Concentric polyhedral assemblies of graphite and diamond panels

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

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

References

1. Octahedron1stEd.pdf The octahedral periodicity of the Atomic Elements and its implications.

http://homepage.mac.com/whitby/FileSharing103.html

2. GraphitePanels.pdf Triangular panels composed of graphite CFUs

http://homepage.mac.com/whitby/Quasicrystals/FileSharing175.html

3. DiamondPanels.pdf Triangular panels composed of diamond CFUs

http://homepage.mac.com/whitby/Quasicrystals/FileSharing176.html

4. QuasicryOcta.pdf Quasicrystalline octahedron having a single C-atom as a facial panel

http://homepage.mac.com/whitby/Quasicrystals/FileSharing69.html

5. TetOctFullerenes.pdf Tetrahedral and octahedral assemblies of graphite and diamond panels

http://homepage.mac.com/whitby/Quasicrystals/FileSharing177.html

6. susana_iglesias.pdf "Fullerenes and bucky onions in the interstellar medium" by Susana Iglesias Groth–a thirty-three page slideshow format document from the internet.

http://homepage.mac.com/whitby/Quasicrystals/FileSharing178.html

Introduction

This document shows how regular polyhedral assemblies of triangular panels of graphite and diamond CFUs assemble concentrically. It was prompted by a reference to concentric fullerenes or "Bucky onions" in the Susana Iglesias Groth document [Reference 6].

Polyhedral assemblies

General

Given the number of CFUs $\boldsymbol{l}$ along an edge of the triangular panel, the edge length $\boldsymbol{L}$ in He-octa edges of the internal polyhedron is given by the equation

$$L = 4(l - 1) + 3$$

Icosahedron

An icosahedral assembly of graphite or diamond panels defines an inner icosahedron and an outer icosahedron. The panels are bounded by the two icosahedra. The internal icosahedron produced by graphite panels is identical to the internal icosahedron produced by diamond panels.

Table 1: Sizes of icosahedra formed by triangular panels of graphite and diamond

Edge length		CFUs/icosa	C-atoms	
panel	icosahedron		graphite	diamond
CFUs	He-octa edges			
1	3	20	60	80
2	7	80	240	320
3	11	180	540	720
4	15	320	960	1280
5	19	500	1500	2000
6	23	720	2160	2880

The distance between the centroid of an icosahedron and the centroid of one of its faces is fixed by its geometry. The thickness ***t*** of the CFUs which constitute the panel adds to the facial radius of the inner icosahedron to produce the facial radius of the outer icosahedron. Given the edge length ***L*** of the inner icosahedron and the thickness of the CFU, the edge length ***E*** of the outer icosahedron can be found.

The edge length of the outer icosahedron is

$$E = (1 + \Delta R) \times L$$

where

$$\Delta R = \frac{t\sqrt{\frac{2}{3}}}{\frac{L\sqrt{7+3\sqrt{5}}}{\sqrt{8}}}$$

which is equivalent to

$$E = L + 0.6237 \times t$$

The thickness ***t*** is ***2*** for a graphite panel and ***3*** for a diamond panel.
The calculated results of the above equations is tabulated here.

Table 2: Outer bounding envelopes of regular icosahedral assemblies

Edge length				Scale factor outer	
panel	inner	outer		graphite	diamond
		graphite	diamond		
1	3	4.2474	4.8711	1.4158	1.6237
2	7	8.2474	8.8711	1.1782	1.2673
3	11	12.2475	12.8712	1.1134	1.1701
4	15	16.2475	16.8712	1.0832	1.1247
5	19	20.2475	20.8712	1.0657	1.0985
6	23	24.2475	24.8712	1.0542	1.0814

Figure 1 shows each of the five internal icosahedra defined by the triangular panels.

Figure 2 shows the icosahedral assemblies arranged in two concentric groups according to whether their panels are composed of graphite CFUs or diamond.

Figure 3 shows graphite panels having either one CFU per edge or two. Each is shown with the inner triangular face it defines in a polyhedral assembly.

Figure 4 shows the inner icosahedral volumes defined by the panels of Figure 3. The outer icosahedral volume of the 1-panel is shown both separately and then concentrically with the internal icosahedral volume of the 2-panel.

