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ORIGINAL PAPER

The architecture of Platonic polyhedral links

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Abstract A new methodology for understanding the construction of polyhedral links has been developed on the basis of the Platonic solids by using our method of the '*n*-branched curves and *m*-twisted double-lines covering'. There are five classes of platonic polyhedral links we can construct: the tetrahedral links; the hexahedral links; the octahedral links; the dodecahedral links; the icosahedral links. The tetrahedral links, hexahedral links, and dodecahedral links are, respectively, assembled by using the method of the '3-branched curves and *m*-twisted double-lines covering', whereas the octahedral links and dodecahedral links are, respectively, made by using the method of the '4-branched curves' and '5-branched curves', as well as '*m*-twisted double-lines covering'. Moreover, the analysis relating topological properties and link invariants is of considerable importance. Link invariants are powerful tools to classify and measure the complexity of polyhedral catenanes. This study provides further insight into the molecular design, as well as theoretical characterization, of the DNA polyhedral catenanes.

Keywords Platonic polyhedra · Polyhedral links · Knot theory · Link invariants · DNA catenanes

1 Introduction

One challenge in supramolecular chemistry is the design of building blocks to attain total control of the arrangement of molecular knots and links [1–6]. Polyhedral links or catenanes, the interlinked and interlocked architectures, have been synthesized by

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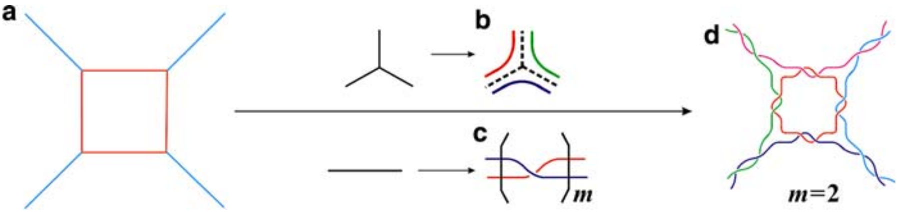


Fig. 1 The method for 'n-branched curves and m-twisted double-lines covering'

using branched DNA molecules [7–13]. DNA three-dimension structures include some Platonic and Archimedean solids and, more recently, DNA bipyramids and buckyballs. These curious objects provide some topological nontrivial structures embedding in 3-space that give us many novel targets for theoretically characterization using mathematical methods [14].

Knot theory is a tool for the study and quantization of configurations of graphs in Euclidean 3-space (R^3) [15–19]. The principles of knot theory have been applied to the modeling substances of different natures [20–26]. Since topologically linked protein catenanes were found in 2000 [27], the method of the 'three-cross-curve and double-twist-line covering' has been developed based on polyhedra and carbon nanotubes which have trihedral vertices [28–30]. This opens a big door to assembling and characterizing links on the basis of the skeleton of a polyhedron [31]. However, the above method is too restrictive to describe polyhedra with arbitrary connectivity of vertices, such as the octahedron has vertices of order four, and the icosahedron has vertices of order five.

In this paper, a more general approach, which is based on the vertices connectivity of the original polyhedron and the principle of DNA branched junctions [32,33] is proposed. In particular, research on platonic solids [34] is of fundamental importance in understanding the new approach. Our study reveals that nontrivial platonic polyhedral links have only rotational point groups [35]. The study of link invariants and symmetry may provide further insight into the theoretical characterization of the DNA polyhedral catenanes. This progress could form the basis of future development of more complex models. Such models can aid synthetic chemists and biologists in testing and developing their synthetic strategies.

2 An approach to the construction of polyhedral links

In our 'n-branched curves and m-twisted double-lines covering' approach, two types of basic building blocks for polyhedral links are needed [36]. One is an n-branched curve designed to replace the vertex of a polyhedron, where n is equal to the vertices degree. Figure 1 shows the example of employing a 3-branched curve to cover a vertex of degree 3. The other is an m-twisted double-line ($m = 0, 1, 2, \ldots$), which is proposed to replace the edge of a polyhedron. Connection of these two building blocks can result in some closed loops. Due to the number of twists, loops may be twisted around the loops that flank it so that trivial or nontrivial link can result.

