XYZ-coordinates of CFUs and He-octas in icosahedral fullerenes

Robert William Whitby
14 March 2006
http://homepage.mac.com/whitby/

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

Reference

1. Octahedron, the Universe defined by Robert William Whitby

A description of the atomic shapes and how they join which follows from the discovery that the periodicity of the atomic elements matches the periodicity of recurring form in which identical regular octahedra combine to form ever larger regular octahedra. Octahedron1stEd.pdf shows that the atomic elements are crystalline assemblies of identical regular octahedra and explores the implications of this discovery. 500 pages.
http://homepage.mac.com/whitby/FileSharing103.html

2. Icosahedral assemblies of triangular graphite panels by Robert William Whitby

The file GraphitePanels.pdf shows the triangular panels which produce the fullerenes having 60, 240, 540, 960, and 1500 C-atoms. Additional panels are shown which are derived by the vertexial truncation of the triangular panels.
http://homepage.mac.com/whitby/Quasicrystals/FileSharing175.html

3. Icosahedral assemblies of triangular panels of diamond CFUs by Robert William Whitby

The file DiamondPanels.pdf shows the triangular panels which produce the fullerenes having 80, 320, 720, 1280, 2000, and 2880 C-atoms.
http://homepage.mac.com/whitby/Quasicrystals/FileSharing176.html

4. C240 icosahedron–triangular panel of four graphite CFUs by Robert William Whitby

The file C240icosa.pdf shows how four graphite CFUs of three C-atoms each can join in the same manner as in a graphite crystal to form a triangular panel. Twenty panels can join to form a regular icosahedral assembly. The file can be downloaded at--
http://homepage.mac.com/whitby/Quasicrystals/FileSharing173.html

5. Icosahedral assembly of graphite CFUs with O-atoms by Robert William Whitby

The file C60fullere.pdf shows how twenty crystal-forming units (CFUs) of graphite, each consisting of three C-atoms, can act as the triangular panels of a regular icosahedral assembly. The file also shows how an O-atom can join with any of the sixty C-atoms of the assembly.
http://homepage.mac.com/whitby/Quasicrystals/FileSharing171.html

Introduction

Each icosahedral fullerene is composed of triangular panels–those consisting of graphite CFUs have been covered in Reference 2; those consisting of diamond CFUs have been covered in Reference 3. This document provides a means of relating the xyz-location of each of the He-octas of an icosahedral assembly of twenty identical panels to the same coordinate system as the unrotated panel.

- Firstly, this document relates the numerical expression of the xyz-location of each of the He-octas of each of the atoms that comprise each of the CFUs of any triangular panel to the tetrahedral centroid of the CFU that is common to each and every panel.
- Secondly, it relates the coordinates of each of the He-octas of a given panel to the centroid of an icosahedral assembly by the addition of offsets.
- Thirdly, it relates the coordinates of each vertex of each He-octa to the icosahedral centroid.
- Fourthly, it provides the angles needed to rotate the panel about the centroid so that it occupies each of the twenty orientations of a structurally coherent icosahedral assembly.

It does this so that the centroid of each vertex of each of the He-octas of each of the C-atoms of each of the CFUs of each of the twenty rotated panels can be expressed as an xyz-location relative to the icosahedral centroid as origin while maintaining the same coordinate system as the unrotated panel. Each coordinate is expressed as a multiple of the edge length of the He-octa. The exact length of He-octa edge is not known. It can be approximated from the improving images of the fullerenes. No allowance has been made for the thermal motions of the CFUs or the atoms that compose them.

He-octa locations of the graphite or diamond CFU relative to its tetrahedral centroid

Each C-atom of the graphite and diamond CFUs acts as a triangular panel. [See Reference 1, Carbon, page 188.] Each panel defines a face of a regular tetrahedron. The diamond CFU has a panel on each face of the defined tetrahedron; the graphite CFU has one less panel. A He-octa fits precisely within the tetrahedron so that its centroid is congruent with that of the tetrahedron. [See Figure 1.] Each of the twelve edges of the centroidal He-octa is congruent with one edge of each of the three He-octas of each of the four C-atoms of the diamond CFU. The centroid of each of the adjoining He-octas is an edgial move from the centroidal He-octa of the tetrahedron. Their locations are given in Table 1.

Table 1: He-octa coordinates of panel CFUs relative to the tetrahedral centroid

Orientation	*A*				*B*			
C-atom	Move	X	Y	Z	Move	X	Y	Z
violet	26,1	0	1	1	52,1	-1	1	0
	52,1	-1	1	0	21,1	0	1	-1
	56,1	-1	0	1	51,1	-1	0	-1
yellow	36,1	1	0	1	34,1	1	-1	0
	46,1	0	-1	1	41,1	0	-1	-1
	34,1	1	-1	0	31,1	1	0	-1
gray	32,1	1	1	0	56,1	-1	0	1
	21,1	0	1	-1	54,1	-1	-1	0
	31,1	1	0	-1	46,1	0	-1	1

Table 1: He-octa coordinates of panel CFUs relative to the tetrahedral centroid

Orientation	*A*				*B*			
C-atom	Move	X	Y	Z	Move	X	Y	Z
green	51,1	-1	0	-1	26,1	0	1	1
	41,1	0	-1	-1	36,1	1	0	1
	54,1	-1	-1	0	32,1	1	1	0

The graphite CFU includes the violet, yellow, and gray C-atoms; the diamond CFU includes the violet, yellow, gray, and green C-atoms. The formation of the panel requires that adjoining CFUs be inverted. The table lists the He-octa locations for each of the two orientations, *A* and *B*.

Locations of the tetrahedral centroids of the CFUs of the triangular panel

Figure 5 shows the spatial arrangement of the tetrahedral centroids of the CFUs that constitute the triangular panel. Each of the two orientations is labeled. Each line represents the distance between the threefold axes of adjoining CFUs. Equation 1 gives the distance between CFUs, *L,* in terms of the edgial length of the He-octa, *S*.

Eq 1 $$L = [4/(\sqrt{3})] \times S$$

Figure 3 shows the relationship between the xyz-locations of the tetrahedral centroids. Figure 3 uses projected vectors to show these inter-CFU relationships and expresses them as both octahedral moves and Δxyzs.

Figure 2 uses an octahedral assembly in which each of the tetrahedral centroids is related to each of the others of the panel.

Figure 4 represents each of the CFUs of a triangular panel as a hexagon. Each hexagon contains the xyz-address of the tetrahedral centroid of the CFU. The hexagons are colored according to the orientation of the CFU.

XYZ-locations of the tetrahedral centroids relative to the icosahedral centroid

For a given triangular panel, the centroid of the icosahedral face it defines is located by the intersection of the three altitudes of the face. [See Figure 9.]

Figure 6 relates the direction and distance, *d*, of the normal to the centroid of the icosahedral face to the tetrahedral centroid of the reference CFU which is given the xyz-address 0,0,0.

Eq 2 $$d = (N-1) \times L$$

Figure 6 also shows the distance, *t*, of the icosahedral face from the tetrahedral centroid of the reference CFU. The value of *t* is the same for every graphite and diamond panel.

Eq 3 $$t = S \times \sqrt{3/2}$$

Figure 7 expresses the octahedral special move as changes in the xyz-coordinates. Figure 9 shows the special move for the 3-triangle panel.

Figure 8 expresses the octahedral facial move as changes in the xyz-coordinates.

The edge length of the icosahedral face, *E*, is determined from the CFU's per edge, *N*.

Eq 4 $$E = S \times (4 \times N - 1)$$

The radius, *R*, that connects the centroid of the icosahedral face to the body centroid is determined using *E*.

Eq 5 $$R = E \times \sqrt{(7 + 3 \times \sqrt{5})/24}$$

Table 2: Icosahedral edge and facial radius for graphite and diamond triangular panels

Panel		Icosahedron		C-atoms/icosahedron	
N	*d*	*E*	*R*	Graphite	Diamond
1	0	3	2.267284	60	80
2	L	7	5.290329	240	320
3	2L	11	8.313374	540	720
4	3L	15	11.336420	960	1280
5	4L	19	14.359465	1500	2000
6	5L	23	17.382510	2160	2880
7	6L	27	20.405555	2940	3920
8	7L	31	23.428601	3840	5120

The xyz-location of the icosahedral centroid is set to 0,0,0 by vectorially subtracting d, t, and R from each of the tetrahedral centroids of the CFUs of the panel.

Icosahedral hinging of panels

Figure 10 shows two graphite panels placed face-to-face and represents their hinge joining as icosahedral facial panels.

Figure 11 shows how the vertex of the icosahedral face relates to the tetrahedral centroid of the nearest CFU.

Orienting twenty panels for an icosahedral assembly

Figure 12 shows a layout for a regular icosahedron. Each triangular face is numbered. Each vertex of each triangular face is numbered with the octahedral vertex that relates it to the orientation of the octahedral panel it represents.

To orient each panel of the icosahedral assembly, the reference panel is rotated through an angle ϕ. [See Figure 13.]

A vertexial diameter of the icosahedral assembly is chosen to be parallel to the 61-diameter of the reference octahedron of the panel. A facial radius of the icosahedron connects the body centroid of the icosahedron with the centroid of the 623-face of the octahedron. [See Figure 13.] This facial radius makes an angle α with the vertexial diameter of the icosahedron

Eq 6 $$.\alpha = \operatorname{atan}\sqrt{2} \sim 54.735610°$$

The radius connecting the body centroid of the icosahedron to the centroid of an icosahedral face at the vertexial cap makes an angle β with the vertexial diameter of the icosahedron.

Eq 7 $$\beta = \operatorname{atan}\sqrt{8/(7+3\sqrt{5})} \sim 37.377368°$$

The radius connecting the body centroid of the icosahedron to the centroid of an equatorial face makes an angle γ with the vertexial diameter of the icosahedron.

Eq 8 $$\gamma = 2 \times \operatorname{atan}\sqrt{[2/(7+3\times\sqrt{5})]} + \beta \sim 79.187952°$$

The panels for each of the five cap faces at the 6-end of the vertexial diameter must be rotated ϕ_1.

Eq 9 $$\phi_1 = 180 - \alpha - \beta \sim 87.887022°$$

The panels for each of the five equatorial faces towards the 1-end of the vertexial diameter must be rotated ϕ_2.

Eq 10 $$\phi_2 = \gamma - \alpha \sim 24.452064°$$

The panels for each of the five cap faces at the 1-end must be rotated ϕ_3.

Eq 11 $$\phi_3 = 180 + \phi_1 \sim 267.887022°$$

The panels for each of the five upper equatorial faces must be rotated ϕ_4.

Eq 12 $$\phi_4 = 180 + \phi_2 \sim 204.452064°$$

An additional rotation θ about the icosahedral vertexial diameter is required for eighteen of the panels. Figure 14 shows each of the φ-rotated octahedra viewed both normally to the rotational plane and parallel to the axis for the θ-rotation.

Figure 15 shows a vertexial view of the icosahedron which shows the directions of the θ-rotations for each of the φ-rotated panels.

Figure 16 shows each of the twenty octahedra in its doubly rotated position labeled according to both its φ and θ rotations.

Figure 17 shows the formation of the icosahedral assembly.

Table 3 shows each of the rotations for each of the twenty panels.

