Polyhedral assemblies of truncated triangular panels of graphite & diamond

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

References

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

2. GraphitePanels.pdf Triangular panels composed of graphite CFUs

3. DiamondPanels.pdf Triangular panels composed of diamond CFUs

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

5. "Structure and energetics of giant fullerenes: An order-N molecular-dynamics study", by Satoshi Itoh, Pablo Ordejon, David A. Drabold, Richard M. Martin, PHYSICAL REVIEW B 15 JANUARY 1996-II VOLUME 53, NUMBER 4

Introduction

This document looks at regular polyhedral assemblies formed by the edgial joining of identical threefold panels consisting solely of graphite CFUs or solely of diamond CFUs which are symmetrically truncated.

Facially incomplete regular polyhedra

Triangular panels can assemble as structurally stable incomplete polyhedra.

Tetrahedron

An open faced tetrahedron is structurally stable. This is the form of the graphite CFU. It includes three panels.

Octahedron

Two open faced octahedra are structurally stable. The seven panel octahedron and the six panel octahedron where the open faces of the latter are opposite to one another.

Icosahedron

The nineteen panel icosahedron and the eighteen panel icosahedra are both stable. The open faces of the latter are opposite to one another.

Panels formed by adding C-atoms to graphite and diamond CFUs

Graphite CFU plus three C-atoms

Figure 2 shows a graphite CFU with a C-atom joined to each of its three C-atoms. Each join is the same as that found between the C-atoms of CFUs in other panels.

Table 1: Polyhedral assemblies whose panels each have six C-atoms

Polyhedron	Panels	C-atoms
tetrahedron	3	18
	4	24
octahedron	6	36
	7	42
	8	48
icosahedron	18	108
	19	114
	20	120

Diamond CFU plus three C-atoms

Figure 3 shows a diamond CFU with a C-atom joined to three of its four C-atoms in the same manner as that between the C-atoms of CFUs in a diamond crystal.

Table 2: Polyhedral assemblies whose panels each have seven C-atoms

Polyhedron	Panels	C-atoms
tetrahedron	3	21
	4	28
octahedron	6	42
	7	49
	8	56
icosahedron	18	126
	19	133
	20	140

C_{70} icosahedron

A C_{70} icosahedron could be formed from facial panels equally distributed between graphite and diamond CFUs. The ten graphite CFUs give thirty C-atoms and the ten diamond CFUs give forty C-atoms for a total of seventy C-atoms. [See Figure 1]

Panels formed by rings of diamond of graphite CFUs

Ring of three graphite CFUs

Figure 4 shows how three graphite CFUs can form a stable ring which can act as a rigid triangular panel. The panel can make a C_{180} icosahedron. The join between any two CFUs is a single He-octa edge.

Ring of three diamond CFUs

Figure 5 shows how three diamond CFUs can form a stable ring which can act as a rigid triangular panel. The panel can make a C_{240} icosahedron. The join between any two CFUs is a single He-octa edge.

Ring of six diamond CFUs

Six diamond CFUs can join as a ring. The rings can join to form a panel which cannot assemble as a polyhedral structure. [See Figure 25.] If the rings are joined to one another by an additional CFU acting as a hub, the panels can assemble as polyhedra. [See Figure 24.]

Truncated triangular panels

Vertexially truncated triangular panels

A CFU may be removed from each of the three vertexes of a triangular panel which has three CFUs per edge or more. The number of CFUs per truncated panel is n^2-3 where n=3, 4, 5,.... For a polyhedron, the number of C-atoms is (n^2-3) * a * b where a is the number of faces of the polyhedron and b = 3 for graphite and 4 for diamond. The table shows the data for icosahedral assemblies.

Table 3: Icosahedral assemblies of triangular panels without vertexial CFUs

CFUs				Atoms/icosa	
edge	panel	truncated panel	icosahedron	graphite	diamond
3	9	6	120	360	480
4	16	13	260	780	1040
5	25	22	440	1320	1760
6	36	33	660	1980	2640

Table 3: Icosahedral assemblies of triangular panels without vertexial CFUs

CFUs				Atoms/icosa	
edge	panel	truncated panel	icosahedron	graphite	diamond
7	49	46	920	2760	3680

Edgially truncated triangular panels

A triangular panel which has an odd number of CFUs along an edge which has five or more CFUs can be symmetrically truncated by removing the middle CFU from each edge. [See Figure11.] Other edgial truncations are possible.

Centroidally truncated triangular panels

Centroidal CFU

A triangular panel whose number of CFUs is n^2 and n>3 with n^2 mod 3 = 1 has a CFU whose centroid lies on the axis of threefold symmetry of the panel. These panels can be truncated by the removal of the centroidal CFU. If n is even, the centroidal CFU is in the same orientation as the three CFUs at the vertexes; if n is odd, the centroidal vertex is oriented obversely to the three CFUs at the vertexes. [See Figure 7 for an example.]

Table 4: Icosahedral assemblies of triangular panels without central CFU

CFUs				Atoms/icosa	
edge	panel	truncated panel	icosahedron	graphite	diamond
4	16	15	300	900	1200
5	25	24	480	1440	1920
7	49	48	960	2880	3840[a]
8	64	63	1260	3780	5040
10	100	99	1980	5940	7920
11	121	120	2400	7200	9600
13	169	168	3360	10080	13440
14	196	195	3900	11700	15600
16	256	255	5100	15300	20400
17	289	288	5760	17280	23040

a. C_{3840} is mentioned in Reference 5

Centroidal triangle

A triangular group of CFUs can be removed from a panel which has four or more CFUs along an edge. The maximum number of CFUs in the removed triangular group is $(n-3)^2$. The number of

Table 5: Icosahedral assemblies of triangular panels without central triangle

CFUs					Atoms/icosa	
edge	inner	panel	truncated panel	icosahedron	graphite	diamond
4	1	16	15	300	900	1200
5	2	25	21	420	1260	1680
6	3	36	27	540	1620	2160
7	4	49	33	660	1980	2640
8	5	64	39	780	2340	3120

C-atoms in the truncated panel is $[n^2 - (n-3)^2]*a$ where n=4,5,6,... and a=3 for graphite and 4 for diamond.

Centroidal ring

A ring of six CFUs can be removed from a triangular panel having $(6 + 3n)^2$ CFUs along an edge. The number of C-atoms in an icosahedron whose panels have been truncated by the removal

Table 6: Icosahedral assemblies of triangular panels without central ring

CFUs				Atoms/icosa	
edge	panel	truncated panel	icosahedron	graphite	diamond
6	36	30	600	1800	2400
9	81	75	1500	4500	6000
12	144	138	2760	8280	11040

of a centroidal six ring is $[(6+3n)^2 - 6]*20*a$ where n=0,1,2,3,... and a =3 for graphite and 4 for diamond.

Assembling larger panels from smaller panels

Smaller panels of graphite or diamond CFUs can assemble as larger panels. [See Figures 19-21 and 23.] Figure 26 shows four ways in which smaller triangular panels can assemble as a 12-triangle panel. Figure 22 shows how a 3-triangle can be assembled from three subassemblies of three CFUs each.

