MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **71** (2014) 175-184

ISSN 0340 - 6253

Topological Construction and Characteristics of Polyhedral Links

Wen-Xing Wang, Xiao-Wei Li and Wen-Yuan Qiu[1]

Department of Chemistry, State Key Laboratory of Applied Organic Chemistry,

Lanzhou University, Lanzhou 730000, People's Republic of China

(Received December 10, 2012)

Abstract

In this paper, the relations between three methods of constructing polyhedral links, '*n*-branched-curve and *m*-twisted double-line covering', '*n*-cross-curve and *m*-twisted double-line covering' and 'tangle-vertex and single-line covering', are discussed. The connection between 'tangle-vertex and single-line covering' and the syntheticism 'star-motif' is showed clearly. In this way the construction models of 'branch-motif' and 'star-motif' are unified. Our results reveal the intrinsic properties of DNA polyhedra and provide new thoughts to DNA polyhedral design.

1. Introduction

Since the discovery of double helix structure of DNA, DNA has been considered as a new synthetic material for its unique structure and property. In 1991, Seeman synthesized the first DNA three-dimensional structure, DNA cube[1], realized the perfect combination between the flexibility of DNA catenanes and rigidity of polyhedra and created a new era for the field of DNA nanotechnology. In the past twenty years, many DNA nanostructures have been synthesized, such as DNA tetrahedron[2-8], DNA cube[9, 10], DNA truncated octahedron[11-13], DNA dodecahedron [4, 14] and DNA icosahedrons[15, 16]. Although brilliant achievements have been achieved in the synthesis of DNA polyhedra, there are only two main synthetic methods: one is to assemble the DNA polyhedra by one step with DNAsingle-chains whose sequences have been predesigned meticulous; the other is to assemble the polyhedra with 'star-motif' in the strategy of 'module hierarchical self-assemble'.

[1] To whom correspondence should be addressed. Email: wyqiu@lzu.edu.cn

DNA polyhedra, which have sprung up like mushrooms, not only enrich the DNA structures database, but also bring new challenges to theoretical characterization. How to describe these complex and intriguing structures and benefit the experimental synthesis? Scientists turn to mathematics for help, and some pioneering work have been done by Qiu et al. DNA polyhedral links provide a powerful mathematical tool for the description of the DNA nanostructures, and meanwhile, present a new set of challenges to synthetic job. This paper utilizes the mathematical model of polyhedral links to unify the existing synthetic strategies of DNA nanostructures. Some import results are presented by a series of transformations, which open a new window for designing and synthesizing of DNA nanostructures.

Mathematical model of DNA polyhedra ---- polyhedral links

In order to describe the structures of DNA polyhedra, Qiu's group replaced the edges and vertices of DNA polyhedra with 'twist double-line' and 'cross-curve', respectively, converting the abstract DNA polyhedra to simple mathematical patterns, and proposed 'n-branched-curve and m-twisted double-line covering' [17, 18], 'n-cross-curve and m-twisted double-line covering' [19-22] and 'tangle-vertex and single-line covering'. [22, 23-24] Among the DNA polyhedra that have been obtained in laboratories, the DNA polyhedra assembled by DNA chains in single-step can be described perfectly by 'n-branched-curve and m-twisted double-line covering', and the DNA polyhedra assembled by 'star-motif' are represented reasonably by 'cross-curve and single-line covering'. This means that a new type of polyhedral link is needed when a new DNA polyhedron arises. In this paper, we will try to connect the methods of constructing DNA polyhedra together, and seek a unified approach to describe all kinds of DNA polyhedra.

2. Three methods of constructing polyhedral links

'N-cross-curve and m-twisted double-line covering' is a method for construction of DNA polyhedral links with n-degree vertices and m-twisted edges (Fig. 1). This method is based on the structure of HK97 capsid.

'N-branched-curve and m-twisted double-line covering' is a method that uses n-branched curves to cover the vertices of the polyhedron and m-twisted double-lines to cover the edges (Fig. 2). This method has been used to describe the topological construction and characteristics of DNA polyhedra synthesized in lab.

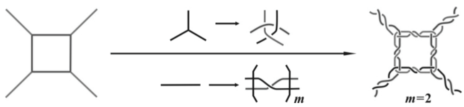


Figure 1: The method for ‘n-cross-curve and m-twisted double-line covering’.

