J Math Chem (2011) 49:2250–2267
DOI 10.1007/s10910-011-9884-6

ORIGINAL PAPER

Nonplanar graphs derived from Gauss codes of virtual knots and links

Slavik Jablan · Ljiljana Radović · Radmila Sazdanović

Received: 4 June 2011 / Accepted: 9 July 2011 / Published online: 12 August 2011

Abstract Virtual knot theory offers the possibility to consider knots and links embedded on different surfaces. This paper analyzes nonplanarity of graphs obtained from Gauss codes of virtual knots and links and their potential applications in chemistry.

Keywords Knot · Link · Nonplanar graph · Virtual knot theory · Gauss code

1 Introduction

After introducing the basics of the virtual knot theory, extended Conway notation for virtual knots and links, and Gauss codes corresponding to virtual knots and links, in Sect. 2 provides an overview of the main properties of nonplanar graphs, including nonplanarity criterion (Kuratowski's Theorem) and the notion of graph crossing number. In order to discuss planarity of graphs obtained from Gauss codes of virtual knots and links, we introduced graph preserving rules (Sect. 2.1). In Sect. 3 we consider some "famous" (named) nonplanar graphs which can be obtained from Gauss codes of the corresponding polyhedral virtual knots and links, in particular the graphs K_5

S. Jablan (✉)
The Mathematical Institute, Knez Mihailova 36, P.O. Box 367, 11001 Belgrade, Serbia
e-mail: sjablan@gmail.com

L. Radović
Faculty of Mechanical Engineering, University of Niš , A. Medvedeva 14, 18000 Niš, Serbia
e-mail: ljradovic@gmail.com

R. Sazdanović
University of Pennsylvania, 209 South 33rd Street, Philadelphia, PA 19104-6395, USA
e-mail: radmilas@math.upenn.edu

and $K_{3,3}$ which correspond to the structure of the first synthesized molecules with non-planar molecular graphs: the Simmons-Paquette molecule and Möbius ladders with three rungs. For named nonplanar 3- and 4-valent graphs with at most 20 vertices we obtained their corresponding virtual knots and links. Different classes of virtual knots and links, rational, pretzel, and Montesinos, and criteria for determining planarity of graphs obtained from their Gauss codes are discussed in Sect. 4. Similar criteria are obtained for virtual knots and links derived from basic polyhedra, in particular from 2-vertex connected basic polyhedra. We also derive virtual knots and links with Gauss codes resulting in nonplanar graphs from the basic polyhedra with at most 12 crossings.

1.1 Basics of virtual knot theory

The *virtual knot theory* introduced by L. Kauffman is a "non-realizable" part of the knot theory and gives the alternative answer to the question about realizability of Dowker-Thistletwaite codes and embedding of knots and links (shortly *KL*s) on different surfaces [1–5].

Virtual crossings are intersection points in the projection of a four-valent graph onto $\mathbb{R}^2$ or S^2, which are not vertices of the original graph. For example, graph with one vertex on a torus, turned into the alternating link, corresponds to the Hopf link, and Borromean rings can be represented as a five-vertex graph on a torus: nonplanar complete graph with five vertices K_5. Projection of a Hopf link onto $\mathbb{R}^2$ has two vertices, where one vertex is the image of the vertex of the original graph, and the other is the "new" virtual vertex (Fig. 1a).

The vertex of the projection corresponding to the vertex of the original graph is called *classical*, and the other vertices are *virtual*. Virtual *KL*-diagrams are obtained by introducing the relation "over-under" in classical vertices of a diagram:

Definition 1.1 A *virtual link diagram* is a 4-valent plane graph of the following structure: each vertex has an overcrossing or undercrossing, or is marked by a virtual crossing.

The equivalence of virtual *KL*s can be described after introducing generalized Reidemeister moves for virtual *KL*s [2–7].