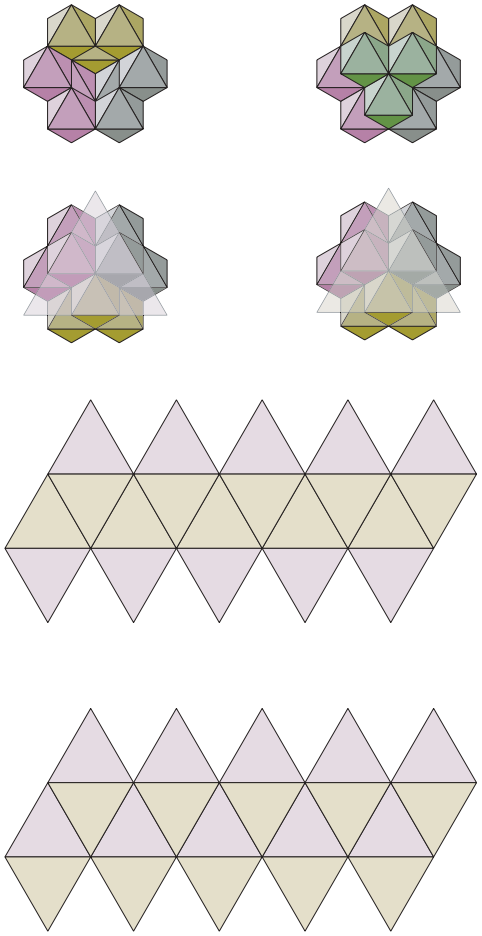


Fig. 1 C_{70} icosahedron

A C_{70} icosahedron might be formed of ten graphite CFUs and ten diamond CFUs. That would give thirty C-atoms for the ten graphite panels and forty for the ten diamond panels. The figure shows two icosahedral layouts in which the panels might be distributed. In either case, if the violet panels are graphite, then the yellow panels are diamond. Two views of each of the CFUs are shown at the top–graphite on the left and diamond on the right.

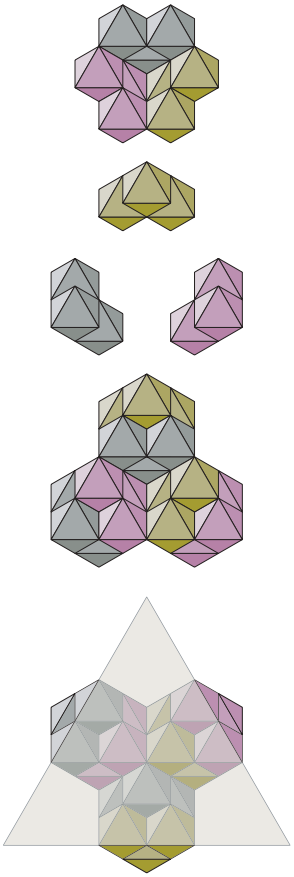


Fig. 2 Graphite CFU with three additional C-atoms

The figure shows a triangular panel consisting of a graphite CFU with a single C-atom in a Mg-join with each of its three C-atoms. The graphite CFU is shown at the top. The additional three C-atoms are shown just below it. The complete assembly is shown next.

The same assembly could be effected by three pairs of Mg-joined C-atoms.

At the bottom, the obverse of the six C-atom assembly is shown with the triangular face it defines.

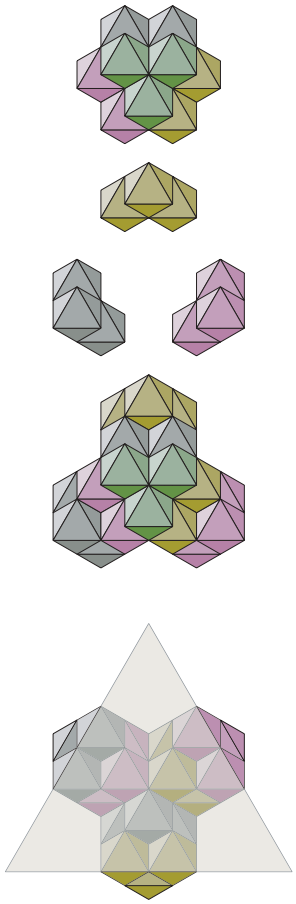


Fig. 3 Diamond CFU with three additional C-atoms

The figure shows the assembly of a triangular panel consisting of a diamond CFU and three single C-atoms. Each of the single C-atoms is Mg-joined to a C-atom of the diamond CFU. The obverse of the assembly is shown at the bottom with the triangular face it defines superimposed upon it.

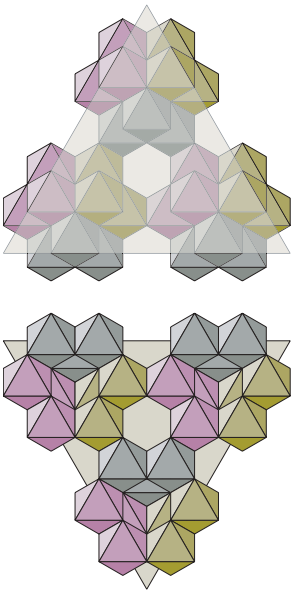


Fig. 4 Triangular panel of three graphite CFUs
The figure shows how three graphite CFUs can assemble as a rigid triangular panel. The join between each pair of CFUs is a single edge of a He-octa. This is the panel which forms the C_{180} fullerene.

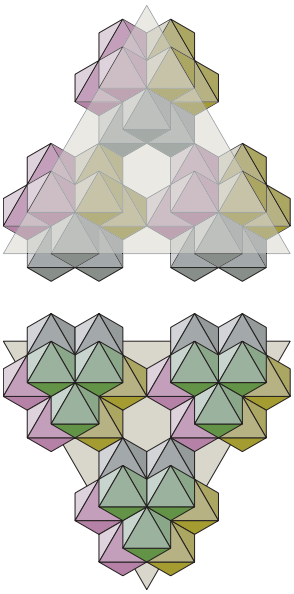


Fig. 5 Triangular panel of three diamond CFUs

The figure shows how three diamond CFUs can assemble as a rigid triangular panel. The join between each pair of CFUs is a single edge of a He-octa. This is the panel which forms the C_{240} fullerene.

