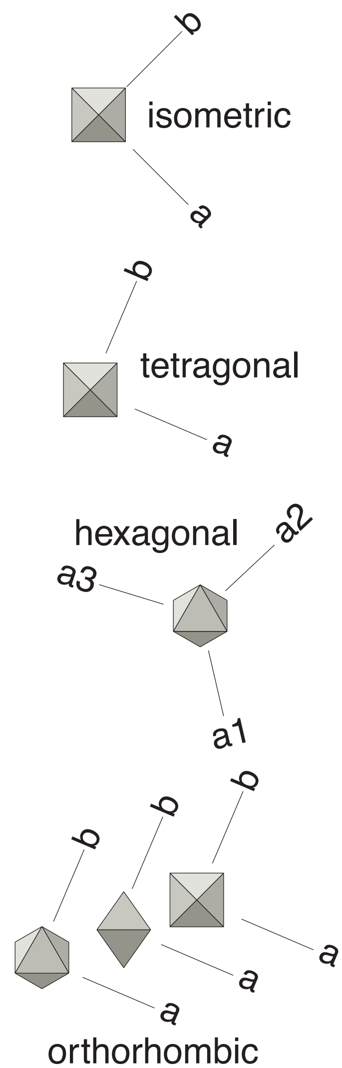
The geometry of the regular octahedron defines the geometry of the crystal. The regular octahedron has three vertexial diameters which intersect at its centroid. These diameters are in the same relationship as the Cartesian coordinates. If there is no motion between adjoining



octahedra in crystalline order, then the position of one relative to another is expressible using integral multiples of the vertexial diameter of the octahedron divided by two. The location of one octahedron relative to another is expressible with three integers which represent the axial directions.

Crystal axes

The symmetry of the crystal class shows the orientation of the octahedra of which its atoms are composed.



Orientation of octahedra in crystals. The symmetries of the crystals within the crystal classes indicates the possible orientations of the octahedra of which its constituent atoms are formed. The views here are parallel to the c-axes.

The **isometric** class is the most well defined in this regard. The crystal axes must be equal in length and at right angles to each other. This condition can only be met if the crystal axes are parallel to the three vertexial diameters of the octahedron. Each of the axial increments is an integral multiple of the vertexial hemi-diameter of the He-octa.

The **tetragonal** class requires the three axes to be mutually perpendicular. Two of the axes must be equal in length. This requires that the c-axis be parallel to a vertexial diameter of the octahedron. The c-axial increment is an integral multiple of the vertexial hemi-diameter of the He-octa.

The **hexagonal** class requires that three axes be equal in length, at 120° , and at right angles to the c-axis. The c-axis must be parallel to a facial diameter of the octahedron to meet these criteria. The c-axial increment is an integral multiple of the facial diameter of the He-octa.

The **orthorhombic** class requires that its three axes be mutually perpendicular. This condition can be met if the c-axis is parallel to an edgial, a facial, or a vertexial diameter of the octahedron.

Moving between octahedral locations

In defining the locations of the parts of the octahedral assembly, the relation of one location to another can be described in terms of *moves*. A reference octahedron is specified and its centroidal address is taken as 0,0,0. Its vertexes are numbered from 1 to 6 and all moves within the assembly are specified in terms of the directions of these vertexes from the centroid. A convention has been adopted wherein the vertexial directions are assigned xyz-directions.

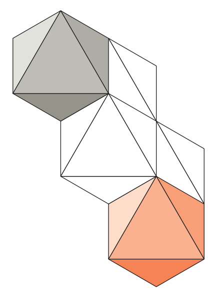
Table 11: Correlation of octahedral directions with Cartesian coordinates

XYZ	Octa vertexial
+x	3
-x	5
+y	2
-y	4
+z	6
-z	1

Table 11: Correlation of octahedral directions with Cartesian coordinates

Edgial move

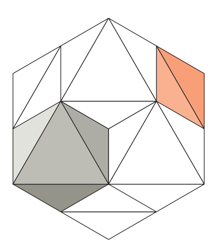
Edgial moves are in the direction from the centroid to the middle of an edge. It is normal to the edge. The direction designation is the pair of numbers of the vertexes which terminate the edge. Each edgial move increments



the values of each of the two coordinates matched by the vertexial numbers by ±1. The move 13,2 adds 2 to the x-coordinate and subtracts 2 from the z-coordinate.

Vertexial move

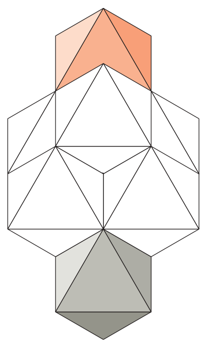
Vertexial moves are in the direction from centroid to vertex. The coordinate is the vertexial number. The vertexial move increments



a single coordinate by ±2. The move 4,1 subtracts 2 from the y-coordinate.

Facial move

The facial move is in the direction from the centroid of the octahedron to the centroid of the octahedral face. It is normal to the face. There is no octahedron whose centroid can lie in the facial direction in the first two layers. It is in the third layer that there can be an octahedron in the requisite crystalline order. The facial move increments the three coordinates



by ±2. The move 546,1 subtracts 2 from the x- and y-coordinates and adds 2 to the z-coordinate.

Planar moves between octahedra

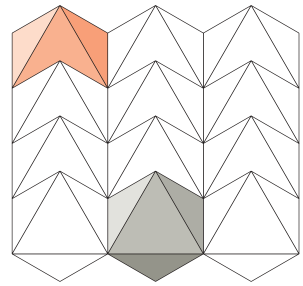
The location of one octahedron is reachable from the location of another octahedron by a series of moves which are in the plane. These are referred to as planar moves. The planes of an octahedral assembly are defined by the topological features of the octahedron. The *vertexial plane* is defined by its vertexes, the *facial plane* by its faces, and the *edgial plane* by its edges. There being no other topological features, any plane is one of these three types.

Vertexial planar moves

The vertexial plane can be normal to a vertexial diameter of the octahedron or at another angle to it. The latter cannot be generalized. The normal and special planes are described.