Table 3: Icosahedral rotations for fullerene panels

Face	Φ	Θ	Face	Φ	Θ
1	ϕ_1	0	11	ϕ_1	216
2	ϕ_1	72	12	ϕ_4	324
3	ϕ_4	252	13	ϕ_3	288
4	ϕ_2	36	14	ϕ_3	144
5	ϕ_4	180	15	ϕ_4	108
6	ϕ_1	144	16	ϕ_4	36
7	ϕ_2	108	17	ϕ_2	180
8	ϕ_3	216	18	ϕ_3	0
9	ϕ_2	324	19	ϕ_3	72
10	ϕ_1	288	20	ϕ_2	252

The effects upon the xyz-coordinates of the rotations of the panel rotations are shown in Figures 18, 19, and 20.

Building an icosahedral assembly

Gather the xyz-addresses of the tetrahedral centroids of the CFUs of the unrotated panel

1. Use Eq. 1 to get L.
2. Use Eq. 3 to get t.
3. Using Table 2 and the number of C-atoms of the fullerene, get N, d, E, and R.
4. Using Figure 4, get the xyz-address of each of the tetrahedral centroids of each of the CFUs of the triangular panel with edge length N.

Displace the panel 0,0,0 to the icosahedral centroid

5. Vectorially subtract d, t, and R from each of the tetrahedral centroids.
6. Using Table 1, add the coordinates of each relevant (graphite or diamond) He-octa to each of the tetrahedral centroids according to its orientation, A or B.

Rotate the unrotated panel into each icosahedral position and add it to the assembly

7. Using Table 3, apply the rotations for each panel to the unrotated He-octa coordinates and add them to the icosahedral assembly.

Example

Given the C540-fullerene, create a database that will include for the unrotated panel and each icosahedral panel–

- the xyz-coordinates of the tetrahedral centroids of each CFU
- the xyz-coordinates of the He-octas of each atom
- the xyz-coordinates of the vertexes of each He-octa.

Procedure

From Table 2 get N=3, E=11, R=8.313374

$$L = [4/(\sqrt{3})] \times S$$

$$t = S \times \sqrt{3/2}$$

$$d = 2 \times L = 4.618802 \times S$$

Let *x0*, *y0*, and *z0* be the coordinates of the tetrahedral centroid of a CFU and *x1*, *y1*, and *z1* be the coordinates of the same tetrahedral centroid relative to the centroid of the icosahedral assembly. Then,

$$x1 = x0 - (t + R) \times \sqrt{1/3} - d \times \sqrt{1/6}$$

$$y1 = y0 - (t + R) \times \sqrt{1/3} - d \times \sqrt{1/6}$$

$$z1 = z0 - (t + R) \times \sqrt{1/3} + d \times \sqrt{2/3}$$

Using the values in Table 1, add the coordinates (*x2*, *y2*, and *z2*) of each He-octa of each C-atom relative to the tetrahedral centroid (*x1*, *y1*, and *z1*) to get its coordinates (*x3*, *y3*, and *z3*) relative to the icosahedral centroid.

$$x3 = x1 + x2$$
$$y3 = y1 + y2$$
$$z3 = z1 + z2$$

To include the coordinates (*x5*, *y5*, and *z5*) of each vertex of the He-octa, add its coordinates (*x4*, *y4*, and *z4*) relative to the He-octa centroid from Table 4 to (*x3*, *y3*, and *z3*).

Table 4: Octahedral vertex relative to octahedral centroid

Vertex	x	y	z
1	0	0	-sqr(1/2)
2	0	sqr(1/2)	0
3	sqr(1/2)	0	0
4	0	-sqr(1/2)	0
5	-sqr(1/2)	0	0
6	0	0	sqr(1/2)

$$x5 = x3 + x4$$
$$y5 = y3 + y4$$
$$z5 = z3 + z4$$

Rotate the tetrahedral centroids, the He-octa centroids, and the He-octa vertexes by using their coordinates for *x*, *y*, and *z* in the following equations.

$$x\phi = \sqrt{[x\sin 45] \wedge 2 + (x\cos 45\cos\phi) \wedge 2} + z\sin\phi\cos 45$$
$$y\phi = \sqrt{[y\sin 45] \wedge 2 + (y\cos 45\cos\phi) \wedge 2} + z\sin\phi\cos 45$$
$$z\phi = (-x)\cos 45\sin\phi + (-y)\cos 45\sin\phi + z\cos\phi$$
$$x\theta = x\phi\cos\theta + y\phi\sin\theta$$
$$y\theta = y\cos\theta - x\sin\theta$$
$$z\theta = z\phi$$

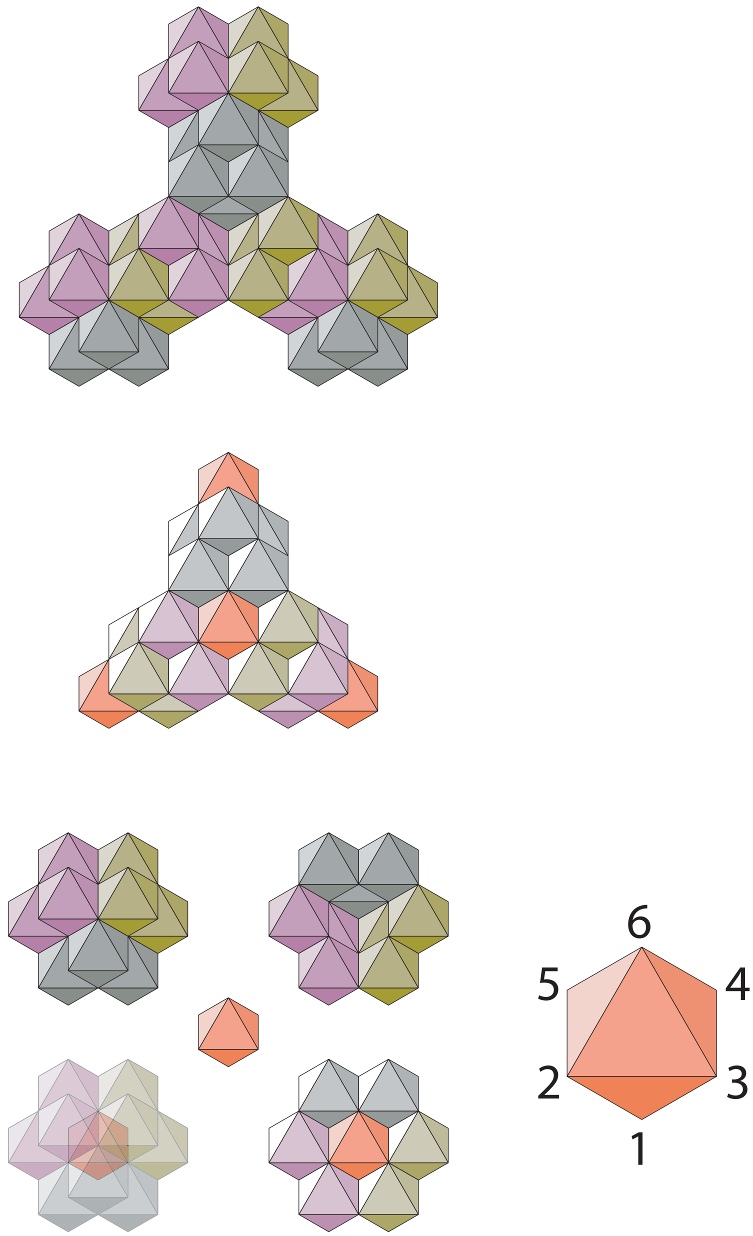


Fig. 1 Centroids of the graphite and diamond CFUs.

Each of the C-atoms of the graphite and diamond CFUs is the facial panel of a regular tetrahedron. A He-octa fits within the tetrahedron defined by the panels so that its centroid is congruent with the centroid of the tetrahedron. In either CFU, an edge of the centroidal He-octa is congruent with an edge of each of the He-octas of each of the enclosing C-atoms.

At top, the figure shows one of the twenty triangular panels of four graphite CFUs from a C240-fullerene.

At bottom, a graphite CFU is shown twice in each of the two orientations required to form the triangular panel–once with the red He-octa occupying the tetrahedral centroid and once without.

At middle, the figure shows the central CFU of the fullerene panel with a red He-octa at its centroid, the adjoining C-atom from each of the adjoining CFUs, and a red He-octa at the centroid of each of the adjoining CFUs.

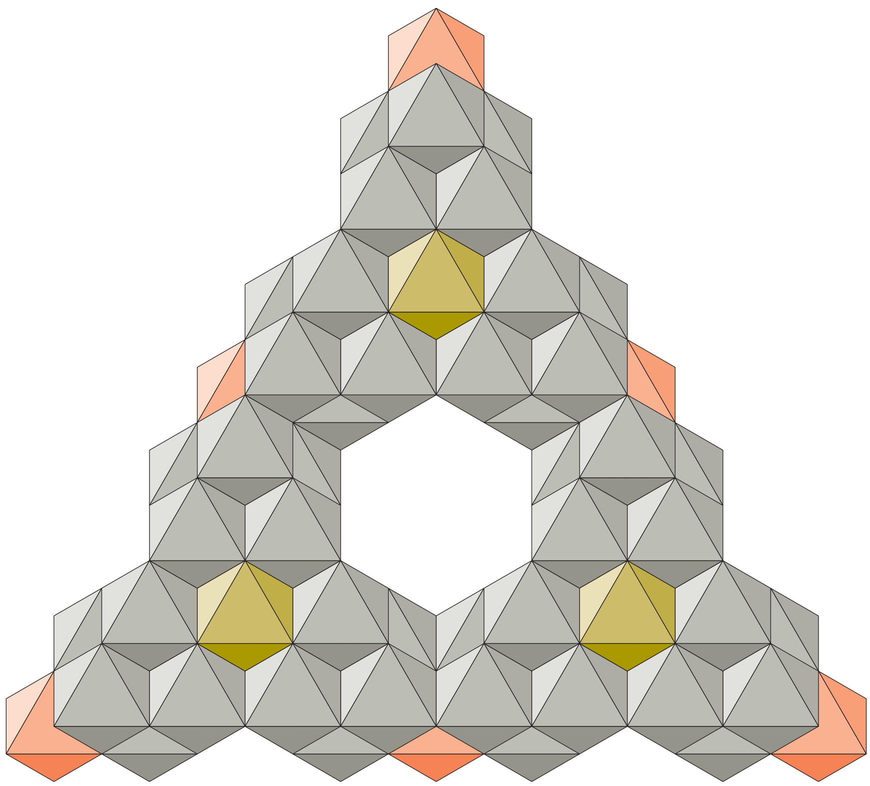


Fig. 2 Triangular panels–spatial relationships of tetrahedral centroids of CFUs
The figure shows the tetrahedral centroid of each of the CFUs of a 3-triangle panel of a fullerene. The centroid of each of the red He-octas coincides with the centroid of the tetrahedron defined by the C-atoms that constitute its faces. The yellow He-octas lie at the centroid of each of the tetrahedra that are defined by the C-atoms of the inverted CFUs.

