Icosahedral assemblies of Si-atoms

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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. See **Octahedron1stEd.pdf.**

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

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

The file **C60fullerene.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. The file may be downloaded at the URL

http://homepage.mac.com/whitby/Quasicrystals/FileSharing171.html

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

Triangular panels consisting solely of graphite CFUs of three C-atoms each produce icosahedral assemblies having 60, 240, 540, 960, 1500, 2160...C-atoms. This series of numbers occurs in fullerenes. The number of CFUs in a triangular panel is the square of the number of CFUs along the panel's edge. The number of C-atoms in a CFU is three. The number of panels per icosahedron is twenty. The number of atoms in an icosahedral assembly is 3*20*n^2 where n is the number of CFUs along the panel's edge.

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. It can be downloaded using the URL--

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

4. The structure and stability of Si60 and Ge60 cages: A computational study by Zhongfang Chen, Haijun Jiao, Gotthard Seifert, Anselm H. C. Horn, Dengke Yu, Tim Clark, Walter Thiel, Paul Von Ragué Schleyer, *Journal of Computational Chemistry,* v. 24, no. 8, pp. 948 - 953, Wiley Periodicals, Inc.,Published Online: 14 Apr 2003

http://www3.interscience.wiley.com/cgi-bin/abstract/104525216/ABSTRACT

Introduction

This file has been prompted by references to a Si60-cluster which resembles the C60-fullerene

such as Reference 4. It shows two ways in which three Si-atoms can form a triplet that can act as one of twenty identical panels in forming a rigidly structural regular icosahedral assembly.

Figure 1 shows two different Si-triplets in which the Si-atoms are identically oriented. It shows how each of the Si-atoms of one triplet can be cleftly joined to the same C-atom. The Si-atoms of the second triplet can be cleftly joined by three C-atoms each of which joins a pair of adjacent Si-atoms.

Figure 2 compares each of the Si-triplets to the C-triplet of the C60-fullerene.

Figure 3 shows each of the icosahedral faces defined by the C-triplet and the two Si-triplets.

Figures 4, 5, and 6 show how twenty of one type of Si-triplet assemble to fully enclose an icosahedral volume.

Figures 7, 8, and 9 show how twenty of the other type of Si-triplet assemble as an open icosahedral cage.

