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The Architecture and Growth of Extended Platonic Polyhedra

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Abstract

The formation of polyhedra has attracted much interest as an attractive research topic that is connected with chemistry. In this paper, we focus on the grow law of so-called Goldberg method based on Platonic polyhedra. There are four classes of extended Platonic polyhedra we can construct: the extended tetrahedra; the extended hexahedra; the extended octahedra; the extended dodecahedra. The extended tetrahedra, extended hexahedra, and extended dodecahedra are, respectively, assembled by using the method of adding hexagons, whereas the extended octahedra are made by means of adding squares. We also prove that this method fails to be applied to icosahedra. The study of the architecture and growth of extended Platonic polyhedra provides further insight into the molecular design and theoretical characterization of chemical molecules.

1. Introduction

The elegant structure of polyhedra makes it one of the basic forms of physical existence in nature. Beautiful crystals, a series of ball-like fullerenes [1, 2] and viral capsids [3, 4] are typical polyhedra in chemistry and biology. Platonic solids, the five simplest polyhedra with all faces regular, have attracted the special attention of chemists as structural models time and again since antiquity [5-7]. The five Platonic polyhedra are tetrahedron, cube, octahedron, dodecahedron and icosahedron. However, the polyhedral world is mysterious and there are more novel polyhedral solids waiting for us to explore [8, 9].

In 1937 [10], Goldberg proposed a mathematical method to generate a kind of 'multi-symmetric' polyhedra. These so-called Goldberg polyhedra have been found as mathematical modes of icosahedral fullerenes science than. Then in 1971 [11], Coxeter also found the same operation in order to explain the structural principle of spherical viral capsids. Deza et al. [12, 13], recently, recalled the Goldberg-Coxeter construction to build a large collection of 3- and 4-valent plane graphs, while some related structural properties, such as zigzags and central circuits, are described in [14, 15]. They decomposed this method into some simpler well-known operations, such as medial, leapfrog, and *k*-inflation [16]. In particular, the chirality of fullerene can be determined during the Goldberg construction [17]. On the other hand, two series of extended Goldberg polyhedra [18-20] were constructed from Goldberg polyhedra, which preserve icosahedral symmetry and are similar to some viral capsids which abide by Caspar-Klug theory [3]. We also proposed two combinatorial operations to generate a kind of chemically potential cages based on Goldberg polyhedra [21].

This paper presents the Goldberg method by adding regular polygons in another point of view, which maintains the symmetry in the operation. In Golberg's seminal paper [10], dodecahedron was used as a case to explain this symmetrical operation. According to this idea, we apply it to other four Platonic polyhedra and generate extended Platonic polyhedra. These extended Platonic polyhedra are assembled by adding hexagons and squares to Platonic solids and they may belong to the subset of some bifaced regular polyhedra discussed by Deza and Grishukin [22], but keep the symmetry of original polyhedra. Therefore, these particular bifaced regular polyhedral modes have already played an important role as models for chemical molecules [23, 24], or will also found their chemical analogues in the future.

2. Goldberg method and Extended Dodecahedra

In this paper, we will introduce the Goldberg method proposed in ref. [10], which consists of three steps: splitting, adding and assembling. In the following, the method will be explained in detail by using dodecahedron as an example.

The first step is splitting, which means to break a dodecahedron down into twelve regular pentagonal pieces, as shown in Figure 1.

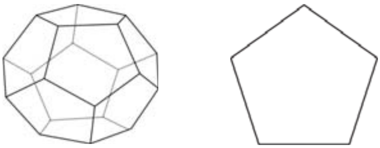

Fig. 1 The operation of breaking a dodecahedron into twelve regular pentagonal pieces.

The second step is adding, which refers to inserting several hexagons in twelve pentagons of a dodecahedron in a coherent way. The fact that hexagons are added to one pentagon of a dodecahedron regularly is shown in Figure 2.

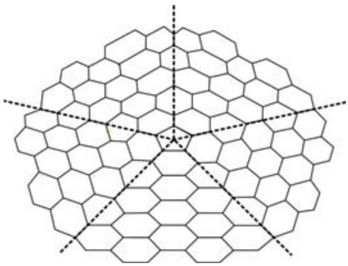

Fig. 2 Adding hexagons to a pentagon in a coherent way.