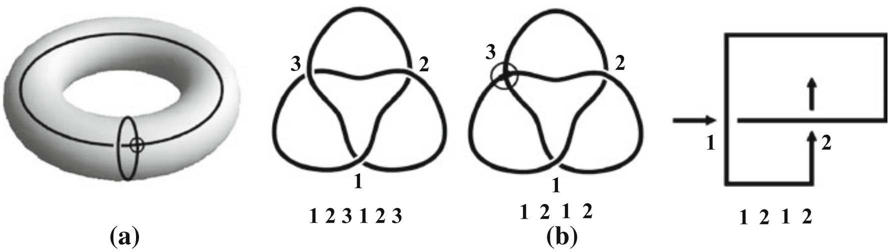

Fig. 1 **a** Hopf link on torus; **b** Gauss code of a trefoil with one virtual crossing

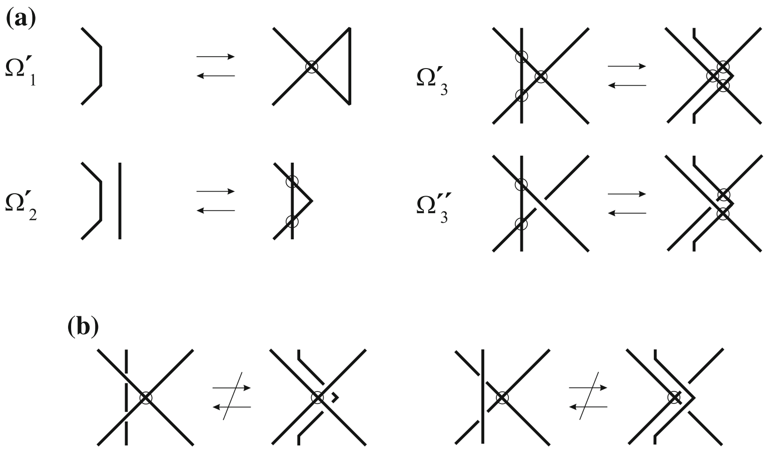

Fig. 2 Generalized Reidemeister moves for virtual *KL*s

Definition 1.2 Generalized Reidemeister moves (Fig. 2a) consist of:

1. classical Reidemeister moves related to classical vertices;
2. virtual versions Ω'_1, Ω'_2, Ω'_3 of Reidemeister moves;
3. the "semivirtual" version Ω''_3 of the third Reidemeister move.

Two virtual diagrams are equivalent if there exists a sequence of generalized Reidemeister moves transforming one diagram to the other one.

Definition 1.3 A *virtual link* is an equivalence class of virtual diagrams modulo generalized Reidemeister moves.

The remaining two versions of the third move (Fig. 2b) are forbidden. Actually, the forbidden move is a very strong one: each virtual knot can be transformed to another one using all generalized Reidemeister moves and the forbidden move [6].

1.2 Extended Conway notation for virtual *KL*s

Conway notation for *KL*s is introduced by J.H. Conway in 1967 [8], and effectively used in [7,9]. Here we introduce so-called *extended Conway notation* for virtual knots and links using expanded Conway symbols, where every *KL* is expressed by elementary tangles 1 and -1 (e.g., trefoil $3 = 1, 1, 1$; figure-eight knot $2\,2 = (1, 1)\,(1, 1), \ldots$), and virtual crossings which are denoted by i. For example, Hopf link with a virtual crossing is denoted as i, 1, a trefoil with a virtual crossing is i, 1, 1, *etc*. In order to make the extended Conway symbols shorter we can use the following rules:

- product $i\,i\,\ldots i$ of the length n is denoted by $i^{\overline{n}}$;
- a sequence of n real positive crossings $1, \ldots, 1$ is denoted by 1^n;
- a sequence of n real crossings of negative sign $-1, \ldots, -1$ by $(-1)^n$.