Octahedron

An octahedral assembly of graphite or diamond panels defines an inner octahedron and an outer octahedron. The panels are bounded by the two octahedra. The internal octahedron produced by graphite panels is identical to the internal octahedron produced by diamond panels

The facial radius ***R*** of the octahedron is one half of its facial diameter. The panel thickness ***t*** adds to the facial radius of the inner octahedron to give the facial radius of the outer octahedron

The edge length ***E*** of the outer octahedron is

$$E = (1 + \Delta R) \times L$$

where

$$\Delta R = \frac{t \times \sqrt{\frac{2}{3}}}{\frac{1}{2} \times L \times \sqrt{\frac{2}{3}}}$$

$$\Delta R = 2 \times \frac{t}{L}$$

which is equivalent to

$$E = L + 2 \times t$$

where ***t*** is ***2*** for a graphite panel and ***3*** for a diamond panel.

The calculated results of the above equations is tabulated here.

Table 3: Outer bounding envelopes of regular octahedral assemblies

Edge length			
panel	inner	outer	
		graphite	diamond
1	3	7	9
2	7	11	13
3	11	15	17
4	15	19	21
5	19	23	25
6	23	27	36

Figure 5 shows an edgial view of each of the five inner octahedra to the same scale.

Figure 6 shows the five octahedral assemblies divided into two groups according to whether the number of CFUs along an edge of a panel of the assembly is odd or even. The assemblies of each group are concentric. For each assembly, only the four panels which are perpendicular to the viewing plane are shown.

Figure 7 shows the five assemblies as a concentric unit. The surfaces of adjacent assemblies abut.

Tetrahedron

The relationships between the tetrahedral assemblies of triangular graphite and diamond panels was done graphically. Figure 8 shows the arrangement of the panels in the regular tetrahedral assemblies. Figure 9 shows that the outer surface of one tetrahedral assembly abuts the inner surface of another tetrahedral assembly when the number of CFUs along an edge of the panel of one differs from that of the other by one.