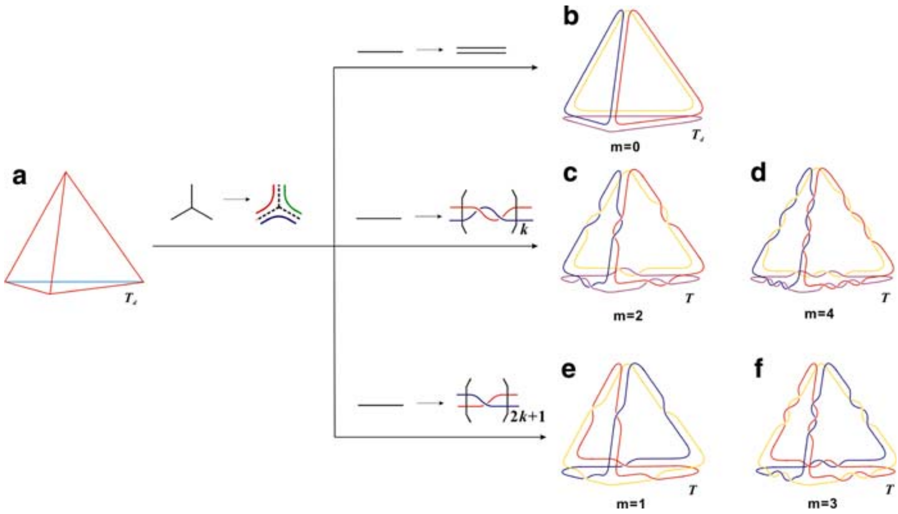


Fig. 2 The construction for the T_m-tetrahedral links by the method of the '3-branched curves and m-twisted double-lines covering'

Depending on its vertex degree, we consider the construction of three classes of platonic polyhedra. The symmetry and some topological properties of relevant links satisfy the following rules:

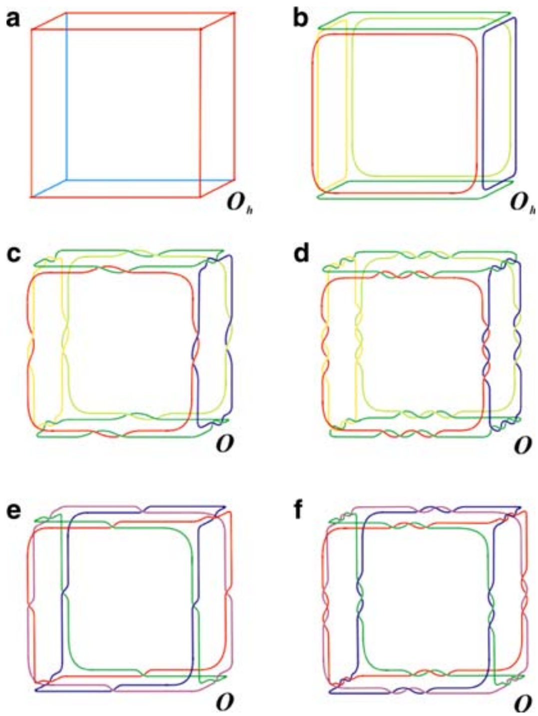
(1) A polyhedral link having m double line twists is called a T_m-polyhedral link;
(2) If $m=0$, the trivial link is obtained and the symmetry of a polyhedron is preserved. If $m>0$, the pattern of twists destroys the reflection symmetry group and, therefore, the nontrivial link is chiral;
(3) Given a polyhedron with F faces, E edges, V vertices of degree n, let L denotes the number of edges that a component covered. If $m=0$ or $m=2$k ($k = 1, 2, \ldots$), the trivial or nontrivial link has F components. If $m = 2k+1 (k = 1, 2, \ldots)$, the number of components C of the nontrivial link can be formalized as $C = \frac{2E}{L} = \frac{nV}{L}$.

3 Three-regular polyhedral links

The tetrahedron, the hexahedron, and the dodecahedron are all regular of degree three. Thus, their links can be obtained by the method of the '3-branched curves and m-twisted double-lines covering'. Note that the similar DNA tetrahedral and hexahedral links have been synthesized already, but except for the DNA dodecahedron, which has been assembled by a different method [11,12].

