

Stable Traces as a Model for Self-Assembly of Polypeptide Nanoscale Polyhedrons

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Abstract

Gradišar et al. [11] recently presented a novel self-assembly strategy for polypeptide nanostructure design that could lead to significant developments in biotechnology. In the present paper, the underlying mathematical model is developed. A construction of a polypeptide polyhedron is modelled with a stable trace in the corresponding graph of the polyhedra. Here a stable trace is a double trace with two additional conditions—having no retracing and no repetition through any vertex. It is proved that the graphs that admit stable traces are precisely graphs with minimum degree 3. Parallel and antiparallel double traces are also introduced and studied. Computational results for several polyhedra are presented.

1 Introduction

The most complex nanostructures known in nature are formed by self-assembly of biopolymers, where polypeptides form most complex structures. Self-assembly of designed DNA into tetrahedron [10, 12], cube [2, 23], octahedron [17], dodecahedron [24], and icosahedron [1, 4] were reported. A related topic is the one of constructing topologically linked proteins, the first such construction being reported in [6]. For some recent developments in this direction see [3, 5] where mathematical models of n -pyramidal links (a link is a finite union of knots), regular links, and semi-regular links are proposed, see also [14].

On the other hand, the design of polypeptide folds is significantly more challenging as the stability of polypeptide assemblies depend on numerous cooperative interactions. Nevertheless, very recently Gradišar et al. [11] presented a novel polypeptide self-assembly strategy for nanostructure design relying on the topological arrangement of interacting modular peptide segments. The main success of their research is a construction of a polypeptide self-assembling tetrahedron by concatenating 12 coiled-coil-forming segments in an exact order. More precisely, a single polypeptide chain was assembled through the 6 edges of the tetrahedron in such a way that every edge was traversed exactly twice. In this way 6 coiled-coil dimers were created and interlocked into a stable structure. This technological procedure seems to be a landmark discovery that could lead to significant developments in biotechnology.

The required mathematical support for the particular case of the tetrahedron in the above research was already given in [11]. The main purposes of this paper are

- (a) to make comprehensive general mathematical model for investigations that could follow the breakthrough from [11],
- (b) to point to related mathematical investigations that exist in the literature, and
- (c) to prove new general results that could be used in the experimental work in the future.

The paper is organized as follows. In the next section we first list basic concepts from graph theory needed throughout the paper. Then we introduce double traces and extend them to stable traces, where the latter traces form the main mathematical model for the self-assembly of polypeptides. In Section 3 we prove (Theorem 3.1) that a connected graph admits a stable trace if and only if its minimum degree is at least 3. This in particular implies that not only the tetrahedron but any polyhedron can be (at least theoretically) constructed from a single coiled-coil-forming segment. In Section 4 we give a new proof (based on the proof idea of Theorem 3.1) of the theorem from [7] asserting that a weaker condition for a graph to contain the so-called proper trace is fulfilled if and only if the minimum degree is at least 2. In Section 5 we consider two special cases of double traces, with either only parallel or only antiparallel edges. We conclude with numerical results that reveal possible varieties in designing polyhedra different from the tetrahedron.

2 Double traces and stable traces

All graphs considered in this paper will be connected and finite. Unless stated otherwise, for instance when doubling every edge of a graph, graphs will also be simple, that is, without loops and parallel edges. If v is a vertex of a graph G , then its degree will be denoted by $d_G(v)$ or $d(v)$ for short if G will be clear from the context. The minimum and the maximum degree of G are denoted with $\delta(G)$ and $\Delta(G)$, respectively. A *subdivision* of a graph G is a graph obtained from G by replacing some of its edges with disjoint paths. A *directed graph* is a graph, whose edges have a direction associated with them. In formal terms, a directed graph is a pair $G = (V, A)$, where V is a set of vertices and A is a set of ordered pairs of vertices, called *arcs*.

An *Eulerian circuit* in G is a circuit which traverses every edge of G exactly once. G is called *Eulerian* if it admits an Eulerian circuit. A fundamental theorem of graph theory, known as Euler's theorem, asserts that G is Eulerian if and only if all of its vertices are of even degree. Its directed version claims that a directed graph G admits an Eulerian circuit if and only if for every vertex u in G , the incoming degree of u is equal to the outgoing degree of u . For other terms and concepts from graph theory not defined here we refer to [22].