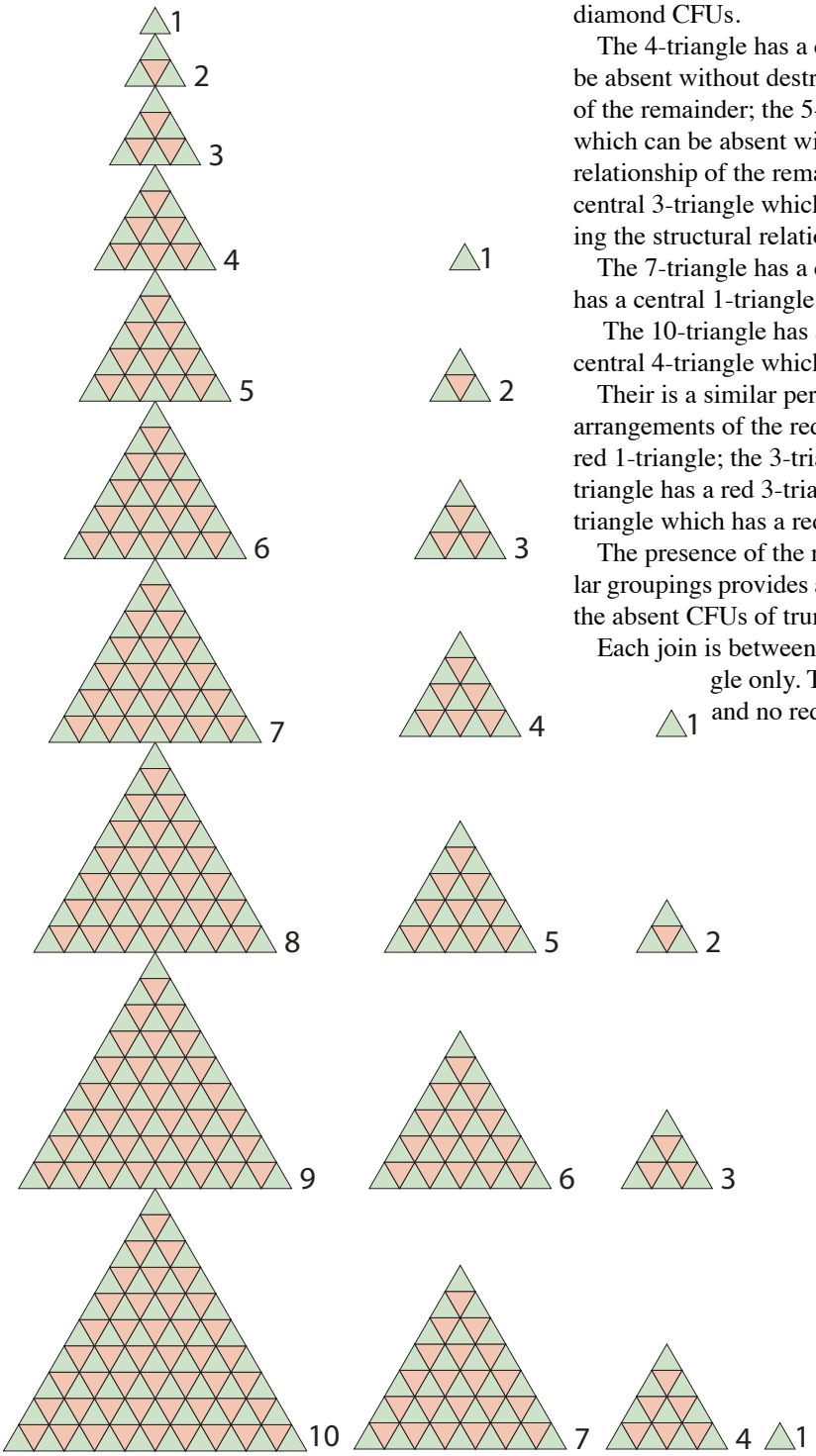


Fig. 6 Truncation index for triangular panels

Each green triangle and each red triangle represents a CFU of graphite or diamond. The red triangle is the obverse of the green. Each of the compound triangles represents a complete triangular assembly of graphite or diamond CFUs.

The 4-triangle has a central green triangle which can be absent without destroying the structural relationship of the remainder; the 5-triangle has a central 2-triangle which can be absent without destroying the structural relationship of the remainder; and the 6-triangle has a central 3-triangle which can be absent without destroying the structural relationship of the remainder.

The 7-triangle has a central 4-triangle which, in turn, has a central 1-triangle.

The 10-triangle has a central 7-triangle which has a central 4-triangle which has a central 1-triangle.

Their is a similar periodic occurrence within the arrangements of the red triangles. The 2-triangle has a red 1-triangle; the 3-triangle has a red 2-triangle; the 4-triangle has a red 3-triangle; the 5-triangle has a red 4-triangle which has a red 1-triangle.

The presence of the red and green intra-panel triangular groupings provides a way to describe the locations of the absent CFUs of truncated triangular panels.

Each join is between a green triangle and a red triangle only. There is no green to green join and no red to red join.

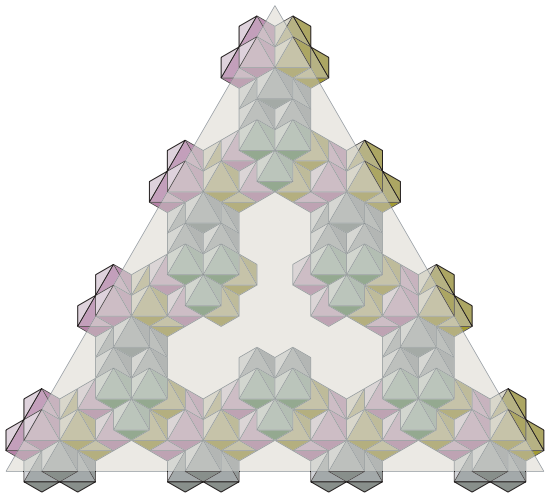


Fig. 7 Truncation of a 4-triangle–center CFU
The figure shows a diamond 4-triangle that is missing its central CFU. Each of the three vertexial CFUs could also be absent without destroying the structural stability of the remaining CFUs.

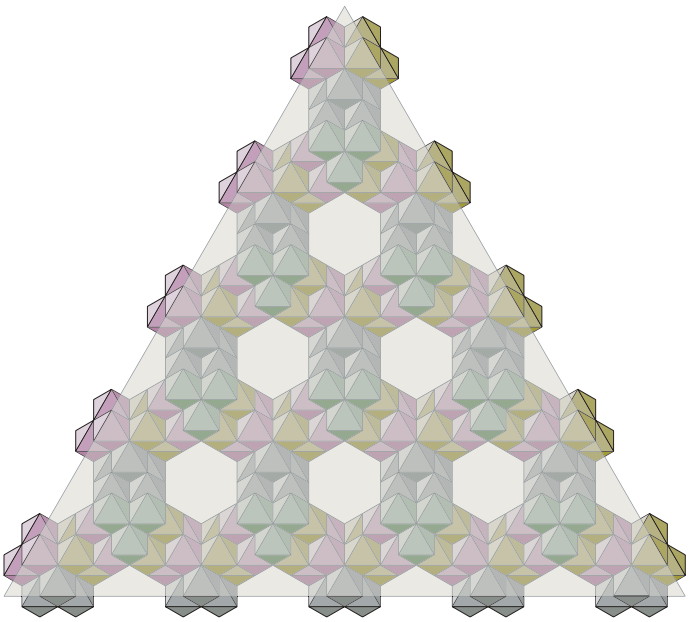


Fig. 8 Untruncated 5-triangle
The figure shows an untruncated 5-triangle of diamond CFUs.

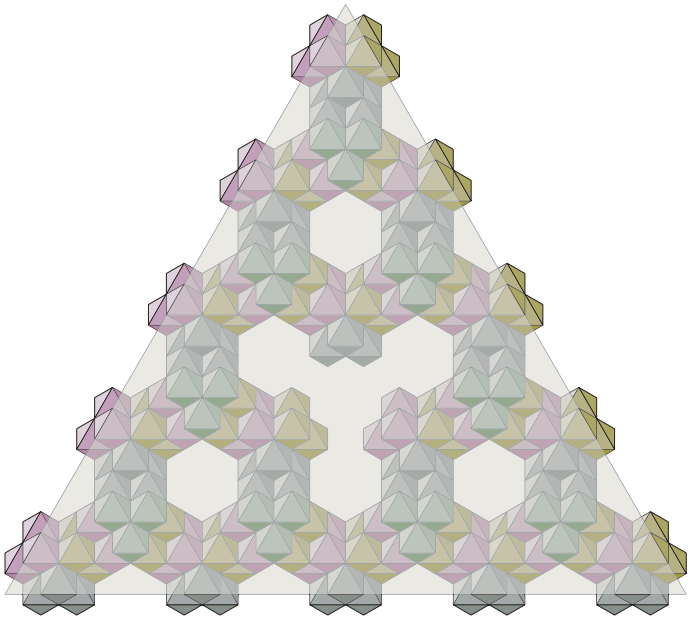


Fig. 9 Truncation of a 5-triangle–central CFU
The figure shows a 5-triangle of diamond CFUs without its central CFU.