For the tetrahedron (Fig. 2a), the T_m-tetrahedral links are obtained, where m is the twisting number of each double-line. If $m=0$ (Fig. 2b), the T_0-tetrahedral link with T_d symmetry has 4 unlinked loops, thus, it is trivial. If $m=2$k, the T_{2k}-tetrahedral links with T symmetry also have 4 linked loops. For instance, the T_2-tetrahedral link and the T_4-tetrahedral link are shown in Fig. 2c, d, respectively. If $m=2k+1$, the resulting T_{2k+1}-tetrahedral links with T symmetry and each component covers across $L=4$

Fig. 3 The T_m-hexahedral links



edges. Hence, the numbers of components equal $C = 3$. The T_1-tetrahedral link and the T_3-tetrahedral link are shown in Fig. 2e, f, respectively.

For the hexahedron (Fig. 3a) and the dodecahedron (Fig. 4a), the T_m-hexahedral and dodecahedral links are obtained. If $m = 0$, the T_0-hexahedral link (Fig. 3b) and the T_0-dodecahedral link (Fig. 4b), with O_h symmetry has 6 unlinked components, as well as, with I_h symmetry has 12 unlinked components, respectively. If $m = 2k$, the T_{2k}-hexahedral links with O symmetry and the T_{2k}-dodecahedral links with I symmetry have 6 and 12 linked components. For instance, the T_2-hexahedral link and the T_4-hexahedral link are shown in Fig. 3c, d, respectively, the T_2-dodecahedral link and the T_4-dodecahedral link are shown in Fig. 4c, d, respectively. If $m = 2k+1$, the resulting links are the T_{2k+1}-hexahedral links with O symmetry and the T_{2k+1}-dodecahedral links with I symmetry, each component covers 6 and 10 edges. Hence, their components have $C = 4$ and 6. The T_1-hexahedral link and the T_3-hexahedral link are shown in Fig. 3e, f, and the T_1-decahedral link and the T_3-dodecahedral link are shown in Fig. 4e, f, respectively.

4 Four- and five-regular polyhedral links

The octahedron (Fig. 5a) and the icosahedron (Fig. 6a) are regular of degree four and five. Thus, their links can be constructed by methods of the '4-branched curves and m-twisted double-lines covering' and the '5-branched curves and m-twisted

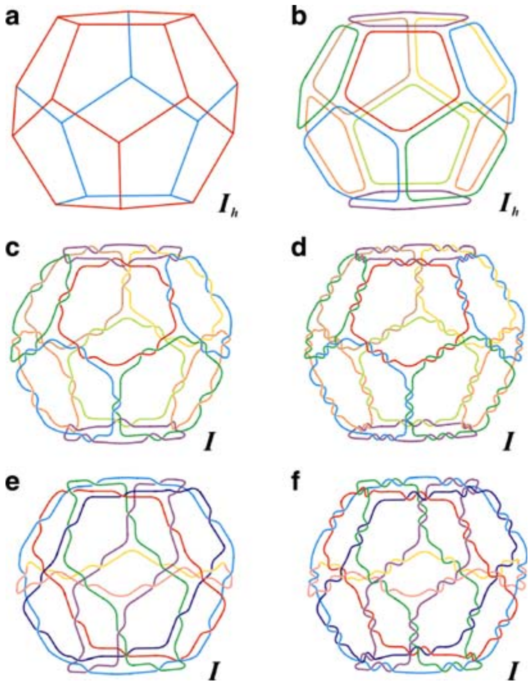


Fig. 4 The T_m-dodecahedral links

double-lines covering', respectively. This means that one uses 4-branched and 5-branched curves to cover V vertices and m-twisted double-lines to replace E edges of the polyhedron which are then glued together. Note that the DNA octahedron [37] reported in the laboratory is connected by six different four-way junctions and contains no catenations or knots.

For the T_m-octahedral links, each distinct m gives different octahedral links. For example, if $m = 0$, it gives the T_0-octahedral link. As Fig. 5b indicates, this is a collection of 8 components which has O_h symmetry. If $m = 2$ and $m = 4$, the T_2- and T_4-octahedral links will be generated (Fig. 5c, d). They are both interlocked cages with 8 components which belong to O symmetry. If $m = 1$ and 3, the resulting T_1- and T_3-octahedral links (Fig. 5e, f) both have O symmetry. Each component covers 6 edges, hence the numbers of components equal $C = 4$.

For the T_m-icosahedral links, $m = 0$ gives the T_0-icosahedral link. As Fig. 6b indicates, this is a collection of 20 components which has I_h symmetry. If $m = 2$ and $m = 4$, the generated T_2- and T_4-icosahedral links are shown in Fig. 6c, d, respectively. They are both interlocked cages with 20 components which belong to I symmetry. If $m = 1$ and 3, the T_1- and T_3-icosahedral links with I symmetry that would result are shown in Fig. 6e, f, respectively. Each component covers 10 edges, hence the numbers of components are $C = 6$.