The third step is assembling, which indicates that assemble all twelve parts in which hexagons are added to pentagons regularly. For example, an extended dodecahedron of 72-hedron [$5^{12}6^{60}$] is assembled from 12 regular pentagons of a dodecahedron to which 5 hexagons are added respectively.

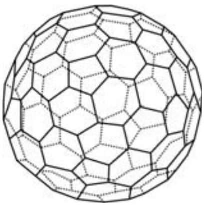

Fig. 3 The 72-hedron contains 12 pentagons and 60 hexagons.

The study of the Goldberg method, from Figure 1 to Figure 3, reveals two outstanding properties:

(1) The resulting polyhedra are vertex regular and the degree of vertex remains unchanged during the construction. For example, the degree of extended dodecahedron is three, the same as the initial dodecahedron.

(2) The symmetrical property of the Platonic polyhedra is one which remains unchanged when adding regular polygons. Given an extended dodecahedron with I or I_h, the initial pentagons lie on axises of rotation of order 5, while the positions of 2- and 3- fold axises are at the edges and centers of hexagons.

Proposition 2.1 *For any extended dodecahedra, the adding polygons are hexagons.*

Proof Suppose that x regular y-gons are added to the dodecahedron, and then the extended dodecahedron will satisfy these conditions as follows:

$$F = 12 + x \tag{1}$$

$$E = 30 + \frac{xy}{2} \tag{2}$$

$$V = 20 + \frac{xy}{3} \tag{3}$$

where F, E and V are the number of faces, edges and vertices respectively.

Then plug these conditions into Euler formula: $\mathrm{F} - \mathrm{E} + \mathrm{V} = 2$ and get $(12 + \mathrm{x}) - (30 + \mathrm{xy}/2) + (20 + \mathrm{xy}/3) = 2$, then $\mathrm{x}(1 - \mathrm{y}/6) = 0$ and finally we can derive the following result: $\mathrm{y} = 6$. This completes the proof.

The adding of hexagons should follow the particular rule in accordance with the symmetrical restraint. The Figure 4 shows how to add hexagons around an initial pentagon. As shown in the figure, the adding hexagons are divided into five identical parts, where the 5-fold symmetry of pentagons maintains in the adding process. Likewise, Figure 5 shows the distribution of adding hexagons to one hexagon. The adding hexagons can be divided into six identical parts to make the 2-fold and 3-fold symmetry unchanged.

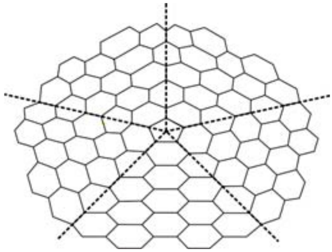

Fig. 4 The adding of hexagons around a pentagon.

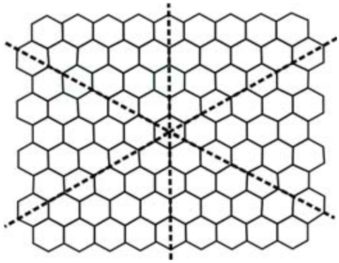

Fig. 5 The distribution of adding hexagons to one hexagon.

Comparing the fact that hexagons are added to the pentagon with that hexagons are added to the hexagon topologically, we will find that they have the same number of hexagons in one part, as is shown in Figure 6. According to the above two rules, the number of hexagons can be calculated by considering the distribution of hexagons in a polar coordinate. The Figure 6 shows the distribution of hexagons in each part.

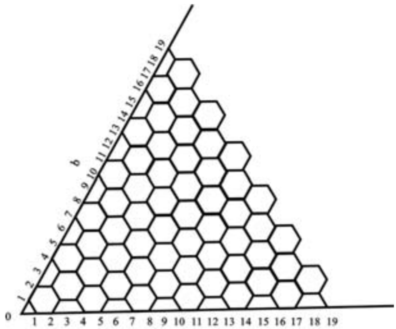

Fig. 6 The distribution of hexagons in one part.