The normal vertexial plane

The location of any octahedron defining the *normal vertexial plane* is reachable by edgial

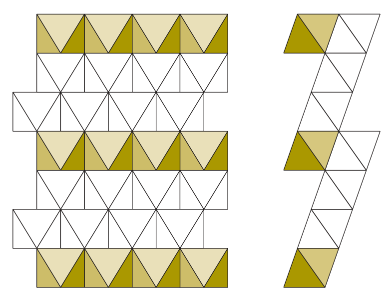


The normal vertexial plane.
The normal vertexial plane is at right angles to the vertexial diameters of each of the octahedra whose vertexes define the plane. The locations of the two octahedra which are colored differ by edgial moves which are parallel to the plane.

moves parallel to the plane. There are four edgial directions in a normal vertexial plane. Some locations are reachable by a vertexial move. The (100) faces of crystals of the isometric system are defined by octahedral vertexes and are normal vertexial planes.

The special vertexial plane

The *special vertexial plane* is a type of vertexial plane which arises from the facial move. There are two edgial moves and two facial

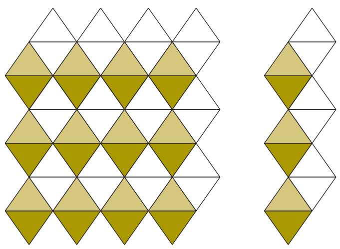


The special vertexial plane.
The view on the left is normal to the plane and parallel to a pair of faces of the octahedra which constitute it. The plane is defined by a vertex of each of the octahedra which is colored yellow. The view on the right is parallel to the plane.

moves in the special vertexial plane. These planes are normal to a pair of faces of the regular octahedron and can occur as hexagonal prisms.

Edgial planar moves

The move from one octahedral location to another in the edgial plane is accomplished

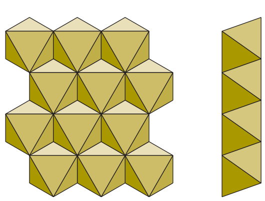


The edgial plane.
The view on the left is normal to the edgial plane. That on the right is parallel to the edgial plane. An edge of each of the octahedra colored yellow defines the edgial plane.

with the two edgial directions, four facial directions, and two vertexial directions. These planes are exemplified by the (110) planes of the isometric system.

Facial planar moves

There are six edgial moves in the facial plane. These planes are exemplified by the (111) planes of the isometric system and the (0001) planes of the hexagonal system.



The facial plane.
The view on the left is normal to the facial plane. That on the right is parallel to the facial plane. A face of each of the octahedra defines the facial plane.

The isometric system

Closed forms

A closed form is defined by crystal planes which are so oriented that they enclose a volume. Each plane of a closed form has axial intercepts which are numerically identical with those of every other plane of the form. Modeling the closed forms is a rigorous test which the shape that defines the forms of the atomic elements must pass. Each of the closed forms of the isometric system is definable through the edge to edge association of regular octahedra. Each of the crystalline planes is defined solely by one of the three topological features of the regular octahedron—edge, vertex, or face.

Crystal planes specified by vertexial axes of the octahedron

For modeling the crystal planes of the isometric system using regular octahedra, the planes may be specified by axes defined by the vertexial diameters of the octahedron. These axes are the same as those used for describing the positions of the He-octas in the atomic elements. Specifying the plane in this way establishes an absolute description of the plane. The axial intercepts of the octahedral plane are expressed as integral lengths of the vertexial hemi-diameters of the He-octa. The vertexial hemi-diameter is equal to the edge of the He-octa divided by $\sqrt{2}$.

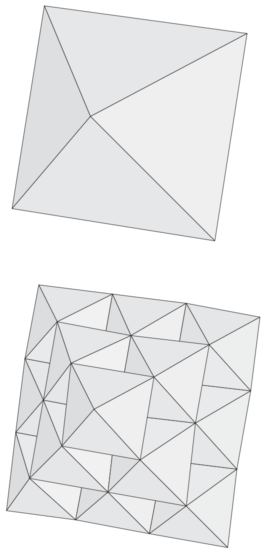
Planes defined by octahedral faces

The (111) planes of the crystals of the isometric system are defined by faces of the epn-octas which make up the atoms of which the crystal is formed. There are two closed forms which have only (111) faces—the regular octahedron and the regular tetrahedron.

Octahedron (111)

Faces of the simple octahedra which compose the compound octahedron define the

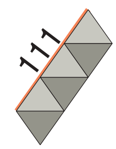
(111) planes of the regular octahedron.



Octahedron (111)

Tetrahedron (111)

Here the faces of the octahedra define the faces of a regular tetrahedron. The octahedron has eight faces which can be seen as two sets of four faces each. Each set includes the faces of a regular tetrahedron.



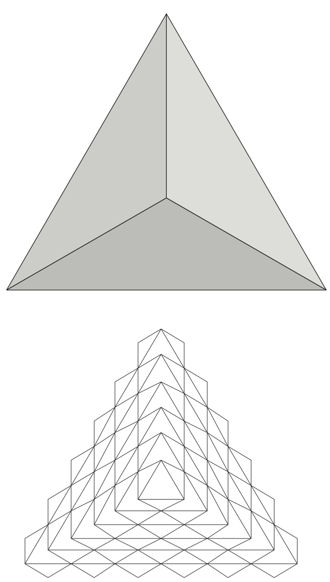
Tetrahedral planes (111)

Planes defined by octahedral edges

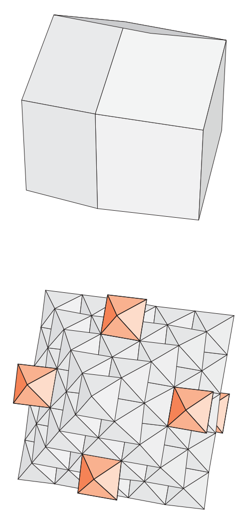
Three closed forms of the isometric system are the *rhombic dodecahedron*, the *trisoctahedron*, and the tetragonal *tristetrahedron*.

Rhombic dodecahedron (hh0)

Each of the rhombic dodecahedral planes is normal to an edgial diameter of the regular octahedron and is defined by the edges of the octahedra. The rhombic dodecahedral assembly depicted here is the minimal such assembly. It is composed of a 5-octa which has 1-octas mounted on its face centers. An edge of 5-octa combines with an edge of each of two of the 1-octas to define each of the rhombic

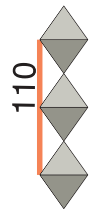


Tetrahedron (111)



Rhombic dodecahedron.

