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A New Euler Formula and Its Characterization of DNA Polyhedra

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Abstract

This paper studies the law of component number of DNA polyhedral links from mathematical and chemical viewpoints. The topological properties of extended Platonic polyhedral links, including component number, Seifert circle number, crossing number, characteristic λ, characteristic$Q$,are characterized intrinsically.We extend the polyhedral links with even half-twistsedges to the ones with odd half-twistsedges, which is helpful for experimenter to design and synthesize various practical DNA polyhedra. Our study indicates that there are some rules to follow for more DNA polyhedra, providing reference materials and some extended examples.

1. Introduction

People have long since been doing research into crystals. The ancient Greek philosopher Plato defined five regular polyhedra: tetrahedron, cube, octahedron, dodecahedron and icosahedron, namely Platonic solids. On the other hand, biologists and chemists would like to

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see polyhedra introduced to general use. In 2000, scientists discovered the peculiarcrystal structure of the double-stranded DNA bacteriophage HK97 mature empty capsid, which is made of 12 pentameric and 60 hexameric rings of covalently joined subunits that loop through each other[1]. Owing to its double helical structure and self-assembly ability, DNA is an ideal programmable building blocks for the assembly of a wide range of nanostructures[2]. Since Seeman utilized nucleic acids to form migrationally immobile junctions[3], a variety of DNA cages [4-6], including some exotic ones [7-9], had been realized. An important first step regarding the application of DNA cages was accomplished by scientists at Oxford University and they showed that artificial DNA cages that could be used to carry cargoes of drugs can enter living cellsefficiently and survive inside, potentially leading to new methods of drug delivery[10]. Recently, a new approach for constructing nanoscale polyhedral surfacesfrom DNA has been reported [11], lowing the barriers to applications of DNA nanotechnology. The novel cross-linked structure of DNA cages appears in new research field constantly.

One great challenge in supramolecular chemistry is the designing of building blocks to attain total control of the arrangement of molecules with polyhedral skeletons [12]. There has been tremendous interest in trying to rationalize the geometries and chemical properties of these novel structures[13-15]. Base on graph theory and knot theory, we proposed the method of “m-inverted twisted double-lines and n-branched curves covering” to construct polyhedral links[16] and thereby brought some topological viewpoints to describe and answer structural characteristics of DNA polyhedra [17-19]. This model actually conforms to the structure of DNA cages.

In our previous work, the Seifert construction of polyhedral links gave a good understanding of DNA nanopolyhedra. It generates a new Euler formula for DNA polyhedra that relates the numbers of Seifert circles s, components$\mu$and crossings c[19].

$$s+\mu=c+2 \quad (1)$$

However, this formula is too restrictive to describe DNA polyhedra in theory because it just considers the case of DNA polyhedra with even half-twists (crossings) along each edge.Here we will study the DNA polyhedra whose edges consist of both even and odd half-twists.

Furthermore, a new formula having a wider significance and two topological characteristics characterizing the DNA polyhedra are proposed, which is helpful for experimenter to design and synthesize various practical DNA polyhedra. Thus, the model of the polyhedral links could adapt itself to more types of DNA polyhedra and some interesting and underlying principles emerge as well. This study reveals the intrinsic properties and paves the way for the topology-aided molecular design of DNA polyhedra.

2. New Formula for DNA Polyhedra

2.1 Methods

To get a full appreciation of what this paper means we must turn first to some basic concepts used in our previous work.

Polyhedral links, the interlinked and interlocked strands based on the skeleton of polyhedra, serve as effective models of DNA polyhedra or cages.

Definition 1 A polyhedral link is an interlinked and interlocked architectures obtained form a polyhedral graph G, by using branches curves and twisted lines to replace the vertices and edges [19].

Definition 2 The crossing number of a polyhedral link c is the least number of crossings that occur in any projection of the polyhedral link [19].

Definition 3 The component number of a polyhedral link μ is the number of loops (rings) knotted with each other [19].

Definition 4 The Seifert circle number of a polyhedral link s is the number of Seifert circles distributed in an orientable surface with the polyhedral link as its only edge [19].

There are two kinds of holes in DNA cages: the large holes are located at vertices and the small holes are located at edges, and Seifert circles are used to fill these holes during the Seifert construction.