Using a,b as the inclined coordinates of the vertex of a part, the square of the distance from the center of the part to the vertex is $\mathrm{a}^2+\mathrm{ab}+\mathrm{b}^2$. With the mathematical method, we can figure out that the number of hexagons added to a pentagon in one part is $(\mathrm{a}^2+\mathrm{ab}+\mathrm{b}^2-1)/6$. Since there are five equal parts, the number of hexagons added to a pentagon is $5(\mathrm{a}^2+\mathrm{ab}+\mathrm{b}^2-1)/6$. Similarly, the number of hexagons added to a dodecahedron is $10(\mathrm{a}^2+\mathrm{ab}+\mathrm{b}^2-1)$ due to twelve symmetrically distributed pentagons and adding twelve pentagons we can easily compute that the total number of faces in this polyhedron is $10(\mathrm{a}^2+\mathrm{ab}+\mathrm{b}^2)+2$.

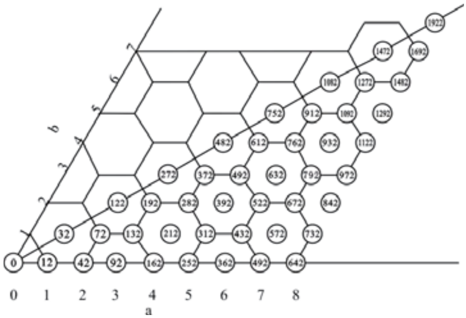

Fig. 7 The number of faces of the extended dodecahedra.

As shown in Figure 7, the numbers in the circles denote the number of faces of extended dodecahedra, which are also called “Goldberg polyhedra” somewhere else [10]. For example, 42-, 72- and 92-hedron are shown in Figure 8.

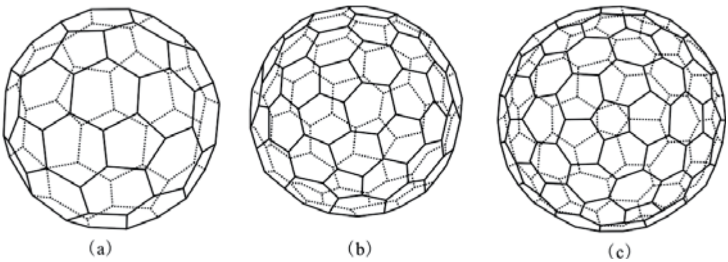

Fig. 8 Three extend dodecahedra. (a) 42, (b) 72 and (c) 92-hedron.

Therefore, the numbers of faces F, vertices V and edges E of the polyhedra derived from

Goldberg's method can be expressed as:

$$F = 10(a^2 + ab + b^2) + 2 \tag{4}$$

$$E = 30(a^2 + ab + b^2) \tag{5}$$

$$V = 20(a^2 + ab + b^2) \tag{6}$$

If $a = 0$ then $b \neq 0$, or vice versa.

3. Extended Tetrahedra

Similar with the extended dodecahedra, the extended tetrahedra also have two properties as follows:

(1) The degree of vertex of the extended tetrahedra is three.

(2) The symmetry of the extended tetrahedra is T or T_d.

Proposition 3.1 *For any extended tetrahedra, the adding polygons are hexagons.*

Proof Suppose that x regular y-gons are added to a tetrahedron, and then the extended tetrahedra will satisfy these conditions as follows:

$$F = 4 + x \tag{7}$$

$$E = 6 + \frac{xy}{2} \tag{8}$$

$$V = 4 + \frac{xy}{3} \tag{9}$$

Plug F, E and V into Euler formula, yield $(4 + x) - (6 + xy/2) + (4 + xy/3) = 2$, then $x(1 - y/6) = 0$ and finally we can get the following result: $y = 6$. This completes the proof.