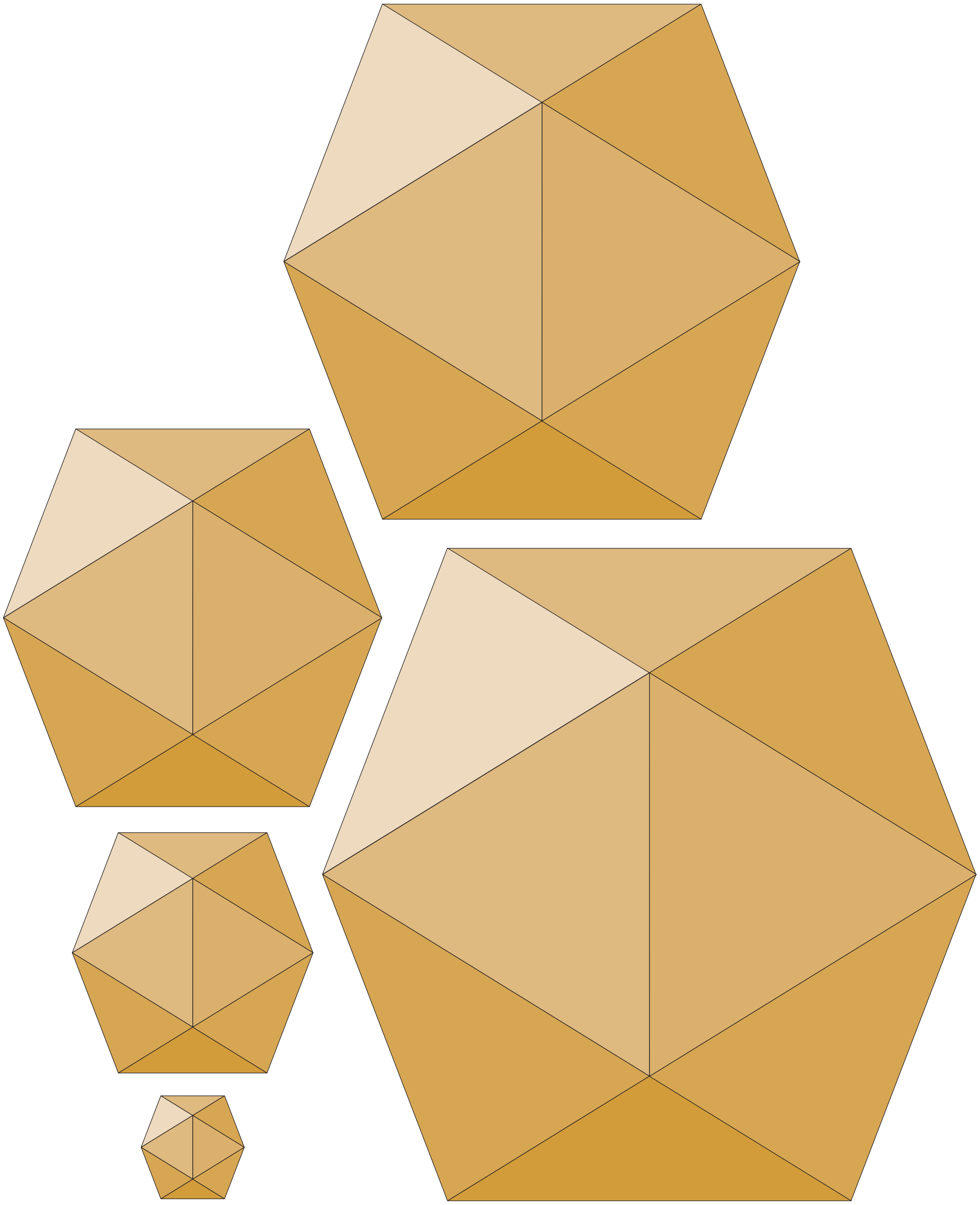

Fig. 1 Internal volumes of icosahedral assemblies of graphite and diamond CFUs
The figure shows the five smallest inner icosahedra defined by triangular panels consisting of either graphite or diamond CFUs.