We now move to the underlying mathematical model for the biotechnological investigations presented in the introduction. A polyhedron P which is composed from a single polymer chain can be naturally represented with the graph $G(P)$ of the polyhedron. Its vertices are the endpoints of segments, two vertices being adjacent if there is a segment connecting them. Since in the technological process every edge of $G(P)$ corresponds to a coiled-coil dimer, exactly two segments are associated with a fixed edge of $G(P)$. We therefore say that a *double trace* in a graph G is a circuit which traverses every edge exactly twice. With this concept in hand we can formulate the following basic:

Fact 2.1 *Suppose that a polyhedron P is composed from a single polymer chain such that coiled-coil dimers were created and interlocked into a stable structure. Then the sequence of coiled-coil segments corresponds to a double trace in $G(P)$.*

It is easy to see (but important) that every graph admits a double trace:

Proposition 2.2 *Every graph G has a double trace.*

Proof. Construct a new graph, called the *double of G* , by replacing every edge of G with two new parallel edges. Obviously any vertex of the double of G has even degree. Hence by Euler's theorem the double of G admits an Eulerian circuit C . The circuit C then represents a double trace of the original graph G . \square

A double trace in $G(P)$ itself does not guarantee that the structure created is stable. In order to have a stable structure, the following condition must be fulfilled:

- (i) no immediate succession of an edge e by its parallel copy occurs.

We say that a double trace contains a *retracing* if it has an immediate succession of an edge e by its parallel copy, see Fig. 1.

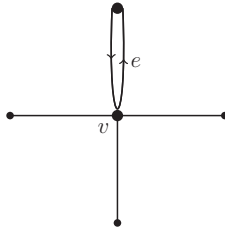


Figure 1. Retracing of an edge e

We therefore make the following:

Definition 2.3 A double trace that fulfils condition (i) is called a proper trace. In other words, a proper trace is a double trace with no retracing.

Hence we are interested in proper traces. The graphs that admit proper traces were first characterized by Sabidussi in [16] and later independently by Eggleton and Skilton in [7] as follows:

Theorem 2.4 A graph G admits a proper trace if and only if $\delta(G) \geq 2$.

In their paper, Eggleton and Skilton also studied infinite graphs, a research also done by Thomassen in [19]. Their results could be useful if the biotechnological progress will allow the design of huge nanostructures.

But also proper traces do not yet guarantee that the structures created are stable. To make them such, we also need the following condition to be fulfilled:

- (ii) a vertex sequence $u \rightarrow v \rightarrow w$ appears at most once in any direction ($u \rightarrow v \rightarrow w$ or $w \rightarrow v \rightarrow u$) on a double trace.

More formally, if v is a vertex of a graph G with a double trace T and u and w are two different neighbors of v , then we say that T contains a *repetition through v* if the vertex sequence $u \rightarrow v \rightarrow w$ appears twice in T in any direction ($u \rightarrow v \rightarrow w$ or $w \rightarrow v \rightarrow u$), see Fig. 2.

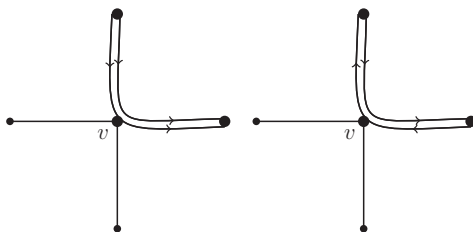


Figure 2. Possible repetitions through vertex v

Conditions (i) and (ii) are now sufficient for a double trace in order that the corresponding polyhedron composed from a single polymer chain forms a stable structure. We therefore make the key definition of this paper:

Definition 2.5 *A double trace that in addition fulfils conditions (i) and (ii) is called a stable trace. In other words, a stable trace is a proper trace without repetitions through its vertices.*

The prime object of our interest are thus stable traces. Graphs that admit such traces will be characterized in the next section.

3 Graphs that admit stable traces

As announced, we next prove the following result. Its message is that theoretically arbitrary stable polyhedrons can be created from a single polymer chain.

Theorem 3.1 *A graph G admits a stable trace if and only if $\delta(G) \geq 3$.*

Proof. Suppose first that G admits a stable trace. Then by Theorem 2.4, G does not contain a vertex of degree 1. Moreover, G does not contain a vertex of degree 2, because such a vertex v clearly forces either two retracings in v or a repetition through v .