Thus, the extended tetrahedra are a kind of polyhedra that contain 3-gons and 6-gons. Combining the symmetrical restraint, the hexagon adding rule is same as the extended dodecahedra, as shown in Figure 5 and 6. The Figure 9 shows the distribution of the faces of hexagons in each part. It is easy to calculate that the number of hexagons added to a regular triangle in one part is $(a^2 + ab + b^2 - 1)/6$. Since there are three equal parts, the number of hexagons added to a regular triangle is $(a^2 + ab + b^2 - 1)/2$. The number of hexagons added to a tetrahedron is $2(a^2 + ab + b^2 - 1)$ because of four symmetrically distributed triangles and adding the four triangles, the total number of faces in this polyhedron is $2(a^2 + ab + b^2) + 2$, which is shown in Figure 9.

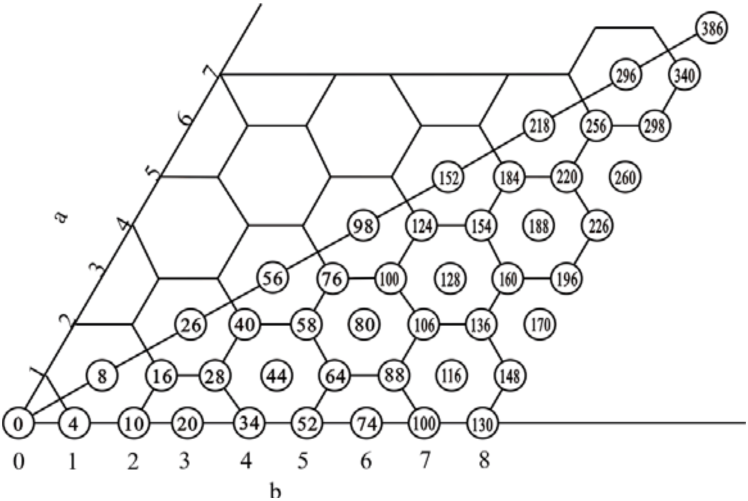

Fig. 9 The numbers of faces of the extended tetrahedra.

The numbers of faces F, vertices V and edges E of this type of polyhedra obtained from Goldberg's method are given by:

$$F = 2(a^2 + ab + b^2) + 2 \tag{10}$$

$$E = 6(a^2 + ab + b^2) \tag{11}$$

$$V = 4(a^2 + ab + b^2) \tag{12}$$

As an example, when $a = b = 1$, the obtained extended tetrahedron is actually truncated tetrahedron of Archimedean polyhedra. Some carbon-containing compounds own this structure. The C_n polyhedra of fullerene (or ball-shaped alkane) with hexagonal and triangular faces possess the highest T_d symmetry [25]. They have relation with their dual polyhedra of closed boron hydride with 3 or 6 edges, as illustrated in Figure 10.

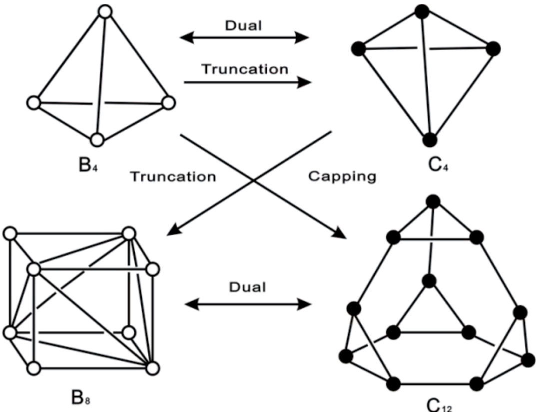

Fig. 10 The dual polyhedra of B_n and C_n with T_d symmetry.

Decahedron, hexadecahedron and icosahedron of this type of polyhedra are shown in Figure 11.

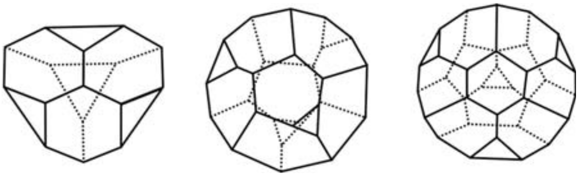

Fig. 11 Decahedron $(a = 2, b = 0)$, hexadecahedron $(a = 2, b = 1)$ and icosahedrons $(a = 3, b = 0)$.

4. Extended Hexahedra

In the case of extended hexahedra, they also have two properties as follows:

(1) The degree of vertex of the extended hexahedra is three.