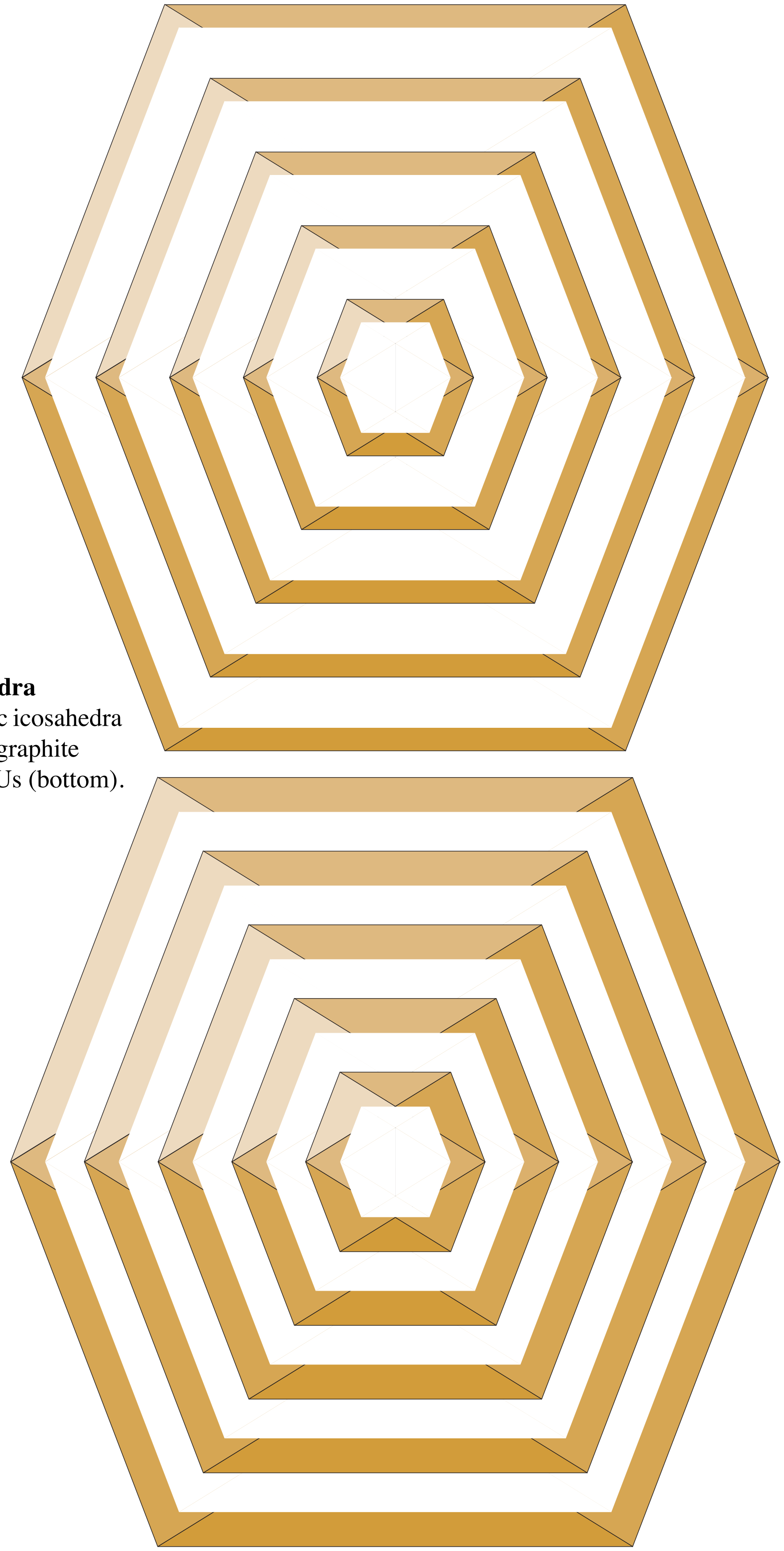

Fig. 2 Concentric icosahedra
The figure shows concentric icosahedra made of triangular panels of graphite CFUs (top) and diamond CFUs (bottom).

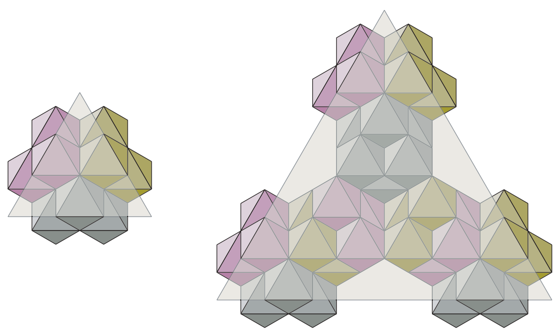

Fig. 3 Graphite panels for compact C_{60} and C_{240} icosahedra

The panel on the left has an edge length which is three times the edge length of a He-octa; the panel on the right has an edge length which is seven times the edge length of a He-octa. Twenty panels identical to those on the left assemble as an icosahedron of sixty C-atoms; twenty panels identical to those on the right assemble as an icosahedron of 240 C-atoms.