Hence, a trefoil knot i, 1, 1 with one virtual crossing can be shortly written as i, 1^2, and the virtual knot 2 i i i 3 can be written as $2\,i^{\overline{3}}\,3$.

Compared with the other notations used for virtual *KL*s [2,3,10], extended Conway notation has a few advantages: it is understandable, very concise, preserves the complete information about real *KL* from which a virtual *KL* is obtained by virtualizing some crossings, and enables a natural extension of particular *KL* symbols to the families and classes of virtual *KL*s.

Conway notation of *KL*s and definitions of all terms used in this paper are given in [7–9]. Here we restate the definitions of a rational *KL*, algebraic *KL*, basic polyhedron, and polyhedral *KL* [7]:

Definition 1.4 A *rational tangle* is any finite product of elementary tangles. A *rational KL* is a numerator closure of a rational tangle.

Definition 1.5 A tangle is *algebraic* if it can be obtained from elementary tangles using the operations of sum and product. *KL* is *algebraic* if it is a numerator closure of an algebraic tangle.

Definition 1.6 *Basic polyhedron* is a 4-regular, 4-edge-connected, at least 2-vertex connected plane graph without bigons.

Definition 1.7 A link L is called *algebraic link* if there exists at least one diagram of L which can be reduced to the basic polyhedron 1^* by a finite sequence of bigon collapses [7]. Otherwise it is a *non-algebraic* or *polyhedral link*.

1.3 Gauss codes of virtual *KL*s and their corresponding graphs

After introducing overcrossings (O), undercrossings (U), and signs of crossings ($+$ or $-$), Gauss code of a virtual trefoil becomes $U1 + O2 + O1 + U2+$ [2,3,5]. In this paper we are interested in Gauss codes of virtual *KL*s treated as graphs. Hence, we assign a simplified code to all of the knots. For example, the trefoil with one virtual crossing corresponds to the code 1 2 1 2, the 4-valent multigraph given by the cycle {{1, 2}, {2, 1}, {1, 2}, {2, 1}}, or by the list of unordered pairs of vertices {{1, 2}, {1, 2}, {1, 2}, {1, 2}}. In the same way, Borromean rings with one virtual crossing 6^*i and with the unsigned Gauss code {{1, 2, 3}, {4, 2, 5}, {1, 4, 3, 5}} give cycles {{1, 2}, {2, 3}, {3, 1}}, {{4, 2}, {2, 5}, {5, 4}}, {{1, 4}, {4, 3}, {3, 5}, {5, 1}} corresponding to the components of these Borromean rings with one virtual crossing. Furthermore, starting with the cycles we obtain the graph given by the list of unordered pairs: {{1, 3}, {1, 2}, {2, 3}, {4, 5}, {2, 4}, {2, 5}, {1, 5}, {1, 4}, {3, 4}, {3, 5}}-the complete graph K_5. Since we restricted our attention to unsigned Gauss codes of virtual *KL*s and their corresponding graphs (in fact, to the shadows of virtual *KL*s), we are working only with alternating virtual *KL*s, i.e., virtual *KL*s derived from alternating *KL*s. In the sense of the extended Conway notation, this means none of the symbols contain negative entries.

If we compare the graphs obtained from a trefoil and Borromean rings, both with one virtual crossing, we notice the fundamental difference: the graph obtained from the virtual trefoil is planar, and the graph obtained from Borromean rings with a virtual crossing is nonplanar. This motivates the main questions of this paper: which virtual *KL*s give Gauss codes resulting in nonplanar graphs and how they can be used for the analysis of nonplanar 4-valent graphs occurring in chemistry. The restriction to 4-valent graphs is inherent to the proposed construction because our graphs originate from knot theory. This restriction is not an essential obstacle for their applications in chemistry, since the most of nonplanar molecules recognized in chemistry are carbon-based.

2 Nonplanar graphs

Definition 2.1 A graph G is *plane* if it is drawn in plane (or on the sphere) with no two edges crossing each other, and it is *planar* if it is isomorphic to a plane graph. Otherwise, it is *nonplanar*.

