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The Architecture of Extended Platonic Polyhedral Links

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Abstract

Polyhedral links proved to be effective mathematical models for new types of polyhedral molecules, especially DNA polyhedra. In this paper, we construct four types of polyhedral links based on extended Platonic polyhedra. By applying a new Euler formula and polyhedral growth law to these polyhedral links, their topological characteristics, including crossing number, component number and Seifert circle number, are computed, thus promoting the understanding of the topological structure and synthesis of extended Platonic polyhedral links. Our study indicates that, the new Euler formula and its three important parameters explain the architectures of most polyhedral links including their Euler characteristics and genus, which facilitates rational design and synthesis of new DNA molecules and intrinsically reveals the basic principles of novel structures.

Introduction

In nature, DNA has been utilized as the main material to perform various biological functions, such as storage and transmission of genetic information. In structural nanotechnology [1-3], DNA molecules have been used to assemble a large variety of three-dimensional (3-D) nanoscale structures [4,5], especially DNA polyhedra [6-12], and potential applications have begun to emerge [3,13]. In spite of the development of more advanced structures, the fact remains that we have a lot of technical issues to address and one of them is how to design and synthesize these DNA polyhedra efficiently. The deeper understanding of these intriguing architectures and topologies not only reveal their potential properties but also accelerate the process of their preparation.

In fact, techniques coming from mathematics have had great impact on chemistry and play an important role in investigating the tricky and complicated questions we are wrestling with. Euler's polyhedron formula, which transcends metric properties to topology, is a simple and important way for characterizing the relationship of three basic quantities of a polyhedron, vertices, edges and faces. Thus, it becomes an effective tool to address many issues related to polyhedra in chemistry. However, when it comes to the new architecture of DNA nanocages or even more complex DNA molecules, Euler's formula may have limitations in characterizing the new architecture. On the other hand, it has been proved that polyhedral links, interlinked and interlocked structures rather than classical polyhedra, are reasonable mathematical models for various DNA polyhedra and viral capsids [14-18], particularly those Qiu's group had constructed using topology and graph theory [19]. Moreover, polyhedral links, which consist of knots, helices, and holes instead of the standard building blocks of vertices, faces and edges, have had a new Euler's formula for DNA polyhedra already [20]. The numbers of components μ, of crossings c, and of Seifert circles s are related in a simple and elegant formula, $s+\mu=c+2$, which unites the basic features of the entangled structures of these more complex DNA polyhedra.

We have had discussed extended Platonic polyhedra and conclude their growth law before [21]. Four extended Platonic polyhedra are obtained, of which 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. The understanding of extended Platonic polyhedra facilitates the architecture of their polyhedral links. Moreover, the understanding of extended Platonic polyhedral links and the new Euler's formula contribute to the characterization and design of DNA cages with higher genus or even more complex DNA nanostructures.

This paper presents extended Platonic polyhedral links designed by four construction methods: type (Ⅰ) three or four branches curves and 2*k*-twisted lines, type (Ⅱ) vertex expansion, type (Ⅲ) three or four crossing curves and 2*k*-twisted lines, and type (Ⅳ) three or four point star and 2*k*-inverted twisted quadruplex-lines. Then, their key elements that construct polyhedral links are computed on the basis of the growth law of extended Platonic polyhedra and some effective topological index are also illustrated by applying the new Euler formula. Our ultimate aim is to assemble DNA polyhedra or similar DNA 3D nanocages by means of these basic features of polyhedral links. Besides, these elements related by the new Euler's formula for DNA polyhedra connect the topological aspects of the DNA cage to the Euler characteristic of the underlying polyhedra. Therefore, this study provides a theoretical framework not only for the design and synthesis of some DNA nanostructures but also for profound description of geometrical and topological structures of more complex DNA molecules.

Extended tetrahedral links

The tetrahedron, hexahedron, and dodecahedron are Platonic polyhedra in which very vertex has degree of three. Based on them, the extended tetrahedra, the extended hexahedra, and the extended dodecahedra are polyhedra with vertices of degree of three and the adding polygons are all hexagons [21]. The extended tetrahedra is the simplest of the extended tetrahedra, hexahedra, and dodecahedra. Thus, its polyhedral links are studied in detail and the same way is also applied to the other two.