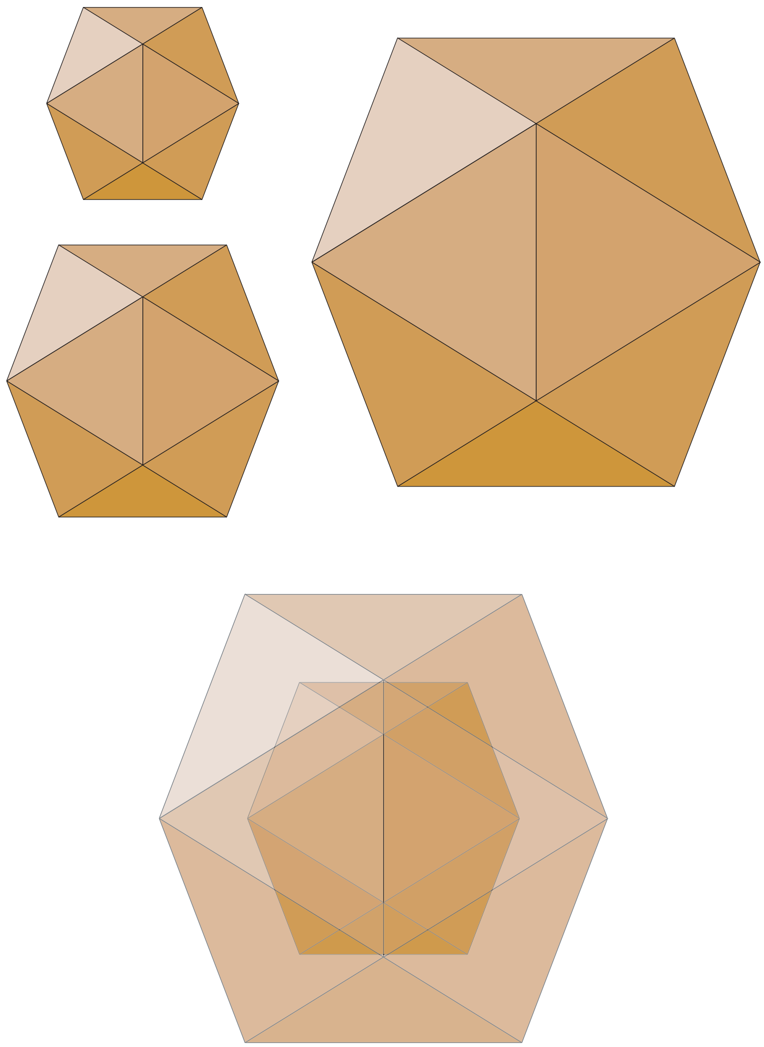

Fig. 4 Comparison of the boundaries of the C_{60} and C_{240} icosahedra

At the top left, the icosahedron represents the internal boundary of the C_{60} icosahedron. The larger icosahedron just below it represents the external boundary of the C60 icosahedron. The difference between the inner and outer boundaries is the domain of the panel thickness.

At the top right, the icosahedron represents the internal boundary of the C_{240} icosahedron. Its edge length is two and one third times that of the C_{60} icosahedron.

At the bottom, the external boundary of the C_{60} icosahedron is placed within the internal volume of the C_{240} icosahedron.

Fig. 5 Octahedra defined by the inner surfaces of triangular panels of graphite or diamond
The figure shows the five smaller inner octahedra defined by triangular panels of either graphite or diamond CFUs.

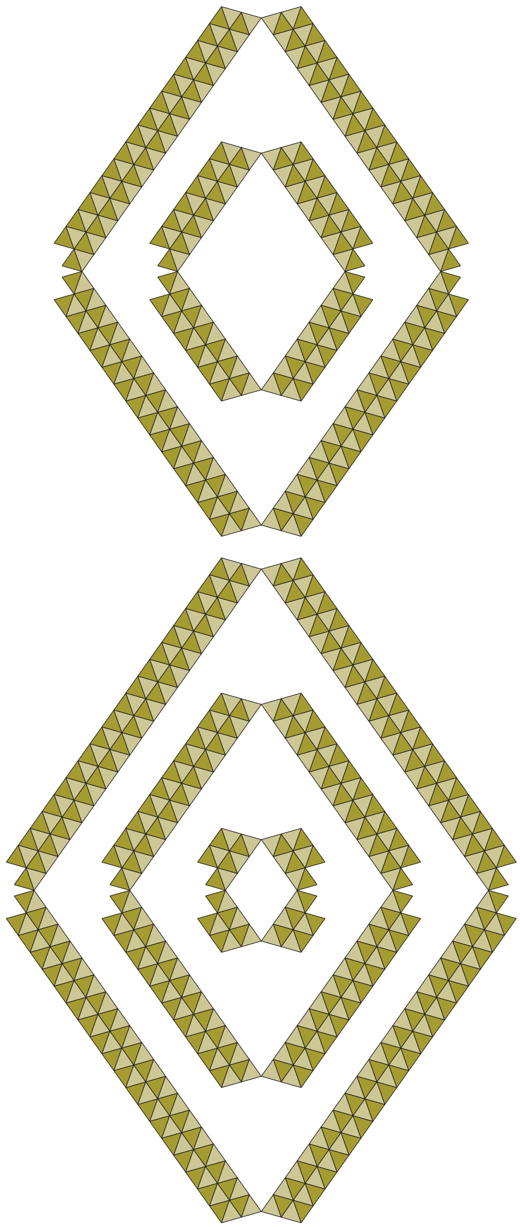

Fig. 6 Edgial views of octahedra formed by triangular panels of graphite CFUs

The figure shows just four panels each of the five octahedral assemblies of triangular panels of graphite CFUs. Each of the panels shown is viewed edge-on in the edgial views of the five octahedra. Each of the panels of the three concentric octahedra at the bottom has an odd number of CFUs along an edge. The innermost has one, the outermost has five, and the intermediate has three. The panels of the two concentric octahedra at the top have two or four CFUs along an edge.