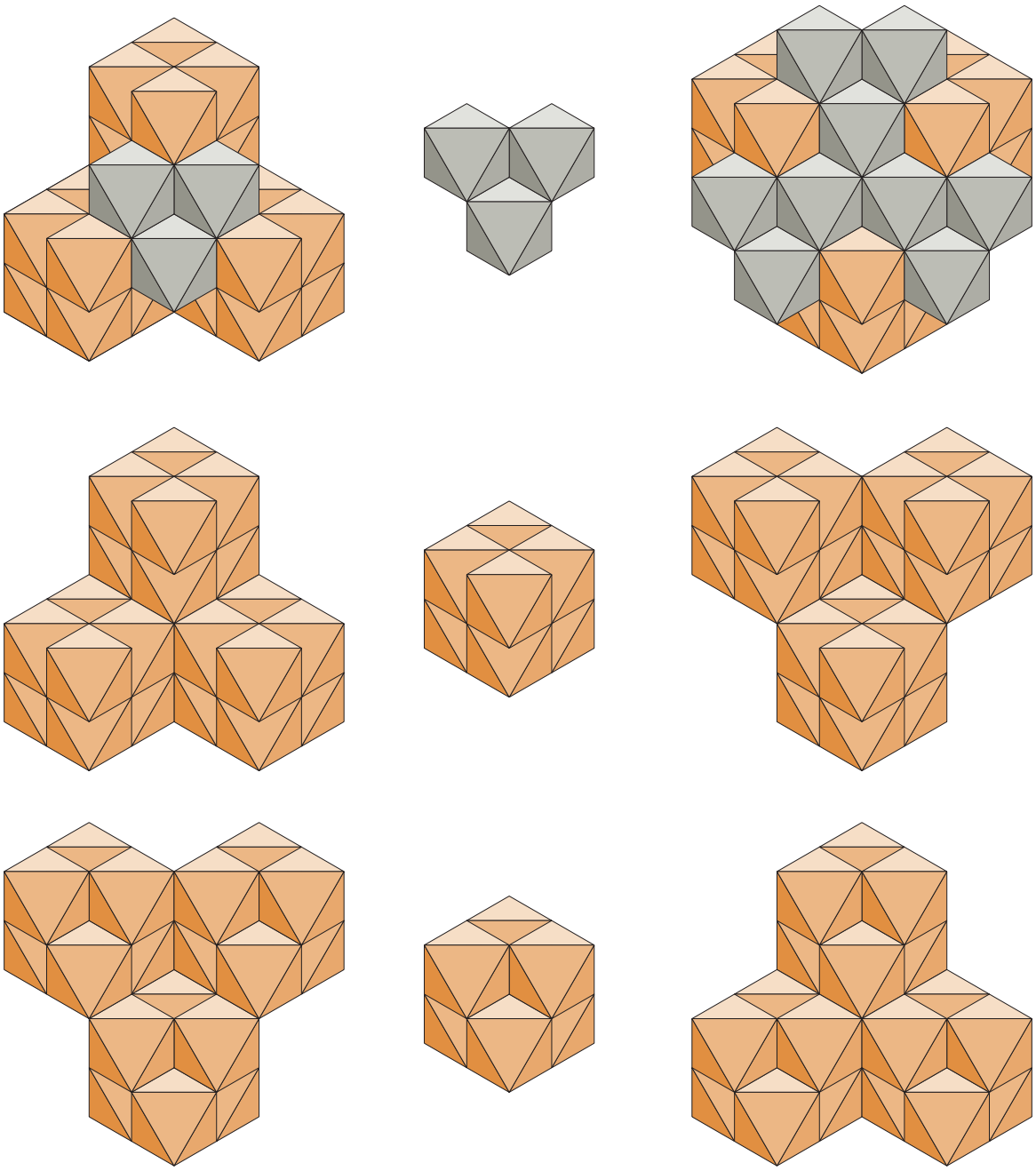

Fig. 1 Two Si-atom triplets

The figure shows two ways in which three Si-atoms can form a triplet that can serve as a panel of an icosahedral assembly of sixty Si-atoms.

In the middle row, each Si-atom is oriented so that its Si-octa is nearest the viewer. A lone Si-atom is in the middle column; the two triplets are in the left and right columns. The orientation of each He-octa of each of the atoms of each of the triplets is the same as each of the other He-octas.

In the bottom row, the two triplets and the Si-atom separating them are inverted.

In the top row, each Si-atom of the triplet on the left is cleftly joined to a common C-atom. Each Si-atom of the triplet on the right is cleftly joined to two C-atoms. A lone C-atom is shown in the middle of the row.