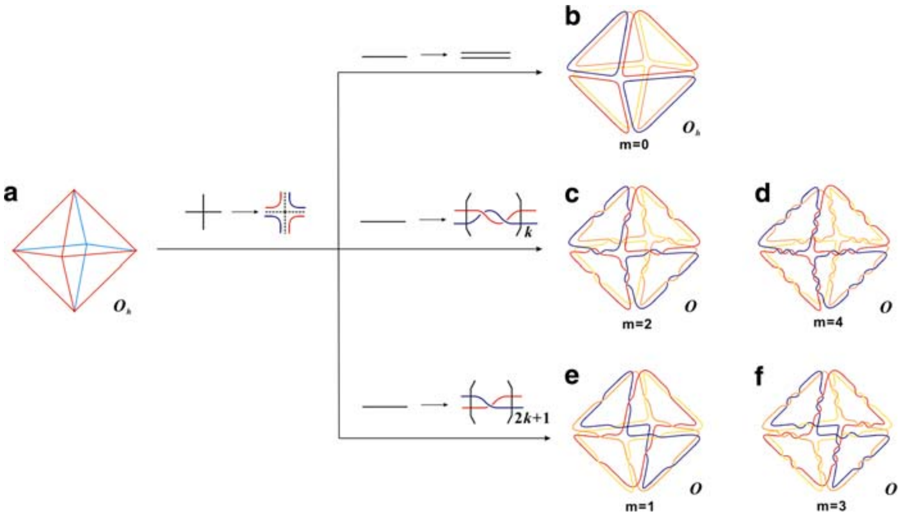


Fig. 5 The construction for the T_m-octahedral links by the method of the '4-branched curves and m-twisted double-lines covering'

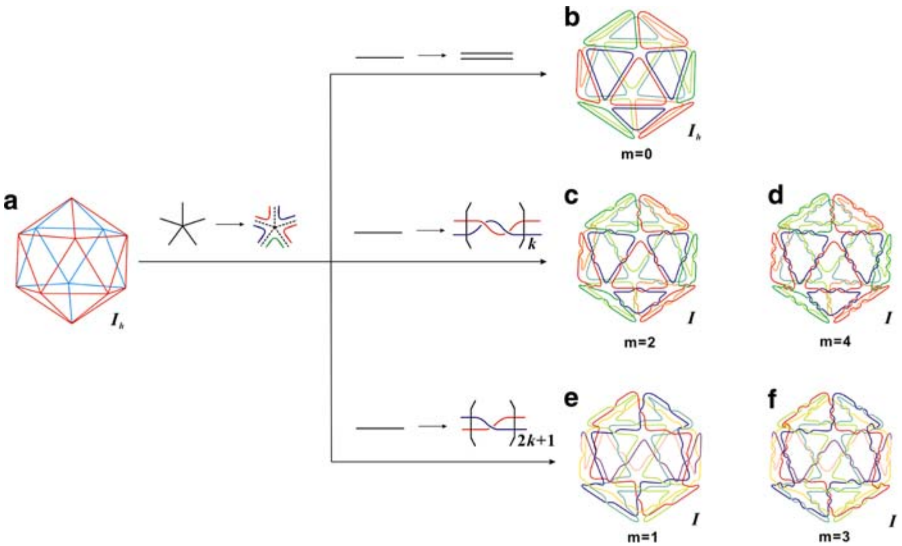
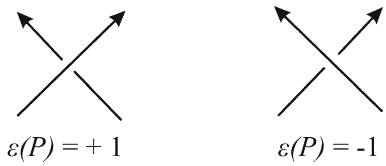


Fig. 6 The construction for the T_m-icosahedral links by the method of the '5-branched curves and m-twisted double-lines covering'

5 Link invariants

A basic problem in knot theory is determining whether two knots or links are equivalent or not. The extremely useful tools are knot and link invariants, which are