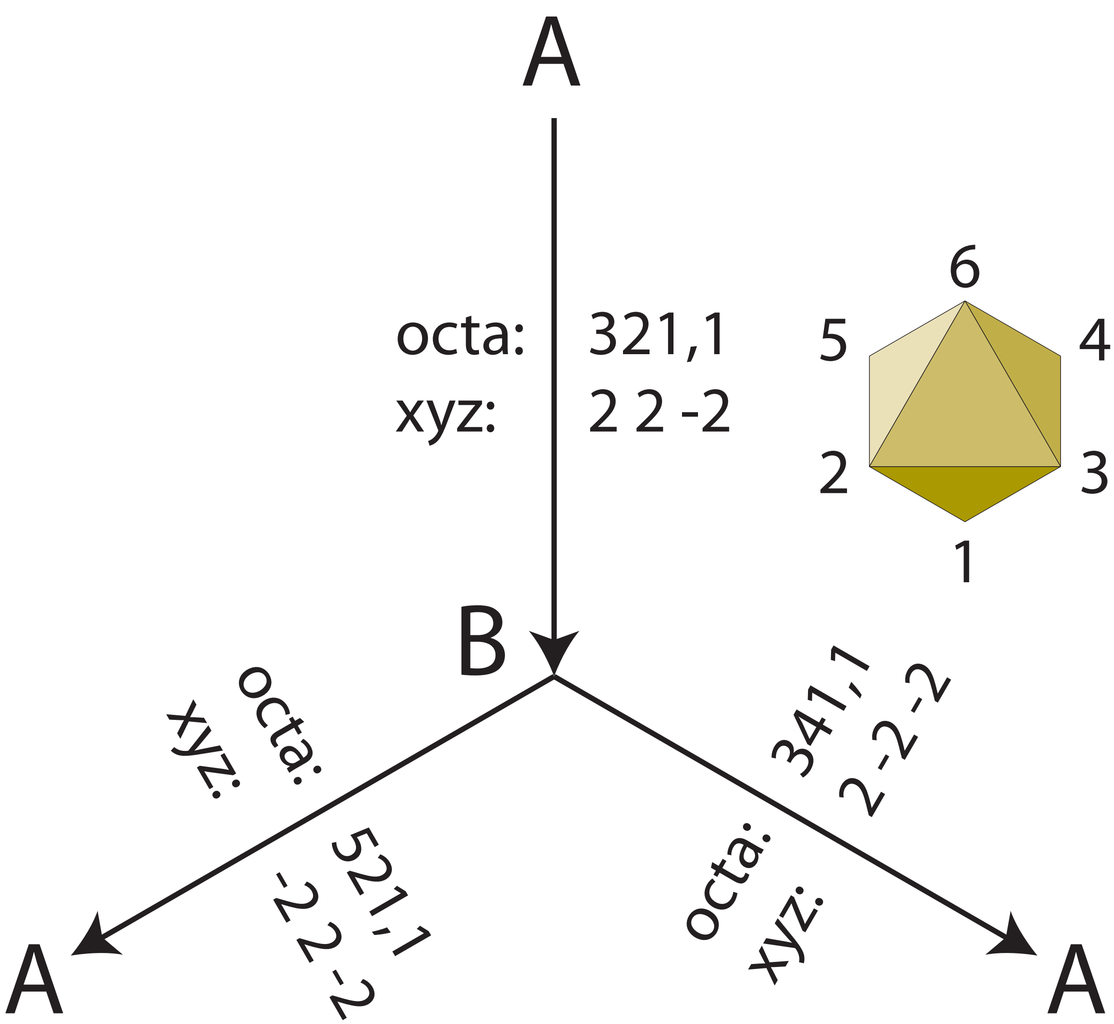


Fig. 3 Triangular panels–octahedral moves between tetrahedral centroids of CFUs
The figure shows a vector for each of the octahedral moves between the tetrahedral centroids of adjoining CFUs of a triangular panel of a fullerene. The two orientations of the CFUs are represented by the labels A and B.

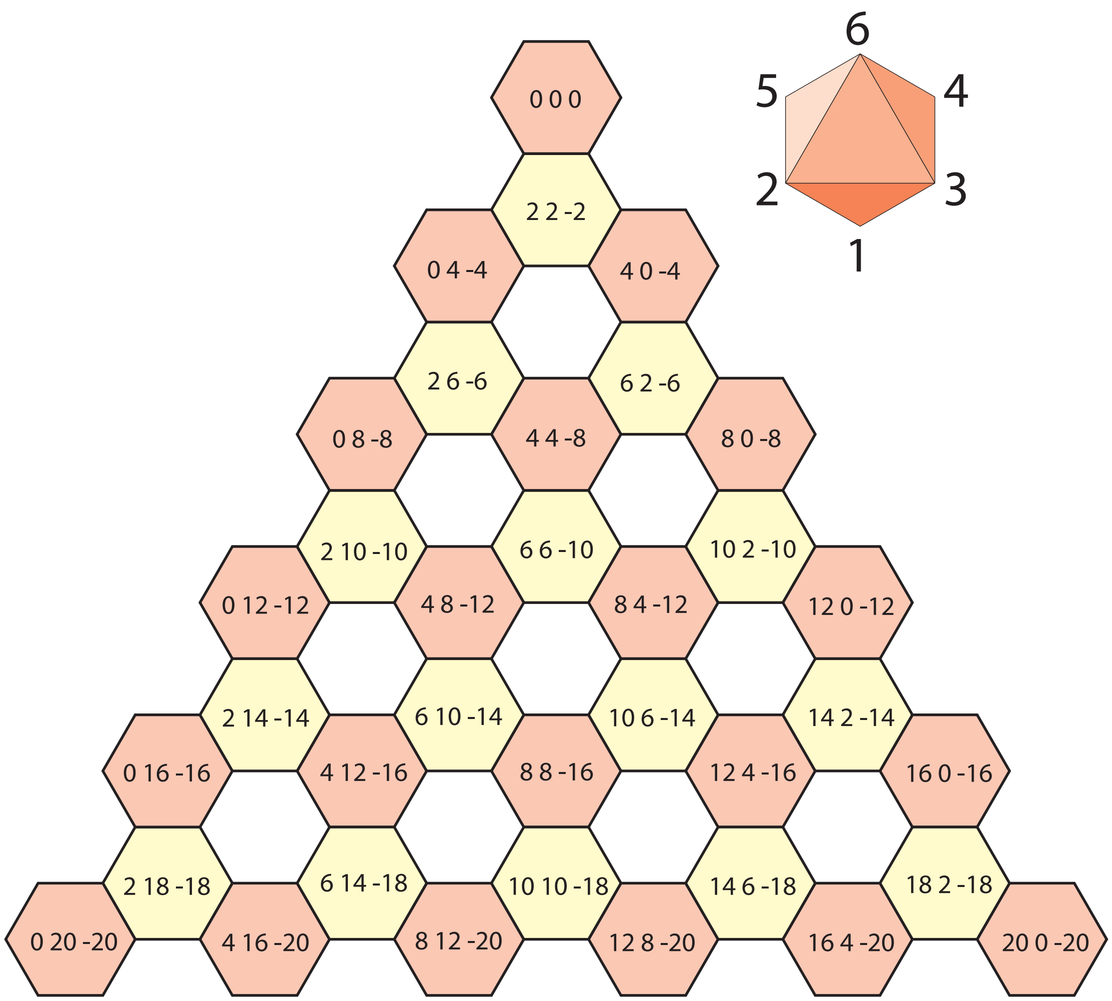


Fig. 4 Triangular panel of graphite or diamond CFUs with tetrahedral centroid xyzs

The figure shows the arrangement of the CFUs of each of the triangular panels having from one to six CFUs per edge. Each CFU is represented by either a red or a yellow hexagon–red for orientation A, yellow for orientation B. Each hexagon is labeled with the xyz-coordinates of the tetrahedral centroid of the CFU it represents.

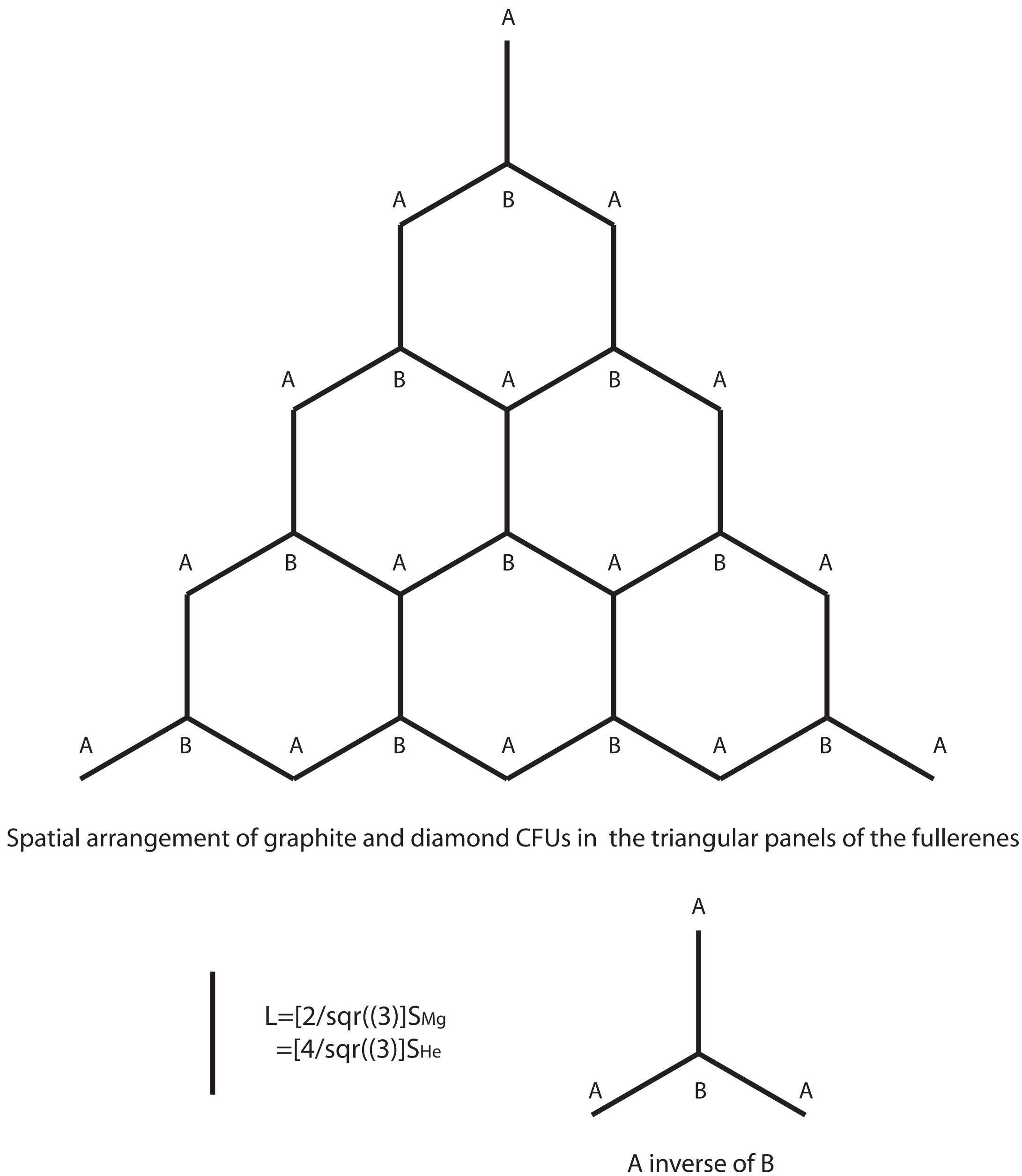


Fig. 5 Triangular panels–spatial arrangement of CFU centroids

The figure shows the spatial arrangement of the diamond and graphite CFUs that constitute the triangular panels of the fullerenes. Each line segment represents the distance L between the normals to the facial plane that pass through the centroids of adjoining CFUs. Each CFU has one of two orientations, A or B. A is inverted relative to B. Adjoining CFUs must be inverted relative to one another to effect a join.