Assume now that G is an arbitrary graph with $\delta(G) \geq 3$. We proceed by induction on $\Delta = \Delta(G)$.

Let $\Delta = 3$. Then $\delta(G) = \Delta(G) = 3$, in other words G is a cubic graph. By Theorem 2.4 we know that G admits a proper trace T . Since all the vertices of G are of degree 3 and T is proper, it is not difficult to see that T is also a stable trace. (This fact was already observed in [11], hence we do not repeat the arguments here.)

Assume now that $\Delta \geq 4$ and that any graph H with $\Delta(H) < \Delta$ and $\delta(H) \geq 3$ admits a stable trace. To make the argument more transparent, assume first that G contains a unique vertex v of degree Δ . Let $v_1, v_2, \dots, v_\Delta$ be the neighbors of v and construct the graph G' from G as follows. Remove from G the vertex v , add two new vertices v' and v'' , connect them by an edge, connect v' with $v_1, \dots, v_{\lceil \frac{\Delta}{2} \rceil}$, and connect v'' with the remaining neighbors of v , see Fig. 3.

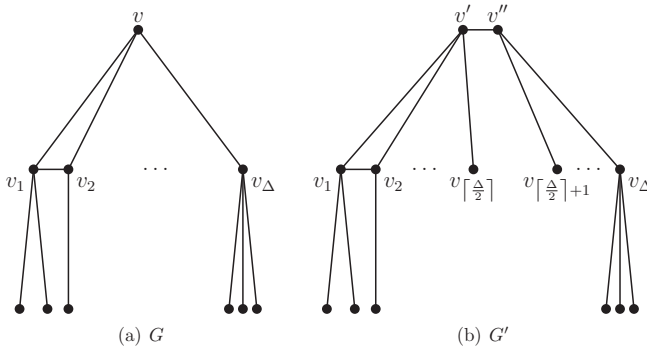


Figure 3. Construction from the proof of Theorem 3.1

Note that in G' all the vertices but v' and v'' are of the same degree as in G , while $d_{G'}(v') = \lceil \frac{\Delta}{2} \rceil + 1$ and $d_{G'}(v'') = \lfloor \frac{\Delta}{2} \rfloor + 1$. It follows that $\Delta(G') < \Delta$. Since $\Delta \geq 4$, we also infer that $\delta(G') \geq 3$, hence by the induction assumption on Δ , G' admits a stable trace T' .

We next construct a trace T in G from T' as follows. Let $e = xy$ be an arbitrary (oriented) edge of T' . If $x, y \in V(G') \setminus \{v', v''\}$ we put xy into T . Let $u \neq v', v''$. If $e = uv'$ then replace e with uv in T . Similarly we replace edges of the form $v'u, uv''$, and $v''u$ with vu, uv , and vu , respectively. Finally, the two occurrences of the edge $v'v''$ (or $v''v'$) from T' are ignored in T .

We claim that T is a stable trace of G . Note first that any edge e that appears in G has its unique corresponding edge e' in G' . Clearly, $e' \neq v'v''$. Since e' is traversed twice in T' , the edge e is traversed twice in T . Hence T is a double trace. It is also clear that T is a proper trace because otherwise T' would not be proper. (If there would be a retracing of edge e in T , it would lead to a retracing of its corresponding edge e' in T' .) Finally we need to verify that T is stable. Let $e = xy$ and $f = yz$ be two consecutive edges of T . If $\{x, y, z\} \cap \{v\} = \emptyset$, then e, f does not give a repetition through y because otherwise we would have a repetition through y in T' . The same conclusion holds if $x = v$ or $z = v$. Assume hence that $y = v$. Let $x = v_i$ and $z = v_j$ and consider two subcases. In the first subcase let $i, j \leq \lceil \frac{\Delta}{2} \rceil$. Then e, f were obtained from the edges $v_iv', v'v_j$ which do not have a repetition through v' hence e, f do not have a repetition through v . Analogous conclusion holds when $i, j > \lceil \frac{\Delta}{2} \rceil$ (just replace v' with v'' in the argument). In the second subcase let $i \leq \lceil \frac{\Delta}{2} \rceil < j$. Then e, f were constructed from $v_iv', v'v'', v''v_j$ in T' . Recall that $v'v''$ is traversed exactly twice in T' . Hence if e, f would have a repetition through v , we would have (in particular) a repetition through v' in T' , a contradiction. We conclude that T is a stable trace of G .

