

Using dual polyhedral links models to predict characters of DNA polyhedra



Jin-Wei Duan, Wen-Yuan Qiu *

Department of Chemistry, State Key Laboratory of Applied Organic Chemistry, Lanzhou University, Lanzhou 730000, People's Republic of China

HIGHLIGHTS

- Dual polyhedral links models are used to predict characters of DNA polyhedra.
- The advantage of self-complementary palindromes are introduced here.
- The symmetries of the dual DNA Platonic polyhedra are recovered.

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ABSTRACT

In this paper, crossed junctions are used to simulate “V” holes of DNA polyhedra, the “sphere-surface-movement” method and dual polyhedral link models are used to character dual DNA polyhedra. The results show that dual polyhedral link models are good enough to describe DNA polyhedra and self-complementary palindromic sequences are useful materials to construct DNA polyhedra.

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1. Introduction

DNA has been considered as an ideal material for its double helix structure to produce addressable, controllable and structure predictable novel structures [1]. In 1991, professor Seeman reported the first architecture DNA polyhedron, a DNA cube [2]. In the following years, scientists have produced more and more novel DNA structures, such as platonic polyhedra [3–11], trigonal bipyramid [12], smile faces [13] and [14–22].

All these experimental results enriches the library of DNA nanostructures. To make further understanding about these structures, theoretical studies are urgently desired to reveal secrets that behind these structures. Mathematical tools, such as knot theory and topology are used to simulate intrinsic properties of these polyhedra. Polyhedral links have been considered as a powerful tool to describe DNA nanostructures [23,24]. Qiu and his colleagues have calculated some invariants of DNA polyhedral links [30–33,36] and brought forward a series of designing methods [25–29,34,35].

Although both experiments and theoretical work have made accomplishments, there still corners are not been concerned. If look at electron micrographs of the reported DNA polyhedra, holes derived from every vertex and every face. To the best of my knowledge, no one pay attention to these holes.

Dual polyhedral links are built and the “sphere-surface-movement” method [34,35] is used to study process of hole forming. At last component strands of dual DNA polyhedral links are reduce to one with self-palindromic sequence. Our results will help scientists to modify their designing and synthesizing strategies.

2. Methods and results

DNA polyhedra are architected by DNA junctions with sticky ends which can paired with each other based on base complementary pairing rules [1]. DNA strands will be bent at vertexes for strands tension and space steric hindrance between bases. Therefore, a vertex generates a “V” hole. The shape of a hole is determined by the vertex degree. For examples, “V” holes of a DNA tetrahedron, hexahedron and dodecahedron are triangles, of a DNA octahedron are squares, of a DNA icosahedron are pentagons. Faces also generates a series of holes that are marked as “F” holes.

* Corresponding author. Tel.: +86 931 8912862

E-mail address: wyqiu@lzu.edu.cn (W.-Y. Qiu).

Table 1

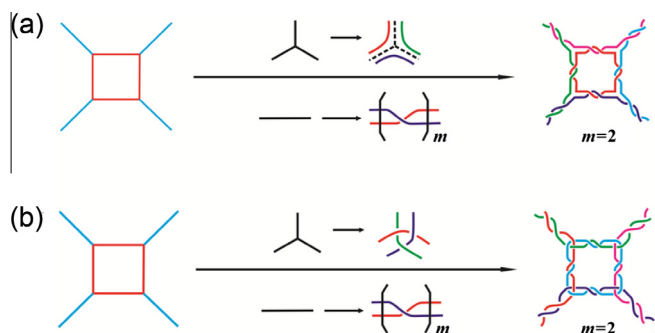
Frameworks analysis of DNA polyhedra.

Polyhedra	V holes		F holes		DNA polyhedra
	Shape	Number	Shape	Number	
Tetrahedra	Triangle	4	Hexagon	4	Irregular octahedron
Hexahedra	Triangle	8	Octagon	6	Tetrakaidecahedron
Octahedra	Square	6	Heptagon	8	Tetrakaidecahedron
Dodecahedra	Triangle	20	Decagon	12	Icosidodecahedron
Icosahedra	Pentagon	12	Hexagon	20	Icosidodecahedron

Table 2

The component numbers of dual DNA polyhedral links.