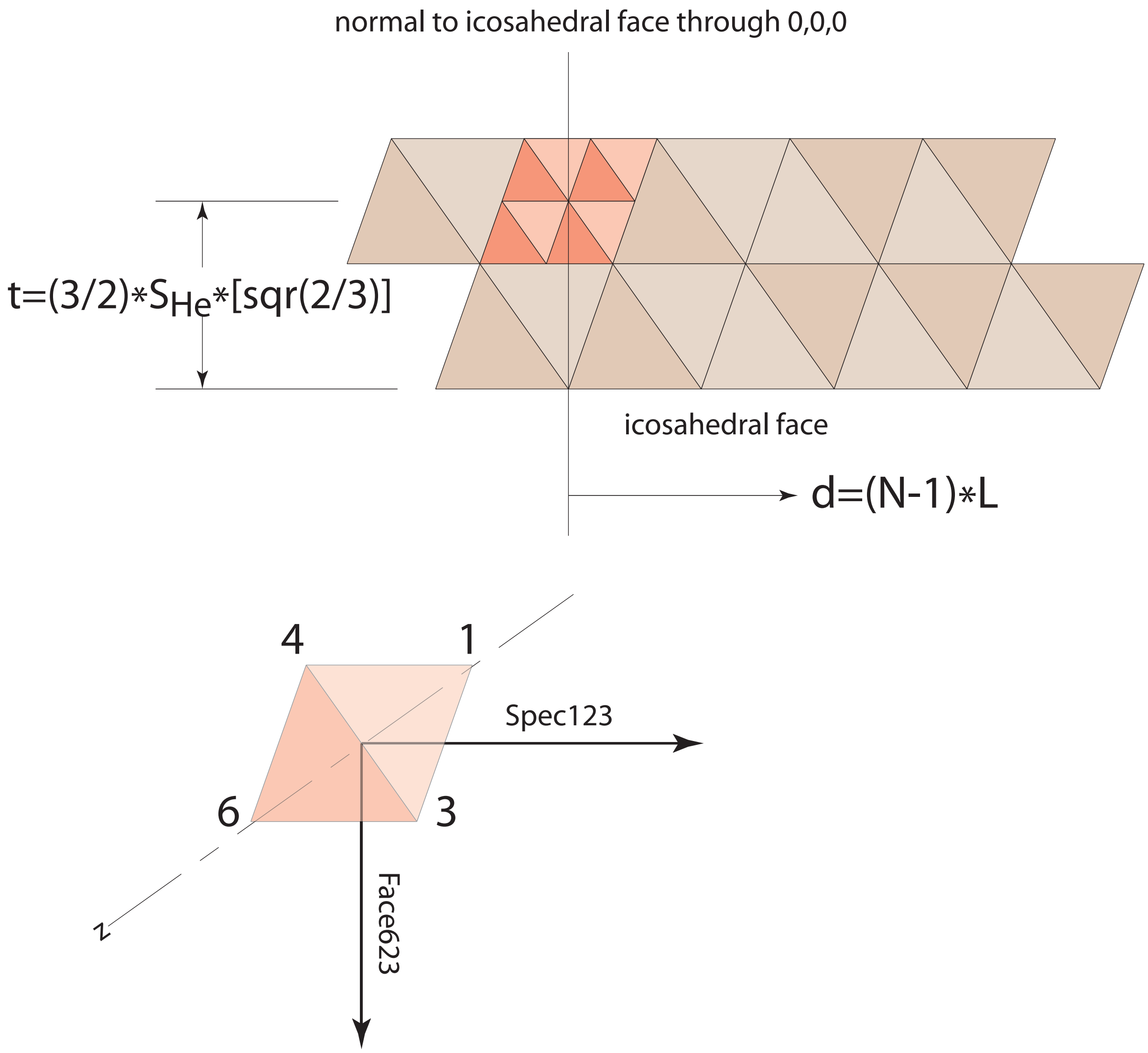


Fig. 6 Panel centroids

The figure shows the relationship between the centroid of the reference CFU of a graphite/diamond panel and the centroid of the icosahedral face that the panel defines. The relationship on the left is between the CFU centroid and the plane of the icosahedral face; the relationship on the right is between the CFU centroid and the centroid of the icosahedral face. N is the number of CFUs along an edge of the triangular panel; L is the distance between the normals to the icosahedral face which pass through adjacent panel centroids.

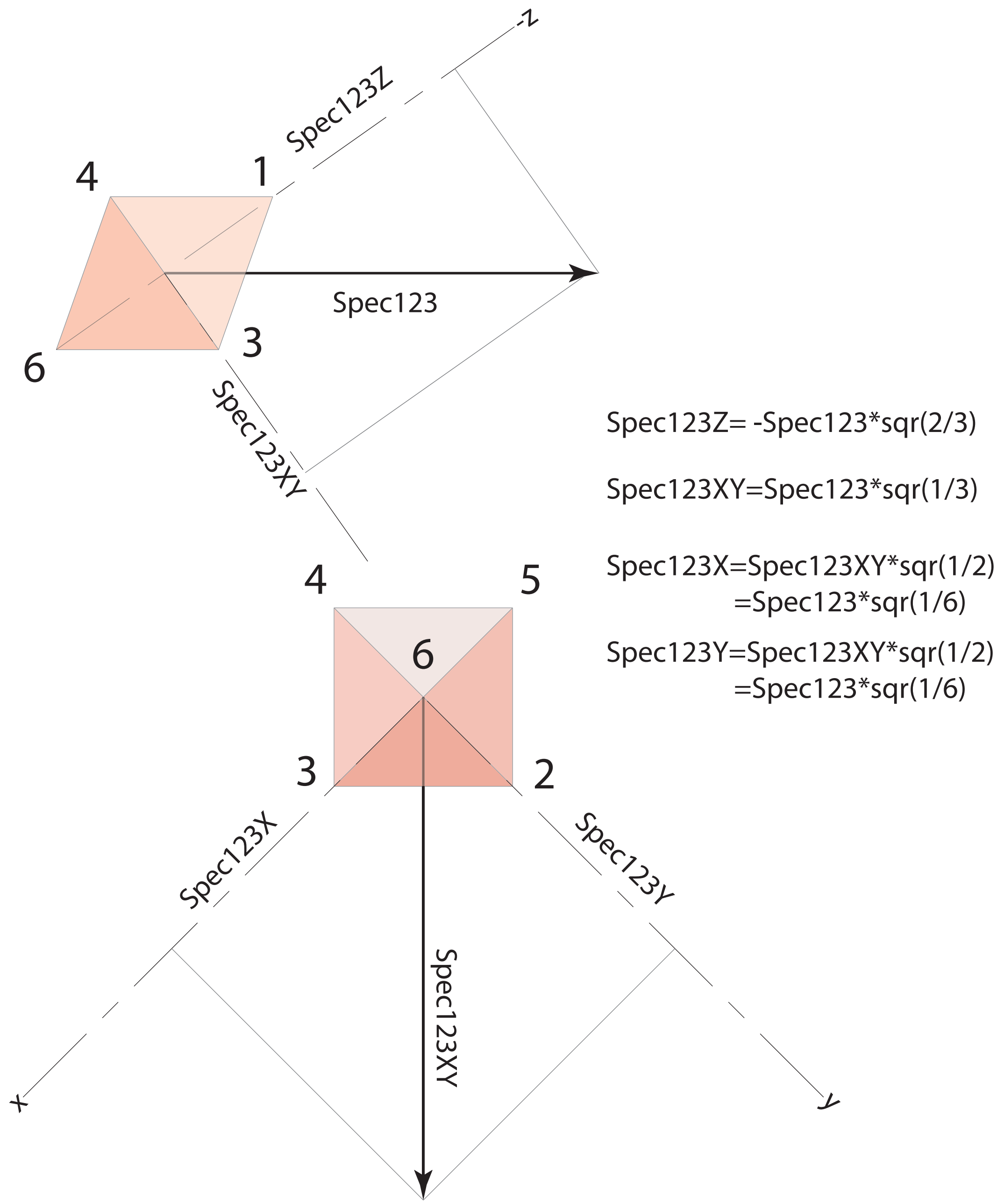


Fig. 7 XYZ-coordinates of the octahedral spec123-move
The figure shows the changes in the xyz-coordinates of two points related by a move parallel to the altitude of the 145-face of the reference octahedron.

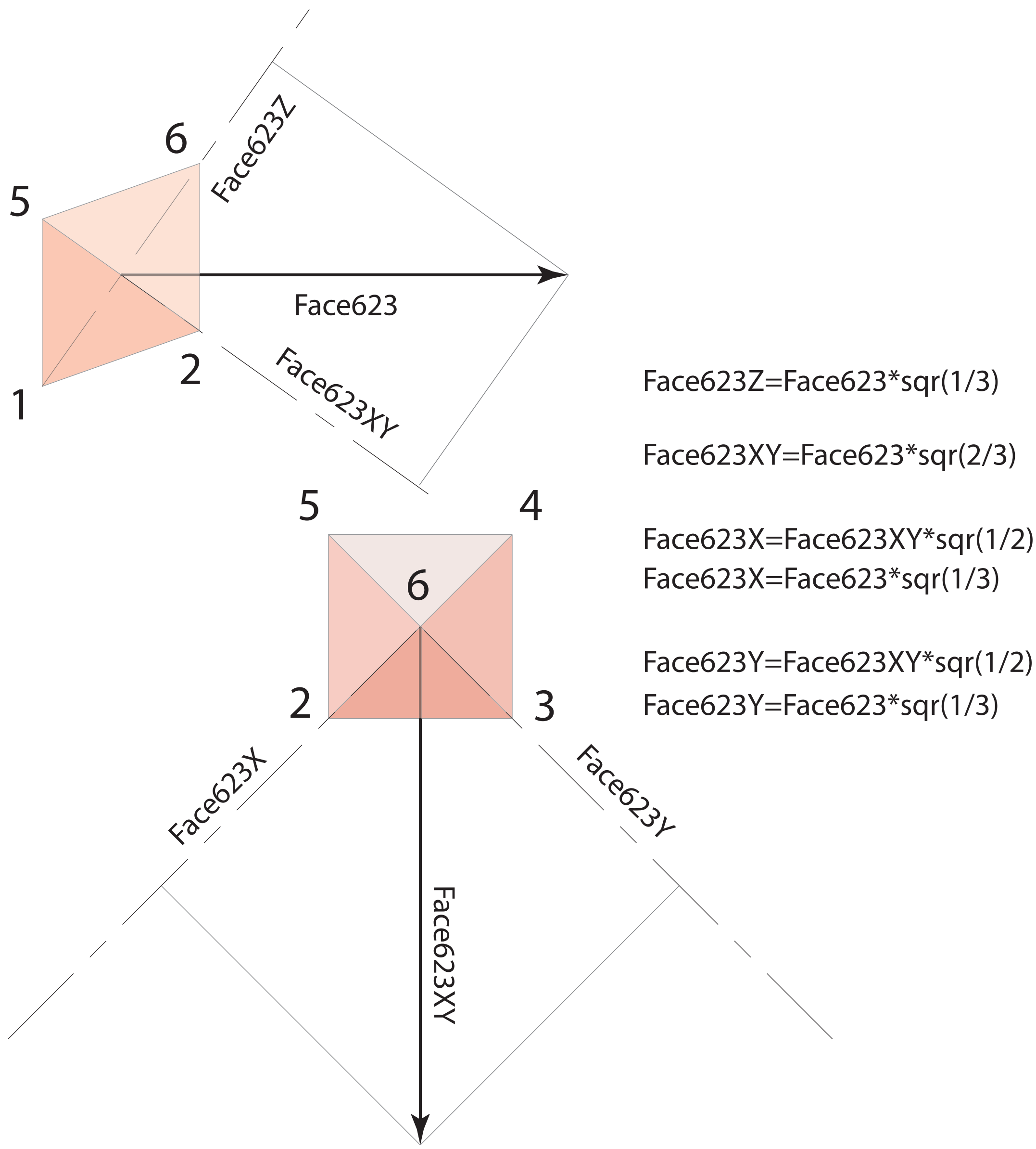


Fig. 8 XYZ-coordinates of the octahedral facial move 623
The figure shows the changes in the xyz-coordinates that result from a move perpendicular to the octahedral face 623.