2.2 New Euler's Formula

If applying the Seifert operation to vertices, each vertex converts into a Seifert circle independent of the degree of vertex, namely,

$$s_v = V \tag{2}$$

Where s_v denotes the number of Seifert circles derived from vertices. In addition to these circles, other Seifert circles are distributed at edges, the number of which is s_e. Therefore, the number of Seifert circles of DNA polyhedral links*s* equals:

$$s = s_v + s_e \tag{3}$$

Then, we will discuss the calculation of s_e. For a DNA polyhedral link, its underlying polyhedral graph has *F* faces, *E* edges and *V* vertices. Suppose that this polyhedral link has *p* edges with even half-twists whose half-twist numbers are m_1, m_2, …, m_p, *q* edges with odd half-twists whose half-twist numbers are n_1, n_2, …, n_q, respectively. We could expect that each edge of the polyhedral link is assembled by DNA double helix with even or odd number of half-twists. Hence,

$$E = p + q \tag{4}$$

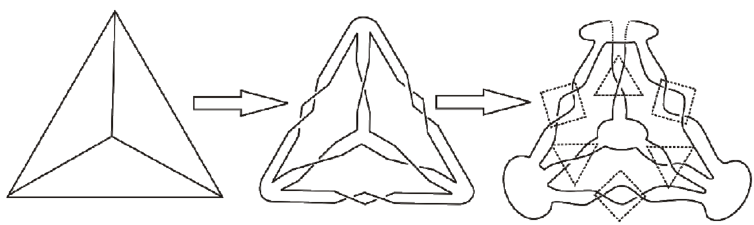

Figure 1 The Seifert construction of a tetrahedron

Look at a tetrahedron's Seifert construction shown in Fig. 1, for example. It has 3 edges with evenhalf-twists (indicated by dotted rectangle), $m_1 = m_2 = m_3 = 2$ and 3 edges with odd half-twists(indicated by dotted triangle), $n_1 = n_2 = n_3 = 1$.Besides, we can also count the number of Seifert circles derived from vertices, $s_v = 4$ and the number of Seifert circles derived from edges, $s_e = 3$, respectively.

Given an edge with *m* twists, *m*-1 Seifert circles are generated. So the number of Seifert circles on the edges is

$$s_e = \sum_{i=1}^{p}(m_i - 1) + \sum_{j=1}^{q}(n_j - 1)$$

$$= \sum_{i=1}^{p} m_i - p + \sum_{j=1}^{q} n_j - q$$

$$= \sum_{i=1}^{p} m_i + \sum_{j=1}^{q} n_j - (p+q) \tag{5}$$

Substituting Eq.(4) into Eq.(5), we obtain

$$s_e = \sum_{i=1}^{p} m_i + \sum_{j=1}^{q} n_j - E \tag{6}$$

Therefore

$$s = s_v + s_e = V + \sum_{i=1}^{p} m_i + \sum_{j=1}^{q} n_j - E \tag{7}$$

Notice that a half-twist corresponds to a crossing, the half-twist number equals to the crossing number on each edge. So we have that

$$c = \sum_{i=1}^{p} m_i + \sum_{j=1}^{q} n_j \tag{8}$$

Let’s plug Eq.(8) into Eq.(7), a more general formula for polyhedral link is put forward.

$$s = V + c - E \tag{9}$$

Substituting the Euler’s formula $V + F = E + 2$ into Eq. (9), we could obtain the following result.

$$s = V + c - E$$

$$= (E + 2 - F) + c - E$$

$$= 2 - F + c$$

Then, we have that

$$s + F = 2 + c \tag{10}$$

Eq. (10), $s + F = 2 + c$, is applied for polyhedral links both with even and odd half-twists on each edge. In fact, Eq.(10) could be regarded as the real new Euler's formula for DNA polyhedra for the reason that it has more general scope of application. To some extent Eq. (1), "a new Euler's formula" reported in [19], is a special form of Eq. (10) for it could only address the case of polyhedral links with even half-twists on edges. Furthermore, Eq. (1) is referred to as new Euler's formula Ⅱ into which Eq. (10), $s + F = 2 + c$, is converted when the component number μ equals the face number F.

In addition, both Eq. (9) and Eq. (1) study the DNA polyhedral links, the former introduces geometric parameter F and the latter introduces topological invariant μ. We believe that they arealso complementary and illustrate each other.