Fig. 7 Sign convention for crossings



Cr (L) = min { Cr (D): D is diagram of L}

w (L) = min { |wD)|: D is diagram of L}

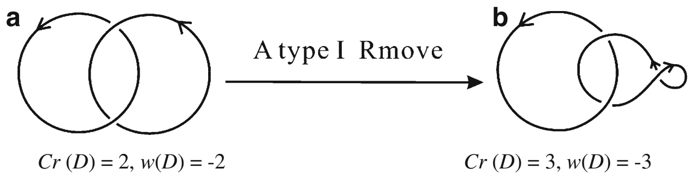


Fig. 8 Two different diagrams of the hopf link derived from each other by a type I Reidemeister move (Rmove)

unchanged under three Reidemeister moves. Here, we have calculated several quantities of links: crossing numbers $Cr(L)$, writhe numbers $w(L)$, linking numbers $Lk(L)$ and HOMFLY polynomials. Detailed definitions can be found in Ref. [15].

By assigning the same direction to each component of links, $\varepsilon(p)$ is given a sign according to the convention, as shown in Fig. 7, the writhe number $w(L)$ and the linking number $Lk(L)$ can be calculated by the two following equations:

$$w(L) = \sum_{p \in C_r(L)} \varepsilon(p); \quad Lk(L) = \frac{1}{2} \sum_{p \in \alpha_i \cap \alpha_j} \varepsilon(p).$$

where $\varepsilon(p)$ defined to be ± 1 if the overpass slants from top left to bottom right or bottom left to top right, $Cr(L)$ is the set of crossings of an oriented link, and $\alpha_i \cap \alpha_j$ is the set of crossings of two different components.

The numbers of crossings and writhe depend on the representation of knot diagram D. For example, two different diagrams of the Hopf link are shown in Fig. 8. They have different crossing numbers $Cr(D)$, and writhe numbers $w(D)$ also change under the type I Reidemeister moves, i.e., adding or removing extra crossing to a circle. However, when $Cr(L)$ and $w(L)$ are defined as following, they immediately become invariants of oriented links L:

$$\begin{aligned} Cr(L) &= \min\{Cr(D) : D \text{ is diagram of } L\} \\ w(L) &= \min\{|w(D)| : D \text{ is diagram of } L\} \end{aligned}$$

Note that linking numbers and HOMFLY polynomials can be used to detect chirality of knots and links. The configuration is D if $Lk(L) > 0$, and it is L if $Lk(L) < 0$

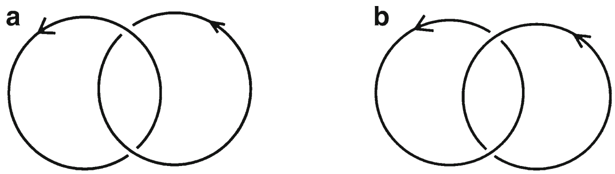


Fig. 9 Two mirror images of hopf link diagrams of **a** D configuration, **b** L configuration

Table 1 Invariants include component numbers $C(L)$, crossing numbers $Cr(L)$, linking numbers $Lk(L)$, writhe numbers $w(L)$, and configurations, of platonic polyhedral links

Platonic polyhedral links	Twist number m	C(L)	$Cr(L)$	$w(L)$	$Lk(L)$	Configuration
Tetrahedral links	0	4	0	0	0	None
	$2k$	4	$12k$	$-12k$	$-6k$	L
	$2k+1$	3	$6(2k+1)$	0	0	Unknown
Hexahedral links	0	6	0	0	0	None
	$2k$	6	$24k$	$-24k$	$-12k$	L
	$2k+1$	4	$12(2k+1)$	$12k$	$6k$	D
Octahedral links	0	8	0	0	0	None
	$2k$	8	$24k$	$-24k$	$-12k$	L
	$2k+1$	4	$12(2k+1)$	$-12k$	$-6k$	L
Dodecahedral links	0	12	0	0	0	None
	$2k$	12	$60k$	$-60k$	$-30k$	L
	$2k+1$	6	$30(2k+1)$	$30k$	$15k$	D
Icosahedral links	0	20	0	0	0	None
	$2k$	20	$60k$	$-60k$	$-30k$	L
	$2k+1$	6	$30(2k+1)$	$-60k$	$-30k$	L

[38]. The HOMFLY polynomial is a 2-variable knot polynomial, the variables being v and z. If the HOMFLY polynomial of a link is not symmetric in v, then the link is topological chiral. Some examples are shown in Fig. 9. For the diagram shown in Fig. 9a, the linking number is +1, so it belongs to D configuration, and the relating HOMFLY polynomial is $p = z^{-1}(-v^3 + v) + zv$. For the diagram shown in Fig. 9b, the linking number is -1, so it belongs to L configuration, and the relating HOMFLY polynomial is $\overline{p} = z^{-1}(-v^{-3}+v^{-1})+zv^{-1}$. It is easy to find that $p(v, z) = \overline{p}(v^{-1}, z)$, this means that these two diagrams are mirror images of one another.