Stereographic projection caries plane embeddings to embeddings on a sphere and *vice versa*.

Definition 2.2 An *embedding* of a graph G is a drawing of G on a certain surface in which the edges do not intersect.

A nonplanar graph can be always embedded on some surface, other then a plane (or sphere). For example, all graphs of polyhedra are planar, and the graphs K_5 and $K_{3,3}$ are nonplanar.

The most celebrated result about the planarity of graphs is *Kuratowski's Theorem* [12]. Two graphs G and G' are *isomorphic modulo vertices of degree 2* if G is isomorphic to a graph G'' obtained from G' by the addition or deletion of vertices with just two incident edges:

Theorem 2.1 (Kuratowski's Theorem) *Let G be a finite graph. G is planar iff it contains no subgraph isomorphic to K_5 or $K_{3,3}$ modulo vertices of degree 2 [12].*

Short proof of the sufficiency part of this theorem is given by Makarychev [13], and the complete proof can be found, e.g., in the book [14].

The transformations described above are *subdivision* and *contraction* of a graph edge. A *subdivision* of a graph G is a graph obtained from G by a finite number of the following operations. Let $v,\ w$ be the vertices of G which are connected by the edge vw. Introduce a new vertex x and replace the edge vw by two edges vx and xw, i.e., insert a vertex x in the middle of an existing edge vw.

Definition 2.3 Replacing two adjacent vertices by a single vertex of a graph is the operation called *elementary contraction*. The new vertex is joined to every other vertex which was joined to one or both original two vertices. A *contraction* of G is any graph that can be obtained from G by a finite sequence of elementary contractions.

These operations, subdivision and contraction, can be applied to any line segment AB in $\mathbb{R}^3$ replacing it by two line segments AC and CB or *vice versa*.

In the language of contraction, Kuratowski's Theorem can be formulated as:

Theorem 2.2 *A graph G is planar iff it contains no subgraph which has K_5 or $K_{3,3}$ as a contraction.*

A special kind of contraction where edges forming a bigon are contracted simultaneously plays an important role in analyzing *KL*s. We call such contraction a *bigon collapse* [7].

Planar embeddings of graphs can contain intersections of edges, called *crossings*, which are not the vertices of the graph. For planar graphs, there is always a plane diagram that avoids such (nugatory) crossings. But an important invariant of nonplanar graphs is their *graph crossing number* (usually denoted by k)—the minimal number of edge crossings among all possible planar diagrammatic representations of the graph [15,16].

Since it is defined over all possible diagrammatic representations of a graph in a plane, the graph crossing number is an invariant very hard to compute. For planar graphs it is always $k(G) = 0$, and if we are able to find a plane diagram of a nonplanar graph G with one crossing, than $k(G) = 1$.

The length of the shortest graph cycle (if any) in a graph is called the *girth* of a graph and denoted by c. For graphs without multiple edges and loops, $c \geq 3$. The girth of a graph G can be computed using *Mathematica* function Girth[G] [17]. If e denotes the number of edges, and c the girth of G, the lower bound of the graph crossing number $k(G)$ is given [15] by the formula:

$$k(G) \geq e - \frac{(v-2)c}{c-2}. \tag{2.1}$$

If the right side of the preceding formula is a negative integer,[1] we conclude that $k \geq 0$.

Since we are interested only in graphs (shadows) of virtual *KL*s, all parameters in their Conway symbols take only non-negative values.

A tangle of the form $p_1\,p_2\,\ldots\,p_n$ where $p_1 \geq 1$ and all other $p_i \geq 0$ is called (positive) *rational tangle*. A tangle of the form $p_1, p_2, \ldots, p_n$ $(n \geq 3)$, where p_i are positive twists is called (positive) pretzel tangle, and a tangle of the form $r_1, r_2, \ldots, r_n$ $(n \geq 3)$, where r_i are (positive) rational tangles not beginning with 1 is called (positive) *Montesinos tangle* [7].