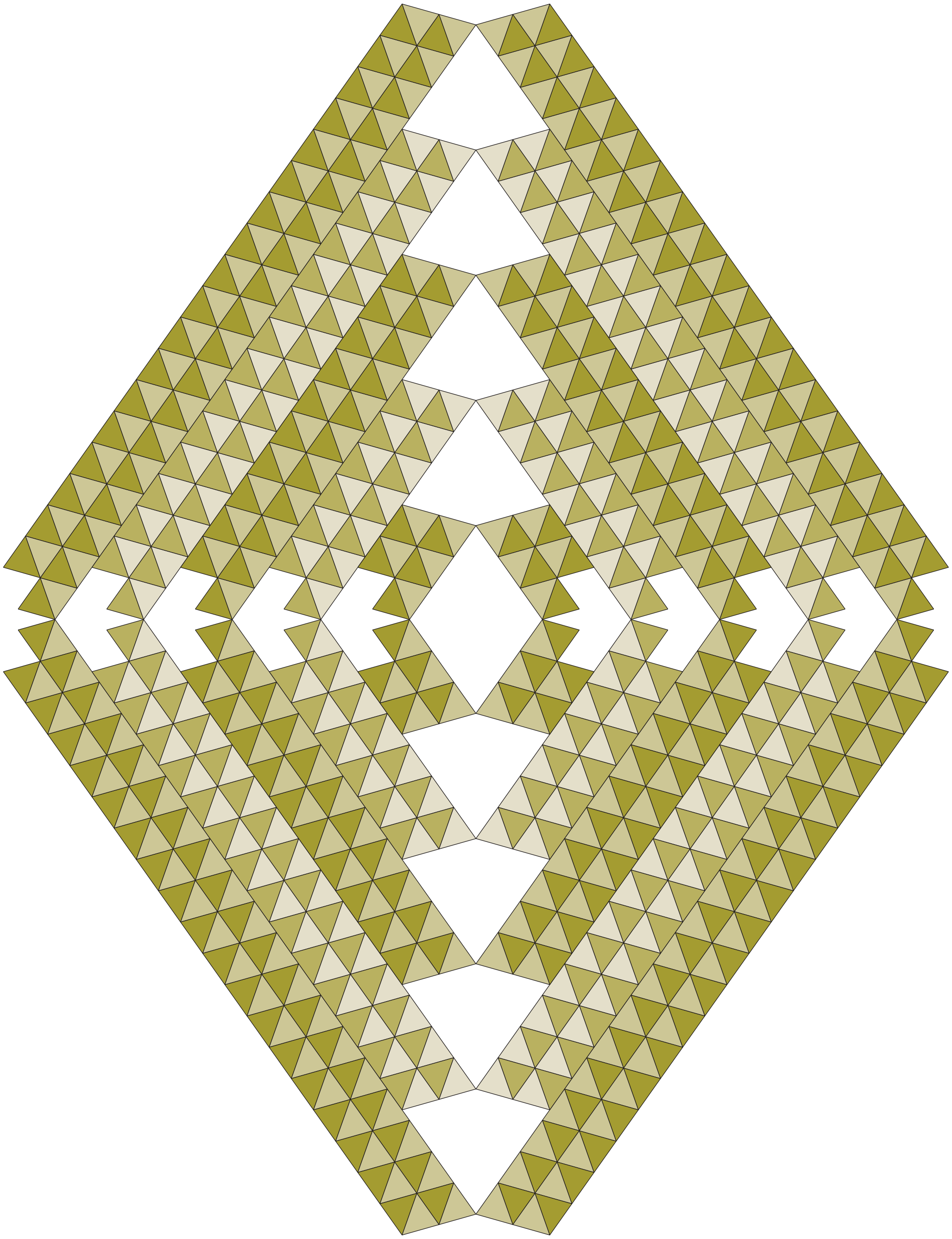

Fig. 7 Concentric octahedral assemblies of graphite panels

Each of the five octahedral assemblies of graphite panels is in contact with each neighboring assembly. The octahedra of adjacent assemblies are not in positions to make edge to edge joins.