Some invariants of platonic polyhedral links are listed in Table 1, whilst some HOMFLY polynomials are given in the Appendix.

If $m=0$, all configurations are trivial. As a consequence, they are achiral and have zero linking numbers. The only invariant is the number of component. If $m = 2k$, the absolute values of writhe numbers are equal to crossing numbers and all are L configuration. If $m = 2k + 1$, the absolute values writhe numbers are equal to the half of crossing numbers except for the tetrahedral links, which have zero writhe numbers and linking numbers. Thus, these configurations are unclassified.

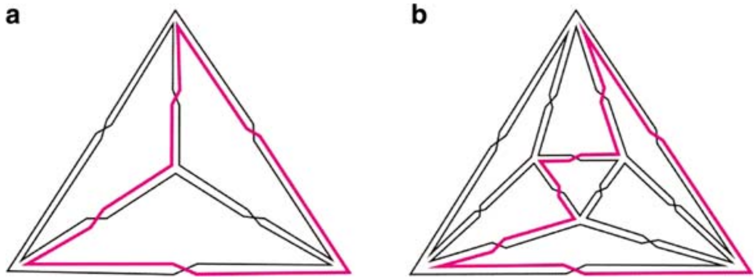


Fig. 10 Two examples of Hamiltonian cycles covering all the vertices of a polyhedral link **a** The T_1-tetrahedral link graph, **b** The T_1-octahedral link graph

6 Conclusion

In summary, we have presented a general approach to construct a polyhedral link based on the platonic polyhedron and its vertices degree and paved the way to understanding the construction of the polyhedral link from an arbitrary polyhedron. This approach cannot only be applied to a polyhedron which possesses trihedral vertices, such as the tetrahedron, hexahedron, and dodecahedron, but also to a polyhedron with any vertices degree, such as the octahedron and icosahedron whose vertices are of order 4 and 5, respectively. The approach can also be applied to irregular graphs.

Furthermore, the symmetrical analysis for platonic polyhedral links shows that the T_0-tetrahedral link, the T_0-hexahedral and T_0-octahedral links, and the T_0-dodecahedral and T_0-icosahedral links possess T_d, O_h, and I_h symmetry, respectively. When the twisting number $m > 0$, the tetrahedral links, the hexahedral and octahedral links, and the dodecahedral and icosahedral links belong to T, O, and I symmetry, respectively, hence, are said to be chiral. On the other hand, the number of components of a polyhedral link also depends on the twisting number m. It is equal to the face number of the polyhedron if m is zero or an even number, and always needs fewer components than the face number of the polyhedron for odd m. In particular, for the T_{2K+1}-tetrahedral and octahedral link graphs, each component corresponds to a Hamiltonian cycle because it hits every vertices exactly once (Fig. 10). These interesting structures inspire some fundamental questions in graph theory. We shall discuss them in detail elsewhere.

Using the knot invariant technique, many of the chemical information of DNA polyhedra which based on its entanglement are obtained. Such as molecules of larger crossing numbers migrate more rapidly in gel electrophoresis; topological stereo-isomers have the same sequence of base pairs but different linking numbers; knot polynomials have already played a significant role in the description and analysis of chirality problems of chemistry [39–41]. This not only can help us theoretical classify and identify these molecules, but also may provide a new insight and new methodology for further synthesis.

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Appendix

The HOMFLY polynomial is defined by the skein relationship

$$v^{-1} P_{L^+} - v P_{L^-} = Z P_{L^0}$$

T_2-tetrahedral link

$$\begin{aligned} & z^{-3}\left(-v^3+3v-3v^{-1}+v^{-3}\right)+z^{-1}\left(-3v^3+9v-9v^{-1}+3v^{-3}\right) \\ & \quad +z\left(-3v^3+15v+v^{-1}+4v^{-3}+v^{-5}\right)+z^3\left(-v^3+12v-18v^{-1}+3v^{-5}\right) \\ & \quad +z^5\left(3v-10v^{-1}-3v^{-3}+v^{-5}\right)+z^7\left(-2v^{-1}-v^{-3}\right) \end{aligned}$$