Polyhedra	Tetrahedra	Hexahedra	Octahedra	Dodecahedra	Icosahedra
Half-turns	Even	Even	Even	Even	Even
Component number	4	6	6	12	12

**Fig. 1.** Uncrossed vertex junctions and crossed vertex junctions. (a) uncrossed vertex junction and (b) crossed vertex junction.

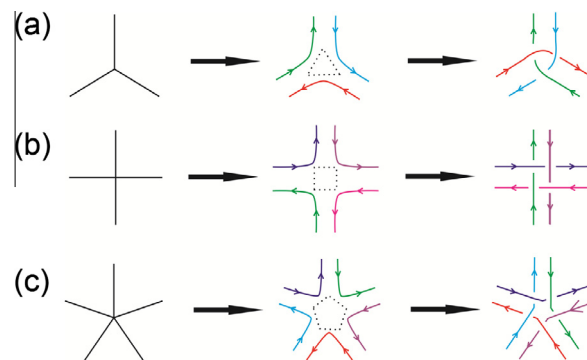
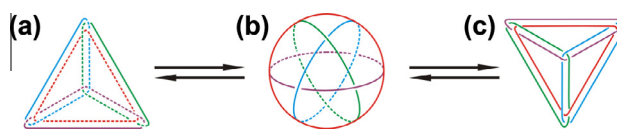
All these derived “V” and “F” holes make the regular polyhedra are not themselves any longer, but some irregular polyhedra frameworks. For an instance, a DNA tetrahedron is a special octahedron with four generated triangles on vertexes, results of other polyhedra are summarized in Table 1. Table 1 shows a amazing result is that DNA cube and octahedron have same framework, a tetrakaidcahedron. As well as this, DNA dodecahedron and icosahedron are icosidodecahedra.

For platonic polyhedra, the vertex (faces) number of a polyhedron is equal to the faces (vertexes) number of other polyhedron when they are dual polyhedra. Tetrahedra are self-dual polyhedra, hexahedra and octahedra are a pair of dual polyhedra, as well as dodecahedra and icosahedra.

In Table 1, the number of “V” holes and “F” holes of tetrahedra are same, the number of “V” holes and “F” holes of hexahedra are same with of the “F” holes and “V” holes of octahedra, the number of “V” holes and “F” holes of dodecahedra are same with of the “F” holes and “V” holes of icosahedra. All these make us try to use dual polyhedral links as models to predict intrinsic properties under these structures, each edge of all structures are covered by even half-turns and their component numbers are shown in Table 2. Table 2 suggests that dual polyhedral links have same components.

In order to describe “V” holes exactly, polyhedral links with no-crossed junctions (Fig. 1a) are not applicative, but crossed junctions (Fig. 1b) are the best choice. In Fig. 1b, a square with four three degree vertexes are shown, here $m = 2$.

Constructing links on “V” holes based on different vertexes, and then junctions as shown in Fig. 2 are gotten. The vertexes of

**Fig. 2.** Vertexes junctions based on vertex degree. (a) crossed 3-junction; (b) 4-junction; and (c) 5-junction.**Fig. 3.** The “sphere-surface-movement” on tetrahedral links.

tetrahedra, hexahedra and dodecahedra are covered by junctions with three degree (3-junction), the vertexes of octahedra are covered by 4-junctions, and that of icosahedra are covered by 5-junctions.

Lu et. put forward a strategy called “sphere-surface-movement” to describe and study characters of dual polyhedral links. The main point is that make a polyhedral link mapping on a sphere though topological methods, which means the operation is consecutive and without no cutting and adhesion [34,35]. For a convenience discussion, the “sphere-surface-movement” on a tetrahedron is shown in Fig. 3. First, a series of topological operations are made to make the tetrahedron mapping on a sphere; second, make the four components move with a direct orientation and an intermediate (Fig. 3b) is gotten; finally, the intermediate is translated into a tetrahedron (Fig. 3c). Obviously, the tetrahedron shown in Fig. 3c can also be translated into tetrahedron shown in Fig. 3a. So, tetrahedra links are self-dual polyhedral links.

As well as tetrahedra links, other polyhedral links also can be obtained. In Fig. 4, translation between hexahedra and octahedra links is diagrammed. The “sphere-surface-movement” on dodeca-

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