2.3 Two characteristics of *Q* and *λ*

In this part, two characteristics are defined to describe the intrinsic properties of DNA polyhedra. According to new Euler's formula, $s + F = 2 + c$, we define Q as its characteristic, thus obtaining $Q = s + F - c$ and Q remains 2 in case of all types of convex polyhedral links, including "even" polyhedral links with their edges even twists, "odd" polyhedral ones with their edges odd twists and "even and odd" polyhedral ones with their edges exiting both odd and even twists, which makes it easy to compute various parameters. For "new Euler's formula Ⅱ" or Eq.(1), $s + \mu = c + 2$, we give a new characteristic of λ to substitute the constant which equals 2 when polyhedral link is a convex one.

$$\lambda = s + \mu - c \tag{11}$$

Using above equation and the polyhedral Euler's formula $V + F = E + 2$, we can derive the following result:

$$\lambda = 2 - F + \mu \tag{12}$$

From this formula, it is easy to compute λ through the face number F and the component number of polyhedral links, avoiding the troubles about counting Seifert circles number using Eq. (1). The value of λ, decreasing from the maximum of 2 to a minus by 2 gradually, is an even whose minimum is

$$2-2\left(\frac{F-2}{2}\right)=4-F \tag{13}$$

2.4 DNA polyhedral links and common polyhedral links

In this part, we will talk about the difference between a common polyhedral link and a DNA polyhedral link.

Firstly, both common polyhedral links and DNA polyhedral links are polyhedral links. As a matter of fact, polyhedral links are made up of DNA polyhedral links and non-DNA polyhedral links, namely common polyhedral links. So DNA polyhedral links belong to polyhedral links, to speak more precisely, a kind of polyhedral links.

Secondly, a common polyhedral link does not have Seifert circle number for its rings or components are not oriented. On the other hand, a DNA polyhedral link has Seifert circle number for all its rings or components are oriented or, more to point, the two strands of duplex DNA are oppositely oriented.

2.5 Three topological invariants for a polyhedral link

For a polyhedron, vertex number V, edge number$E$ and face number$F$ arethree fundamental geometrical parameters.Correspondingly, crossing number c, component number$\mu$and Seifert circle number $s$are three important topological invariants for a polyhedral link.

For convenience, we assume that $m$equals 2 and 1 when the number of half-twists is even and odd in the case that "m-inverted twisted double-linesand "n-branched curvescovering" is used. Let a denote the number of edges with even half-twists and $b$denote the number of edges with odd half-twists. Then, we have:

$$s=V+a \tag{14}$$

As for component number, a common polyhedral link has at most *F* components when it has even half-twists on its edges. So, the component number is between 1 and *F*.

$$1 \le \mu \le F \tag{15}$$

The component number of a DNA polyhedral link must be an even because of itsdouble helix structure. Therefore, there are some small differences in the component number between the DNA polyhedral links and the common polyhedral links.

$$2 \le \mu \le F \; (\mu \text{is an even }) \tag{16}$$

A common polyhedral link and a DNA polyhedral link have the same method to compute the number of crossings.

$$c = 2a + b \tag{17}$$

3. Practical examples

In our previous work, we studied the architecture and growth of extended Platonic polyhedra[17] and constructed various extended Platonic polyhedral links[18]. We select the truncated tetrahedron,the truncated octahedron and the cuboctahedron from three types of extended Platonic polyhedra [17], to demonstrate the above rules and laws we concluded. The analysis and method can also be applied in all the other polyhedra. We will talk about it through computer program in the future.

3.1 The truncated tetrahedron [$3^4 6^4$]

The truncated tetrahedron [$3^4 6^4$] (*E*=18, *V*=12, *F*=8), one of Archimedean solids, is made by adding four hexagons to a tetrahedron [17]. The data about the common links and DNA links of the truncated tetrahedron are listed in Table 1. The Seifert circle number and component numberof this link coincide with the Eqs. (15) and (16). More, the component number of a common link varies from 1 to 8, the DNA polyhedral link occurs only when μ is an even. It is also possible that both a common polyhedral link and a DNA polyhedral link occur when μ is an even. In order to describe DNA polyhedral links, a new characteristic *Q* is introduced based on Eq. (10), $s+F=2+c$. Let's give characteristic Q to describe this formula.

$$Q=s+F-c \tag{18}$$

As both Eq. (9) and Eq. (10)can be applied to DNA polyhedral links having odd or even half-twists on their edges, the characteristic Q in Eq.(18) remains 2 undervarious conditions, which makes it easy to compute any parameter. In contrast, the Eq. (1) can only fit polyhedral links with even half-twistsbecause the Euler characteristic λin Eq. (11) could not keep a constant when odd half-twistsoccur. Besides, we find that the characteristics of $\lambda$and Q exist only in DNA polyhedral links which have Seifert circles. The value of λ decreases to a minus by 2 gradually anditsmaximum is 2 andminimum is $4-F$ according toEq. (13).