2.1 Graph preserving transformations

To shadows of virtual *KL*s, i.e., virtual *KL*s shown as plane graph diagrams with virtual crossings and with real crossings without introduced relation "over"–"under" we can apply graph transformation rules described in the following theorem, restricted to positive tangles:

[1] For some graphs, e.g., Petersen graph or Heawood graph given as the examples in the paper [15], this formula gives the lower bound coinciding with known graph crossing numbers from *Mathematica* data base. However, for Tietze graph with $e = 18,\ v = 12,\ c = 3$, whose crossing number is known to be equal to $k = 2$, the approximation $k \geq -12$ is essentially useless saying only that $k \geq 0$.

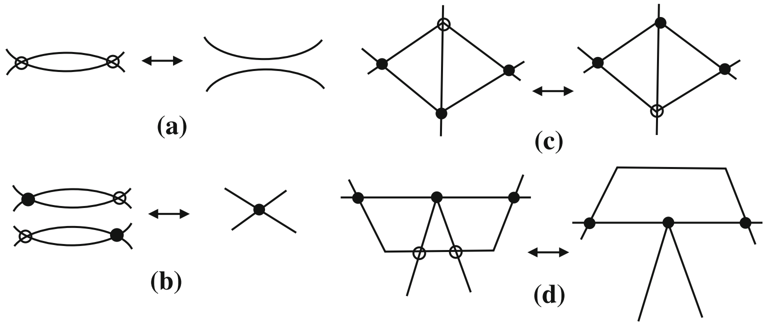

Fig. 3 Graph preserving moves

Theorem 2.3 *The following transformation rules applied to virtual KLs containing only positive tangles preserve the graphs obtained from their Gauss codes:*

1. $1, i = i, 1 = 1$ *(Fig. 3a);*
2. $i^2 = 0$ *(Fig. 3b);*
   Parts of positive rational tangles of the form $p\, i^{\overline{n}}\, q$ *satisfy the following rules:*
3. $p\, 0\, q = p + q;$
4. $p\, i^{\overline{n}}\, q = p + q$ *for* $n = 3k + 2$ $(k \geq 0)$*, and* $p\, q$ *otherwise.*
   The following rules hold for every positive rational tangle r*:*
5. $r\, i^{\overline{3k}} = r;$
6. $r\, i^{\overline{3k+1}} = r\, i;$
7. $r\, i^{\overline{3k+2}} = r\, i^{\overline{2}} = r\, 0;$
8. $i^{\overline{n}}\, r = i^{\overline{2}}\, r = 0\, r$ *for* $n = 3k + 2$ $(k \geq 0)$*, and* $i^{\overline{n}}\, r = r$ *otherwise;*
   Positive Montesinos tangles $r_1, r_2, \ldots, r_n$ *satisfy the rule*
9. $r_1\, i, r_2, \ldots, r_n = r_1, r_2, \ldots, r_n, i.$
   Transformation rules also include the rules shown in Fig. 3c,d.

Rules $i^{2k} = 0$ and $i^{2k+1} = i$ follow from the rule 2).

These rules preserve every graph G obtained from the Gauss code of a virtual *KL* and can be used to reduce number of virtual crossings and draw virtual *KL*s with diagrams in which the number of virtual crossings is equal to the graph crossing number $k(G)$ of the graph G. Since plane diagrams of nonplanar graphs can have different number of crossings, any nonplanar graph can be obtained from Gauss codes of two or more different virtual *KL*s. For example, the complete graph K_5 can be obtained from the virtual knot $10^*i : i : i : i : i$, as well as from the virtual link 6^*i, and the other representation with one virtual crossing corresponds to the diagram of G with graph crossing number $k(G) = 1$ (see Fig. 4d, e).