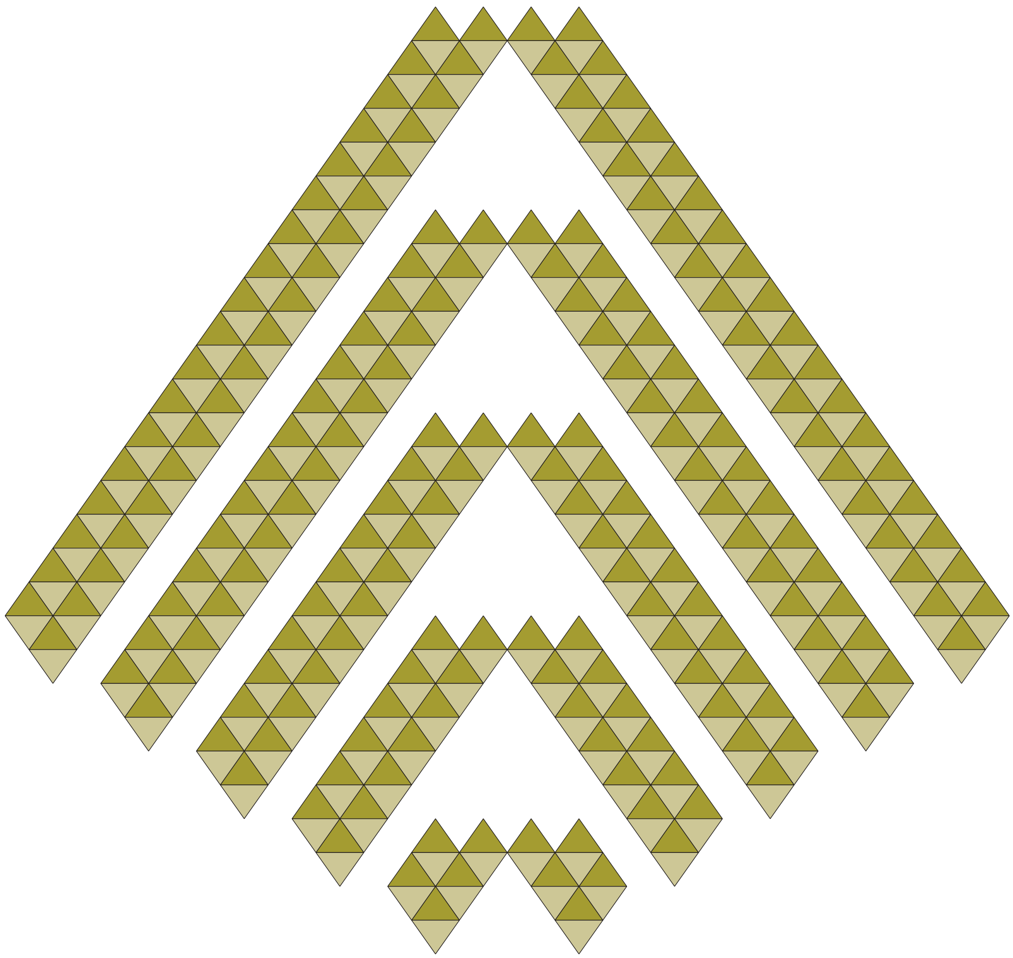

Fig. 8 Tetrahedral assemblies of triangular panels of graphite CFUs
The figure shows just two panels of five tetrahedral assemblies of triangular panels of graphite CFUs. Each of the panels is viewed edge-on, parallel to the plane of the panel. Each tetrahedron is viewed parallel to an edge. The edge length of each triangular face of the tetrahedron at the bottom of the figure is three He-octa edges. The edge lengths of the faces of the other four tetrahedra are 7, 11, 15, and 19 He-octa edges.