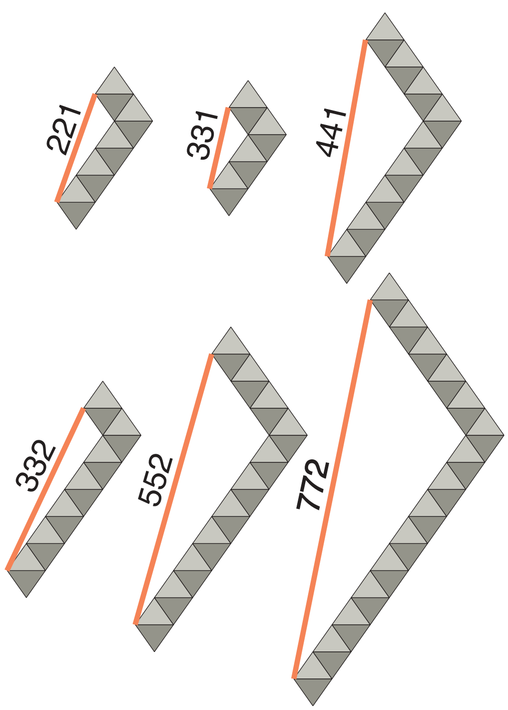
dodecahedral planes.



Rhombic dodecahedral plane (110)

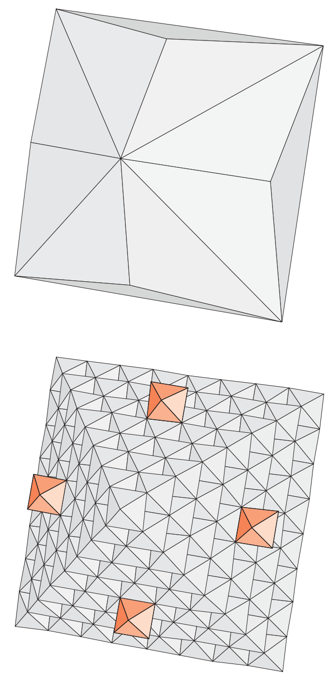
Trisoctahedron (hhk)

The trisoctahedron features a tetrahedron upon each of the eight faces of a regular octahedron. The threefold-axis of the tetrahedron is colinear with the facial centroid to octahedral



Trisoctahedral planes, *hhk*

centroid vector of the face upon which it is situated. The figure shows the minimal trisoctahedron which can be built of identical octahedra. The base octahedron is an 8-octa.

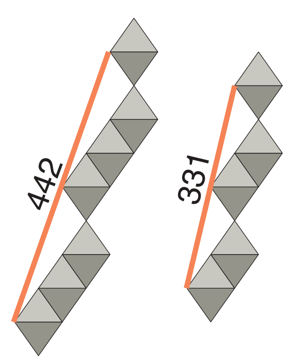


Trisoctahedron (331)

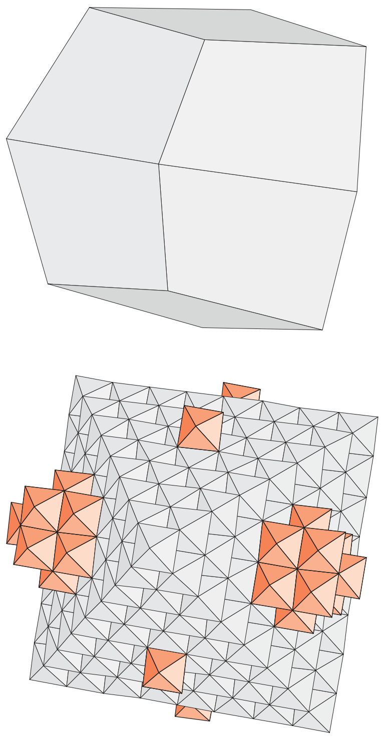
This compound octahedron has faces which each have a facial centroidal position where a simple octahedron can join. The next smaller compound octahedron which has facial centroidal attachment positions is the 5-octa. The faces produced thereon are rhombic dodecahedral as is shown above.

Tetragonal tristetrahedron (hhk)

The tetragonal tristetrahedron has twelve faces of four edges each. Each face is parallel to a pair of octahedral edges. The plane is



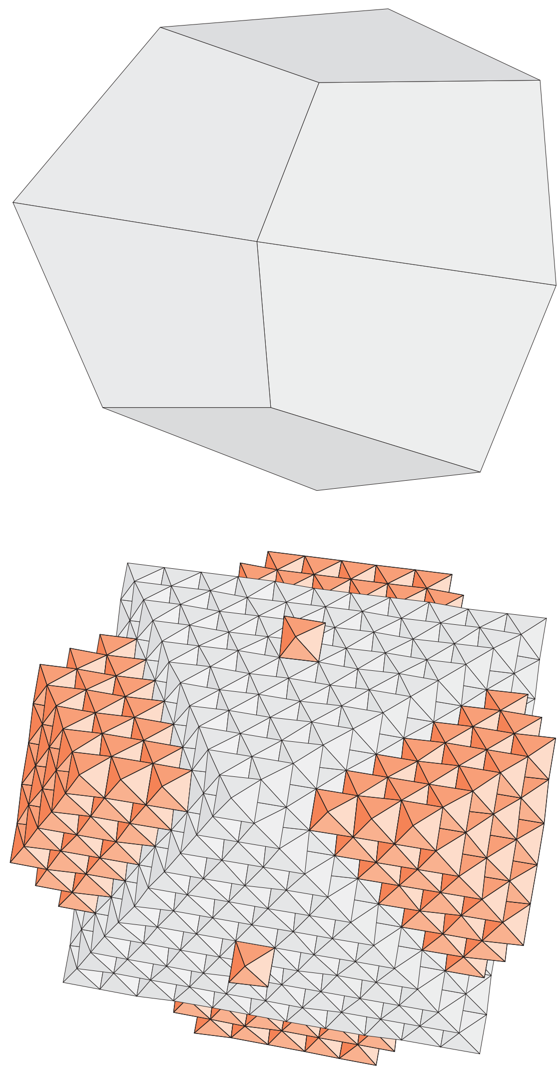
defined by one of these edges. The faces meet at two different types of vertexes—three plane and four plane. The two types alternate. The three-plane vertexes lie on facial-centroidal axes. The four-plane vertexes lie on vertexial diameter axes.



Tetragonal tristetrahedron (331)

The structure of the tetragonal tristetrahedron can be seen in the two examples. The first of these, the (331) is minimally modeled using a single octahedron on four faces which together define a regular tetrahedron. The other four faces have a two layer pyramidal group which is symmetrical about the facial centroid axis. The faces they occupy define a regular tetrahedron as well. The 331-planes are defined by an edge of one octahedron of this group, an edge of the lone octahedron on an adjacent face and an edge of the eight octahedra which define the intervening edge of the 8-octa which is the foundation of the crystal model.