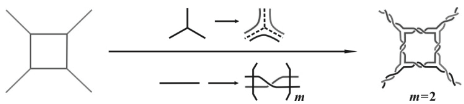


Figure 2: The method for ‘n-branched-curve and m-twisted double-line covering’.

‘Tangle-vertex and single-line covering’ is a method to construct polyhedral links based on four-degree polyhedra by using an even or odd twisted ‘tangle’ (Fig. 3) to cover a vertex and using single-line to cover an edge. A non-four-degree polyhedron can be half-truncated into four-degree by cutting off the corners of the polyhedron along the midpoint of the edges.

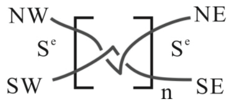


Figure 3: The projection of a tangle.

3. Topological transformation between n-branched polyhedral links and tangle-vertex polyhedral links

Fig. 3 shows the projection of a tangle, i.e. the module of the tangle-vertex polyhedral link. Pulling the lines denoted by NW and SW into parallel lines, and taking the same operation on the lines NE and SE, the tangle will be converted into one-twisted double lines. If we take this operation on every tangle of a tangle-vertex polyhedral link, each edge on the face, enclosed by lines NW and SW (or NE and SE) of several tangles, will shrink to the center of the face, and the face will be transformed into a branched vertex, shown in Fig. 4. In this way the vertices and some of faces of the tangle-vertex polyhedral link will change into twisted edges and branched vertices，respectively, transforming the link into a branched polyhedral link.

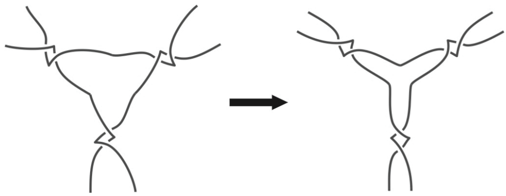


Figure 4: The transformation of a tangle-vertex link and a branched link.

A tetrahedron will be taken for an example to show the process of the transformation.

(1) First a tangle-vertex polyhedral link from the tetrahedron is needed. For its vertices are of 3 degrees, the tetrahedron will be half-truncated into 4-degree. An octahedron will be obtained after the truncation (Fig. 5).

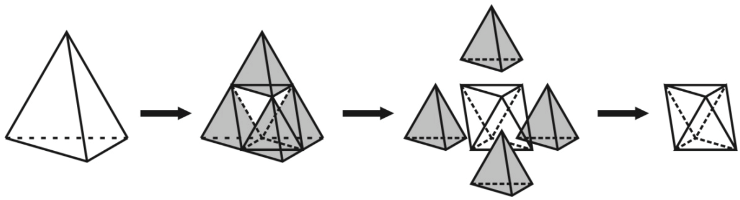
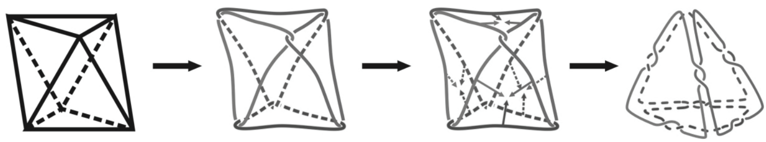


Figure 5: The tetrahedron is half-truncated into the octahedron.

(2) The octahedral link is constructed with the method of 'tangle-vertex and single-line covering' (Fig. 6).

(3) The edges are pulled to the center of the faces following the directions of the arrows shown in Fig. 6(c). In this way the four faces in the octahedral link are transformed into three-branched vertices, while the six vertices are transformed into twisted double-lines, and the octahedral link is transformed topologically into the branched tetrahedral link (Fig. 6(d)).



(a) (b) (c) (d)

Figure 6: The construction and topological transformation of the octahedral link.

The hexahedron and the octahedron are dual to each other. Half-truncating the two polyhedra will get the same four-degree tetrakaidecahedron, or cuboctahedron. The cuboctahedral links are constructed by the method of 'tangle-vertex and single-line covering'. The difference in placements of the tangles will lead to two different cuboctahedral links, which are composed of quadrilateral rings and trilateral rings, respectively (Fig. 7). After the transformation shown in Fig. 4, the two cuboctahedral links change into branched hexahedral link and octahedral link, respectively.