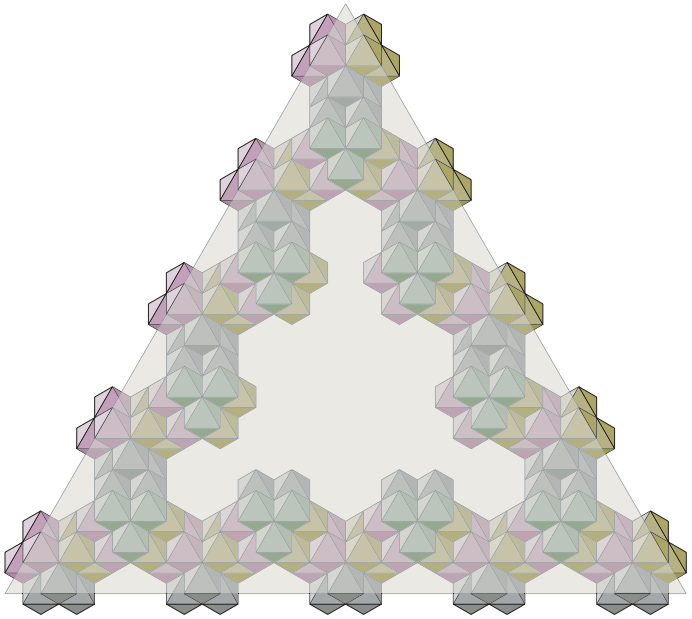


Fig. 10 Truncation of a 5-triangle–central 2-triangle
The figure shows a 5-triangle of diamond CFUs which is missing a central 2-triangle.

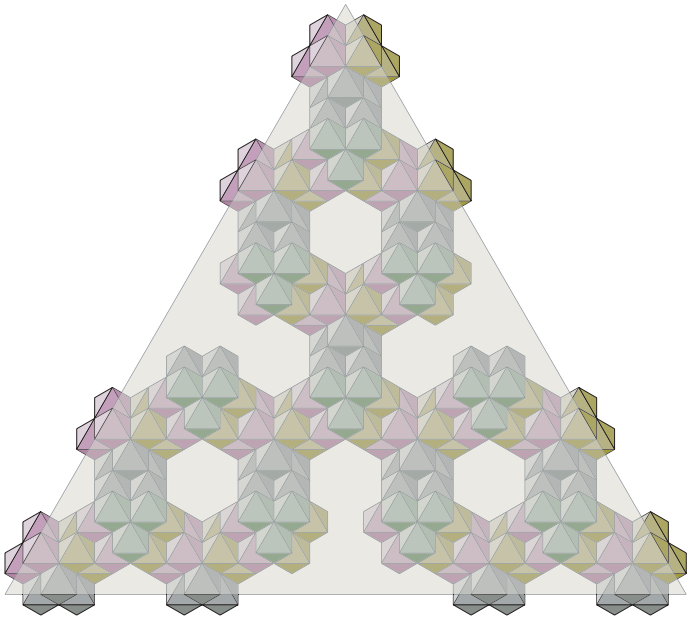


Fig. 11 Truncation of a 5-triangle–mid-edgial CFU

The figure shows a triangular panel of five diamond CFUs to an edge which has been truncated by the removal of one CFU from each mid-edge. It has twenty-two diamond CFUs remaining.

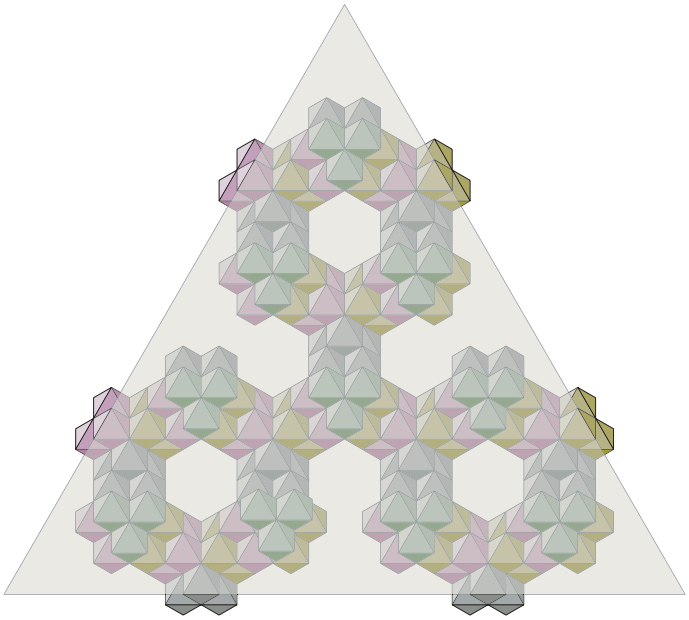


Fig. 12 Truncation of a 5-triangle–midedge and vertexial
The figure shows a 5-triangle of diamond CFUs which is missing a CFU from each of its vertexes and each of its midedges.

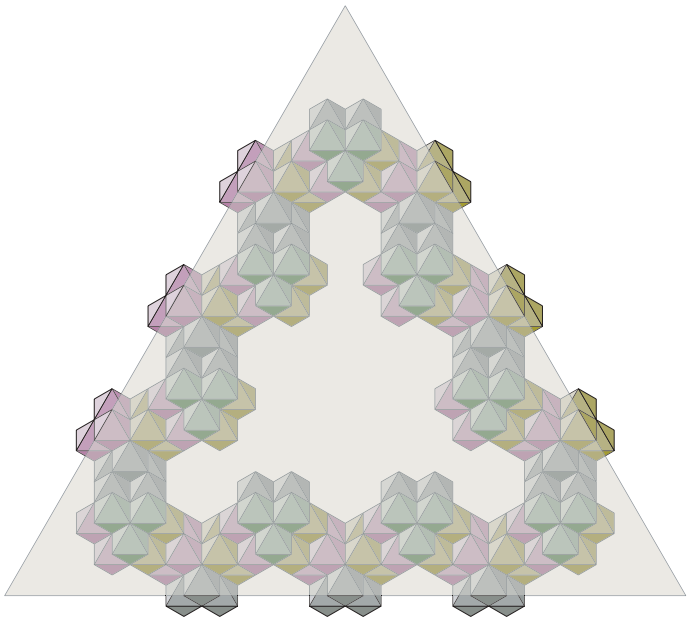


Fig. 13 Truncations of a 5-triangle–center 2-triangle and vertexial

The threefold panel shown in the figure can be seen as a triangular panel of five CFUs to an edge which has been truncated by removing a CFU from each of its three vertexes and four CFUs from its center. It has eighteen CFUs remaining.

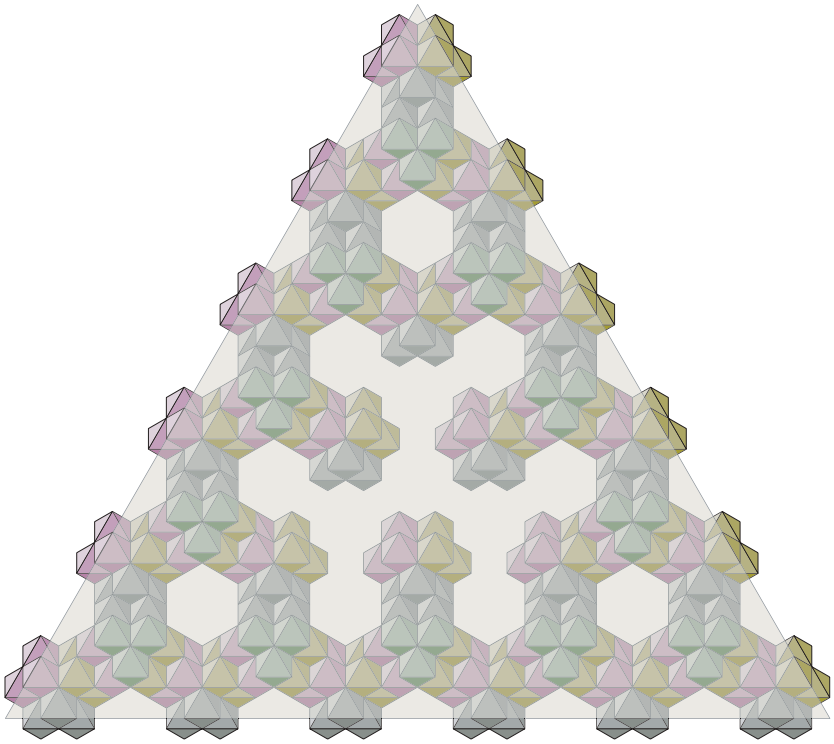


Fig. 14 Truncation of a 6-triangle
The figure shows a 6-triangle of diamond CFUs which is missing its centroidal 2-triangle