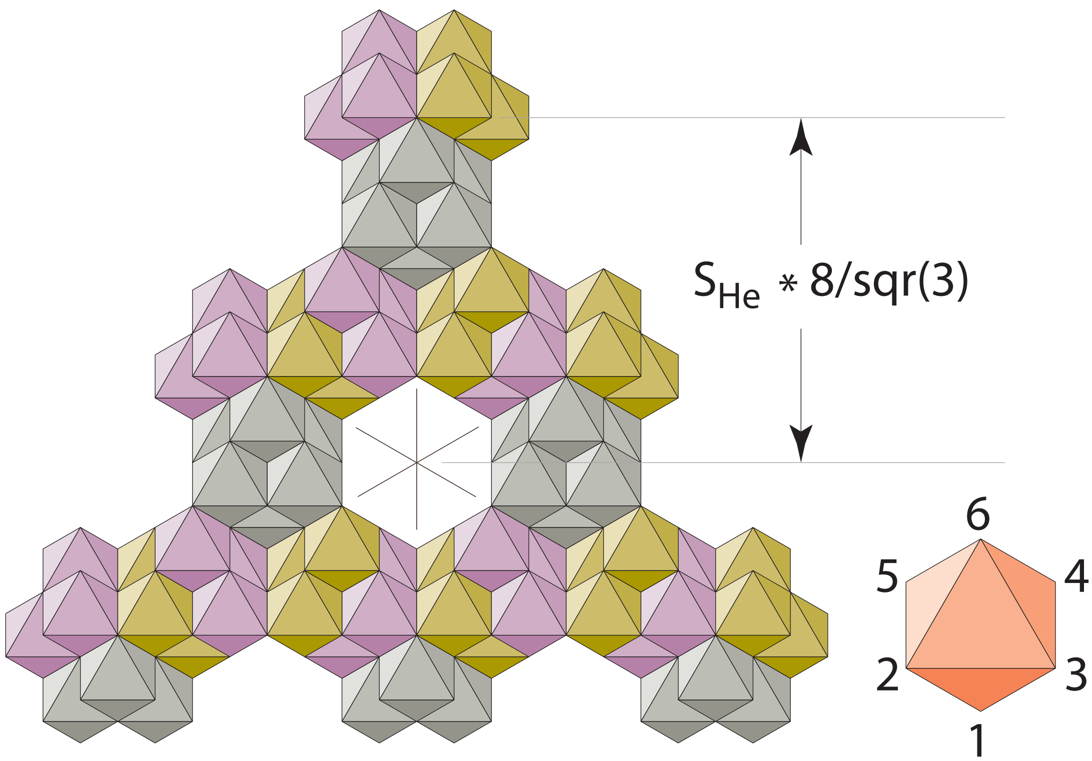


Fig. 9 Distance between plane normals through centroids of panel and reference CFU.
The figure shows a 3-triangle of graphite CFUs suitable as the facial panel of an icosahedral assembly. The reference CFU is at the top. Its centroid is set at 0,0,0. The centroid of the panel is indicated by the three line segments which differ by a rotation of one-third turn. The distance between the centroid of the reference CFU and the centroid of the panel is 2*L or S_{He}*8/sqr(3).

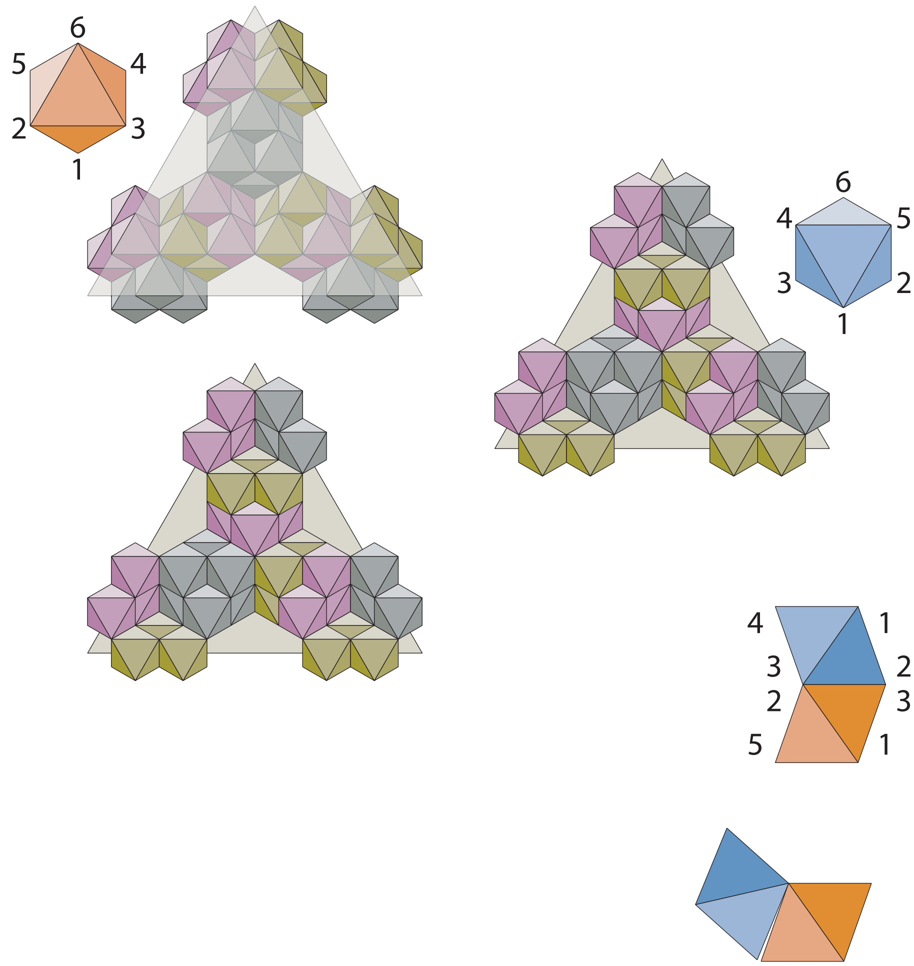


Fig. 10 Icosahedral hinging of identical graphite panels

The figure shows the hinge join between identical graphite panels.

At top left, a four CFU panel is shown with the triangular face it defines superimposed upon it. The orange octahedron shows its orientation.

At top right, the same panel is shown after a one-half turn rotation about the altitude of the 623-face which joins the 6-vertex to the 23-edge. The blue octahedron shows its orientation.

At bottom left, the rotated panel lies atop the reference panel.

At bottom right, each of the two panels is represented by their orientation octas which are first shown joined 623-face to 623-face. The 26-edge of the orange octa and the 36-edge of the blue octa are congruent and act as the hinge between the two panels. Beneath the facially joined pair, the blue octa has been rotated about the hinge through the dihedral angle of the regular icosahedron.

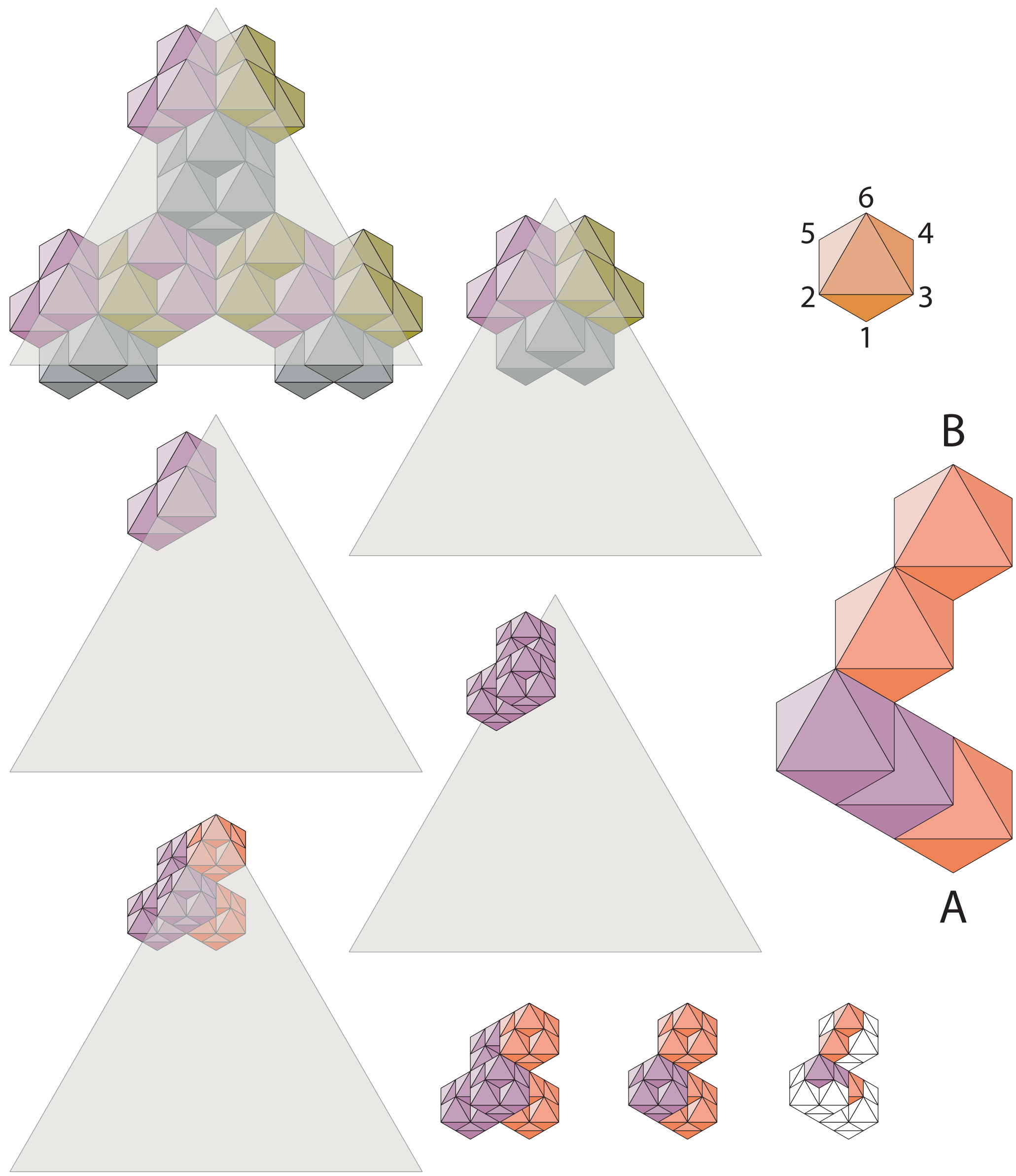


Fig. 11 Relating the icosahedral vertex to the CFU centroid

The figure shows the relationship between the centroid of the reference CFU of the graphite panel and the nearest icosahedral vertex. The panel is shown with the icosahedral face it defines at the top left. Three of the CFUs are removed leaving the reference CFU. The yellow and gray C-atoms are removed leaving the violet C-atom. Each He-octas of the C-atom is replaced with its six epn-octas. Two red reference octahedra of six epns each are added–one at the CFU centroid, the other to continue the bridge the gap between the violet C-atom and the icosahedral vertex. The icosahedral face is removed. Two of the violet He-octas are removed leaving the centroidal He-octa, one violet He-octa, and the bridging He-octa. The color is removed from all but the five epn-octas. These five epn-octas are shown in the enlarged view on the right. The epn vertex A is at the tetrahedral centroid; the epn vertex B is at the icosahedral vertex. Moving from A to B requires the octahedral moves 62,3 and 64,3.which puts the xyz coordinates of B at 0,0,3.