The numbers of faces *F*, vertices *V* and edges *E* of the extended tetrahedra, its growth law, can be expressed as:

$$F = 2\left(a^2 + ab + b^2\right) + 2 \qquad (1)$$

$$E = 6\left(a^2 + ab + b^2\right) \qquad (2)$$

$$V = 4\left(a^2 + ab + b^2\right) \qquad (3)$$

Of course, these three quantities perfectly satisfy Euler's formula: $V + F = E + 2$.

2.1. Three branches curves type

Some nanostructures, whose faces are made of interlocked DNA rings, whose edges are made of double-helices [22] or quadruplex-helices [5, 10] DNA strands, and vertices are formed from multi-arm junctions, have been synthesized recently and these interlinked and interlocked structures could be modeled as "polyhedral links" [6, 14, 23]. The extended tetrahedral links are developed using "three branches curves and $2k$-twisted lines" [14] to cover extended tetrahedra. Specifically, the building blocks of "three branches curves" and "$2k$-twisted lines" replace the vertices and edges of the polyhedra respectively. Extended tetrahedra are assembled from four triangles and several hexagons. Consequently, the extended tetrahedral links are made up of four triangular and several hexagonal rings (loops) which are actually component circuits. In the process of transforming the extended tetrahedra into this type of extended tetrahedral links, triangular and hexagonal faces become triangular and hexagonal rings respectively, edges change into $2k$-twisted lines, and vertices turn out to be three branches curves. According to the growth law of the extended tetrahedra above, a series of characteristics, which can describe its architecture of the extended tetrahedral links of "three branches curves and $2k$-twisted lines", is computed as follows.

The number of triangular rings μ_t: 4

The number of hexagonal rings μ_h: $F-4=2\left(a^2+ab+b^2\right)-2$

The number of crossings c: $2kE=12k\left(a^2+ab+b^2\right)$

Using the mathematical method [20] to examine the specific details, this type of extended tetrahedral links meets new Euler's formula for DNA polyhedra: $s+\mu=c+2$. Utilizing it we may reveal some important intrinsic mathematical properties and even control the supramolecular design of DNA polyhedra.

The number of Seifert circles s:

$$s=c-\mu_t-\mu_h+2 = 2kE-F+2=2(6k-1)\left(a^2+ab+b^2\right)+2$$

The new Euler's formula, $s+\mu=c+2$, connects three most important variants for polyhedral links, component number μ, crossing number c and Seifert circles number s, which is similar to that Euler's formula, $V+F=E+2$, relates three fundamental geometrical parameters, face number F, vertex number V, edge number E. Furthermore, $V+F-E=\lambda=2-2g$, λ denotes Euler characteristic, a topological term, depends on its genus g that is regarded as the "tunnels" or "holes" of a polyhedron. As such, the new Euler formula based on polyhedral links can be generalized to $s+\mu-c=\lambda=2-2g$. For this type of polyhedral links, Euler characteristic is 2, so we get $g=0$, it indicates that DNA polyhedral catenanes synthesized are homeomorphic to a sphere. We will talk about this in future.

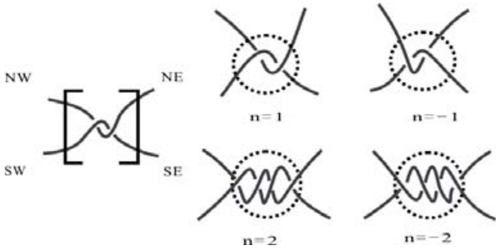

Figure 1. Even tangles obtained by 2*n* half-twists

Besides, tangles covering edges result in different polyhedral links. Fig. 1 illustrates four different tangles with *n* of ±1 and ±2 [16]. The resulting polyhedral link is defined as D configuration if $n>0$, otherwise it is defined as L configuration. Moreover, the D and L polyhedral links are mirror images of one another, in other words, a pair of topological enantiomorphs.