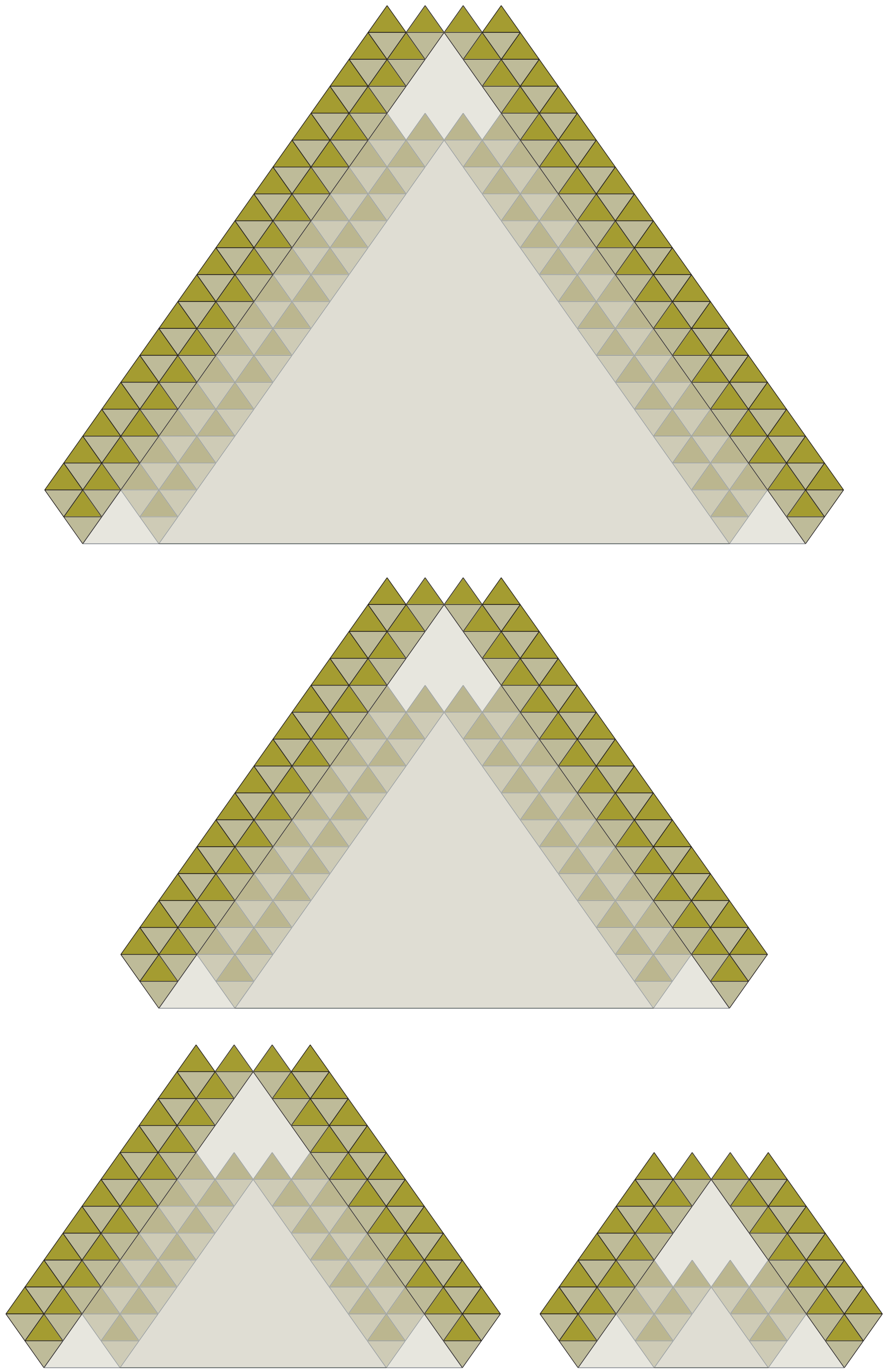

Fig. 9 Concentric regular tetrahedral assemblies of triangular graphite panels

The figure shows four concentric pairs of regular tetrahedral assemblies of triangular graphite panels.

At lower right, a tetrahedron of 1-panels is enclosed by a tetrahedron of 2-panels.

At lower left, a tetrahedron of 2-panels is enclosed by a tetrahedron of 3-panels.

In the middle, a tetrahedron of 3-panels is enclosed by a tetrahedron of 4-panels.

At top, a tetrahedron of 4-panels is enclosed by a tetrahedron of 5-panels

It follows that a smaller tetrahedron can be enclosed by each of the larger tetrahedra and that the five tetrahedra can be included in a single concentric assembly. The He-octas of the triangular panels at the contact surfaces of adjacent tetrahedra are positioned to join edge to edge.