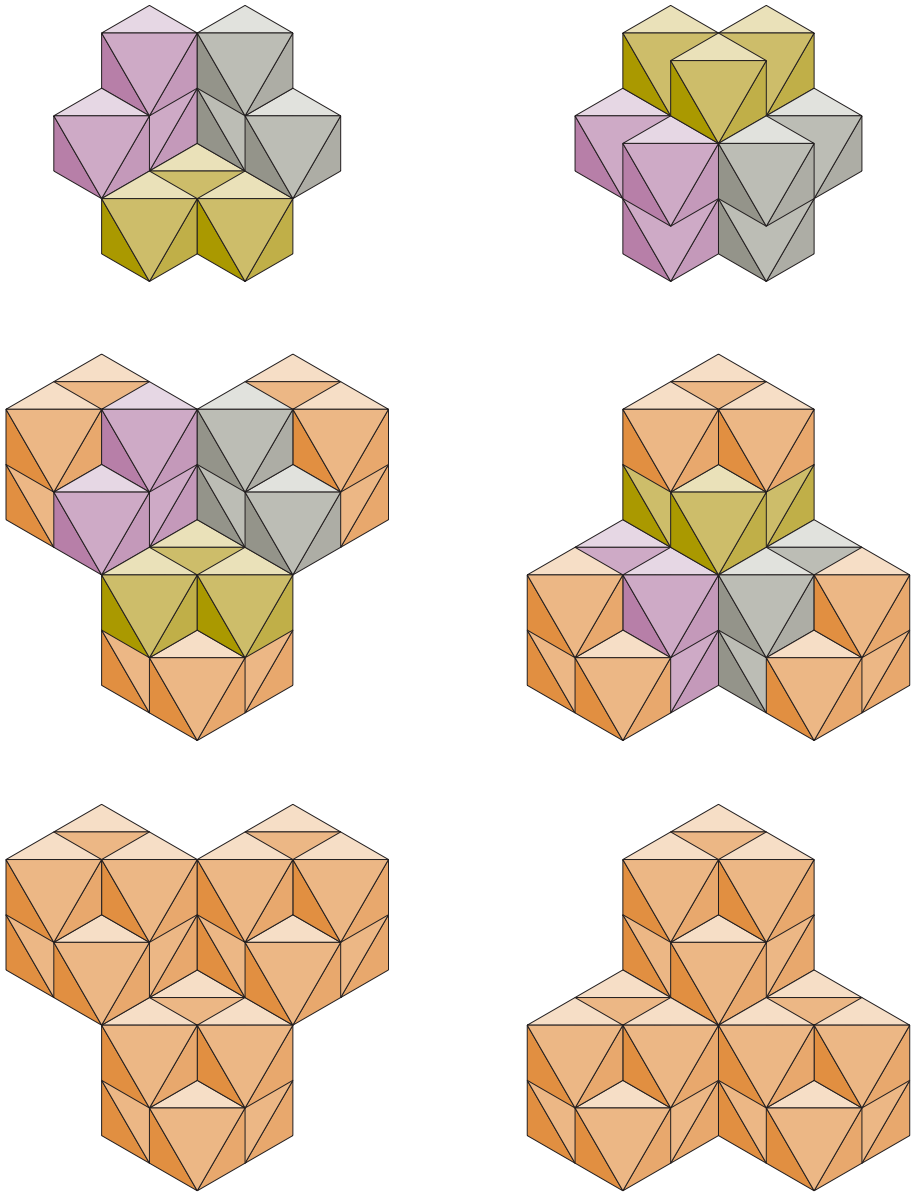

Fig. 2 Comparison of the C60 and Si60 panels

The figure compares the three-atom panels that form the icosahedral assemblies of sixty C-atoms or sixty Si-atoms. Each panel is shown as it would appear from the centroid of the assembly.

Two views of the three C-atom graphite CFU are shown in the top row. Twenty of these CFUs assemble as the facial panels of two types of regular icosahedral C60 assemblies.

In the bottom row, two types of three Si-atom panels of regular icosahedral Si60 assemblies are shown.

In the middle row, each type of carbon panel is substituted for its equivalent portion of the corresponding type of silicon panel.

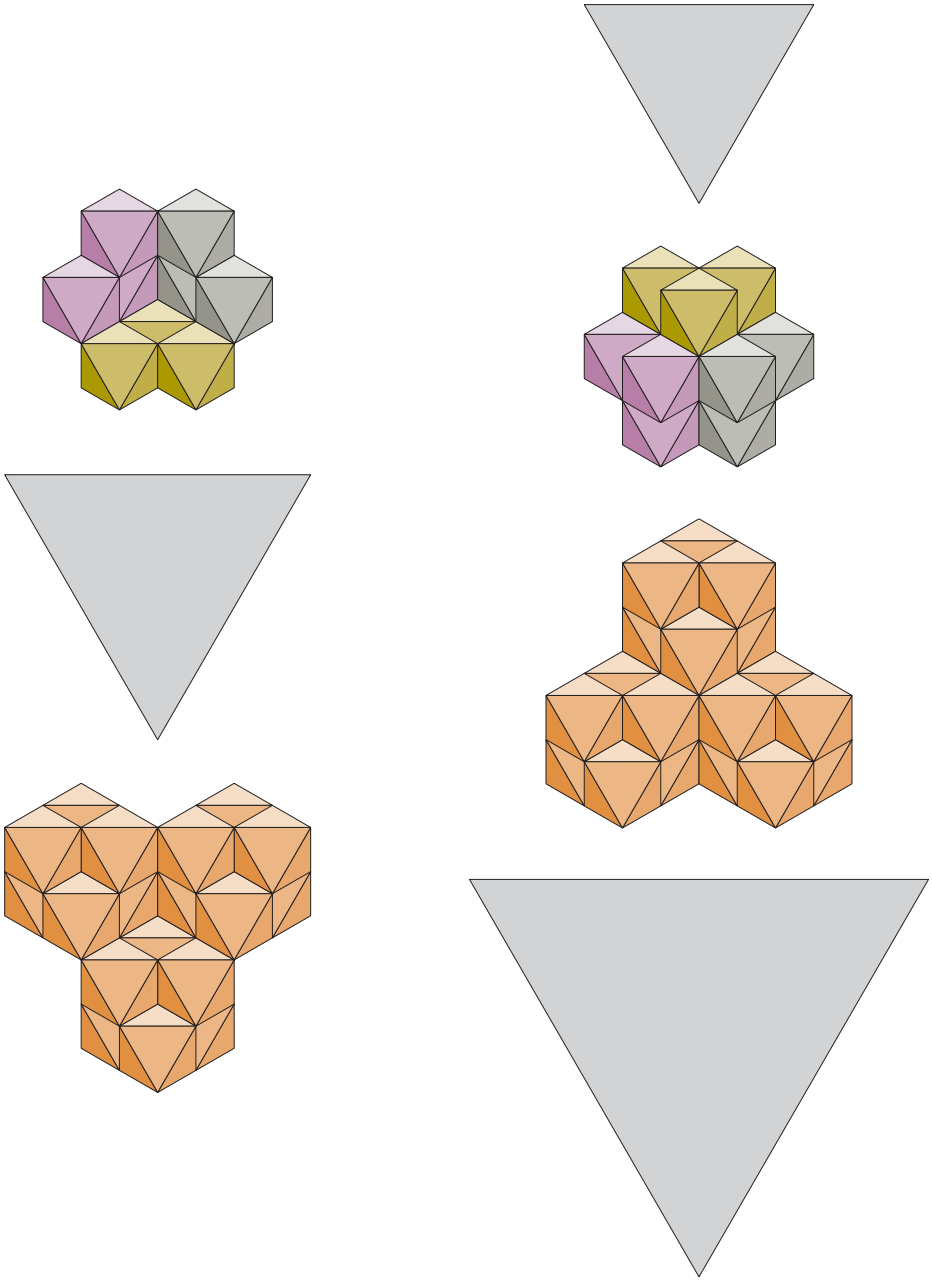

Fig. 3 Comparisons of sizes of icosahedral faces defined by C60 and Si60 panels

The figure shows the icosahedral face defined by the two types of C3 panel and the two orientations of the Si3 panel.