The (442) tetragonal tristetrahedron has an 11-octa for its foundation. A tetrahedral group of the 8-octa faces have a single octahedron at their centroids. The remaining four tetrahedral faces have a pyramidal assembly which is three layers high. Each of the tetragonal tristetrahedral faces is defined by a edge of four octahedra of the three layer pyramidal group, an edge of the lone octahedron on an adjacent face, and an edge of each of the eleven octahedra which define the intervening edge of the 11-octa.

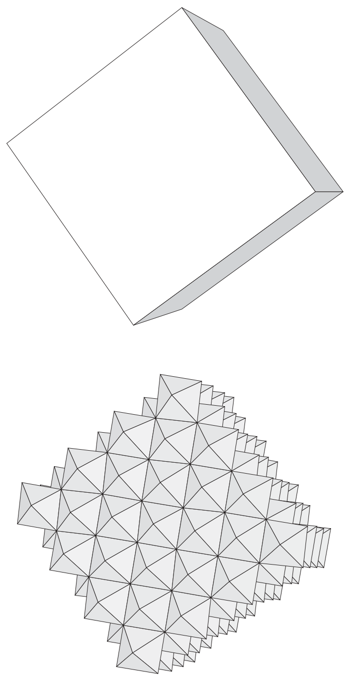


Tetragonal tristetrahedron (442)

Planes defined by octahedral vertexes

Vertexes of the octahedra define these closed forms of the isometric system—the *cube*, the *tetrahexahedron*, the *trapezohedron*, the *tristetrahedron*, the *pyritohedron*, the *gyroid*, the *diploid*, and the *hexoctahedron*

Cube (h00)

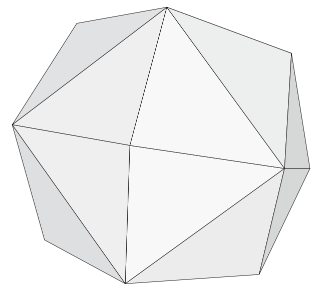


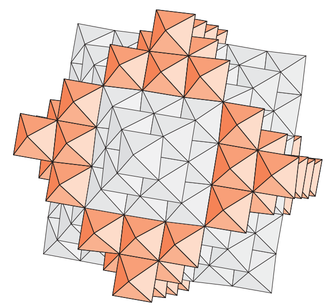
Cube (h00)

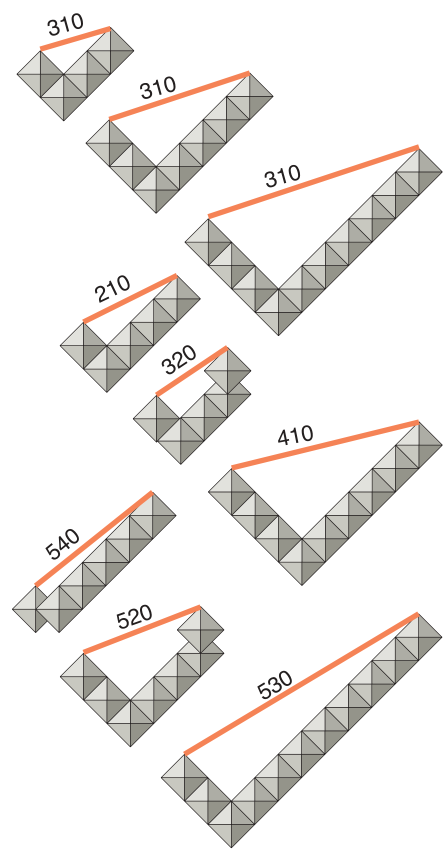
A cube has six (100) faces. The cube faces are defined by octahedral vertexes. Each cube face is perpendicular to a vertexial diameter of each of the octahedra which define it. The octahedral model shown here defines a cube with a facial diameter of four octahedral vertexial diameters.

Tetrahexahedron (hk0)

The tetratexahedron is modeled using a 5-octa foundation. Upon each face of the 5-octa is placed a two layer pyramidal group which is symmetric about a facial centroidal diameter. Each face of the tetrahexahedron is defined by a vertex of the 5-octa and a vertex of each of two octahedra of a pyramidal group on adjacent 5-octa faces.



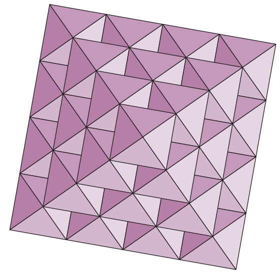




The plane of the tetrahexahedron is parallel to a vertexial diameter of the regular octahedron. This is seen when the plane is viewed edge-on.

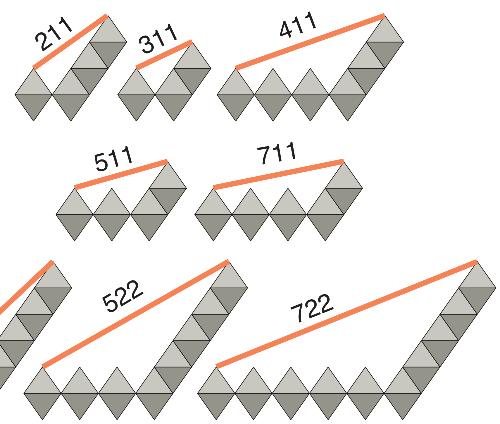
Trapezohedron (hkk)

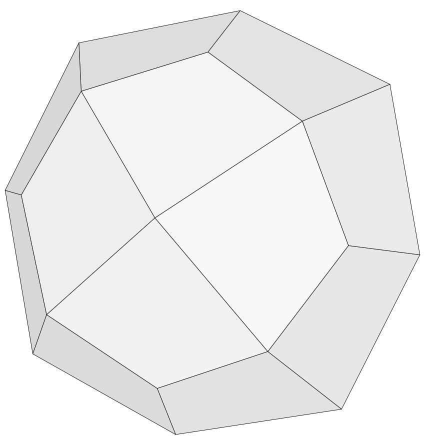
The trapezohedron has twenty-four faces. The model of the trapezohedron (211) has an 11-octa for a foundation. A single octahedron has been placed upon the centroid of each face of the 11-octa. A one octahedron thick square pyramidal cap has been removed from each 11-octa vertex which exposes a portion of a 9-octa. Each face of the trapezohedron is defined by a vertex of the 9-octa and a vertex of a lone facial octahedron and a vertex of each of five 11-octa octahedra which form the edge where the cap was removed.