$$\lambda_{\max}=2, \lambda_{\min}=4-F \tag{19}$$

Table 1 Polyhedral links of the truncated tetrahedron[$3^4 6^4$]

μ	s	c	$\lambda=2-F+\mu$	$Q=s+F-c$	**Notes**
8	30	36	2	2	18 even 0 odd, **a DNA polyhedral link**
7		35			17 even 1 odd, a common polyhedral link
6	26	32	0	2	14 even 4odd, **a DNA polyhedral link**
6		34			16even 2odd, a common polyhedral link
5		33			15even 3odd, a common polyhedral link
4	23	29	-2	2	11even 7odd, **a DNA polyhedral link**
4	21	27	-2	2	9even 9odd, **a DNA polyhedral link**
4	18	24	-2	2	6even 12odd, **a DNA polyhedral link**
4		32			14even 4odd, a common polyhedral link
3		31			13even 5odd, a common polyhedral link
2	19	25	-4	2	7even 11odd, **a DNA polyhedral link**
2		30			12even 6odd, a common polyhedral link
1		29			11even 7odd, a common polyhedral link

We could draw the projections of the DNA polyhedral links of the truncated tetrahedron which can describe the real DNA polyhedral links effectively and clearly.

The projections of three DNA polyhedral links of the truncated tetrahedron are illustrated in Fig.2. Note that “X even Y odd” means there are X edges having even half-twists and Y ones having odd half-twists in this polyhedral link. For instance, the DNA link in Figure 2(c) has six edges that have even half-twists (two crossings) and twelve edges that have odd half-twists (one crossing).

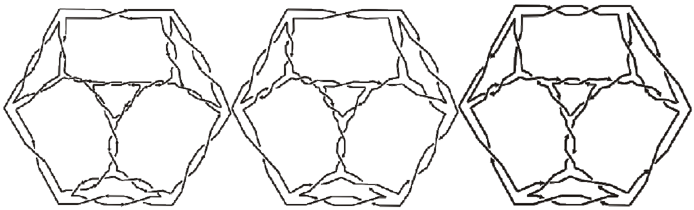

Figure2(a) Figure 2(b)Figure2(c)

Figure 2 The projections of three DNA polyhedral links of the truncated tetrahedron $[3^4 6^4]$: (a) μ=6, 14 even 4 odd; (b)μ=4, 9 even 9 odd; (c)μ=4, 6 even 12 odd

3.2 The truncated octahedron $[4^6 6^8]$

The truncated octahedron $[4^6 6^8]$ (E=36, V=24, F=14), also one of Archimedean solids, is made by adding eight hexagons to a hexahedron [17]. The data about DNA polyhedral links of the truncated octahedron $[4^6 6^8]$ are listed in Table 2. The above rules about DNA polyhedral links can also be applied in this type of DNA polyhedral links. At the same time, the component numbers of the common polyhedral links of the truncated octahedron $[4^6 6^8]$ accord with the Eq. (15), ranging from 1 to 14. To simplify the process, only the data about DNA polyhedral links are listed in Table 2. From Table 1and Table 2, we realize that the truncated octahedron has more DNA polyhedral links than the truncated tetrahedron. It is more likely that the truncated octahedron has more faces and vertices, thus forming more DNA polyhedral links. Three DNA polyhedral links of the truncated octahedron $[4^6 6^8]$ are showed in Fig. 3.

Table 2 DNA polyhedral links of the truncated octahedron [$4^6 6^8$]

$\boldsymbol{\mu}$	$\boldsymbol{s}$	$\boldsymbol{c}$	$\lambda = 2 - F + \mu$	$Q = s + F - c$	**Notes**
14	60	72	2	2	36 even 0odd
12	56	68	0	2	32even 4odd
10	52	64	-2	2	28even 8odd
8	48	60	-4	2	24even 12odd
6	49	61	-6	2	25even 11odd
6	44	56	-6	2	20even 16odd
6	36	48	-2	2	12even 24odd
6	24	36	-6	2	0even 36odd
4	47	59	-8	2	23even 13odd
4	34	46	-8	2	10even 26odd
2	46	58	-10	2	22even 14odd
2	32	44	-10	2	8even 28 odd

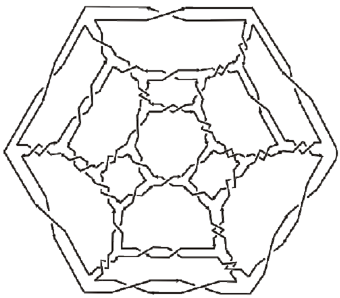

Figure3(a)