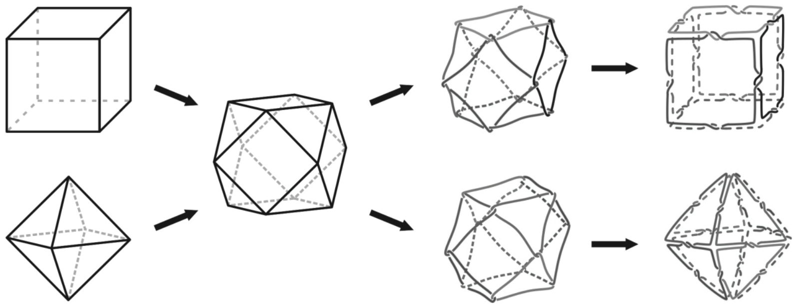


Figure 7: The construction of hexahedral and octahedral links

As similar to the above, the dodecahedron and the icosahedron are also dual to each other. Half-truncating them will get the same four-degree icosidodecahedron. The icosidodecahedral links composed of pentagonal rings and trilateral rings respectively will transform to branched dodecahedral link and icosahedral link (Fig. 8).

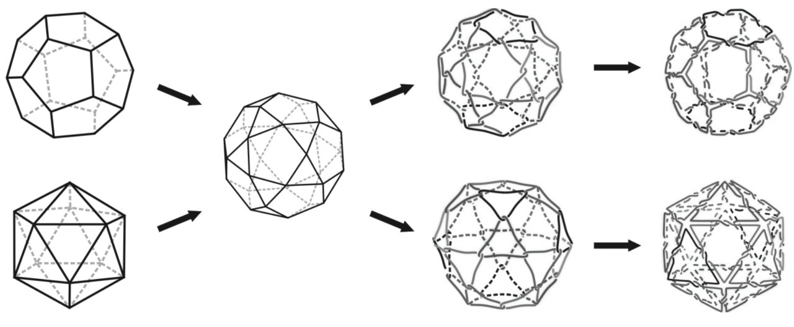


Figure 8: The construction of dodecahedral and icosahedral links.

From the above examples, we can figure out that branched polyhedral link can be transformed topologically to the tangle-vertex polyhedral link constructed from the half-truncated polyhedron. The transformation also builds connection between the two branched polyhedral links constructed from two dual polyhedra.

4. Topological transformation between crossed polyhedral links and tangle-vertex polyhedral links

Fig. 9 shows a four-cross octahedral link, the vertices of which are covered with 4-cross curves. If we pull the four curves outward at the same time, one vertex will change into four, which are half-twist tangle-vertices. The edges of the new polyhedral link are covered with single-line. Therefore, the octahedral link transform into a tangle-vertex polyhedral link which is constructed from the rhombicuboctahedron.

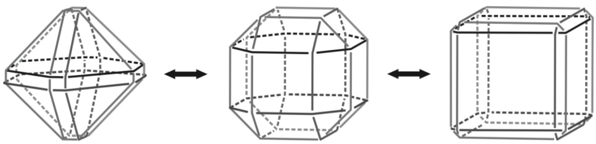


Figure 9: The topological transformation between 4-cross octahedral link and 3-cross hexahedral link.

Note that the rhombicuboctahedron is obtained from the octahedron being half-truncated twice. For the octahedron and the hexahedron are dual to each other, we can also get the rhombicuboctahedron from the hexahedron by half-truncating it twice (Fig. 10). Therefore the 3-cross hexahedral link and the 4-cross octahedral link can topologically transform to each other, and the tangle-vertex rhombicuboctahedral link is the intermediate of this topological transformation.

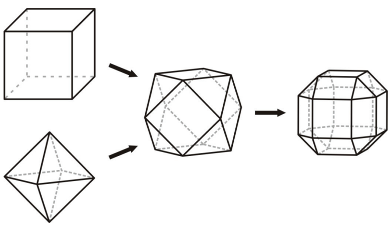


Figure 10: The hexahedron and the octahedron are half-truncated twice into the rhombicuboctahedron.

As similar to the above, the 3-cross dodecahedral link and the 5-cross icosahedral link can be topologically transformed to each other, and the intermediate of the transformation is the tangle-vertex polyhedral link constructed from the rhombicosidodecahedron (Fig. 11), which is gotten from the dodecahedron or icosahedron being half-truncated twice (Fig. 12).