The two panels in the left column define the same size icosahedral face. The face has an edge length of four He-octa edges.

The icosahedral face defined by the orientation of the C3 panel is shown at the top of the column on the right; the icosahedral face defined by the second type of Si3 panels is shown at the bottom of the same column. The face at the top has an edge length of three He-octa edges; the face at the bottom has an edge length of six He-octa edges.

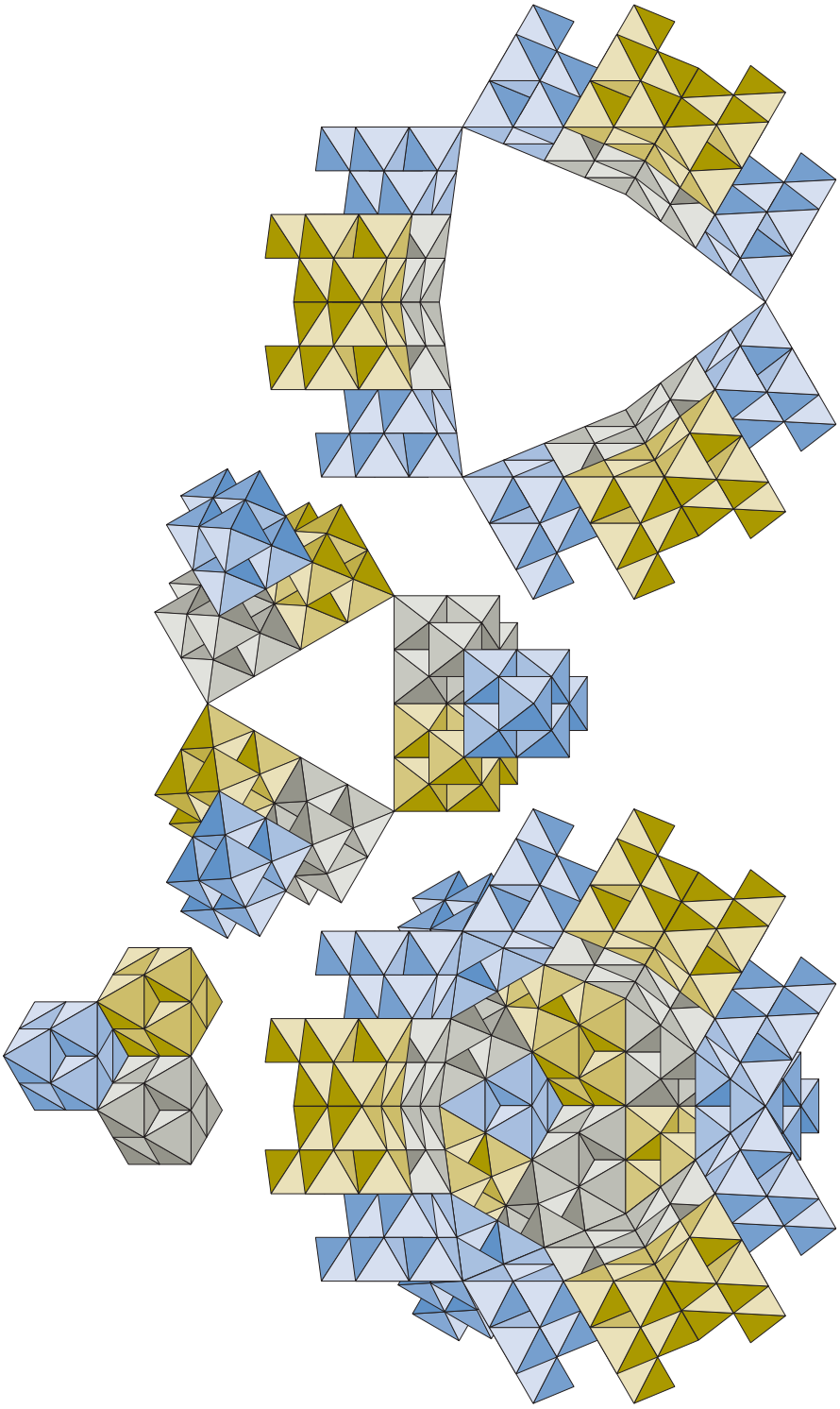

Fig. 4 Assembly of the lower half of a Si60-icosahedron of edge length four He-octa edges

The figure shows the ten panels of the lower half of the four He-octa edge length icosahedron running from the lower left to the upper right. The assembly itself is shown in the lower right. Each Si-atom of the triplet is colored either blue or yellow or gray. The icosahedral view is facial.