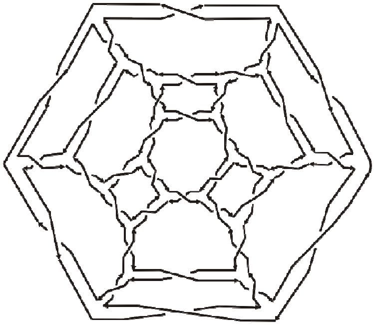

Figure3(b)

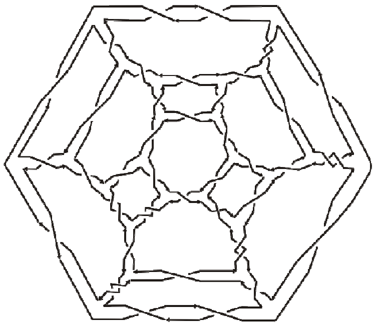

Figure3(c)

Figure 3 The projections of three DNA polyhedral links of the truncated octahedron $[4^6 6^8]$: (a)μ=6, 20 even 16 odd; (b)μ=6, 0 even 36 odd; (c)μ=2, 8 even 28 odd

3.3 The cuboctahedron $[3^8 4^6]$

The cuboctahedron $[3^8 4^6]$ (E=24, V=12, F=14), also one of Archimedean solids, is made by adding six squares to an octahedron[17]. The data about the DNA polyhedral links of the cuboctahedron $[3^8 4^6]$ are listed in Table 3. Compared with the truncated octahedron $[4^6 6^8]$ showed in Fig. 3, the cuboctahedron $[3^8 4^6]$ is also a 14-hedron but has vertices of degree 4. Besides, the cuboctahedron has fewer DNA polyhedral links than the truncated octahedron as we can see from Table 3. We can speculate that it is harder to construct DNA polyhedrallinks with vertices of degree 4 than that with vertices of degree 3. It is possible that the chance of forming DNA polyhedral links gets smaller as polyhedral vertices number increases. In other words, the more vertices a polyhedron has, the more likely DNA polyhedral links it can form. The component numbers of the common polyhedral links of the cuboctahedron [$3^8 4^6$] accord with the Eq. (15), ranging from 1 to 14. Three DNA polyhedral links of the cuboctahedron [$3^8 4^6$] are showed in Fig. 4.

Table 3 DNA polyhedral links ofthe cuboctahedron [$3^8 4^6$]

μ	s	c	$\lambda = 2 - F + \mu$	$Q = s + F - c$	**Notes**
14	36	48	2	2	24 even 0 odd
12	32	44	0	2	20 even 4 odd
10	30	42	-2	2	18 even 6 odd
8	28	40	-4	2	16 even 8 odd
6	24	36	-6	2	12 even 12 odd
4	24	36	-8	2	12 even 12 odd
4	22	34	-8	2	10 even 14 odd
4	20	32	-8	2	8 even 16 odd

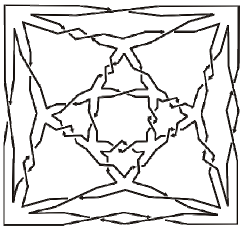

Figure4(a)

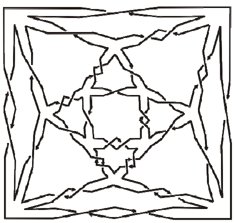

Figure4(b)

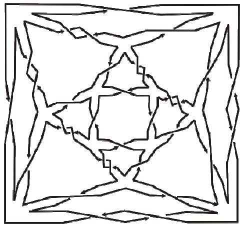

Figure4(c)

Figure 4 The projections of three DNA polyhedral links of the cuboctahedron $[3^8 4^6]$: (a) μ=6, 12 even 12 odd; (b) μ=4, 12 even 12 odd; (c) μ=4, 8 even 16 odd

4. Conclusions

This paper discusses the component numbers of common polyhedral links and DNA polyhedral links which are expressed by Eqs. (15) and (16). We find that the component number of DNA polyhedral links is prone to be an even. Furthermore, a new characteristic Q, describing the relation between Seifert circle number, face number and crossing number of a polyhedral link, is defined to clarify the intrinsic attribute of real DNA polyhedral links with even or odd twists, which facilitates computation of the parameters of the polyhedral links. We take three typical DNA extended Platonic polyhedral links (the truncated tetrahedral links $[3^4 6^4]$, the truncated octahedronal links $[4^6 6^8]$ and the cuboctahedronal links $[3^8 4^6]$) for examples, characterizing their component number, Seifert circle number, crossing number, characteristic Q, the edges of odd or even half-twists. Meanwhile, some of their projections are showed, which make it convenient to observe the components of links. The Eqs. (10)-(19) in this paper, as well as the Eq. (1) reported previously [19], are important tools for designing DNA polyhedral links.