We have thus proved that if G has a single vertex of degree Δ , then G admits a stable trace. We now proceed by the second induction on the number $D_{\max}(G)$ of vertices of maximum degree of a graph G . Let $D_{\max}(G) \geq 2$ and let v be an arbitrary vertex of degree Δ . Then construct a graph G' from G in the same way as above by replacing v with two adjacent vertices such that the neighbors of v are evenly distributed among the two new vertices. Note that $D_{\max}(G') < D_{\max}(G)$ and hence G admits a stable trace by the induction on $D_{\max}(G)$. \square

4 New proof of Theorem 2.4

Based on the proof idea of Theorem 3.1 we next give a new proof of Theorem 2.4. We first state the following lemma which readily follows from the fact that if v is a vertex of G of degree 2 and T is a proper trace of G , then after we reach v on T from u , the trace T continues to the neighbor of v different from u .

Lemma 4.1 *A graph G admits a proper trace if and only if an arbitrary subdivision G' of G admits a proper trace. In particular, the number of proper traces in G is the same*

as the number of proper traces in G' .

The last assertion of Lemma 4.1 follows because every proper trace T of G uniquely lifts to a proper trace of G' .

In the rest of the section we prove Theorem 2.4. Suppose first that G admits a proper trace. Then G does not contain a vertex of degree 1, because such a vertex v clearly forces a retracing in v .

Conversely, let G be an arbitrary graph with $\delta(G) \geq 2$. We proceed by induction on $\Delta = \Delta(G)$. Let $\Delta = 2$. Then $\delta(G) = \Delta(G) = 2$ and as G is connected, G is a cycle. It is straightforward to construct a proper trace of a cycle by starting in an arbitrary vertex and twice traversing the cycle. If $\delta(G) = \Delta(G) = 3$, then it is easy to see (see [11] for an argument) that G admits a stable trace and thus a proper trace as well.

Let next $\delta(G) = 2$ and $\Delta(G) = 3$. By Handshaking lemma, the number D of vertices of degree 3 is even. Suppose first that $D = 2$ and let $d(v_1) = d(v_2) = 3$. Then G contains exactly three internally disjoint paths P' , P'' , and P''' whose endpoints are v_1 and v_2 . These paths are either all between v_1 and v_2 , or, without loss of generality, P' starts and ends in v_1 , P'' starts and ends in v_2 , while P''' is a v_1, v_2 -path. In the first case, we may without loss of generality assume that P'' and P''' are of length at least 2. Then the sequence $v_1 \rightarrow P' \rightarrow v_2 \rightarrow P'' \rightarrow v_1 \rightarrow P''' \rightarrow v_2 \rightarrow P'' \rightarrow v_1 \rightarrow P' \rightarrow v_2 \rightarrow P''' \rightarrow v_1$ gives a proper trace. In the second case the paths P' and P'' are of length at least 2, hence the sequence $v_1 - P' \rightarrow v_1 \rightarrow P' \rightarrow v_1 \rightarrow P''' \rightarrow v_2 \rightarrow P'' \rightarrow v_2 \rightarrow P'' \rightarrow v_2 \rightarrow P''' \rightarrow v_1$ does the same. We point that the subsequence $P' \rightarrow v_1 \rightarrow P'$ is not a retracing because P' is a cycle. Assume now that $\Delta(G) = 3$, $D \geq 4$, and $\delta(G) = 2$. If G is a subdivision of a cubic graph, then it admits a proper trace by Lemma 4.1 and the already known fact that cubic graphs admit proper traces. Otherwise G has a vertex v , $d(v) = 3$, and a path P starting and ending in v and having all inner vertices of degree 2. Note that P is of length at least 2. Suppose first that v and P are the unique vertex and path with described properties. Let e be the edge of G incident with v that is not on P . Since $\delta(G) = 2$, there exists a path Q internally disjoint with P that starts in v , contains e , and ends in a vertex u with $d(u) = 3$. Note that $u \neq v$. Let G' be the graph obtained from G by removing all the vertices from the paths P and Q but the vertex u . Note that in G' all the vertices except u are of the same degree as in G , while $d_{G'}(u) = 2$. Hence G' is a subdivision of a cubic graph and it admits a proper trace T' . Decompose the proper

trace T' as $T'_1 \rightarrow u \rightarrow T'_2$ (note that T'_1 and T'_2 are not disjoint). Then we claim that $T = T'_1 \rightarrow u \rightarrow Q \rightarrow v \rightarrow P \rightarrow v \rightarrow P \rightarrow v \rightarrow Q \rightarrow u \rightarrow T'_2$ is a proper trace in G , see Fig. 4.