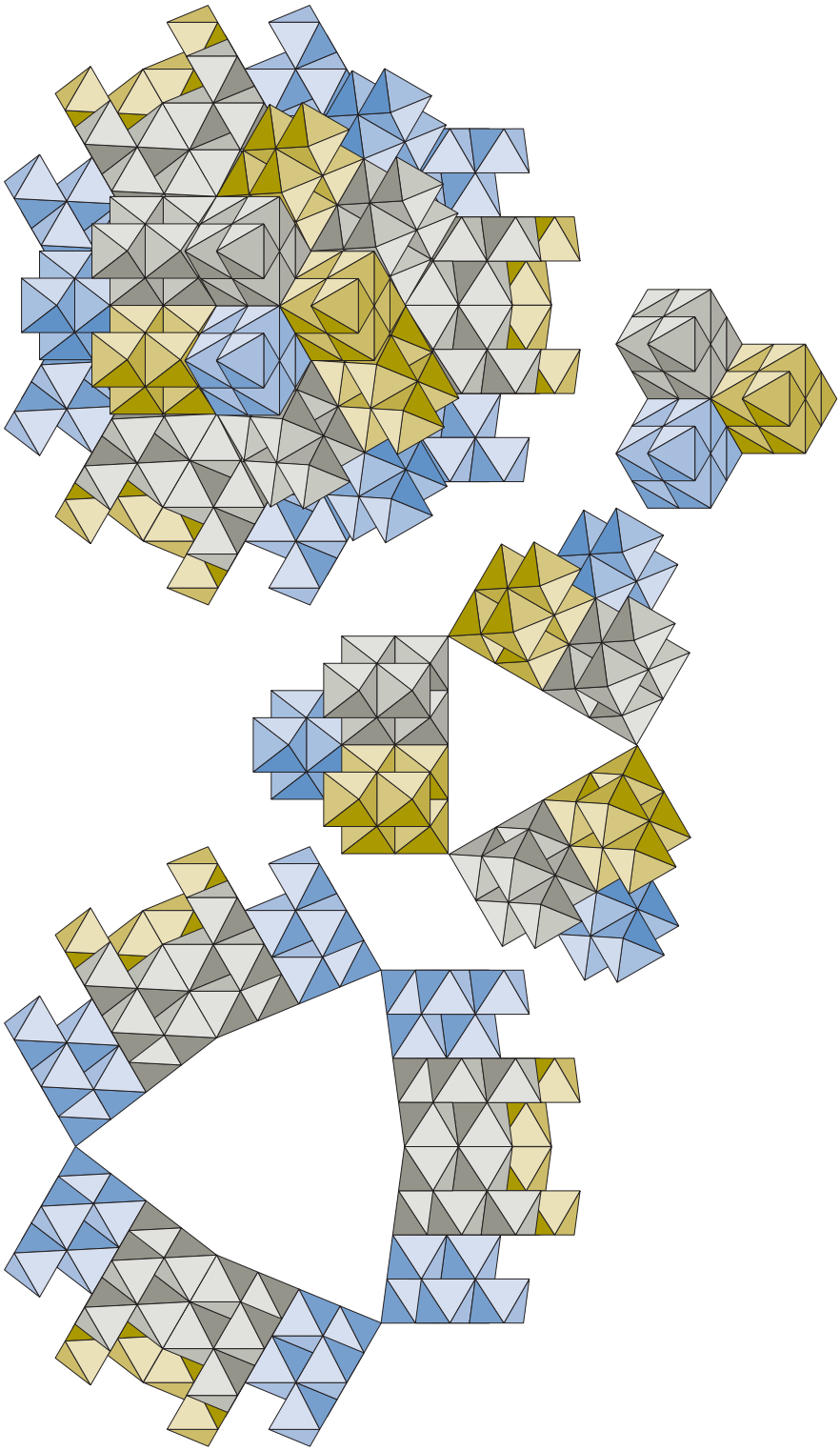

Fig. 5 Assembly of the upper half of a Si60-icosahedron of edge length four He-octa edges
The upper half of the Si60-icosahedron is shown in the upper left of the figure. The panels which compose it are shown running from the lower left to the upper right.