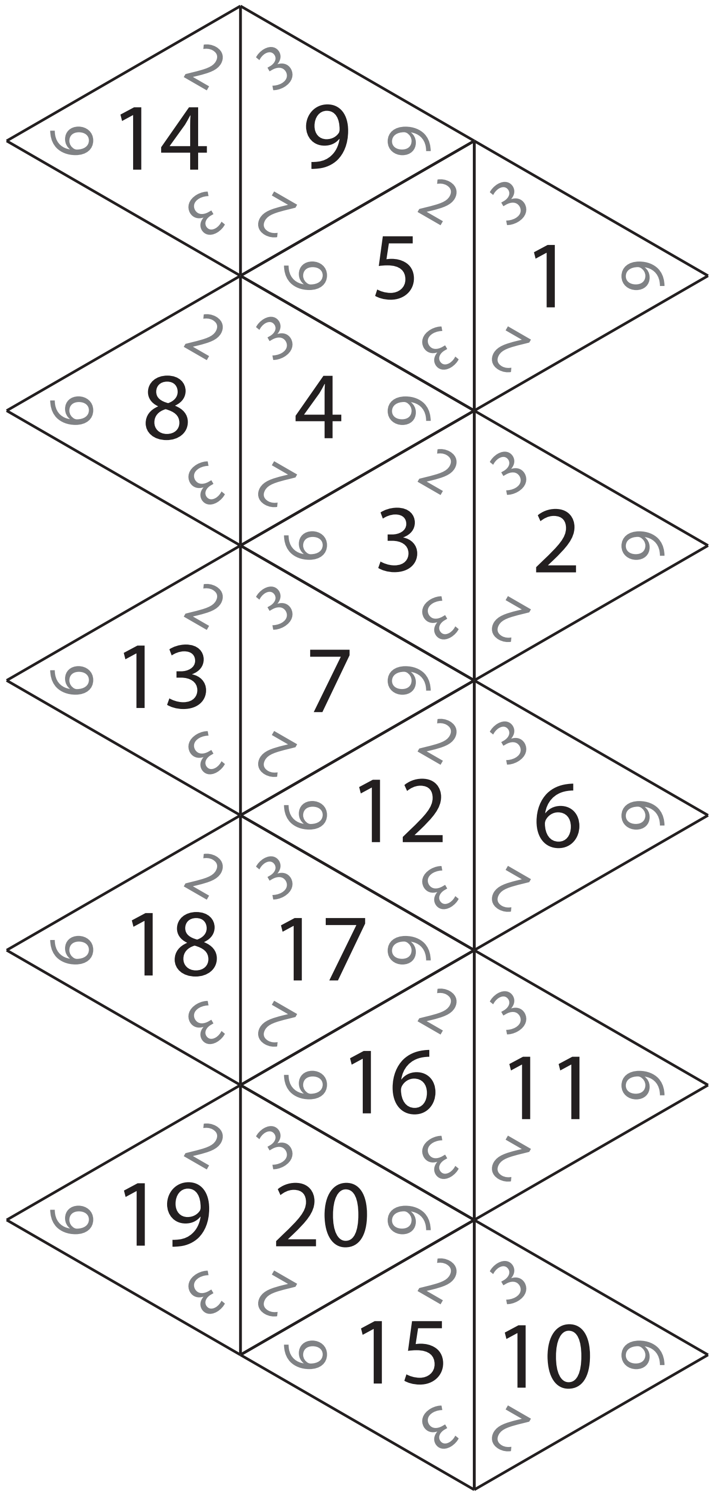


Fig. 12 Panel layout with octahedral facial vertexes and icosahedral numbering

Each face of an icosahedral assembly of fullerene panels is represented by a triangle. Each vertex of each triangle is labeled with the vertexial labels of the octahedral face that is directed towards the icosahedral centroid.

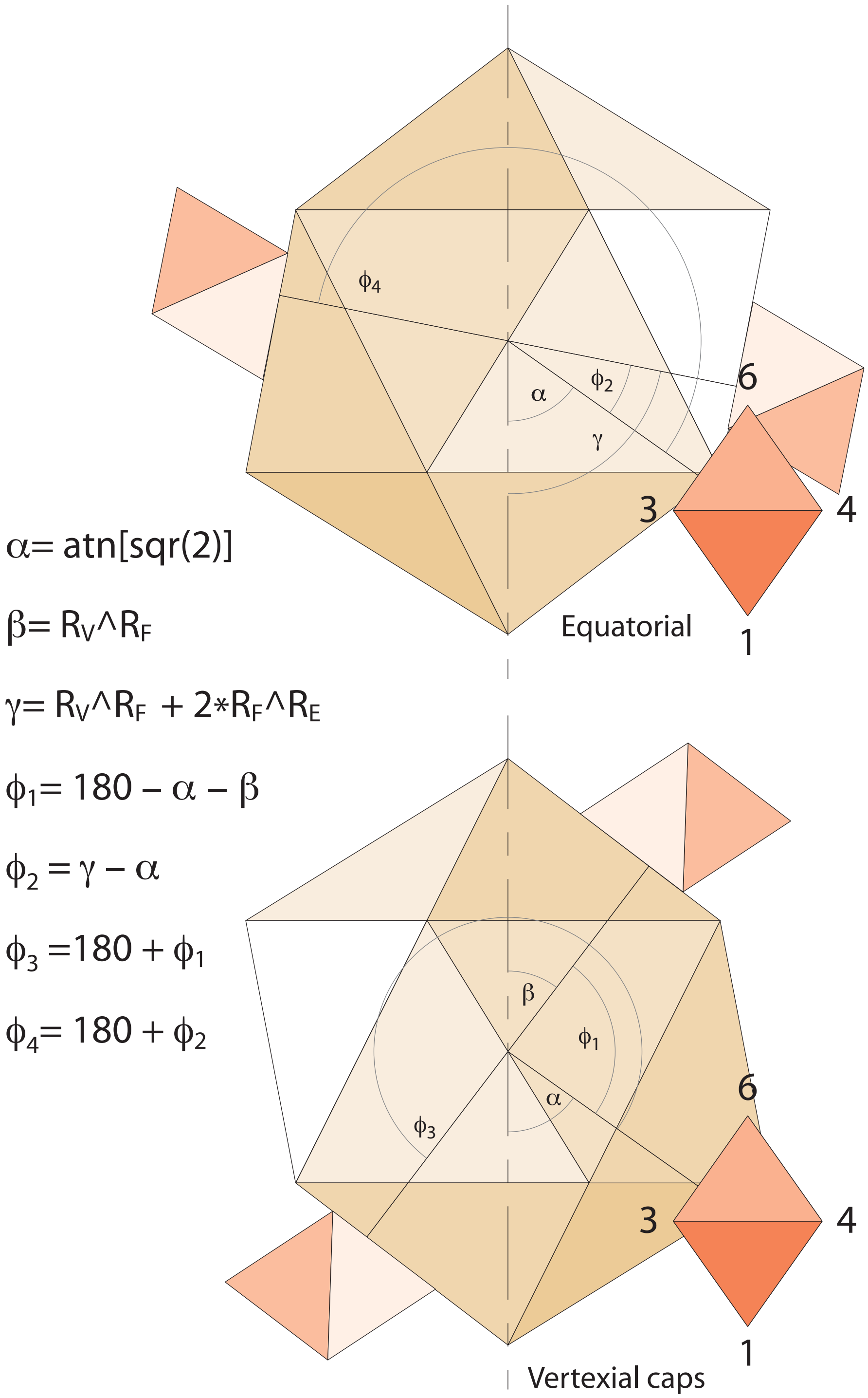


Fig. 13 Φ-rotations of graphite panels

The figure shows the ϕ-rotations of the graphite panels of an icosahedral fullerene. The equatorial panels are shown at the top; the vertexial panels are shown at the bottom. The icosahedron at the bottom is rotated by a one-tenth turn about the fivefold axis relative to the icosahedron at the top.