3 Some "famous" nonplanar graphs

The complete graph K_5, a 4-valent graph with $n = 5$ vertices, corresponds to the simplest regular simplex in four dimensions: pentatope. Usually it is drawn on the plane as a graph with five crossings (Fig. 4a). However, its graph crossing num-

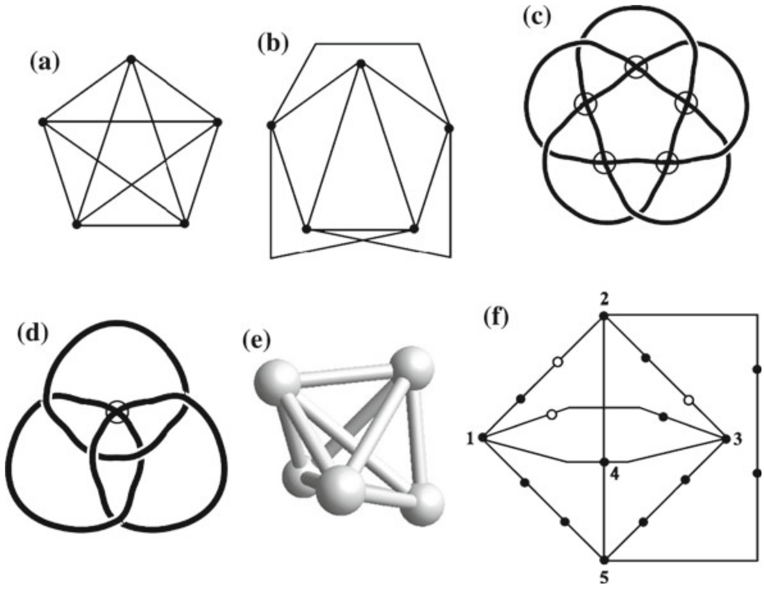

Fig. 4 Complete graph K_5: **a** its drawing with 5 crossings; **b** its drawing with one crossing; **c** virtual knot $10^*i : i : i : i : i$; **d** virtual link 6^*i; **e** $3D$ graph; **f** molecular graph of Simmons-Paquette molecule

ber is $k = 1$ (Fig. 4b). The first representation of this graph can be obtained from the virtual knot $10^*i : i : i : i : i$ with the Gauss code $\{1, 2, 3, 4, 2, 5, 4, 1, 5, 3\}$ (Fig. 4c), but its minimal crossing number representation is obtained from the virtual link 6^*i, Borromean rings with one virtual crossing and with the Gauss code $\{\{1, 2, 3\}, \{4, 2, 5\}, \{1, 4, 3, 5\}\}$ (Fig. 4d). Figure 4e shows its $3D$ representation. In chemistry, graph K_5 corresponds to the molecular graph of the Simmons-Paquette molecule, which was independently synthesized in 1981 by the laboratories of Simmons and Magio [18,19] and of Paquette and Vazeux [19,20], the first synthesized topologically nonplanar molecule. In the molecular graph of Simmons-Paquette molecule (Fig. 4f) hydrogen atoms are omitted, and three white circles represent oxygen atoms. The vertices 1–5 define complete graph K_5 with the graph crossing number 1.

The next family of nonplanar graphs consists of Möbius ladders with k rungs ($k \geq 3$) [19]. The first member of this family is the complete bipartite graph $K_{3,3}$. This graph is usually drawn in the plane with seven crossings, where one of them is the triple crossing (Fig. 5a). However, the crossing number of the graph $K_{3,3}$ is 1 (Fig. 5b). Graph $K_{3,3}$ with the crossing number 1 can be obtained from the Gauss code $\{\{1, 2, 3, 4\}, \{2, 5, 6, 1\}, \{5, 4, 3, 6\}\}$ of the virtual link $2, 2, 2, i$ (Fig. 5c), and represents Möbius ladders with three rungs which are bigons, with $3D$ graph shown in Fig. 5d. In 1982, Walba et al. [22] synthesized the first molecular Möbius ladder with three rungs, the molecule which resembles a Möbius strip in which the surface of the strip is replaced by a ladder. This molecule is a polyether chain of 60 carbon and oxygen atoms, where the rungs are C=C double bonds. Construction of numerous *KL*s based on molecular Möbius ladders become possible when Q.Y. Zheng managed to add twists to the Möbius ladders in 1990 [21]. In fact, after breaking the rungs,