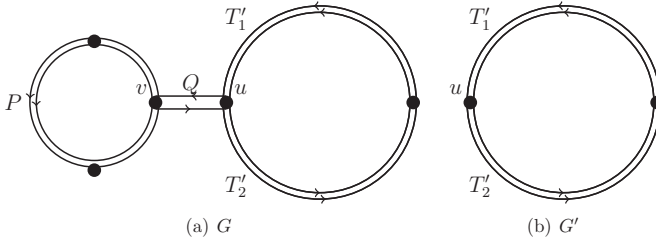


Figure 4. Construction of proper trace in G from the proof of Theorem 2.4

Indeed, every edge on P and Q is traversed twice in T while the edges from G are traversed twice in T because T' is proper. Since T' had no retracing and in the construction of T no new retracing was constructed, T is proper. We conclude that G admits a proper trace if it has a unique vertex v of degree 3 with a path starting and ending in v and having all inner vertices of degree 2.

If G has more than one such vertex, then we proceed by induction on the number of such vertices. Exception appears if all the vertices of degree 3 in graph G have the above described property. While proceeding the induction we are left with a graph G' which has exactly two disjoint cycles and exactly two vertices u, v of degree 3. Each of these two vertices lies in a cycle, the two cycles being disjoint, in which all the other vertices are of degree 2. Vertices u and v are adjacent and are internal vertices one for the first and the other for the second cycle of G' , see Fig. 5. Clearly, G' contains a proper trace.

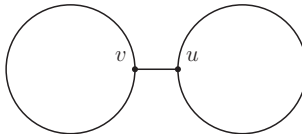


Figure 5. Particular case from the proof of Theorem 2.4

To conclude the proof we assume that the assertion is true for all graphs H with $\delta(H) \geq 2$ and $\Delta(H) \leq \Delta$, where $\Delta \geq 3$. Let G be a graph with $\delta(G) \geq 2$ and $\Delta(G) = \Delta + 1$. Now make the same construction as in the proof of Theorem 3.1, by

splitting every vertex of G of degree $\Delta + 1$ into two vertices of smaller degree. The constructed graph G' has $\delta(G') \geq 2$ and $\Delta(G') = \Delta$. Using induction assumption and the conclusions from the proof of Theorem 3.1 we see that G admits a proper trace. Theorem 2.4 is thus proved.

5 Parallel and antiparallel proper traces

In the forthcoming design of polypeptides, two particular designs could be of special interest: either on every edge of a polyhedra the two coiled-coil-forming segments would be aligned in the same direction, or on every edge the two coiled-coil-forming segments would be aligned in the opposite direction. Because parallel coiled-coil dimers are easier to construct, especially designs of the first type would be useful. We thus introduce the following additional concepts.

Let T be a double trace of a graph G . Then every edge $e = uv$ of T is traversed exactly twice. If in both cases e is traversed in the same direction (either both times from u to v or both times from v to u) we say that e is a *parallel edge* (with respect to T). If this is not the case we say that e is an *antiparallel edge* (with respect to T). Then we put:

Definition 5.1 *Let T be a double trace of a graph G . Then T is a parallel double trace if every edge of T is parallel and an antiparallel double trace if every edge of T is antiparallel.*

The above particular designs of polyhedra can thus be represented with parallel stable traces and antiparallel stable traces, respectively. In the rest of the section we either prove or recall characterizations of graphs that admit (anti)parallel double traces and (anti)parallel proper traces. We begin with the antiparallel case. The following observation goes back to Tarry [18]:

Proposition 5.2 *Every graph admits an antiparallel double trace.*

Proof. Let G be a graph, let G' be the double of G (cf. the proof of Proposition 2.2), and direct the edges of G' such that each parallel pair of its edges is directed antiparallel. Then by Euler's theorem for directed graph, the constructed digraph admits an Eulerian circuit C' . The circuit C' then represents an antiparallel double trace in the original graph G . □

A characterization of graphs that admit antiparallel proper traces is more involved. The problem was posed back in 1951 by Ore in [15], partially solved in [21], and completely solved by Thomassen [20] as follows:

Theorem 5.3 *A graph G admits an antiparallel proper trace if and only if $\delta(G) \geq 2$ and G has a spanning tree T such that each connected component of $G - E(T)$ either has an even number of edges or contains a vertex v , $d_G(v) \geq 4$.*

Theorem 5.3 was generalized by Fan and Zhu in [8]. Moreover, they presented a polynomial recognition algorithm of graphs that admit antiparallel proper traces. Another study in this direction is [13] where graphs that do not admit antiparallel proper traces are studied and the minimum number of retracings needed is expressed in terms of other graph invariants.