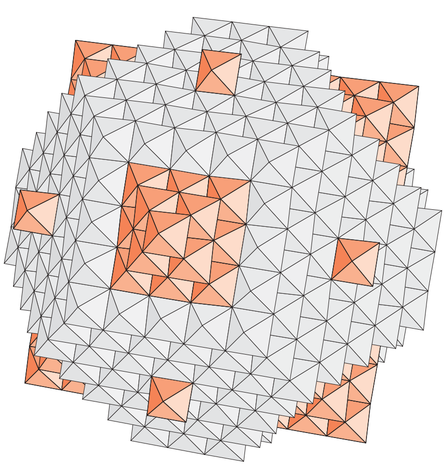


Vertexial cap removed from 11-octa in modeling trapezohedron.

The planes of the trapezohedron are parallel to a pair of edges of the octahedron whose vertexes define it.

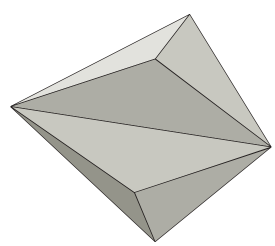


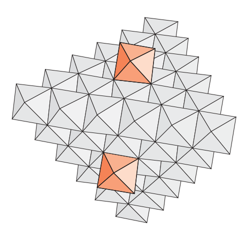




Tristetrahedron (hkk)

A regular tetrahedron constructed with identical octahedra and having six octahedra along each edge is the foundation for the tristetrahedron model. A single octahedron is mounted



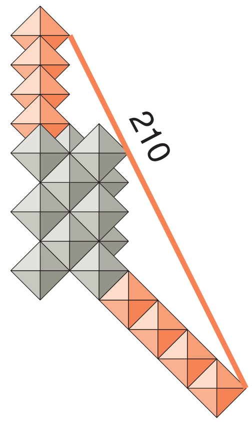


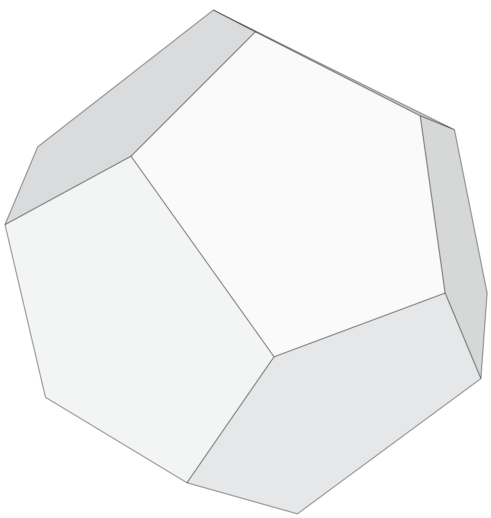
centroidally on each of the four faces. A vertex of the facially mounted octahedron and a vertex of each of the six edgial octahedra of the tetrahedron define the tristetrahedral plane. The formation is such that a triangular pyramid is mounted on each of the tetrahedral faces.

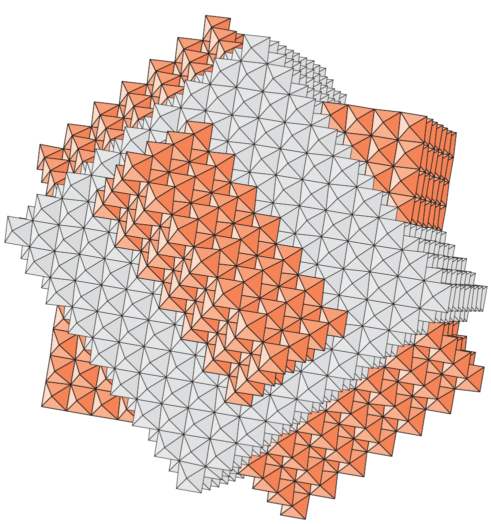
Pyritohedron (hk0)

The foundation for the pyritohedron (210) model is a cube composed of identical octahedra. The cube edge is defined by nine octahedra. A triangular prism which is seven octahedron vertexial diameters long and four vertexial layers high is mounted on each face of the cube. The prisms on opposite faces are mirrored. The three pairs of prisms are mutually perpendicular. The pyritohedral face is defined by an octahedral vertex at the end of the top layer of one prism, a vertex of each of the octahedra in the top layer of a prism on an adjoining face, and a vertex of each of the octahedra along the edge between the faces.

The pyritohedral planes are parallel to a vertexial diameter of the regular octahedra which define it. Each of the defined planes is an irregular pentagon.

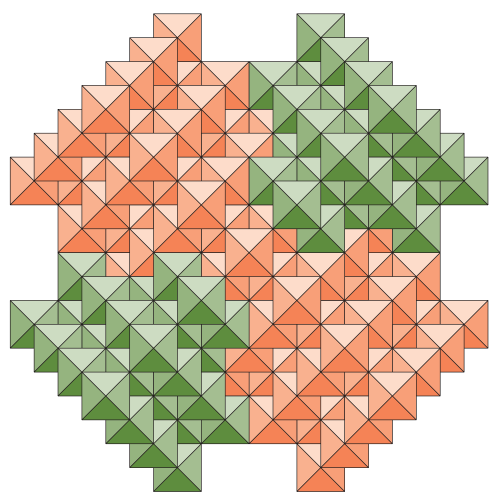




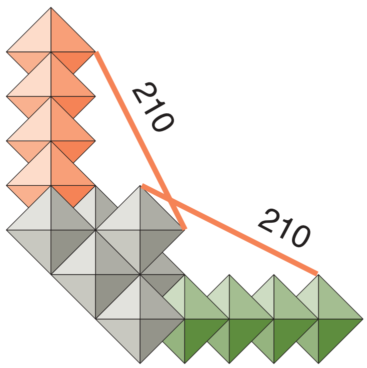


Iron cross twin

The iron cross twin of the pyritohedron has the same base. But the triangular prism on each of the cube faces is replaced by a an interpenetrant triangular prismic cross. The cross



has the same triangular prism which is shown in red with the green additions which make the cross. The planes of the iron cross twin are the same as the pyritohedron. But the planes are now defined by a vertex of an octahedron at the end of the top layer of one leg of the cross and a vertex of each of the nine octahedra which define the cube edge. The planes on either side of a cube edge are shown in the next figure.