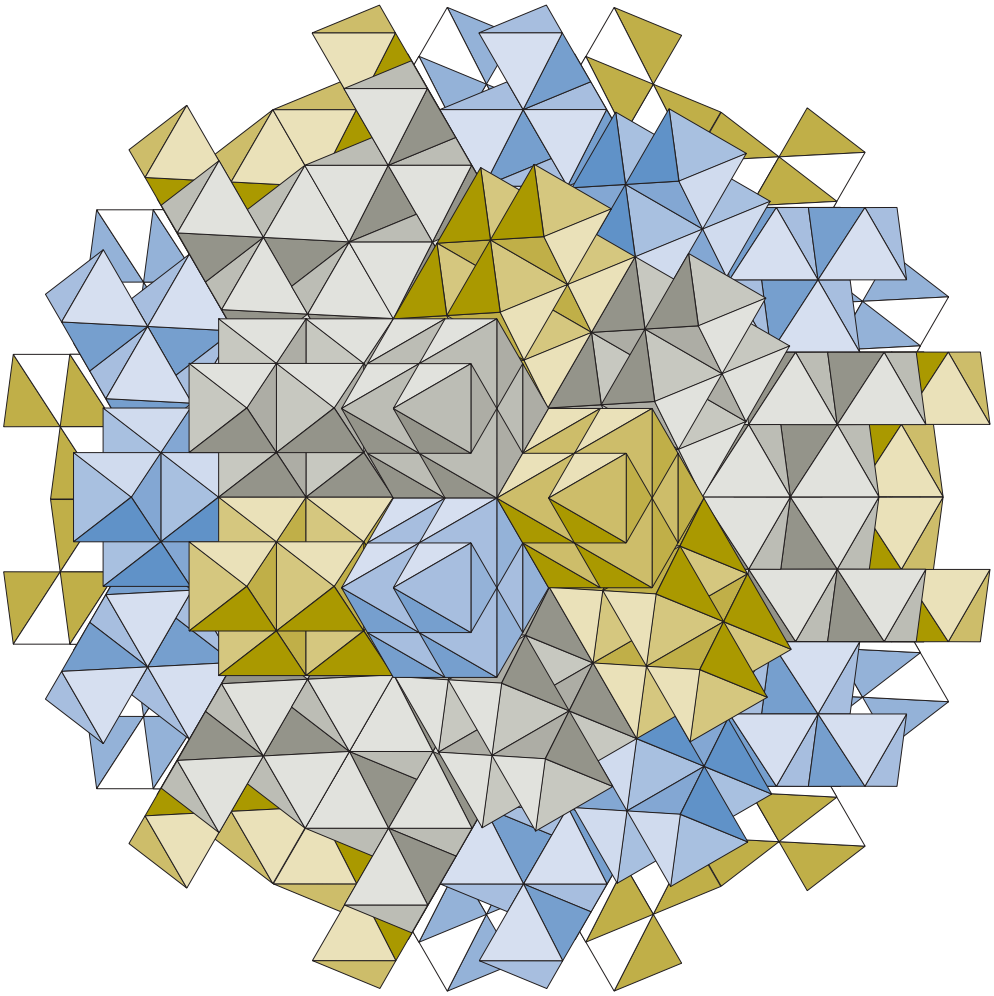

Fig. 6 Si60-icosahedron whose edge length is four He-octa edges–facial view
The figure shows the facial view of a an Si60-icosahedron whose edge length is four He-octa edges.