The information obtained above may help in faster and cheaper DNA design and synthesis. In DNA nanotechnology, crossing number c and component (ring) number μ are two experimentally accessible quantities in that crossing number c depends on the base number of DNA duplexes: c ≈ base pair number /5 and component number μ equals the number of circular DNA strands (DNA loops)[20]. To synthesize one of this type of DNA polyhedra, we can retrieve the value of a and b associated with face number of the polyhedron, then compute crossing number and component number of the resulting polyhedral link. At last, the corresponding DNA polyhedra could be made on the basis of this model.

If wanting 10-hedron link of this type of extended tetrahedral links whose edge is replaced by twisted lines ($k=1$, two crossings), we locate its position on face growth law of extended tetrahedra shown in Fig. 2, getting the value of its polar coordinates a and b. Then, plug 2 and 0 into the expression above and obtain the following information.

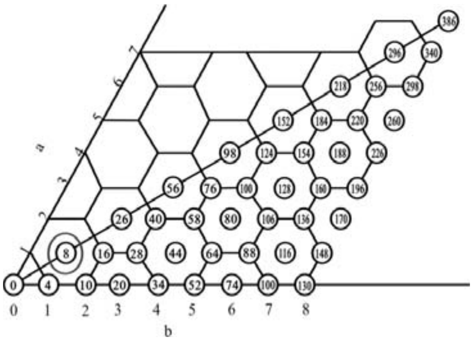

Figure 2. Face growth law of extended tetrahedra

The number of triangular rings μ_t: 4

The number of its hexagonal rings μ_h: $F-4=2\left(a^2+ab+b^2\right)-2=6$

The number of its crossings c: $2kE=12k\left(a^2+ab+b^2\right)=48$

So this DNA polyhedron has 10 circular DNA strands and about 240 base pairs.

The number of Seifert circles s: $s=c-\mu+2=2kE-F+\ 2=48-10+2=40$

By the end, the 10-hedral link of "three branches curves and 2k-twisted lines covering" type of extended tetrahedral links is shown in Fig. 3.

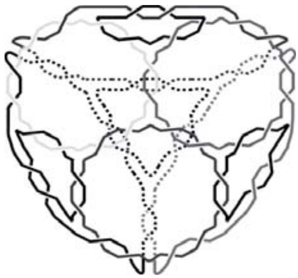

Figure 3 10-hedronal link of three branches curves type

2.2. Vertex expansion type

The extended tetrahedral links are obtained by using "three branches curves and 2k-twisted lines covering". However, their vertices, as we see them, are not stable due to their loose structure. If stretching the strands at vertices, this type of links would transform into another unique polyhedral links, which is the variant of original one above. We call it vertex expansion type. In the process of topology transformation, $2k$-twisted lines are converted into new vertices like nodes; new triangular patches occur in the position of three branches curves; hexagonal rings keep hexagonal ones, their vertices and edges, on the contrary, are located in the position of the former $2k$-twisted lines and three branches curves, respectively; triangular rings also keep triangular ones, their vertices and edges take the place of the former $2k$-twisted lines and three branches curves, respectively. Fig. 4 illustrates 10-hedronal link of vertex expansion type that derives from the basic type.

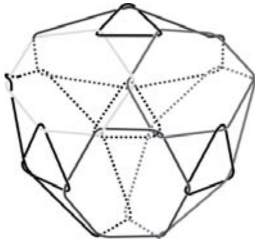

Figure 4. 10-hedronal link of vertex expansion type

In the process of topological transformation, most attributes don't change.

The number of triangular rings μ_t: 4

The number of hexagonal rings μ_h: $F-4=2\left(a^2+ab+b^2\right)-2$

The number of crossings c: $2kE=12k\left(a^2+ab+b^2\right)$

The number of Seifert circles s: $s=c-\mu_t-\mu_h+2=2(6k-1)(a^2+ab+b^2)+2$

In addition, new triangular patches occur in the position of three branches curves of the extended tetrahedral links of basic type.