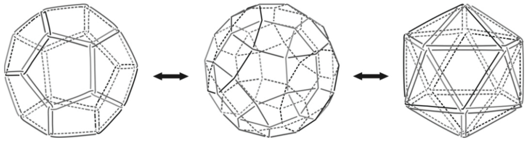


Figure 11: The topological transformation between 3-cross dodecahedral link and 5-cross icosahedral link.

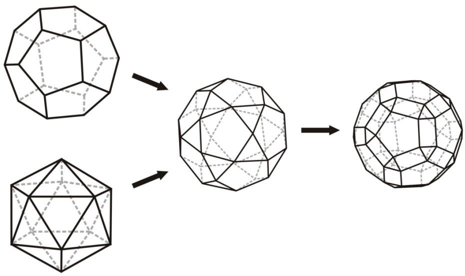


Figure 12: The dodecahedron and the icosahedron are half-truncated twice into the rhombicosidodecahedron.

From the above, we can figure out that two dual cross polyhedral links can be topologically transformed to each other, and the intermediate of the transformation is the tangle-vertex polyhedral link constructed from the polyhedron, which is gotten from the two dual polyhedra being half-truncated twice.

5. The construction of polyhedral links with star-motifs

Mao's group synthesized a number of DNA polyhedra with star-motifs. These DNA polyhedra cannot be described by 'n-branched-curve and m-twisted double-line covering' or 'n-cross-curve and m-twisted double-line covering'. However, we can use the method of 'tangle-vertex and single-line covering' to depict these polyhedra perfectly.

In this paper, the dodecahedron will be taken for example to show the process of constructing the dodecahedral link by the way of 'tangle-vertex covering'.

As shown in Fig. 13, the dodecahedron is half-truncated twice into rhombicosidodecahedron, with each vertex replaced by a triangle and each edge replaced by a quadrangle. A fragment of the rhombicosidodecahedron is taken for further analysis. First the vertices are replaced by even-half-twisted tangles. Then the edges shared by the quadrangle and pentagon are cut off and reconnected by two even-half-twisted tangles. Notice that the two tangles are also connected together. Finally a basic module is obtained as Fig. 14. A 'tangle-vertex and modified edge' dodecahedral links is obtained by applying the basic module to the whole dodecahedron. The 'tangle-vertex and modified edge' dodecahedral link is the mathematical model of DNA dodecahedron synthesized with star-motifs.

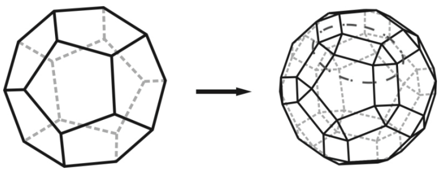


Figure 13: The dodecahedron is half-truncated twice into rhombicosidodecahedron.

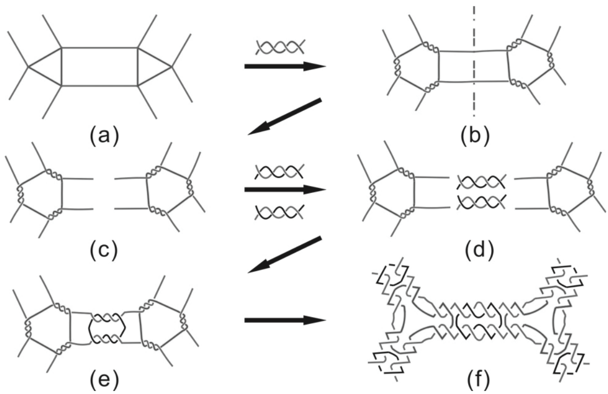


Figure 14: The process of constructing the dodecahedral link by the way of 'tangle-vertex covering'.

From the above example, a general method to build DNA polyhedra synthesized with star-motifs is presented. First, the target polyhedron is half-truncated twice. Second, the vertices of half-truncated polyhedron are replaced by tangles. Third, the edges are cut off and reconnected by tangles.

With the rapid development of DNA polyhedral synthetic technique, theoretical scientists have proposed several mathematical models to describe these novel structures. However, these methods of theoretical construction cannot depict all the DNA polyhedral structures. In this paper, we start with the method of 'tangle-vertex covering', get branched polyhedral links and cross polyhedral links by proper topological transformation, construct the DNA polyhedra synthesized with star-motifs, and accomplish the construction of all the DNA polyhedra with the method of 'tangle-vertex and modified edge'. The methods for polyhedral construction have been unified, and a general method for construction has been obtained.