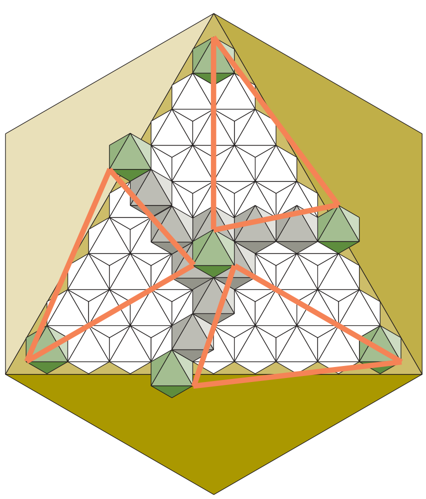


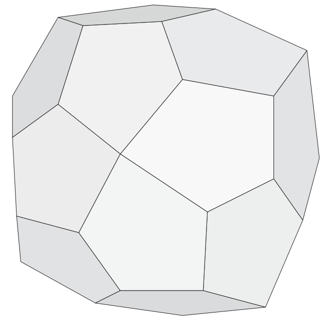
Pyritohedral planes of iron cross twin. The gray colored octahedra belong to the base cube. The red colored octahedra belong to one cross and the green to another cross.

Gyroid (hkl)

Left handed gyroid

The left handed gyroid can be modeled by mounting an assembly which is shown in the figure upon each face of a 10-octa so that it is symmetrical about the facial centroidal axis.





Right handed gyroid

The right handed gyroid can be modeled by mounting an assembly which is shown in the

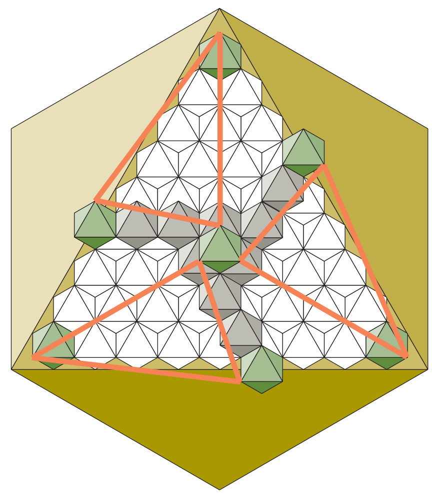
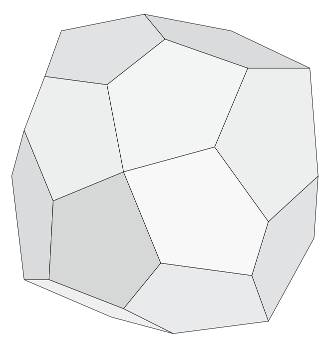
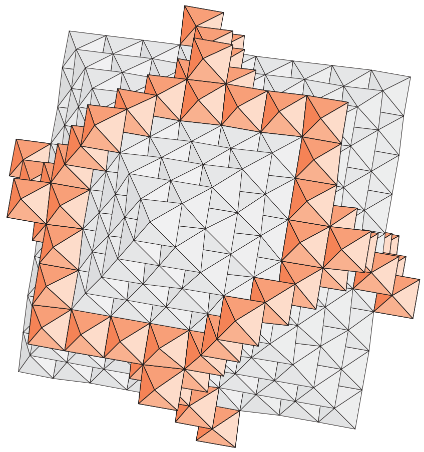


figure upon each face of a 10-octa so that it is symmetrical about the facial centroidal axis.



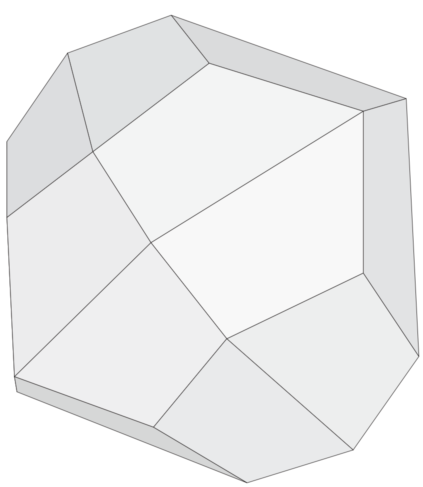
Diploid (hkl)

The diploid model has a 9-octa for its foundation. A two layer octahedral pyramid is



mounted on the centroid of each 9-octa face. Along a pair of opposite edges at a 9-octa vertex there is an octahedron joined to the *fourth* octahedron of each of the two edges. Along each edge of the remaining pair of edges which join to form the vertex there is an octahedron joined to the *fifth* octahedron of each edge.

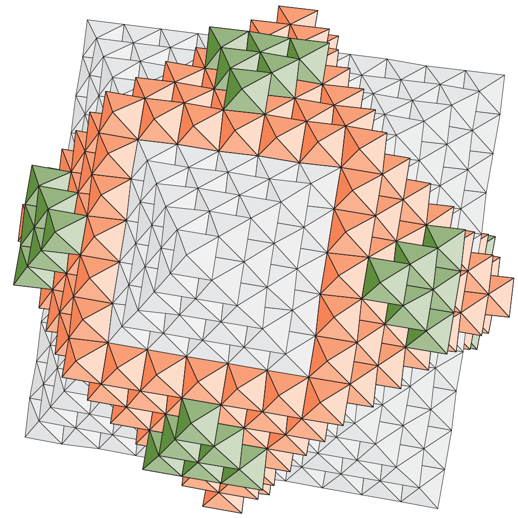
The diploid plane is defined by a vertex of



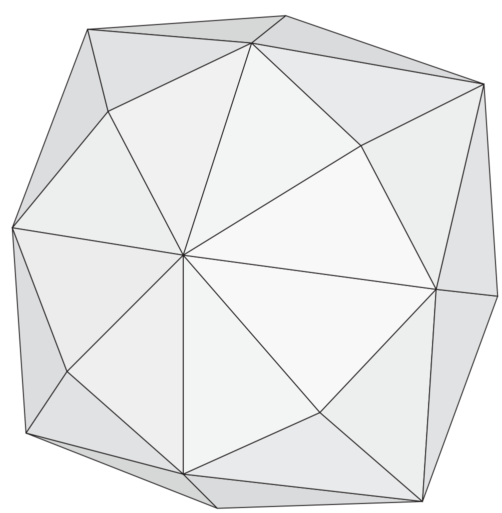
the top layer of the facial pyramid, the vertex which is at the vertex of the 9-octa, and a vertex of each of the two octahedra which are joined to the 9-octa edges.