The number of new triangular patches p_t: $4\left(a^2+ab+b^2\right)$

2.3. Three crossing curves type

Another extended tetrahedral links are constructed using "three crossing curves and 2*k*-twisted lines" to cover extended tetrahedra. Specifically, the building blocks of "three crossing curves" and "2*k*-twisted lines" replace the vertices and edges of the polyhedra respectively. Although this type of polyhedral links is made up of four triangular and hexagonal rings (loops), the building blocks of "three crossing curves" are different from the ones of "three branches curves". When transforming the extended tetrahedra into this type of extended tetrahedral links, triangular and hexagonal faces become triangular and hexagonal rings respectively, edges change into 2*k*-twisted lines, and vertices turn out to be three crossing curves. According to the growth law of the extended tetrahedra, a series of characteristics of the extended tetrahedral links of "three crossing curves and 2*k*-twisted lines" are computed as follows.

The number of triangular rings μ_t: 4

The number of hexagonal rings μ_h: $F-4=2\left(a^2+ab+b^2\right)-2$

Crossings of this type of polyhedral links are scattered in vertices and edges. Like the basic type, it is easy to figure the number of crossings of vertices. As for the number of crossings of vertices, each vertex contributes three.

The number of crossings c:

$$c=2kE+3V=12k\left(a^2+ab+b^2\right)+3\times 4\left(a^2+ab+b^2\right)=12\left(k+1\right)\left(a^2+ab+b^2\right)$$

For all the polyhedra having vertices of degree 3 and edges of 2*k*-twisted lines, three crossing curves at each vertex result in two Seifert circles and 2*k*-twisted lines on each edge make for 2*k*–1 ones, which is shown in Fig. 5.

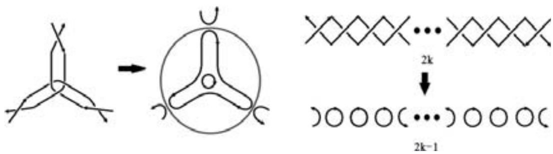

Figure 5. Seifert circles on vertices and edges

The number of Seifert circles s:

$$s=2V+(2k-1)E \ =2\times4\ (a^2+ab+b^2)+(2k-1)\times6(a^2+ab+b^2)=(12k+2)(a^2+ab+b^2)$$

$s+\mu_t+\mu_h-c=2V+(2k-1)E+F-2kE-3V=F-V-E$ .Here plus $V+F=E+2$ into $F-V-E$, then $s+\mu_t+\mu_h-c=2-2V=2-2\times4(a^2+ab+b^2)$. On the other hand, $s+\mu_t+\mu_h-c=2-2g$, where g is equivalent to V and $s+\mu_t+\mu_h-c=2-2V$. In a word, the Euler characteristic of "three crossings curves type" polyhedra mainly depends on its vertices number.

The 10-hedronal link of three crossing curves and $2k$-twisted lines type of extended tetrahedral links is shown in Fig. 6.

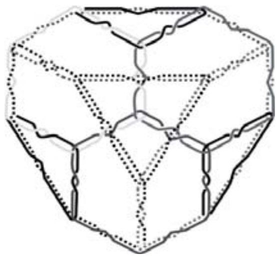

Figure 6. 10-hedronal link of three crossing curves type

2.4. Star motif type

Recently, some more complex DNA polyhedra have emerged [5, 10, 24] and these closed polyhedral structures are assembled from DNA star motifs through two anti-parallel DNA duplexes. "n-point star curves" is used to take place of the vertex of a polyhedron, where n is the degree of vertex. And here DNA star motif, shown in Fig. 7(a), is a symmetric three-point star curves linked by a single-stranded DNA loop, which replaces vertices of a polyhedron and two anti-parallel DNA duplexes, shown in Fig. 7(b), is $2k$-inverted twisted quadruplex-line(k donotes the integer number of full-twists on each edges) linked by a single-stranded DNA crossover, which replaces edges of a polyhedron. Finally, these two building blocks are connected as shown in Fig. 7(c).

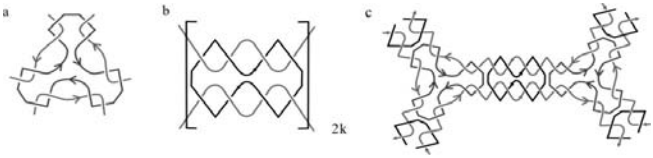

Figure 7. The building blocks of three-point star polyhedral links

Similarly, star polyhedral links of extended tetrahedra are constructed on the basis of extended tetrahedra. As we see, each face corresponds to a single-stranded DNA that forms duplexes while each vertex as well as edge also contains a DNA single strand.