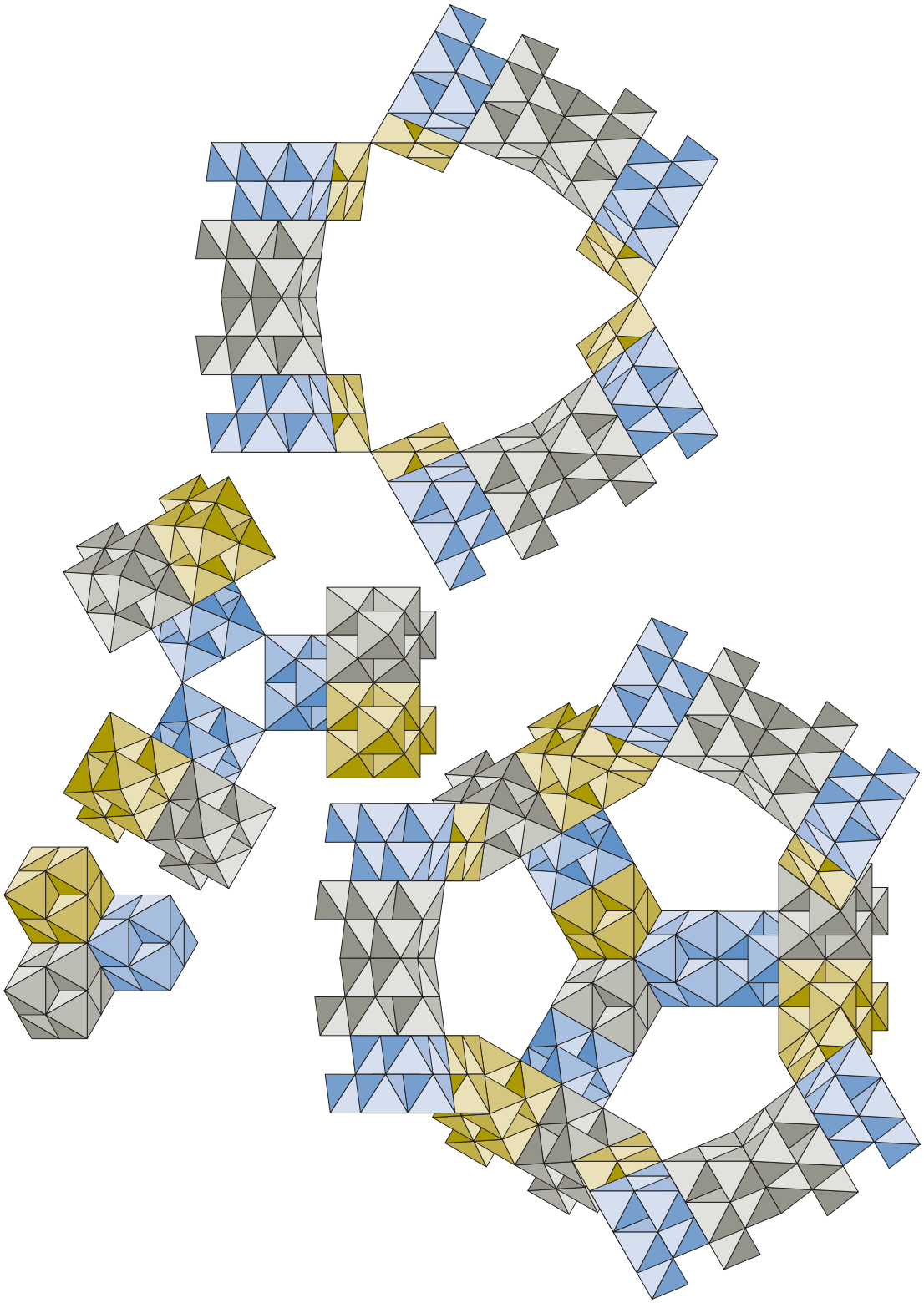

Fig. 7 Assembly of the lower half of a Si60-icosahedron of edge length six He-octa edges
The figure shows the assembly of the lower half of a six He-octa edge Si60 icosahedron.