(2) The symmetry of the extended hexahedra is O or O_h.

Proposition 4.1 *For any extended hexahedra, the adding polygons are hexagons.*

Proof Suppose that x regular y-gons are added to a hexahedron, and then the extended hexahedron will satisfy these conditions as follow:

$$F = 6 + x \tag{13}$$

$$E = 12 + \frac{xy}{2} \tag{14}$$

$$V = 8 + \frac{xy}{3} \tag{15}$$

Then substitute F, E and V into Euler formula, and get $(6 + \mathrm{x}) - (12 + \mathrm{xy}/2) + (8 + \mathrm{xy}/3) = 2$, then $\mathrm{x}(1 - \mathrm{y}/6) = 0$ and finally solving for y we get the following result: $\mathrm{y} = 6$. This completes the proof.

Thus, the extended hexahedra are a kind of polyhedra that contain 4-gons and 6-gons. Combining the symmetrical restraint, the hexagon adding rule is same as the extended dodecahedra, as shown in Fig 5 and 6. Therefore, the number of hexagons added to a square in one part is $(\mathrm{a}^2 + \mathrm{ab} + \mathrm{b}^2 - 1)/6$. Since there are four equal parts, the number of hexagons added to a square is $2(\mathrm{a}^2 + \mathrm{ab} + \mathrm{b}^2 - 1)/3$. The number of hexagons added to a hexahedron is $4(\mathrm{a}^2 + \mathrm{ab} + \mathrm{b}^2 - 1)$ because of 6 symmetrically distributed squares and adding the 6 squares, the total number of faces in this polyhedron is $4(\mathrm{a}^2 + \mathrm{ab} + \mathrm{b}^2) + 2$, which is shown in Figure 12.

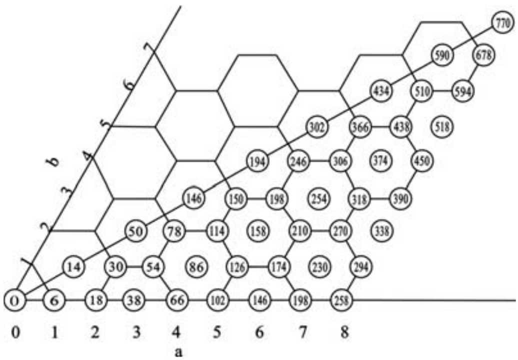

Fig. 12 The numbers of faces of the extended hexahedra.

Thus the numbers of faces F, vertices V and edges E of this type of polyhedra obtained from Goldberg's method are described as

$$F = 4(\mathrm{a}^2 + ab + b^2) + 2 \tag{16}$$

$$E = 12(a^2 + ab + b^2) \tag{17}$$

$$V = 8(a^2 + ab + b^2) \tag{18}$$

As an example, when a = b = 1, the obtained extended hexahedron is actually truncated octahedron of Archimedean polyhedra. Some carbon-containing compounds also own this structure. The C_n polyhedra of fullerene (or ball-shaped alkane) that with hexagonal and quadrilateral faces have the highest O_h symmetry [25]. They have relation with their dual polyhedra of blocked boron hydride with 4 or 6 edges, as illustrated in Figure 13.

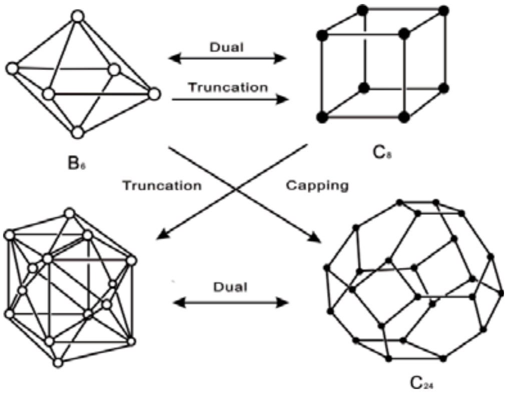

Fig. 13 The dual polyhedra of B_n and C_n with O_h symmetry.