The number of triangular rings μ_t: 4

The number of hexagonal rings μ_h: $F-4=2\left(a^2+ab+b^2\right)-2$

The number of vertex loops μ_v: $4\left(a^2+ab+b^2\right)$

The number of edge crossover μ_c: $6\left(a^2+ab+b^2\right)$

Each vertex corresponds to three-point star where each branch has four crossings. The crossings on edges can also be calculated.

The number of vertex crossings c_v:

$$c_v = 4nV = 8E = 4\times3\times4\left(a^2+ab+b^2\right) = 48\left(a^2+ab+b^2\right)$$

The number of crossings c_e:

$$c_e = (2k+2)E = (2k+2)\times6\left(a^2+ab+b^2\right) = 12(k+1)\left(a^2+ab+b^2\right)$$

This type of extended tetrahedral links satisfies new Euler's formula: $s+\mu=c+2$ as well.

The number of Seifert circles s: $s=\sum c_x - \sum \mu_x + 2$

The 10-hedronal link of star motif type of extended tetrahedral links is shown in Fig. 8.

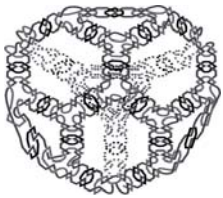

Figure 8. 10-hedronal link of star motif type

Extended octahedral links

Unlike extended tetrahedra, hexahedra, and dodecahedra, the degree of vertex of extended octahedra is four, the adding polygons are squares.

The numbers of faces *F*, vertices *V* and edges *E* of the extended octahedra are given by.

$$F = 6\left(a^2 + b^2\right) + 2 \tag{4}$$

$$E = 12(a^2 + b^2) \tag{5}$$

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

3.1. Four branches curves type

If we have extended octahedral links involved, it's pretty similar, but now what we use to cover extended octahedra is “four branches curves and 2*k*-twisted lines”. Specifically, the building blocks of “four branches curves” and “2*k*-twisted lines” replace the vertices and edges of the extended octahedra respectively. Accordingly, the extended octahedral links are made up of eight triangular and several square rings (loops). Triangular and square faces become triangular and square rings respectively, edges change into 2*k*-twisted lines, and vertices turn out to be four branches curves. According to the growth law of the extended tetrahedra above, a series of characteristics, which can describe its architecture of the extended octahedral links of “four branches curves and 2*k*-twisted lines”, is computed as follows.

The number of triangular rings μ_t: 8

The number of square rings μ_s: $F - 8 = 6\left(a^2 + b^2\right) - 6 = 6\left(a^2 + b^2 - 1\right)$

The number of crossings *c*: $c = 2kE = 24k\left(a^2 + b^2\right)$

The number of Seifert circles *s*:

$s = c - \mu_t - \mu_s + 2 = 2kE - F + 2 = 6\left(4k - 1\right)\left(a^2 + b^2\right)$

Extended octahedral links also have a pair of topological enantiomorphs of D and

L.

To synthesize one of this type of DNA polyhedra, we still retrieve the value of a and b associated with face number of the polyhedron, then compute crossing number and component number of the resulting polyhedral link. Finally, the corresponding DNA polyhedra could be made based on this model.

If wanting 14-hedronal link of this type of extended octahedral links whose edge is replaced by twisted lines ($k=1$), we find its position on face growth law of extended octahedra shown in Fig. 9, getting the value of its polar coordinates $a=1$ and $b=1$. Then, plug 1 and 1 into the expression above and obtain the following information.

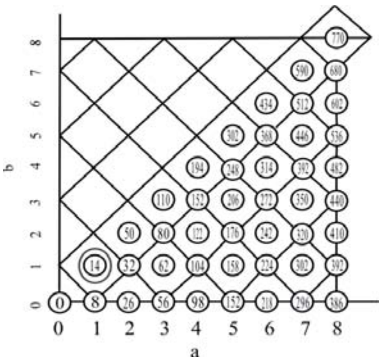

Figure 9. Face growth law of extended octahedra

The number of triangular rings μ_t: 8

The number of its squares rings μ_s: $F-8=6\left(a^2+\ b^2-1\right)=6$

The number of its crossings c: $2kE=24k\left(a^2+b^2\right)=48$

So this DNA polyhedron has 14 circular DNA strands and about 240 base pairs.