Hexoctahedron

An 11-octa is the foundation for the model of the hexoctahedron (321). A two layer pyramid

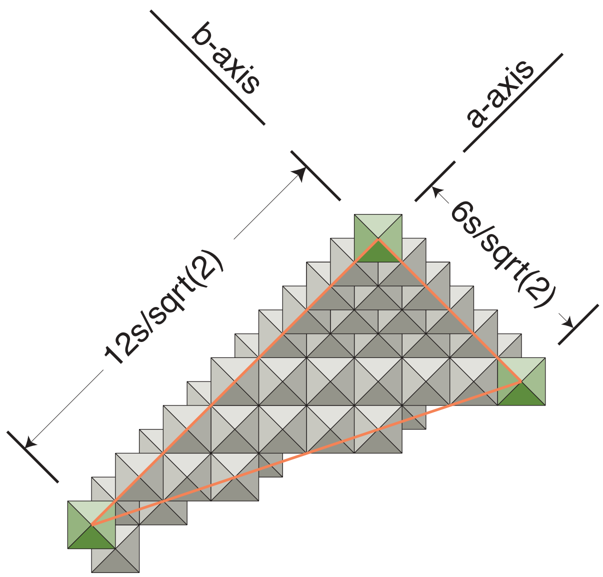


is mounted on the centroid of each face. An octahedron is mounted at the middle of each edge. The hexoctahedral plane is defined by a vertex of the 11-octa, a vertex of the octahedron at a mid-edge and a vertex of an octahedron in the top layer of the facial pyramid.



Hexoctahedron (321)

The isometric (123) plane.

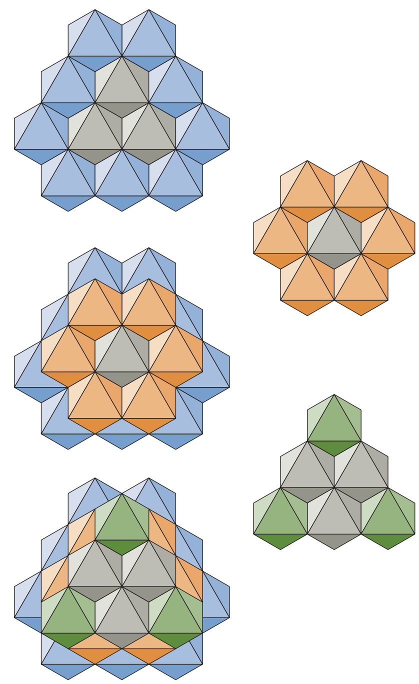


The isometric (123) plane can be modeled so that each of the three octahedra which provide a vertex which defines the plane is lying on a planar axis. The value of each of the axial intercepts is found by counting the vertexial hemi-diameters between the defining vertexes in the three axial directions. From the figure, the distances along the axes are 12 for **a**, 6 for **b** and 4 for **c**. The Miller indices are found by dividing the distances by the highest value 12 and taking the reciprocal. 12/12, 6/12, 4/12 becomes 1,1/2,1/3 with the reciprocals being **1**,**2**,**3**.

Hexagonal forms

It can be seen that the orthographically projected perimeter of the facial view of the regular octahedron is a regular hexagon. The facial diameter through the centroid appears, then, as an axis of sixfold symmetry. This diameter is parallel to the axis of symmetry of the hexagonal crystals which is designated the *c*-axis. The c-plane (0001) is perpendicular to this axis which means that it is defined by octahedral faces. The octahedra which make up the crystal are in layers normal to the c-axis. It follows from this that the c-axis is an integral multiple of the facial diameter of the octahedron which makes it up. This has the value $\sqrt{\frac{2}{3}} \times \text{edge}$.

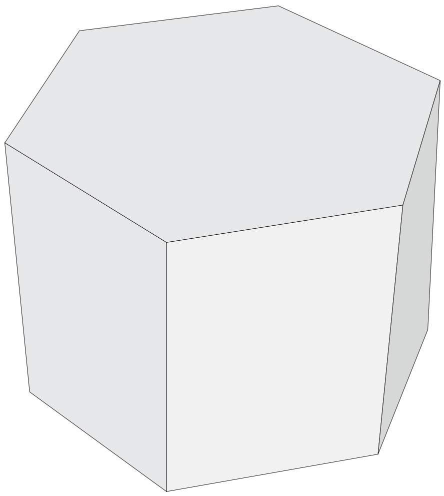
Hexagonal layers



Octahedral layers in hexagonal crystals.

The layers of octahedra which form an hexagonal crystal are normal to the c-axis. The relationship of an octahedron in one layer to that in another is shown in the figure. The middle layer with the orange colored octahedra has an octahedron at the layer centroid. Each of the other two layers has a vertexial junction of three octahedra at the centroid of the layer.

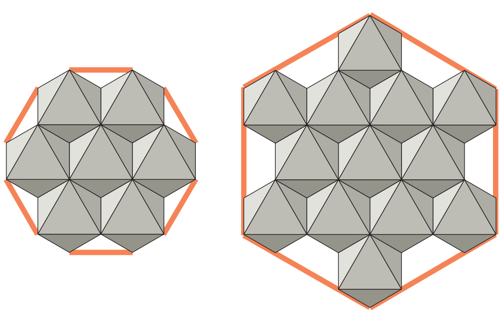
The three layer assembly can join crystally with identical assemblies in the c-axial direction. An octahedron in one blue layer will differ from an octahedron in an identical planar position by a translation parallel to the c-axis.



Hexagonal prisms

The planes which are parallel to the c-axis are called the m-planes. These are defined either by octahedral edges or by octahedral vertexes.

Prisms defined by octahedral edges have axes which are integral multiples of one half of the edgial diameter of the regular octahedron.

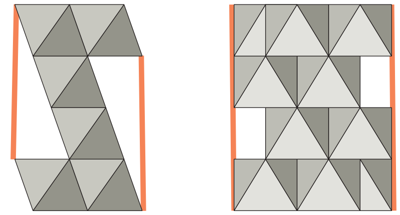


Hexagonal prisms are edgial or vertexial planes.

On the left, the prisms are defined by octahedral vertexes.

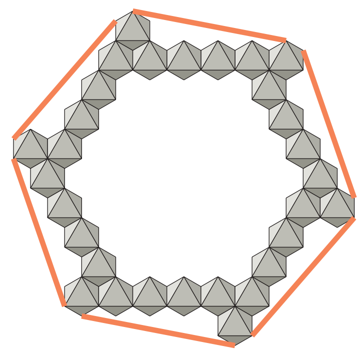
On the right, the prisms are defined by octahedral edges.