5. Extended Octahedra

Goldberg [10] didn't refer the case of adding polygons to an octahedron, instead, we find that the way of constructing the above three polyhedra can also be applied to octahedron. The difference is that the adding polygons for extended octahedra are squares, rather than hexagons. This is because the degree of vertex of octahedron is four.

For the extended octahedra, they have two properties as follow:

(1) The degree of vertex of the extended octahedra is four.

(2) They belong to the octahedrite family [13], with the symmetry of O or O_h.

Proposition 5.1 *For any extended octahedra, the adding polygons are squares.*

Proof Suppose that x regular y-gons are added to a hexahedron, and then the obtained extended octahedra will satisfy these conditions as follow:

$$F = 8 + x \tag{19}$$

$$E = 12 + \frac{xy}{2} \tag{20}$$

$$V = 6 + \frac{xy}{4} \tag{21}$$

Then plug F, E and V into Euler formula, and get $(8 + \mathrm{x}) - (12 + \mathrm{xy}/2) + (6 + \mathrm{xy}/4) = 2$, then $\mathrm{x}(1 - \mathrm{y}/4) = 0$ and finally solving for y we get the following result: $\mathrm{y} = 4$. This completes the proof.

Combining the symmetrical restraint, the adding of squares should follow the particular rule. The Figure 14 shows how to add squares around an initial triangle. As shown in the figure, the adding squares are divided into three identical parts, which the 3-fold symmetry of pentagons maintains in the adding process. Likewise, the Figure 15 shows the distribution of adding squares to one square. The adding squares can be divided into four identical parts to make the 2-fold and 4-fold symmetry unchanged. Accordingly, the extended octahedra keep the symmetry of octahedra, O or O_h. Similarly, comparing the fact that hexagons are added to the regular triangle with that hexagons are added to the hexagon topologically, we will find that they have the same number of hexagons in one part. Accordingly, the number of squares can also be calculated by considering the distribution of squares in a polar coordinate. The Figure 16 shows the distribution of squares in each part. As such, we can calculate that the number of squares added to a triangle in one part is $(\mathrm{a}^2 + \mathrm{b}^2 - 1)/4$. Since there are three equal parts, the number of squares added to a triangle is $3\,(\mathrm{a}^2 + \mathrm{b}^2 - 1)/4$. The number of squares added to an octahedron is $6(\mathrm{a}^2 + \mathrm{b}^2 - 1)$ because of eight symmetrically distributed triangles and adding the eight triangles, the total number of faces in this polyhedron is $6(\mathrm{a}^2 + \mathrm{b}^2) + 2$, which is shown in Figure 17.

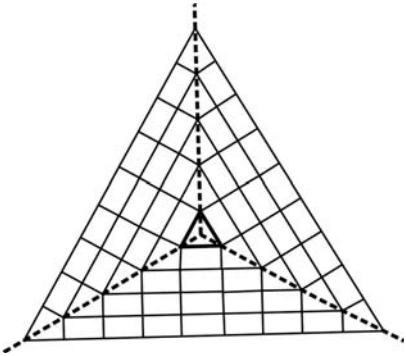

Fig. 14 The distribution of adding squares to one triangle regularly.

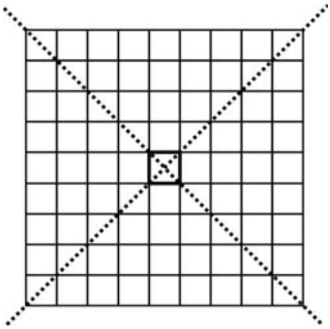

Fig. 15 The distribution of adding squares to one square regularly.

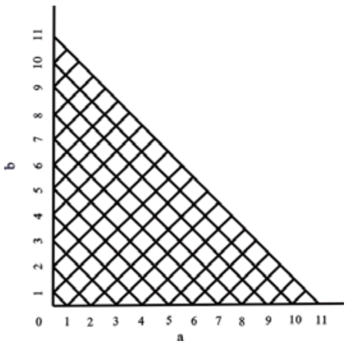

Fig. 16 The distribution of squares in one part.