The number of Seifert circles s: $s=c-\mu+2=48-14+2=36$.

14-hedral link of four branches and 2k-twisted lines type of extended octahedral links is shown in Fig. 10.

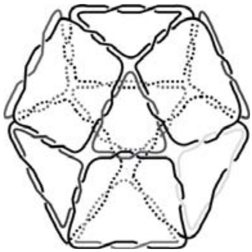

Figure 10. 14-hedronal link of four branches curves type

3.2. Vertex expansion type

If stretching the strands at vertices, extended octahedral links of "four branches curves and $2k$-twisted lines" type would transform into their vertex expansion type. Like the extended tetrahedral links, $2k$-twisted lines grow new vertices; new rectangle patches occur in the position of four branches curves; square rings keep square ones, their vertices and edges, on the contrary, are located in the position of the former $2k$-twisted lines and four branches curves, respectively; triangular rings also keep triangular ones, their vertices and edges take the place of the former $2k$-twisted lines and four branches curves, respectively. Fig. 11 shows 10-hedronal link of vertex expansion type that derives from the basic type.

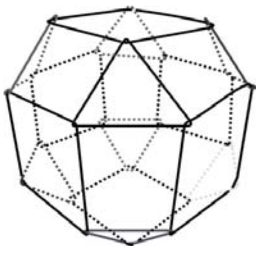

Figure 11. 14-hedronal link of vertex expansion type

The number of triangular rings μ_t: 8

The number of square rings μ_s: $F-8=6\left(a^2+b^2\right)-6=6\left(a^2+b^2-1\right)$

The number of crossings c: $2kE=24k\ \left(a^2+\ b^2\right)$

The number of Seifert circles s:

$$s = c - \mu_t - \mu_s + 2 = 2kE - F + 2 = 6(4k-1)(a^2+b^2)$$

New rectangle patches occur in the position of four branches curves of the extended octahedral links of basic type.

The number of new rectangle patches p_r: $6(a^2+b^2)$

3.3. Four crossing curves type

Likewise, extended octahedral links of four crossing curves and 2*k*-twisted lines type are built. The building blocks of "four crossing curves" and "2*k*-twisted lines" cover the vertices and edges of the extended octahedra respectively. When transforming the extended octahedra into this type of extended octahedra links, triangular and square faces become triangular and square rings respectively, edges change into 2*k*-twisted lines, and vertices turn out to be four crossing curves. According to the growth law of the extended octahedra, a series of characteristics of the extended octahedral links of "four crossing curves and 2*k*-twisted lines" are computed as follows.

The number of triangular rings μ_t: 8

The number of square rings μ_s: $F - 8 = 6(a^2+b^2) - 6 = 6(a^2+b^2-1)$

Multiply edge number by 2*k* to determine the number of crossings of vertices. Likewise, since each vertex has degree four, number of crossings of vertices is $4V$.

The number of crossings c:

$$c = 2kE + 4V = 24k(a^2+b^2) + 4\times 6(a^2+b^2) = 24(k+1)(a^2+b^2)$$

For all the polyhedra having vertices of degree 4 and edges of 2*k*-twisted lines, four crossing curves at each vertex result in four or two Seifert circles, shown in Fig. 12. And 2*k*-twisted lines on each edge still make for 2*k*–1 ones.

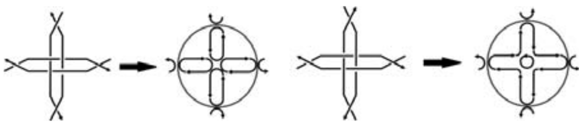

Figure 12. Seifert circles on vertices

The number of Seifert circles:

$$s_1 = 2V + (2k-1)E = 2\times 6(a^2+b^2) + (2k-1)\times 12(a^2+b^2) = 24k(a^2+b^2)$$

$$s_2 = 4V + (2k-1)E = 4\times 6(a^2+b^2) + (2k-1)\times 12(a^2+b^2) = (24k+12)(a^2+b^2)$$

$s+\mu_t+\mu_s-c = 2V+(2k-1)E+F-2kE-4V = F-2V-E$. Plus $V+F=E+2$ into $F-V-E$, then $s+\mu_t+\mu_s-c = 2-3V = 2-3\times 6(a^2+b^2) = 2-18(a^2+b^2)$.