Acknowledgements: This work was supported by grants from the National Natural Science Foundation of China (Nos. 20973085, 10831001, and 21173104) and Specialized Research Fund for the Doctoral Program of Higher Education of China (No. 20090211110006).

References

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

[2] R. P. Goodman, R. M. Berry, A. J. Turberfield, The single-step synthesis of a DNA tetrahedron, *Chem. Commun.* **12** (2004) 1372–1373.

[3] R. P. Goodman, 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.

[4] Y. He, T. Ye, M. Su, C. Zhang, A. E. Ribbe, W. Jiang, C. -D. Mao, Hierarchical self-assembly of DNA into symmetric supramolecular polyhedral, *Nature* **452** (2008) 198–202.

[5] C. Zhang, M. Su, Y. He, Y. -J. Leng, A. E. Ribbe, G. S. Wang, W. Jiang, C. D. Mao, Exterior modification of a DNA tetrahedron, *Chem. Commun.* **46** (2010) 6792–6794.

[6] R. P. Goodman, M. Heilemann, S. Doose, C. M. Erben, A. N. Kapanidis, A. J. Turberfileld, Reconfigurable, braced, three dimensional DNA nanostructures, *Nat. Nanotechnol.* **3** (2008) 93–96.

[7] Y. G. Ke, J. Sharma, M. H. Liu, K. Jahn, Y. Liu, H. Yan, Scaffolded DNA origami of a DNA tetrahedron molecular container, *Nano Lett.* **9** (2009) 2445–2447.

[8] Z. Li, B. Wei, J. Nangreave, C. X. Lin, Y. Liu, Y. L. Mi, H. Yan, A Replicable tetrahedral nanostructure self-assembled from a single DNA strand, *J. Am. Chem. Soc.* **131** (2009) 13093–13098.

[9] N. C. Seeman, DNA in a material world, *Nature* **421** (2003) 427–431.

[10] C. Zhang, S. H. Ko, M. Su, Y. J. Leng, A. E. Ribbe, W. Jiang, C. D. Mao, Symmetry controls the face geometry of DNA polyhedra, *J. Am. Chem. Soc.* **131** (2009) 1413–1415.

[11] W. M. Shih, J. D. Quispe, G. F. Joyce, A 1.7-kilobase single-stranded DNA that folds into a nanoscale octahedron, *Nature* **427** (2004) 618–621.

[12] F. F. Andersen, 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.

[13] Y. He, M. Su, P. A. Fang, C. Zhang, A. E. Ribbe, W. Jiang, C. D. Mao, On the chirality of self-assembled DNA octahedra, *Angew. Chem. Int. Ed.* **49** (2010) 748–751.

[14] J. Zimmermann, M. P. J. Cebulla, S. Münninghoff, G. von Kiedrowski, Self-assembly of a DNA dodecahedron from 20 trisoligonucleotides with C_{3h} linkers, *Angew. Chem. Int. Ed.* **47** (2008) 3626–3630.

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

[16] D. Bhatia, S. Mehlab, R. Krishnan, S. S. Indi, A. Basu, Y. Krishnan, Icosahedral DNA nanocapsules by modular assembly, *Angew. Chem. Int. Ed.* **48** (2009) 4134–4137.

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

[18] G. Hu, W. Y. Qiu, X. S. Cheng, S. Y Liu, The complexity of Platonic and Archimedean polyhedral links, *J. Math. Chem.* **48** (2010) 401–412.

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

[20] W. Y. Qiu, X. D. Zhai, Y. Y. Qiu, Architecture of Platonic and Archimedean polyhedral links, *Sci. China Ser. B: Chemistry* **1** (2008) 13–18.

[21] X. S. Cheng, W. Y. Qiu, H. P. Zhang, A novel molecular design of polyhedral links and their chiral analysis, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 115–130.

[22] D. Lu, G. Hu, Y. Y. Qiu, W. Y. Qiu, Topological transformation of dual polyhedral links, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 67–78.

[23] G. Hu, W. Y. Qiu, Extended Goldberg polyhedral links with even tangles, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 737–752.

[24] G. Hu, W. Y. Qiu, Extended Goldberg polyhedral links with odd tangles, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 753–766.