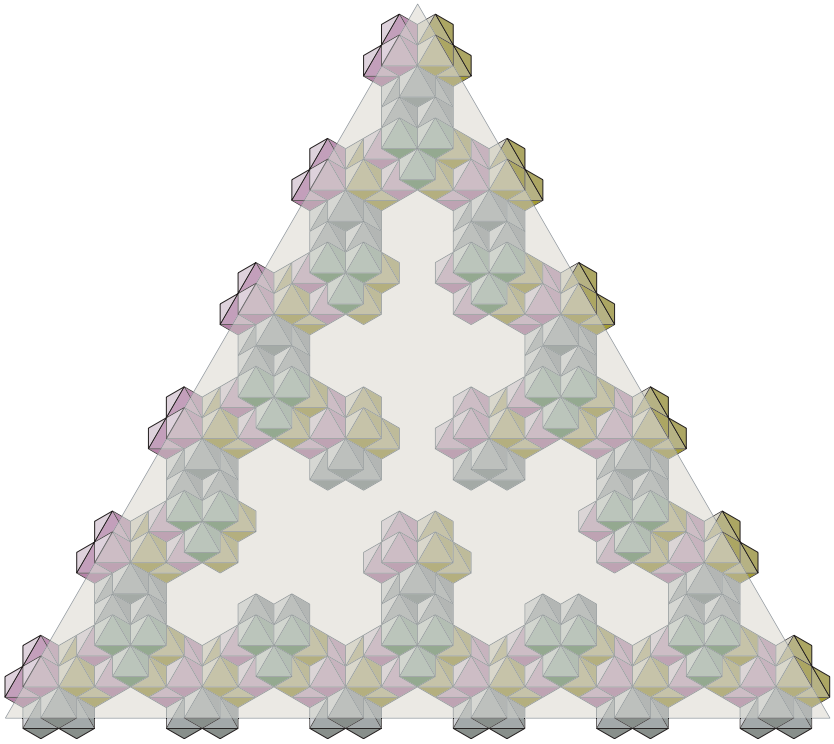


Fig. 15 Truncations of a 6-triangle–central 3-triangle
The figure shows a 6-triangle of diamond CFUs which has been truncated by removing the CFUs of the central 3-triangle except for those at the midedges.

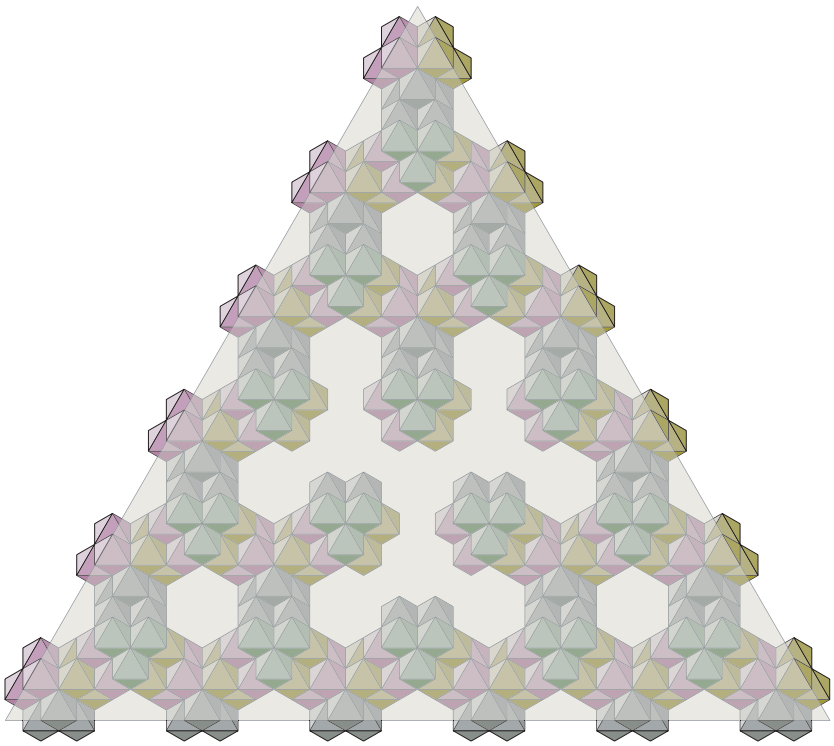


Fig. 16 Truncation of a 6-triangle–midedges of the central 3-triangle

The figure shows a 6-triangle of diamond CFUs which is missing the midedgial CFUs of its central 3-triangle.

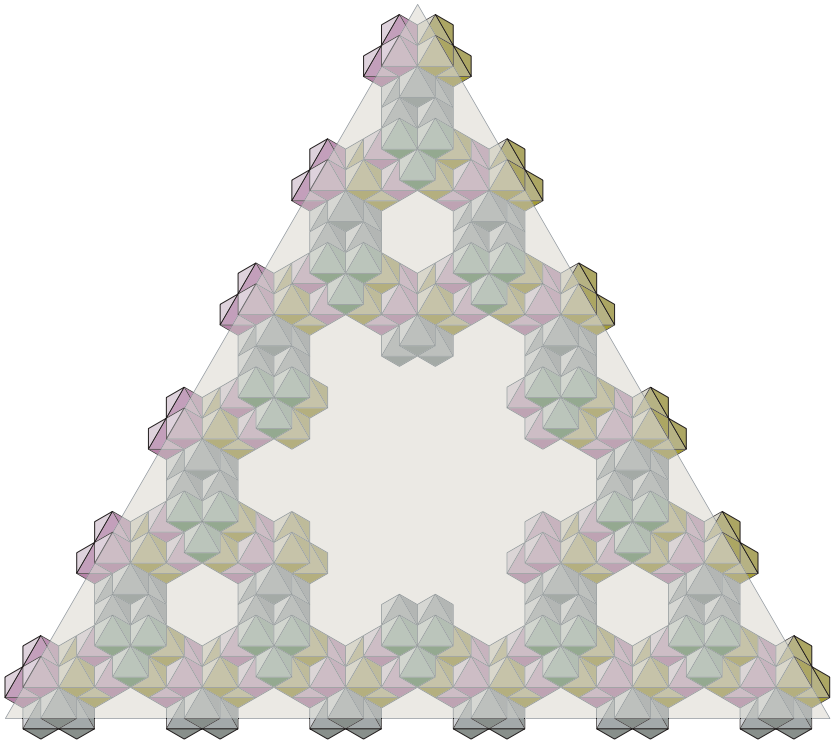


Fig. 17 Truncation of a 6-triangle–central hexagonal ring
The figure shows a 6-triangle of diamond CFUs which is missing the CFUs of its central 3-triangle except for those at the three vertexes. The six missing CFUs form a ring.