The 14-hedronal link of four crossing curves and 2*k*-twisted lines type of extended octahedral links is shown in Fig. 13.

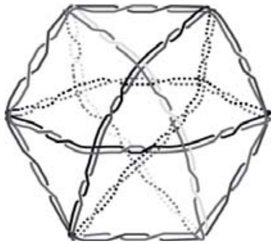

Figure 13. 14-hedronal link of four crossing curves type

3.4. Star motif type

We have been discussing "three-point star curves" of star motif type with which we could yield polyhedra having degree-three vertices, such as extended tetrahedra, hexahedra, and dodecahedra. And what's more, "four-point star curves" serves as materials to assemble polyhedra with vertices of degree four, such as extended octahedra. So, DNA star motif, shown in Fig. 14(a), is a symmetric four-point star curves linked by a single-stranded DNA loop, which replaces vertices of a polyhedron and two anti-parallel DNA duplexes, shown in Fig. 14(b), is 2*k*-inverted twisted quadruplex-line linked by a single-stranded DNA crossover, which replaces edges of a polyhedron. Finally, these two building blocks are connected as shown in Fig. 14(c).

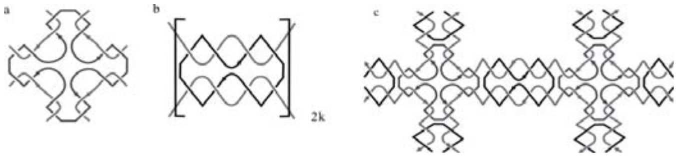

Figure 14. The building blocks of four-point star polyhedral links

As a result, we yield star polyhedral links of extended tetrahedra based on extended octahedra. Obviously, each face corresponds to a single-stranded DNA that forms duplexes, each vertex as well as edge contains a DNA single strand.

The number of triangular rings μ_t: 8

The number of square rings μ_s: $F-8=6\left(a^2+b^2\right)-6=6\left(a^2+b^2-1\right)$

The number of vertex loops μ_v: $6\left(a^2+b^2\right)$

The number of edge crossover μ_c: $12\left(a^2+b^2\right)$

Each vertex yields to four-point star where each branch has four crossings. The crossings on edges can also be calculated.

The number of vertex crossings c_v: $4nV=4\times4\times6\left(a^2+b^2\right)=96\left(a^2+b^2\right)$

The number of edge crossings c_e:

$$c_e=\left(2k+2\right)E=\left(2k+2\right)\times12\left(a^2+b^2\right)=24\left(k+1\right)\left(a^2+b^2\right)$$

The number of Seifert circles s: $s=\sum c_x-\sum\mu_x+2$

The 14-hedronal link of "star motif" type of extended octahedral links is shown in Fig. 15.

Figure 15. 14-hedronal link of star motif type

Conclusion

In this paper, we have constructed four types of polyhedral links based on extended Platonic polyhedra discussed before. These four types of polyhedral links, including three or four branches curves type, vertex expansion type, three or four crossing type and three or four point star type, are described by examples of the extended tetrahedra and octahedra links and their characteristics, such as crossing number, component number and Seifert circles number, are calculated in light of the growth law of the underlying polyhedra and new Euler's formula. These elegant structures of polyhedral links and the related topological characters may guide scientists in the field to build a variety of 3-D nanoscages and even more complex molecules. Furthermore, the mathematical descriptors requiring further investigation pave the way for the connection between underlying polyhedron and entangled polyhedral links, quantifying the geometry and topology of DNA polyhedra. Our work associates some issues of structural chemistry with those of mathematical chemistry, addressing some of them, still, it poses some new questions and challenges. We also hope that researchers from other field, materials science, chemistry, mathematics, biology and computer science, come together to tackle these problems.

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