In the next figure, the two views are normal to



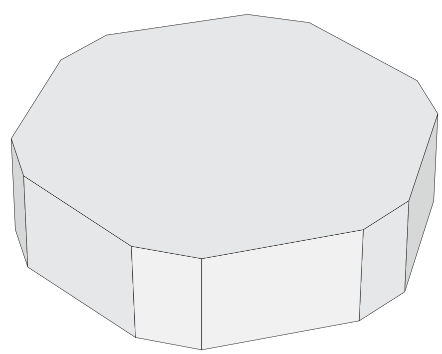
the c-axis The prism planes of the assembly on the left are defined by the vertexes of the octahedra.The assembly on the right has prism planes which are defined by octahedral edges.

Prisms defined by vertexes can be parallel to an edge of the octahedra which define it as shown above, or at an angle to the edge as the next figure shows.

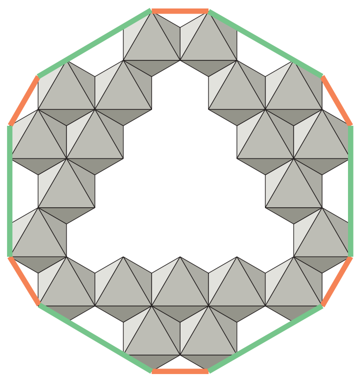


Hexagonal diprisms

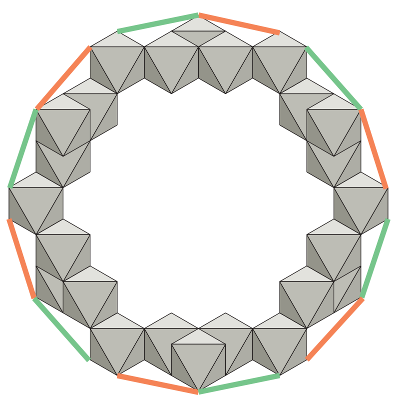
Hexagonal diprisms have two sets of prisms each of which is hexagonal. The octahedral



assembly shown here has two sets of prisms.



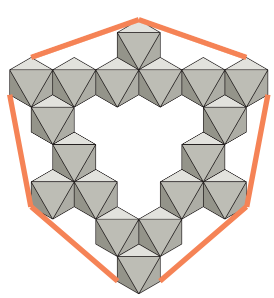
One set is defined by octahedral edges and the other is defined by octahedral vertexes. The two sets of prisms in the next figure are defined



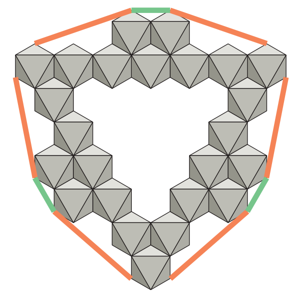
by octahedral vertexes.

Scalenohedral base

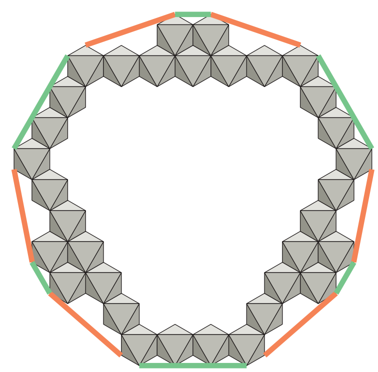
The scalenohedral base has double threefold symmetry. In the octahedral assembly of the figure, alternate faces are 120° to one another.



Adjacent faces are symmetrical. The next figure has the same faces as the previous figure

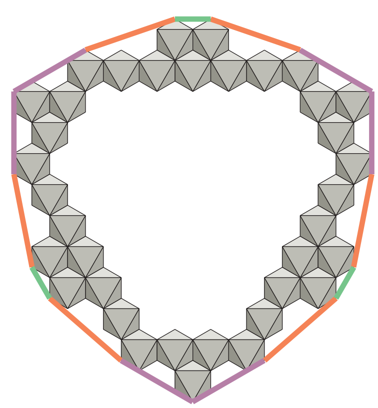


with the addition of three faces which also have threefold symmetry. Three additional faces have been added in the next figure. These



are colored green and combine with the previous green faces to provide a group of sixfold faces to go with the double threefold group. Each of the faces of the octahedral assembly are defined by octahedral vertexes.

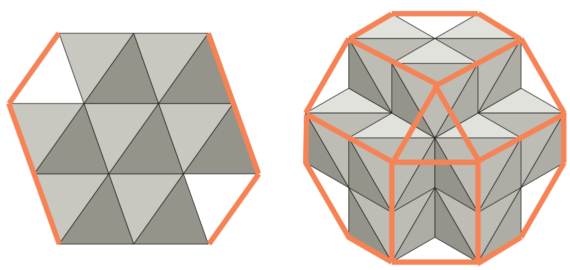
The next figure has five sets of threefold



faces. The first three sets are defined by octahedral vertexes. The two additional sets are defined by octahedral edges.

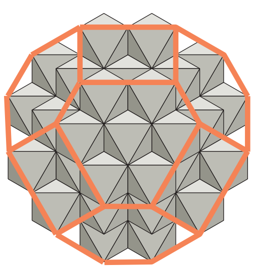
Hexagonal dipyramid

Pyramidal faces are inclined to the c-axis. If the pyramids share the same base, the result is the dipyramid. The figure shows two views of



the same dipyramid. On the left is a view normal to the c-axis. On the right the view is along the c-axis. The alternate planes of this dipyramid are defined by octahedral faces. The other planes are defined by octahedral vertexes.

The octahedral assembly in the next figure produces a hexagonal dipyramid which has planes defined by octahedral vertexes alternating with planes defined by octahedral edges. Planes which are defined by edges in the near

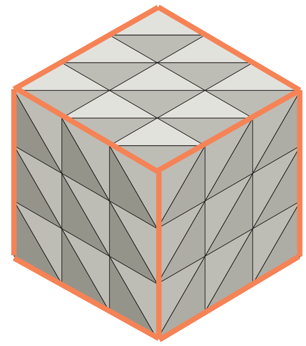


pyramid are defined by vertexes in the pyramid below. The same is true for the other planes.

Rhombohedron

A rhombohedron is a closed form which has threefold symmetry about one axis. Its name derives from the shape of its six identical faces each of which has four edges of equal length.

The planes of the rhombohedron depicted below are defined by the faces of regular octa-



hedra.

The rhombohedron depicted here has its planes defined by octahedral vertexes. The set of planes is identical to the planes of the isometric cube.