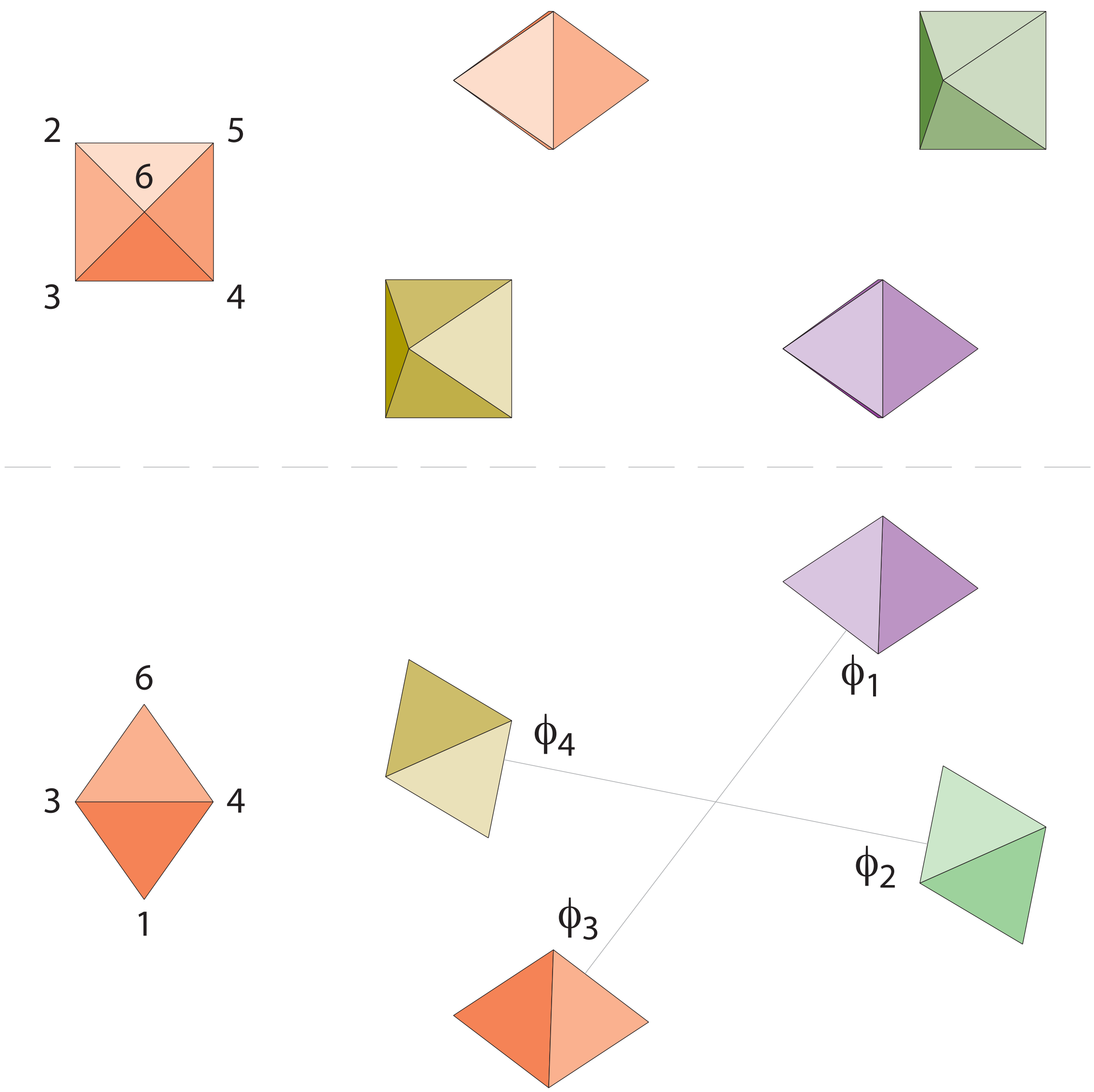


Fig. 14 Orientations of the panel octahedra after their ϕ-rotations

The figure shows the orientations of the panel octahedra due to their ϕ-rotations. The view perpendicular to the axis of rotation is below the view parallel to the axis of rotation. The octahedron on the left of each view is unrotated. Its three vertexial diameters are the xyz-axes of the icosahedral assembly. Each ϕ-rotated octahedron has been given the same coloration in each view.

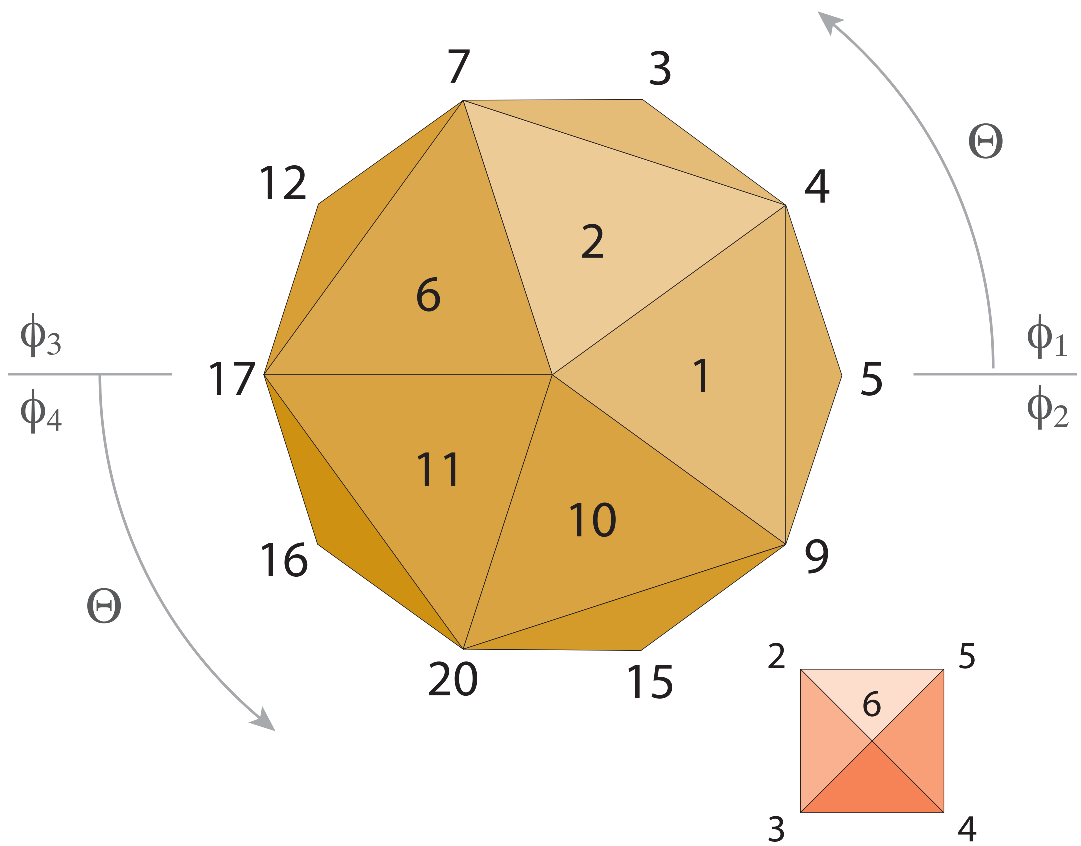


Fig. 15 Panel rotation Θ

The figure shows an icosahedron that is defined by twenty triangular panels of either graphite or diamond CFUs. The view is parallel to a vertexial diameter. After the reference panel is rotated through the required ϕ, it may require a second rotation θ about the vertexial diameter in the sense shown in the figure. For $\phi 1$ and $\phi 2$, θ is measured from the axial normal on the right; for $\phi 3$ and $\phi 4$, θ is measured from the axial normal on the left.

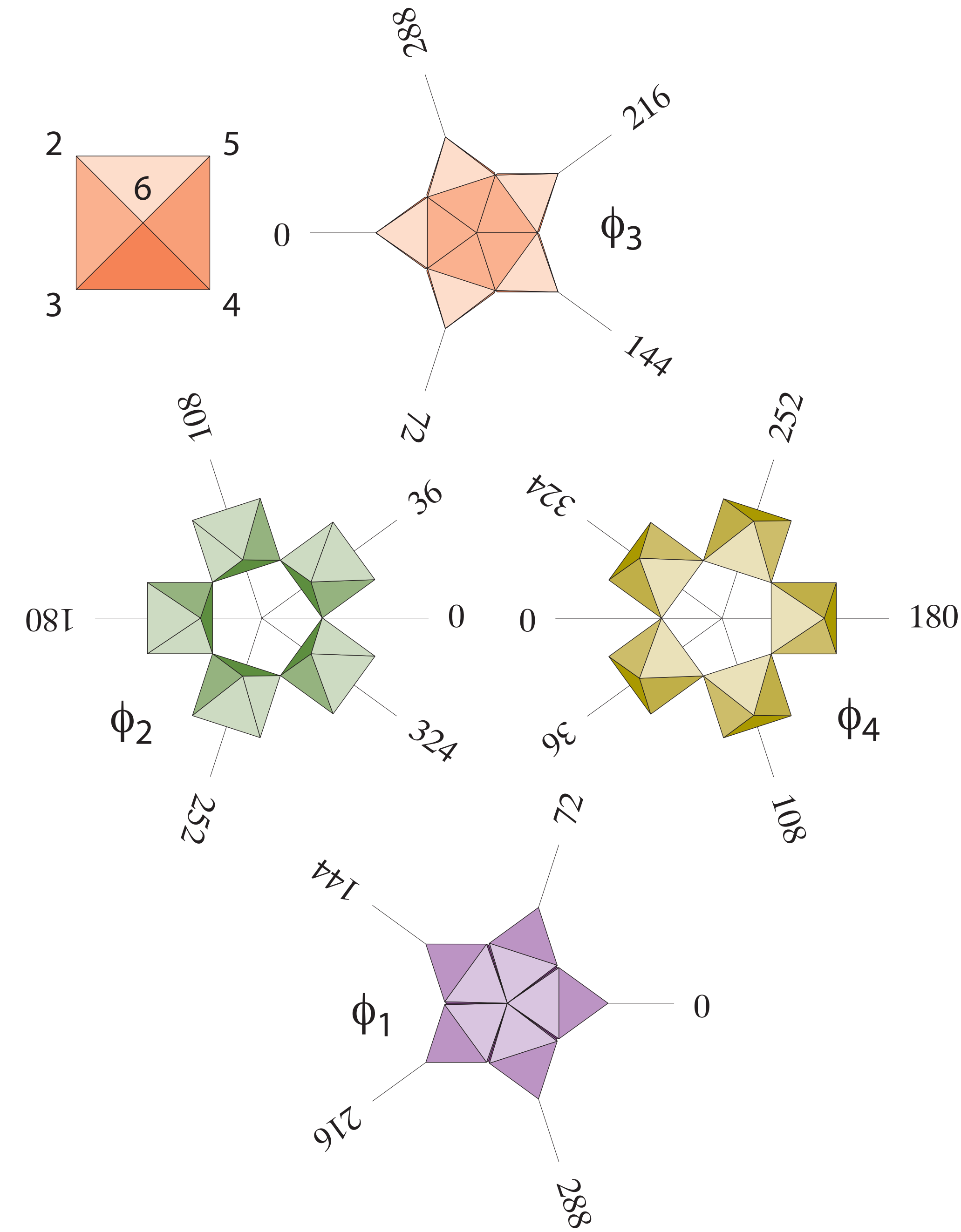


Fig. 16 Θ-rotations of the ϕ-rotated octahedra of the icosahedral fullerene

The figure shows each of the octahedral orientations required for an icosahedral assembly. Each octahedron within each of the four groups has the same ϕ-orientation. Each octahedron of each group has received the θ-orientation indicated by the labeled lines radiating from the center of each group.