Turning to parallel traces we first observe:

Proposition 5.4 *A graph G admits a parallel proper trace if and only if G is Eulerian.*

Proof. Suppose that T is a parallel proper trace of G . Considering T in the double of G we infer that the incoming and the outgoing degree in each vertex are the same. Therefore, each vertex of G is of even degree. Conversely, let G be an Eulerian graph and let T be an Eulerian circuit in G . Traversing T twice we get a double trace. It is clearly parallel and has no retracting. \square

Note that a graph with a vertex of odd degree does not admit a parallel double trace. Since by definition a proper trace is a double trace, we also have:

Corollary 5.5 *A graph G admits a parallel double trace if and only if G is Eulerian.*

Suppose now that a graph G admits a parallel stable trace. Then by Proposition 5.4, G is Eulerian and hence by Theorem 3.1 we also have $\delta(G) \geq 4$. We wonder whether these conditions are also sufficient and hence pose:

Problem 5.6 *Is it true that a graph G admits a parallel stable trace if and only if G is Eulerian and $\delta(G) \geq 4$?*

For the case of antiparallel stable traces we have no suggestion what could be a characterization and thus pose:

Problem 5.7 *Characterize graphs that admit antiparallel stable traces.*

The next section contains some numerical indications that could help with this problem.

6 Conclusions and numerical results

In Table 1 conditions required for graphs to admit double and related traces are collected. To make the presentation short, let us call a spanning tree from Theorem 5.3 *special spanning tree* (SST).

		CONDITION		
		none	parallel	antiparallel
TRACE	double	$\forall G$ (Proposition 2.2)	Eulerian (Corollary 5.5)	$\forall G$ (Proposition 5.2)
	proper	$\delta(G) \geq 2$ (Theorem 2.4)	Eulerian (Proposition 5.4)	$\exists \text{SST} \wedge \delta(G) \geq 2$ (Theorem 5.3)
	stable	$\delta(G) \geq 3$ (Theorem 3.1)	? (Problem 5.6)	? (Problem 5.7)

Table 1. Required conditions for graphs to admit presented double traces

To conclude the paper we present enumeration results for six polyhedra: the tetrahedron and five additional ones. The latter polyhedra whose graphs are shown in Fig. 6 could be the next candidates to be constructed from coiled-coil-forming segments.

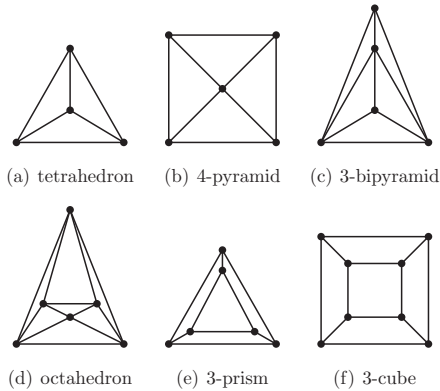


Figure 6. Graphs of the six polyhedra from Table 2

These computations were in part already presented in [11], here we extend them by computing the number of proper traces, antiparallel proper traces, and parallel proper traces. The results are collected in Table 2, where PT and ST stand for the number of

proper traces and stable traces, respectively, while “a” and “p” stand for antiparallel and parallel, respectively.

graph	PT	aPT	pPT	ST	aST	pST
tetrahedron	3	0	0	3	0	0
4-pyramid	101	5	0	82	5	0
3-bipyramid	925	24	0	470	0	0
octahedron	53372	668	1352	22246	0	275
3-prism	25	2	0	25	2	0
3-cube	40	0	0	40	0	0

Table 2. Number of proper traces (PT), antiparallel proper traces (aPT), parallel proper traces (pPT), stable traces (ST), antiparallel stable traces (aST), and parallel stable traces (pST)

We note that in Table 2 only non-equivalent traces are counted, where traces T and T' are called *equivalent* if T' can be obtained from T by reversion T , by shifting T , by applying a permutation on T induced by an automorphisms of G , or using any combination of the previous three operations.