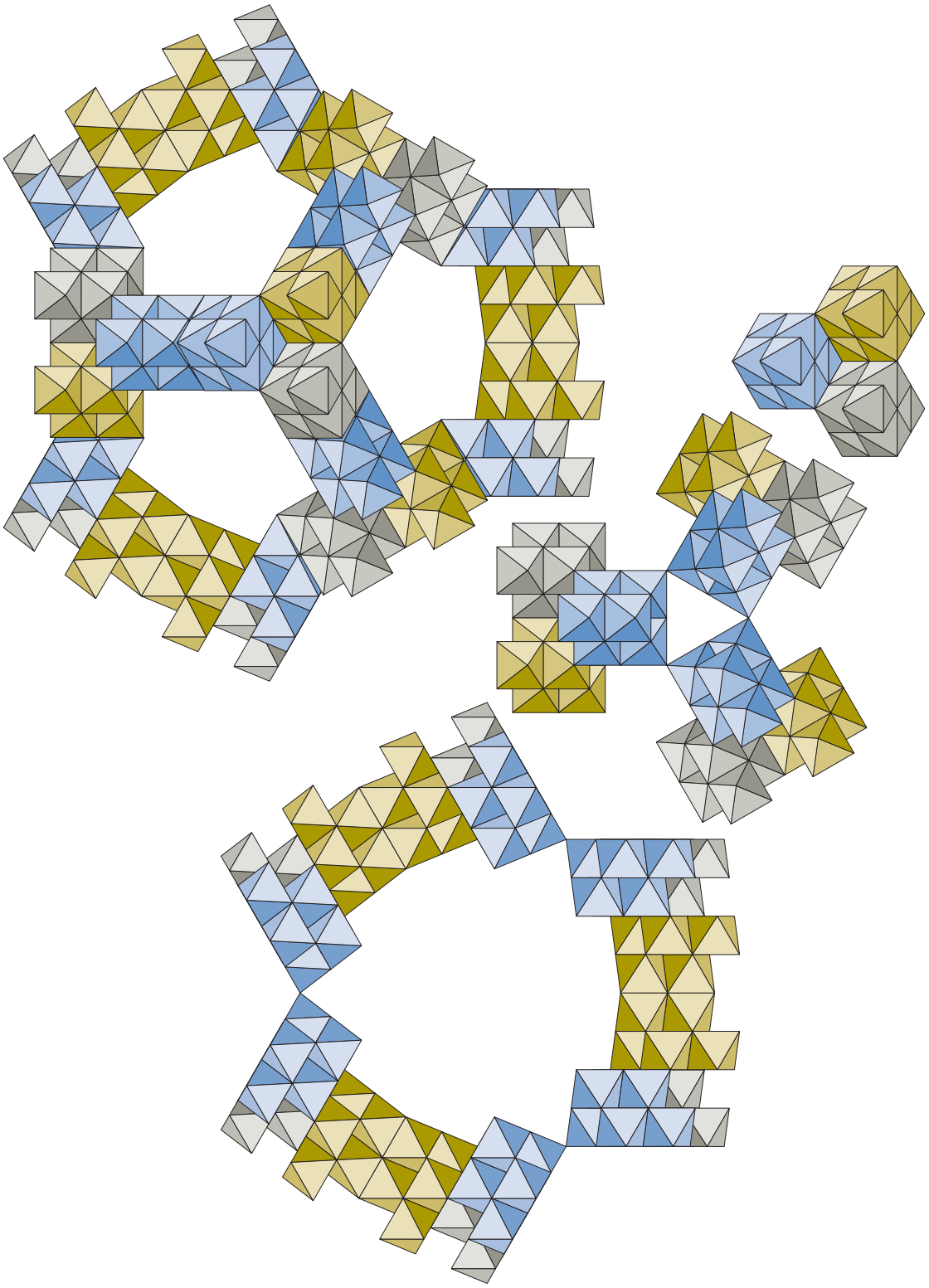

Fig. 8 Assembly of the upper half of a Si60-icosahedron of edge length six He-octa edges
The figure shows the assembly of the upper half of a six He-octa edge Si60 icosahedron.

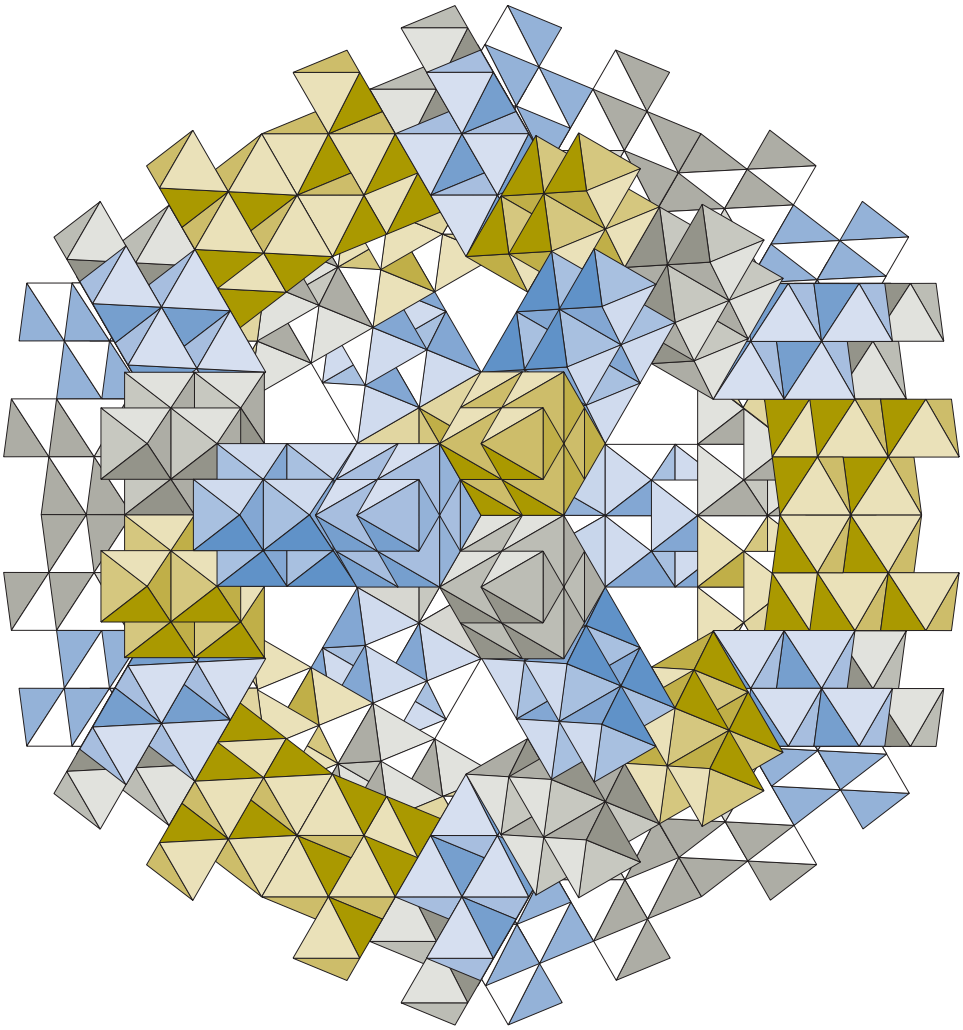

Fig. 9 Si60-icosahedron of edge length six He-octa edges
The figure shows a facial view of a six He-octa edge Si60-icosahedron.