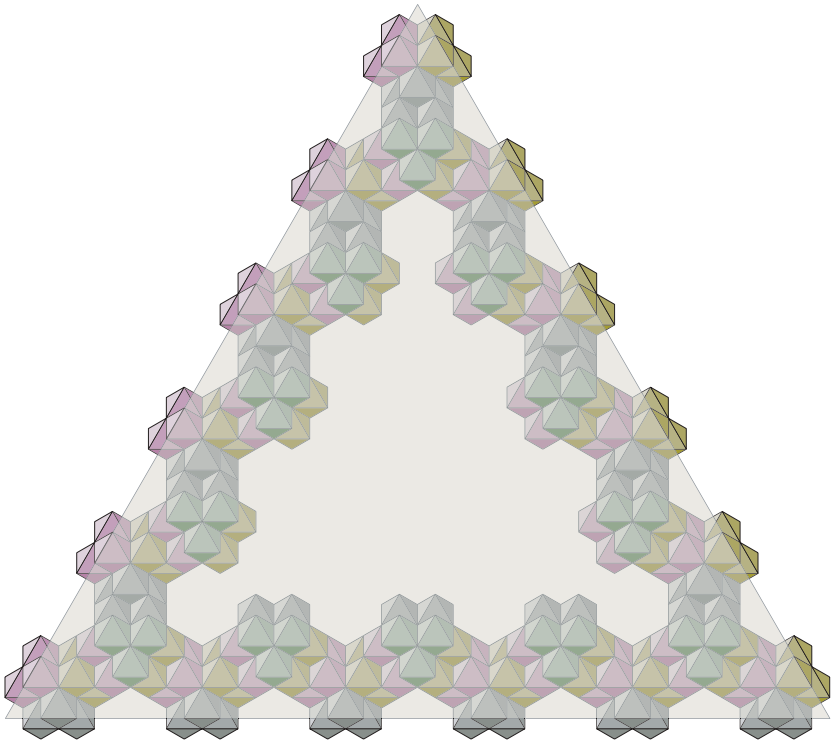


Fig. 18 Truncation of a 6-triangle–center 3-triangle
The figure shows a 6-triangle of diamond CFUs which is missing its central 3-triangle.

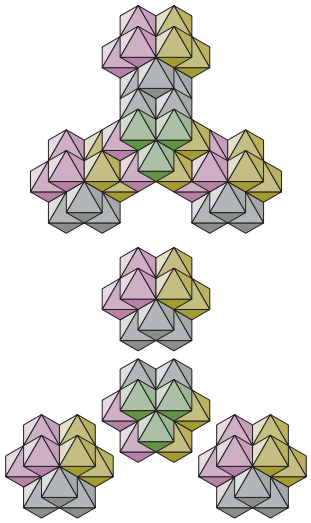


Fig. 19 Assembly of a 2-triangle–four diamond CFUs
The figure shows a 2-triangle of diamond CFUs at the top. Below it, the four diamond CFUs it contains are shown separately.

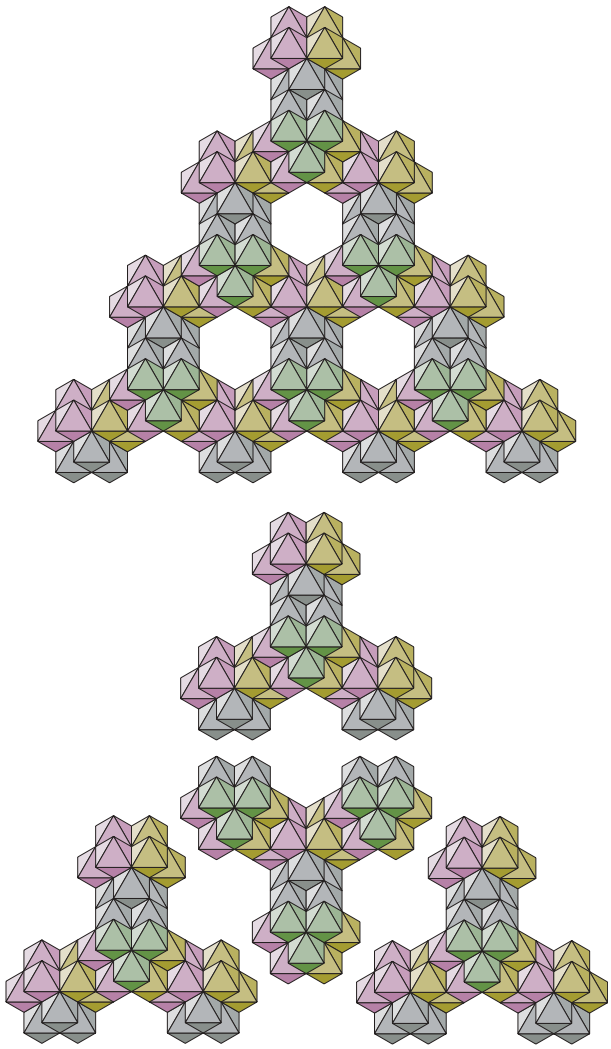


Fig. 20 Assembly of a diamond 4-triangle–four 2-triangles
The figure shows a 4-triangle of diamond CFUs at the top. Below it, the four 2-triangles are in position to assemble as the 4-triangle above.

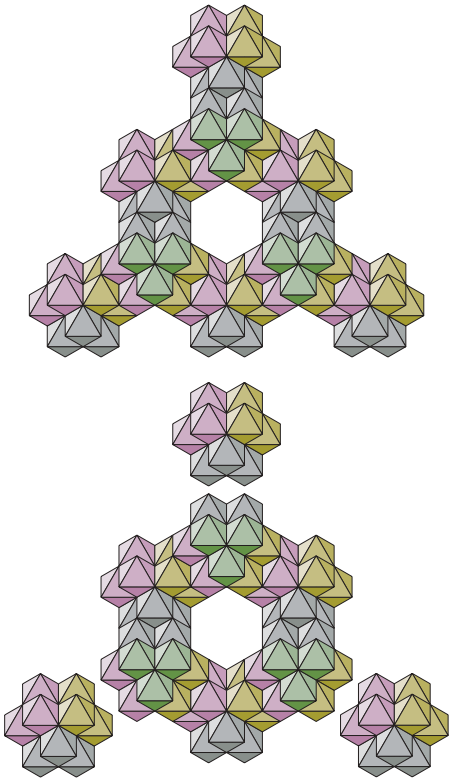


Fig. 21 Assembly of a diamond 3-triangle–ring of six CFUs plus three singles
The figure shows a 3-triangle of diamond CFUs at the top. The ring of six CFUs and the three single CFUs are in position to form the 3-triangle.

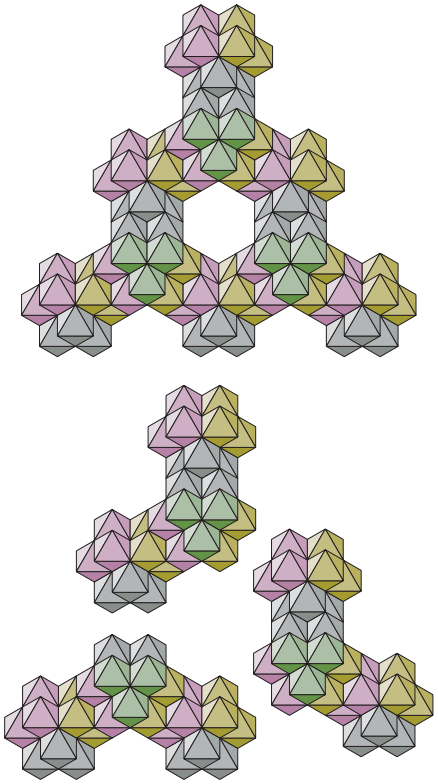


Fig. 22 Assembly of a 3-triangle–three groups of three diamond CFUs
The figure shows a 3-triangle of diamond CFUs at the top. The three groups of three CFUs each are in position to assemble as the 3-triangle.

Fig. 23 Assembly of a 6-triangle–four 3-triangles of diamond CFUs
The 6-triangle of diamond CFUs can be assembled from the four 3-triangles beneath it.