We close the paper by another open problem:

Problem 6.1 *Analytically enumerate ((anti)parallel) proper and stable traces in graphs, in particular in polyhedra.*

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References

- [1] D. Bhatia, S. Mehtab, R. Krishnan, S. S. Indi, A. Basu, Y. Krishnan, Icosahedral DNA nanocapsules by modular assembly, *Angew. Chem. Int. Ed. Engl.* **48** (2009) 4134–4137.
- [2] J.-H. Chen, N. C. Seeman, Synthesis from DNA of a molecule with the connectivity of a cube, *Nature* **350** (1991) 631–633.
- [3] X. S. Cheng, S. Y. Liu, H. Zhang, W. Y. Qiu, Fabrication of a family of pyramidal links and their genus, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 623–636.
- [4] S. M. Douglas, H. Dietz, T. Liedl, B. Högberg, F. Graf, W. M. Shih, Self-assembly of DNA into nanoscale three-dimensional shapes, *Nature* **459** (2009) 414–418.
- [5] J. W. Duan, Z. Zheng, P. P. Zhou, W. Y. Qiu, The architecture of DNA Sierpinski links, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 817–832.
- [6] R. L. Duda, Protein chainmail, *Cell* **94** (1998) 55–60.

- [7] R. B. Eggleton, D. K. Skilton, Double tracings of graphs, *Ars Combin.* **17A** (1984) 307–323.
- [8] H. Fan, X. Zhu, Oriented walk double covering and bidirectional double tracing, *J. Graph Theory* **29** (1998) 89–102.
- [9] H. Fleischner, *Eulerian Graphs and Related Topics*, North–Holland, Amsterdam, 1991.
- [10] R. P. Goodman, R. M. Berry, A. J. Turberfield, The single–step synthesis of a DNA tetrahedron, *Chem. Commun.* **12** (2004) 1372–1373.
- [11] H. Gradišar, S. Božič, T. Doles, D. Vengust, I. Hafner Bratkovič, A. Mertelj, B. Webb, A. Šali, S. Klavžar, R. Jerala, Design of a single chain polypeptide tetrahedron self-assembled from concatenated coiled-coil-forming segments, *Nature Chem. Biol.* **9** (2013) 362–366.
- [12] 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.
- [13] Y. Q. Huang, Y. P. Liu, Y. M. Chu, Bidirectional double tracings and the maximum genus of a graph (Chinese), *Acta Math. Sci. Ser. A Chin. Ed.* **24** (2004) 530–536.
- [14] S. Y. Liu, H. Zhang, W. Y. Qiu, The HOMFLY polynomial for a family of polyhedral links, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 65–90.
- [15] O. Ore, A problem regarding the tracing of graphs, *Elemente der Math.* **6** (1951) 49–53.
- [16] G. Sabidussi, Tracing graphs without backtracking, *Operations Research Verfahren XXV*, Symp. Heidelberg, Teil 1 (1977) 314–332.
- [17] 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.
- [18] G. Tarry, Le problème des labyrinthes, *Nouv. Ann. (3) XIV* (1895) 187–190.
- [19] C. Thomassen, Retracting–free double tracings of graphs, *Ars Combin.* **19** (1985) 63–68.
- [20] C. Thomassen, Bidirectional retracting–free double tracings and upper embeddability of graphs, *J. Combin. Theory B* **50** (1990) 198–207.
- [21] D. J. Troy, On traversing graphs, *Amer. Math. Month.* **73** (1966) 497–499.
- [22] D. B. West, *Introduction to Graph Theory*, Prentice Hall, Upper Saddle River, 1996.
- [23] C. Zhang, S. H. Ko, M. Su, Y. Leng, A. E. Ribbe, W. Jiang, C. Mao, Symmetry controls the face geometry of DNA polyhedra, *J. Amer. Chem. Soc.* **131** (2009) 1413–1415.
- [24] J. Zimmermann, M. P. J. Cebulla, S. Mönninghoff, G. von Kiedrowski, Self–assembly of a DNA dodecahedron from 20 trisoligonucleotides with C_{3h} linkers, *Angew. Chem. Int. Ed. Engl.* **47** (2008) 3626–3630.