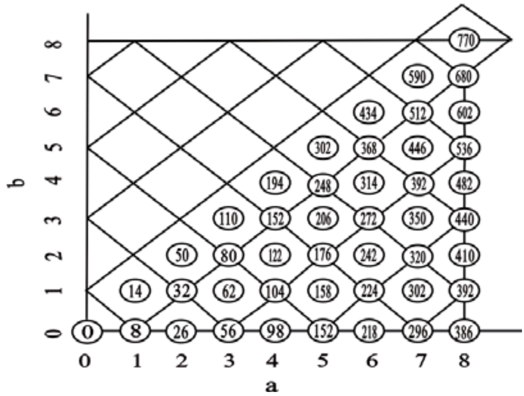

Fig. 17 The numbers of faces of the extended octahedra.

The numbers of faces F, vertices V and edges E of this type of polyhedra obtained from Goldberg's method are described as

$$F = 6(a^2 + b^2) + 2 \tag{22}$$

$$E = 12(a^2 + b^2) \tag{23}$$

$$V = 6(a^2 + b^2) \tag{24}$$

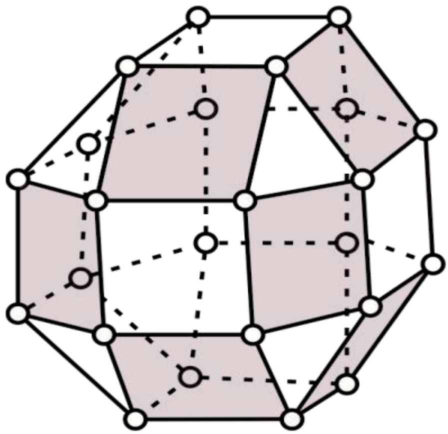

Fig. 18 Parallelogram faces of AgO_4 radical from 26-hedron.

As an example, when $a = b = 1$, the obtained extended octahedra are actually cuboctahedron of Archimedean polyhedra. Cluster nucleus atoms in transition-metal cluster compound form similar tetrakaidecahedron [$4^6 3^8$], such as $[Rh_{13}H_2(CO)_{24}][P(CH_2Ph)Ph_3]_3$. If $a = b = 2$, then the resulting 26-hedron is rhombicuboctahedron of Archimedean polyhedra. Ag_6O_8 in crystal of $Ag(Ag_6O_8)NO_3$ is similar to these structure in which Ag ion and O atoms make parallelogram faces of AgO_4 radical by dsp^2 hybridized orbit. These parallelogram faces form 26-hedron [4^{18} 3^8] by shared vertices, which is shown in Fig. 18.

6. Applying Goldberg method to Icosahedron

Unfortunately, we find that Goldberg method can't be applied to the icosahedron. It is assumed that Goldberg method be used in the icosahedron and the resulting polyhedra will satisfy these properties.

(1) The degree of vertex of this type of polyhedra is five.

(2) The symmetry of this type of polyhedra is I or I_h.

Supposing that x regular y-gons are added to an icosahedron, then the resulting polyhedron will satisfy these conditions as follow:

$$F = 20 + x \tag{25}$$

$$E = 30 + \frac{xy}{2} \tag{26}$$

$$V = 12 + \frac{xy}{5} \tag{27}$$

Substitute F, E and V into Euler formula, and get $(20 + x) - (30 + xy/2) + (12 + xy/5) = 2$, then $x\,(10 - 3y) = 0$ and finally solving for y we get the following result: $y = 10/3$. It means that polygons of a single type can't be added to the icosahedron according to Goldberg method.

7. Conclusion

Research on the Goldberg method based on dodecahedron reveals three construction steps: splitting, adding and assembling. This method can be applied to other Platonic polyhedra of regular tetrahedron, regular hexahedron and regular octahedron, but except regular icosahedron. Therefore, the extended tetrahedra, extended hexahedra and extended octahedra are proposed. According to their construction method and structures, we deduced their growth law and cited some actual examples of molecules in various disciplines. Although these polyhedra have been partly discussed in pervious works, our work indicates that the combination of Goldberg method for polyhedra and chemistry can be extended into a number of new areas for theories and methods in structural chemistry, and enrich the study of topological stereochemistry and be widely used in many fields.

Acknowledgments

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