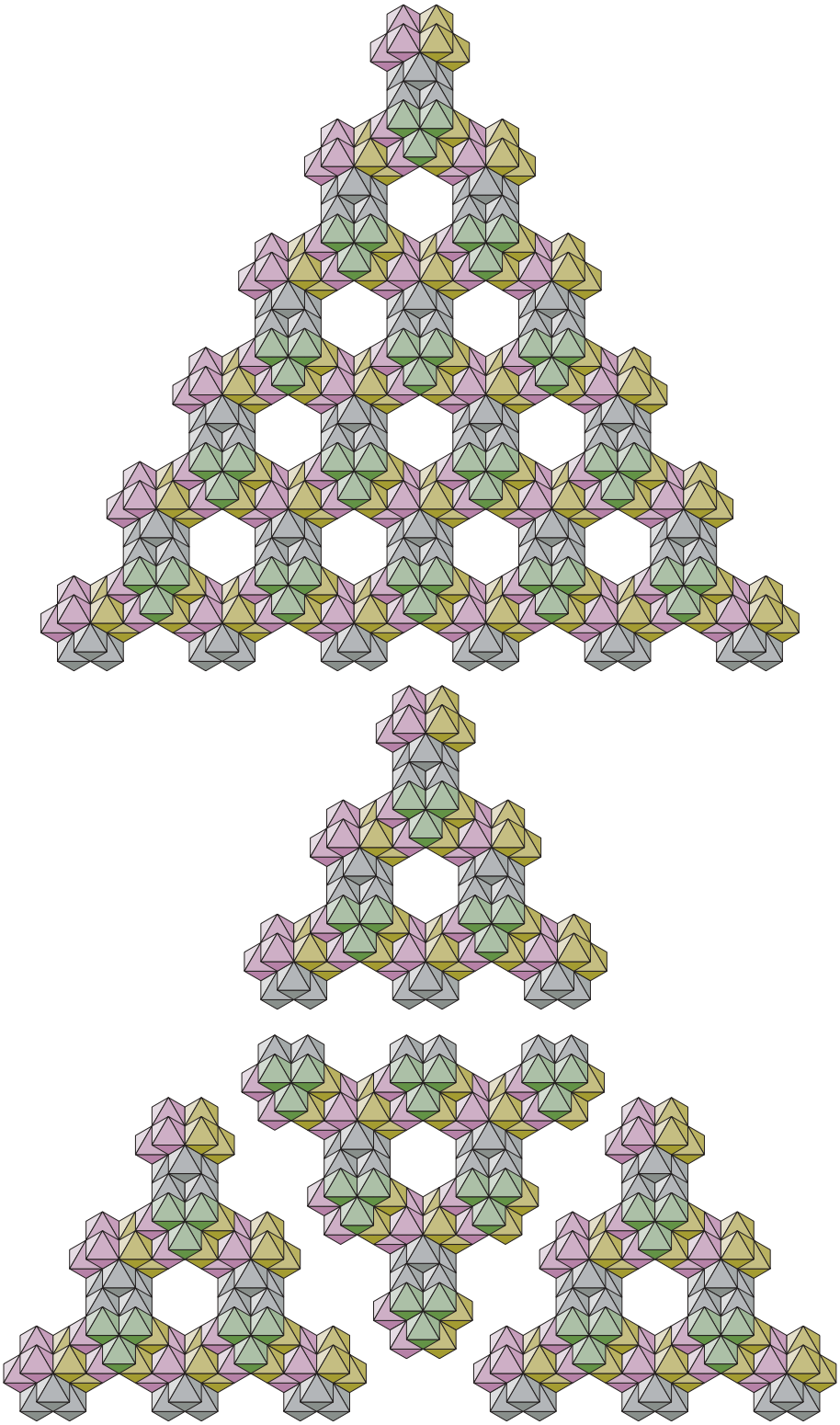


Fig. 24 Ring and hub assemblies of diamond CFUs
The figure show triangular panels of diamond CFUs which have been assembled for rings of six joined

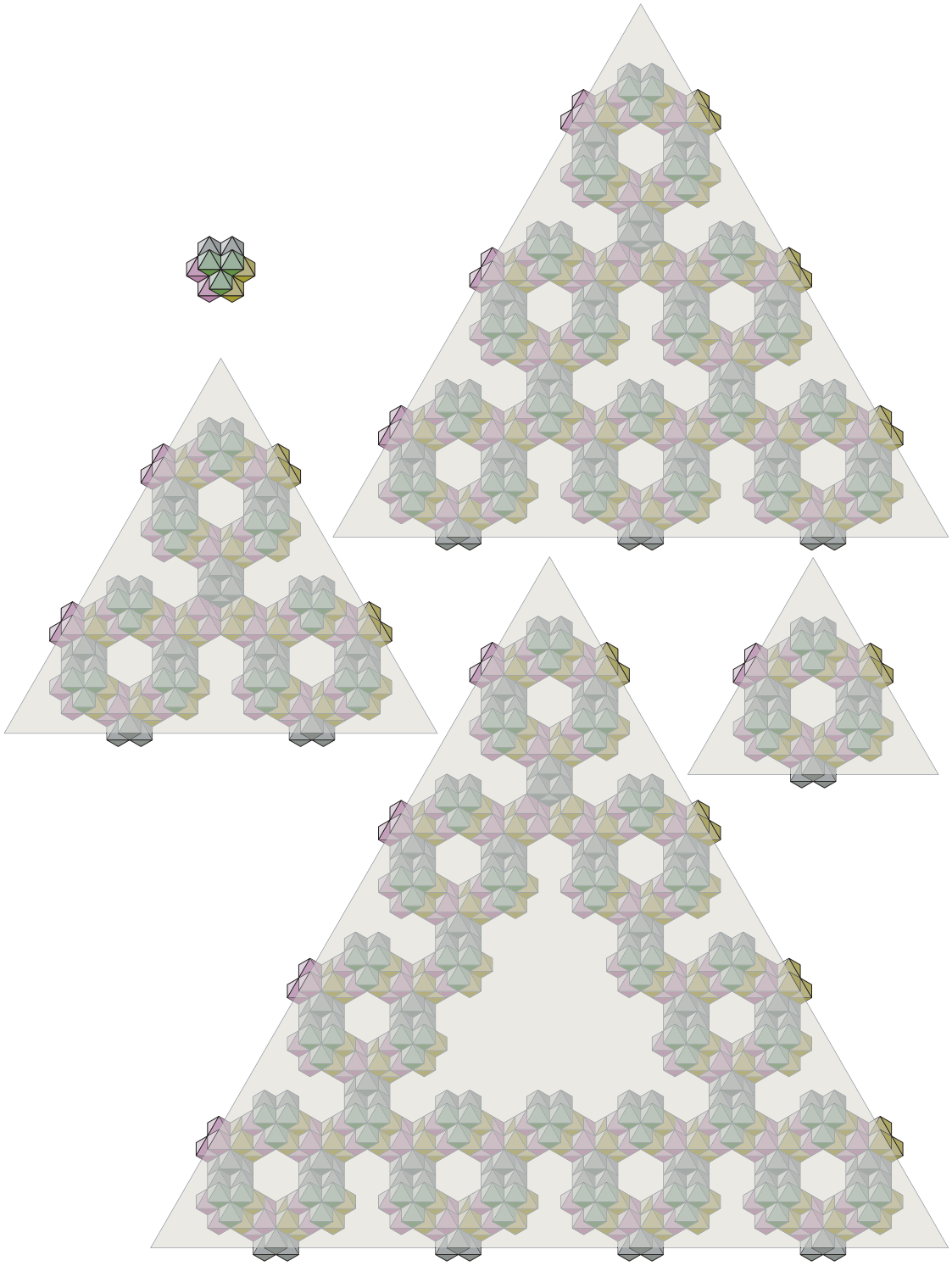
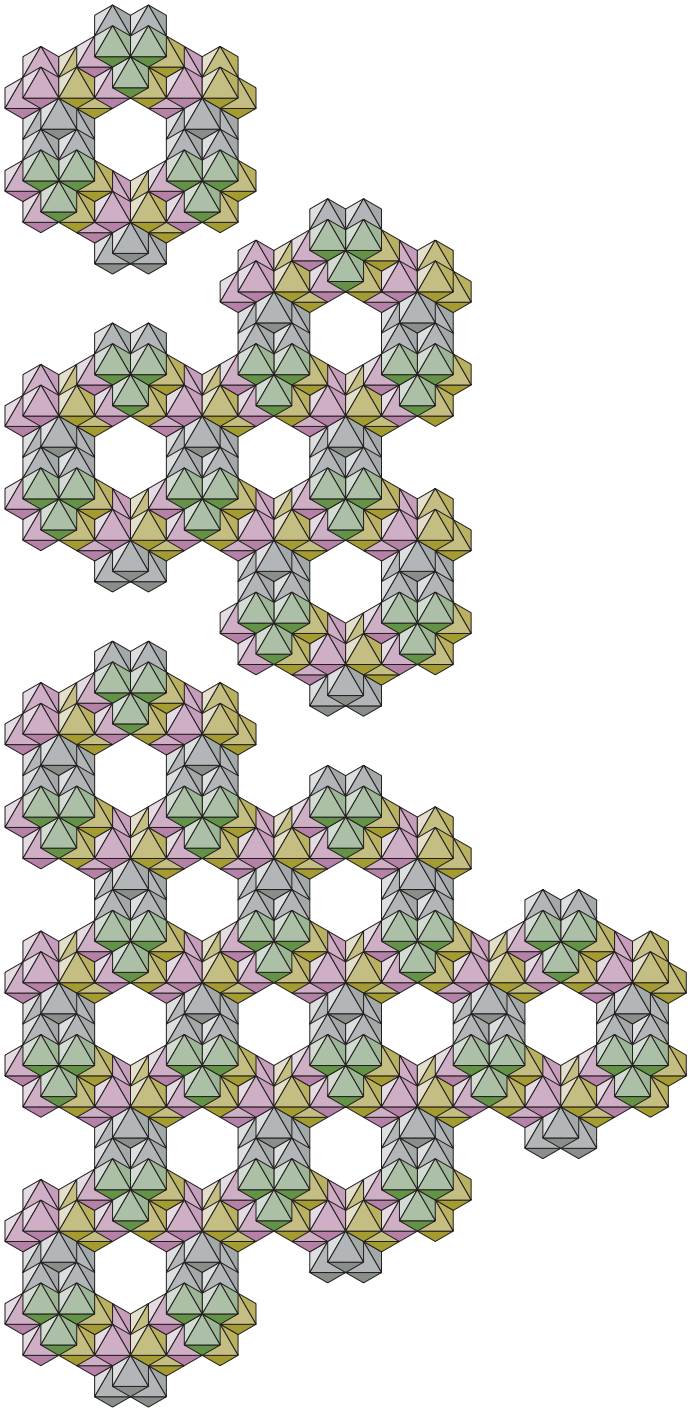