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References

[1] W. R. Wikoff, L. Liljas, R. L. Duda, H. Tsuruta, R. W. Hendrix, J. E. Johnson, Topologically linked protein rings in the Bacteriophage HK97 Capsid, *Science* **289** (2000) 2129–2133.

[2] F. A. Aldaye, A. L. Palmer, H. F. Sleiman, Assmebling materials with DNA as the guide, *Science* **321** (2008) 1795–1799.

[3] N. C. Seeman, Nucleic acid junctions and lattices, *J. Theor. Biol.* **99** (1982) 237–247.

[4] J. Chen, N. C. Seeman, Synthesis from DNA of a molecule with the connectivity of a cube, *Nature* **350** (1991) 631–633.

[5] R. P. Goodman, I. A. T. Schaap, C. F. Tardin, C. M. Erben, R. M. Berry, C. F. Schmidt, A. J. Turberfield, Rapid chiral assembly of rigid DNA building blocks for molecular nanofabrication, *Science* **310** (2005) 1661–1665.

[6] F. F. Anderson, B. Knudsen, C. L. P. Oliveira, R. F. Frøhlich, D. Krüger, J. Bungert, M. Agbandje–McKenna, R. McKenna, S. Juul, C. Veigaard, J. Koch, J. L. Rubinstein, B. Guldbrandtsen, M. S. Hede, G. Karlsson, A. H. Andersen, J. S. Pedersen, B. R. Knudsen, Assembly and structural analysis of a covalently closed nano-scale DNA cage, *Nucleic Acids Res.* **36** (2008) 1113–1119.

[7] Y. He, T. Ye, M. Su, C. Zhang, A. E. Ribbe, W. Jiang, C. Mao, Hierarchical self-assembly of DNA into symmetric supramolecular polyhedra, *Nature* **452** (2008) 198–201.

[8] Y. He, M. Su, P. A. Fang, C. Zhang, E. R. Alexander, W. Jiang, C. Mao, On the chirality of self-assembled DNA octahedra, *Angew. Chem. Int. Ed*. **122** (2010) 760–763.

[9] C. Zhang, M. Su, Y. He, X. Zhao, P. A. Fang, E. R. Alexander, W. Jiang, C. Mao, Conformational flexibility facilitates self-assembly of complex DNA nanostructures, *Proc. Natl. Acad. Sci*. **105** (2008) 10665–10669.

[10] A. S. Walsh, H. Yin, C. M. Erben, M. J. A. Wood, A. J. Turberfield, DNA cage delivery to mammalian cells, *ACS Nano* **5** (2011) 5427–5432.

[11] E. Benson, A. Mohammed, J. Gardell, S. Masich, E. Czeizler, P. Orponen, B. Högberg, DNA rendering of polyhedral meshes, *Nature* **523** (2015) 441–444.

[12] A. T. Balaban, From chemical topology to 3D geometry, *J. Chem. Inf. Comput. Sci.* **37** (1997) 645–650.

[13] J. Rudnick, R. Bruinsma, Icosahedral packing of RNA viral genomes, *Phys. Rev. Lett.* **94** (2005) 038101.

[14] W. Y. Qiu, X. D. Zhai, Molecular design of Goldberg polyhedral links, *J. Mol. Struct. (THEOCHEM)* **756** (2005) 163–166.

[15] W. Y. Qiu, Z. Wang, G. Hu, *The Chemistry and Mathematics of DNA Polyhedra*, NOVA, New York, 2010.

[16] G. Hu, X. D. Zhai, D.Lu, W. Y. Qiu, The architecture of Platonic polyhedral links, *J. Math. Chem.* **46** (2009) 592–603.

[17] T. Deng, M. L.Yu, G. Hu, W. Y. Qiu, The architecture and growth of extended Platonic polyhedra, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 713–730.

[18] T. Deng, W. Y. Qiu, The architecture of extended Platonic polyhedral links, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 347–364.

[19] G. Hu, W. Y. Qiu, A. Ceulemans, A new Euler's formula for DNA polyhedra, *PLoS ONE* **6** (2011) e26308.