T_2- hexahedral link

$$\begin{aligned} & z^{-5}\left(-v^5+5v^3-10v+10v^{-1}-5v^{-3}+v^{-5}\right) \\ & \quad +z^{-3}\left(-6v^5+30v^3-60v+60v^{-1}-30v^{-3}+6v^{-5}\right) \\ & \quad +z^{-1}\left(-15v^5+87v^3-190v+196v^{-1}-93v^{-3}+13v^{-5}+2v^{-7}\right) \\ & \quad +z\left(-20v^5+154v^3-396v+446v^{-1}-211v^{-3}+19v^{-5}+7v^{-7}+v^{-9}\right) \\ & \quad +z^3\left(-15v^5+171v^3-580v+744v^{-1}-385v^{-3}+10v^{-5}+18v^{-7}+7v^{-9}\right) \\ & \quad +z^5\left(-6v^5+114v^3-569v+982v^{-1}-526v^{-3}-52v^{-5}+31v^{-7}+26v^{-9}\right) \\ & \quad +z^7\left(-v^5+41v^3-337v+828v^{-1}-511v^{-3}-146v^{-5}+21v^{-7}+41v^{-9}\right) \\ & \quad +z^9\left(6v^3-105v+419v^{-1}-349v^{-3}-169v^{-5}-11v^{-7}+29v^{-9}\right) \\ & \quad +z^{11}\left(-13v+112v^{-1}-156v^{-3}-99v^{-5}-20v^{-7}+9v^{-9}\right) \\ & \quad +z^{13}\left(12v^{-1}-39v^{-3}-28v^{-5}-8v^{-7}+v^{-9}\right) \\ & \quad +z^{15}\left(-4v^{-3}-3v^{-5}-v^{-7}\right) \end{aligned}$$

T_1-dodecahedral link

$$\begin{aligned} & z^{-5}\left(-v^{-1}+5v^{-3}-10v^{-5}+10v^{-7}-5v^{-9}+v^{-11}\right) \\ & \quad +z^{-3}\left(-9v^{-1}+42v^{-3}-78v^{-5}+72v^{-7}-33v^{-9}+6v^{-11}\right) \\ & \quad +z^{-1}\left(-31v^{-1}+137v^{-3}-235v^{-5}+193v^{-7}-74v^{-9}+10v^{-11}\right) \end{aligned}$$

$$
\begin{aligned}
&+z\left(-42v^{-1}+208v^{-3}-357v^{-5}+206v^{-7}-71v^{-9}+2v^{-11}\right)\\
&+z^{3}\left(27v^{-1}+58v^{-3}-231v^{-5}+138v^{-7}+38v^{-9}-30v^{-11}\right)\\
&+z^{5}\left(74v^{-1}-124v^{-3}-62v^{-5}-65v^{-7}+191v^{-9}-62v^{-11}\right)\\
&+z^{7}\left(3v^{-1}-31v^{-3}-182v^{-5}+77v^{-7}+40v^{-9}-7v^{-11}\right)\\
&+z^{9}\left(-32v^{-1}+105v^{-3}-395v^{-5}+698v^{-7}-551v^{-9}+166v^{-11}\right)\\
&+z^{11}\left(56v^{-3}-453v^{-5}+1289v^{-7}-1161v^{-9}+317v^{-11}\right)\\
&+z^{13}\left(6v^{-1}+6v^{-3}-402v^{-5}+1375v^{-7}-1265v^{-9}+300v^{-11}\right)\\
&+z^{15}\left(-v^{-1}+31v^{-3}-315v^{-5}+1006v^{-7}-868v^{-9}+171v^{-11}\right)\\
&+z^{17}\left(-3v^{-1}+36v^{-3}-204v^{-5}+531v^{-7}-399v^{-9}+60v^{-11}\right)\\
&+z^{19}\left(-v^{-1}+17v^{-3}-92v^{-5}+208v^{-7}-122v^{-9}+12v^{-11}\right)\\
&+z^{21}\left(3v^{-3}-25v^{-5}+59v^{-7}-23v^{-9}+v^{-11}\right)\\
&+z^{23}\left(-3v^{-5}+11v^{-7}-2v^{-9}\right)\\
&+z^{25}v^{-7}
\end{aligned}
$$

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