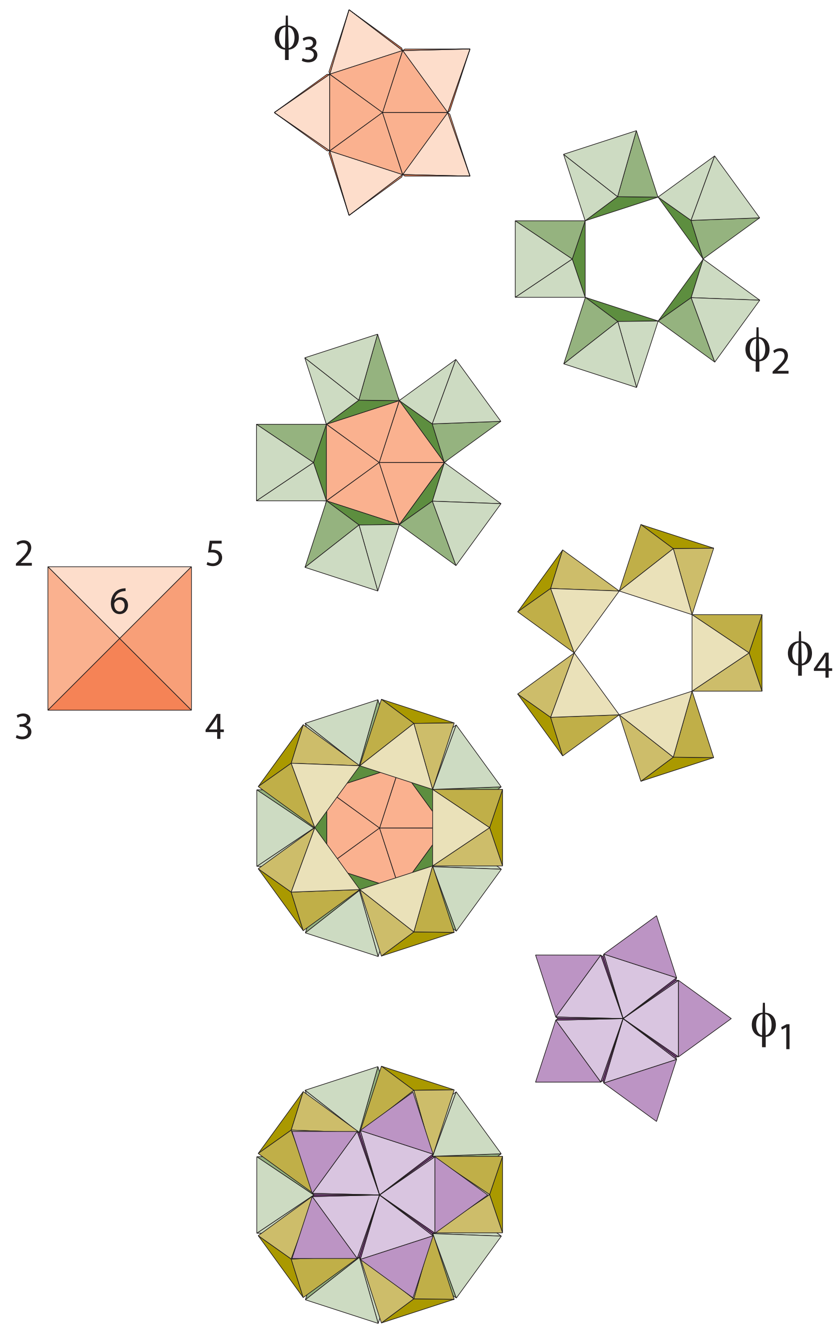


Fig. 17 Icosahedral assembly of $\phi-$ and $\theta-$rotated octahedra

The figure shows each of the four groups of five octahedra each that result from the ϕ and θ rotations required for an icosahedral assembly. The assembly begins at the top with the group of five red-colored octahedra labelled ϕ_3 and ends with the group of violet-colored octahedra labelled ϕ_1.

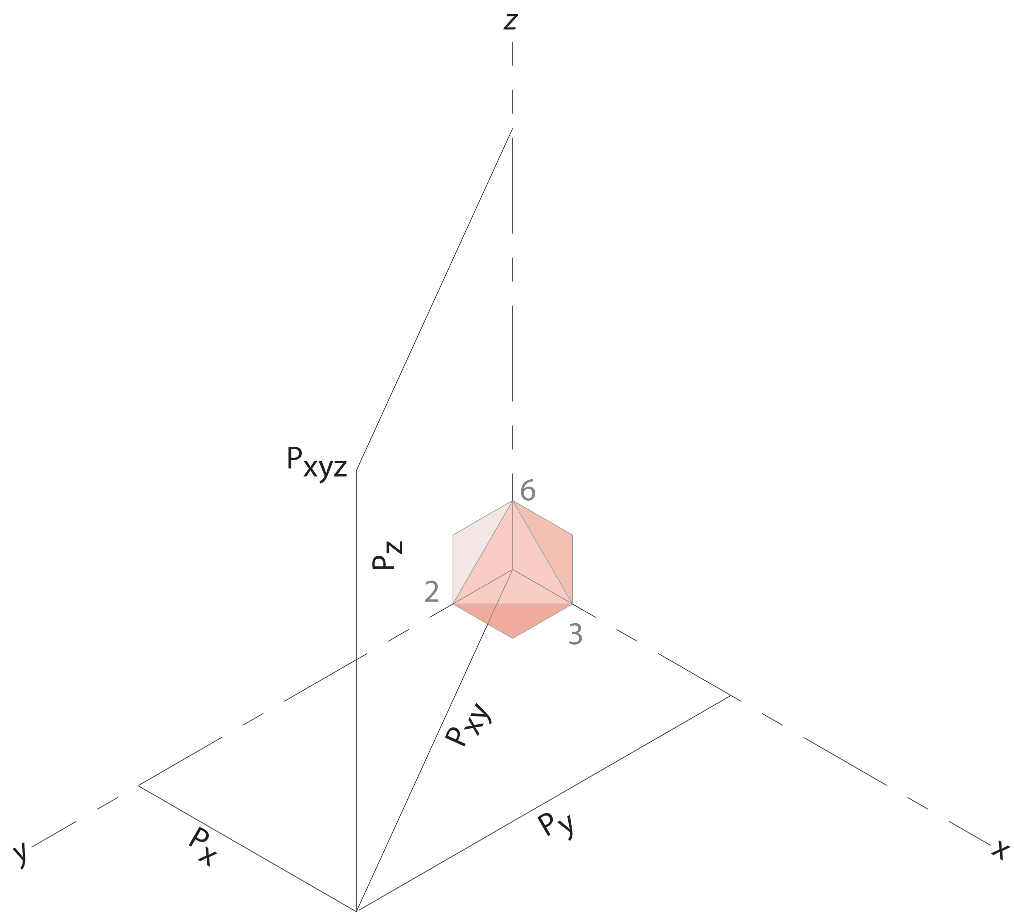
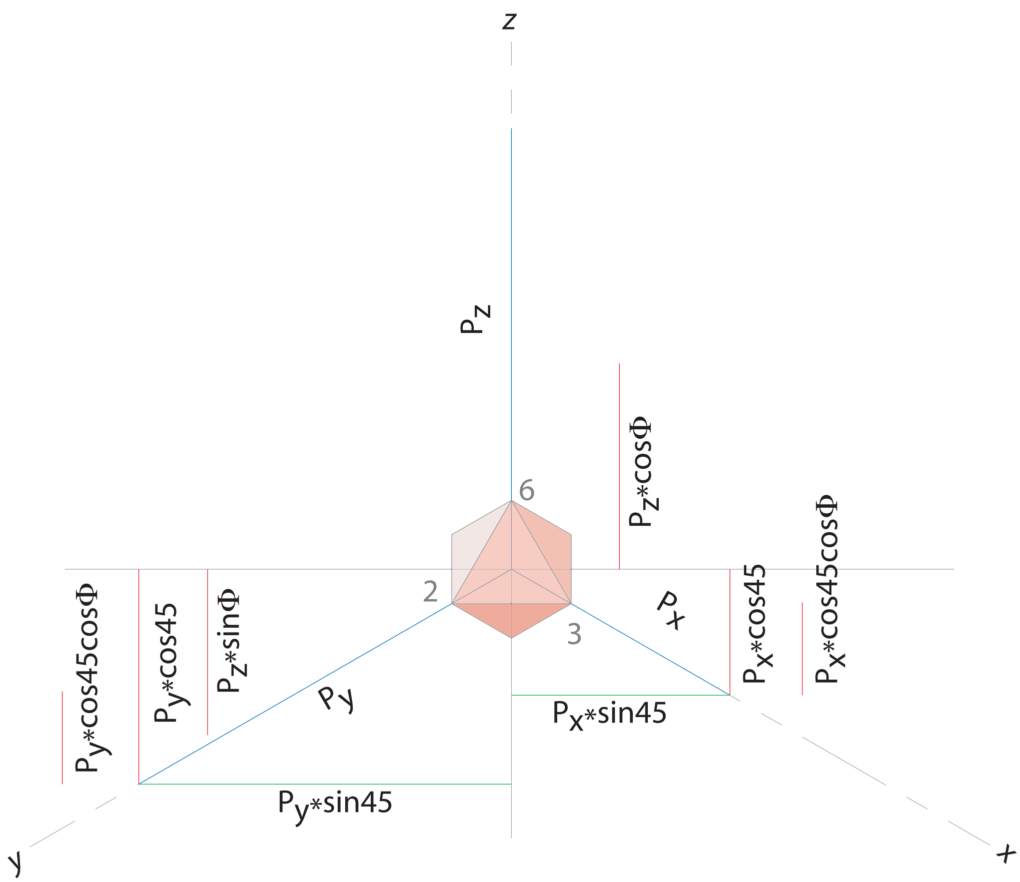


Fig. 18 Coordinate system of the octahedral assembly

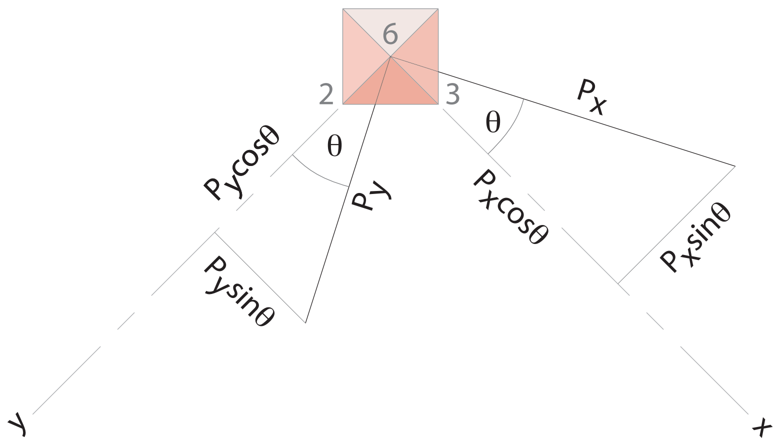
The figure shows the relationship of the regular octahedron to the Cartesian xyz-system. Pxyz represents the terminus of the vector between any point of interest in the assembly relative to the point chosen as the origin. Pxy is the projection of the vector Pxyz upon the xy-plane. Px is the projection of Pxy upon the x-axis; Py is the projection of Pxy upon the y-axis; and Pz is the projection of Pxyz upon the z-axis. The x-axis is collinear with the 35-vertexial diameter of the octahedron; the y-axis is collinear with the 24-vertexial diameter of the octahedron; and the z-axis is collinear with the 61-vertexial diameter of the octahedron.



$$rotatedx=sqr\{[(P_x*sin45)\wedge 2]+[(P_x*cos45cos\Phi)\wedge 2]\}+P_z*sin\Phi*cos45$$
$$rotatedy=sqr\{[(P_y*sin45)\wedge 2]+[(P_y*cos45cos\Phi)\wedge 2]\}+P_z*sin\Phi*cos45$$
$$rotatedz=P_x*cos45sin\Phi+P_y*cos45sin\Phi+P_z*cos\Phi$$

Fig. 19 Coordinates resulting from a ϕ-rotation

The figure shows the effect of a ϕ-rotation upon the xyz-coordinates of the He-octas of the C-atoms of the CFUs of the graphite or diamond CFUs of the unrotated triangular panel of an icosahedral fullerene.



$$rotatedx = P_x\cos\theta + P_y * \sin\theta$$
$$rotatedy = P_y\cos\theta - P_x * \sin\theta$$
$$rotatedz = Pz$$

Fig. 20 Coordinates resulting from a θ-rotation

The figure shows the effect of a θ-rotation upon the xyz-coordinates of the He-octas of the C-atoms of the CFUs of the graphite or diamond CFUs of the ϕ-rotated triangular panel of an icosahedral fullerene.