Fig. 25 Triangular assemblies of rings of six diamond CFUs

The figure shows triangular assemblies of rings of six diamond CFUs each. The lone ring can join with identical rings to form polyhedral assemblies. The multiple ring assemblies do not seem likely to make polyhedral assemblies.



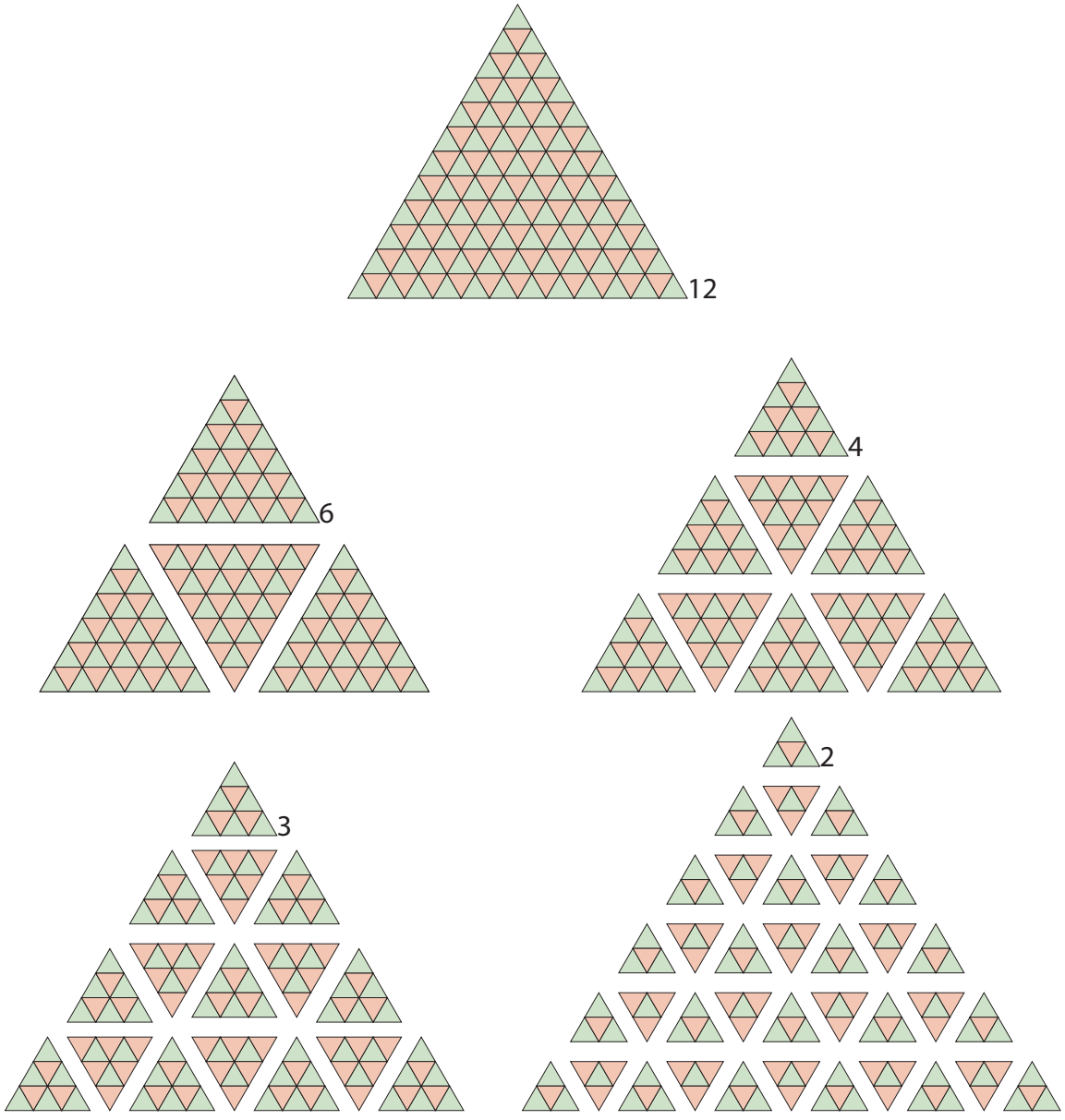


Fig. 26 Assembling a 12-triangle panel from smaller triangular panels

The figure shows four ways in which smaller triangular panels can assemble as the 12-triangle shown at the top–four 6-triangles (middle left), nine 4-triangles (middle right), sixteen 3-triangles (bottom left), thirty-six 2-triangles (bottom right).