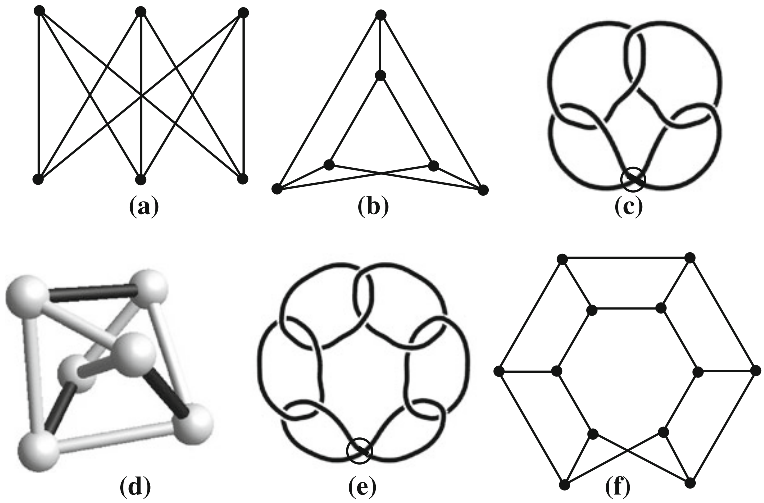

Fig. 5 Complete bipartite graph $K_{3,3}$: (a) its drawing with 7 crossings; (b) with one crossing; (c) virtual link 2, 2, 2, i; (d) graph 3D; (e) virtual link 2, 2, 2, 2, 2, i; (f) Möbius ladder with 5 rungs

Möbius multi-strand twisted ladder becomes molecular closed braid representation of a *KL*. Möbius ladder with k rungs are obtained as the Gauss code of the virtual link $2, 2, 2, \ldots, 2, i$, where number 2 occurs k times ($k \geq 3$) (Fig. 5e).[2]

Since we are dealing with nonplanar graphs that originate from virtual knot theory as Gauss codes of virtual *KL*s, we restrict our consideration to 3- and 4-regular nonplanar graphs with at most $n = 20$ vertices. The number of nonplanar graphs with n vertices ($n \geq 5$) is given by the sequence $1, 14, 222, 5380, 194815, \ldots$, the sequence A145269 from N. Sloane's "The Online Encyclopedia of Integer Sequences" [23], and the number of 3- and 4-regular nonplanar graphs is also very large even for relatively small values of n. Hence, we consider only selected "famous" (or named) 3- and 4-regular graphs with $n \leq 20$ vertices. For all of them we computed their representations coming from virtual knot theory, as graphs corresponding to Gauss codes of virtual *KL*s. Our goal was to obtain graphs with the minimal number of crossings and succeeded in that for all graphs except "$MoebiusKantorGraph$".[3]

The following list contains selected named nonplanar 3- and 4-regular graphs, given by their number of vertices n ($10 \leq n \leq 20$), name, vertex valence, known or estimated graph crossing number k, virtual knot or link from which the graph in question is obtained from its Gauss code, and its number of components c (Figs. 6, 7). The names of the graphs are taken from *Mathematica* GraphData base [24].

[2] Double bonds are represented by bold (black) edges, respectively, in both graph diagrams and graph 3D images.

[3] Notice that for Möbius Kantor graph the lower bound of graph crossing number obtained from formula (2.1) is 3, and in the paper [16] is mentioned that the 4-crossing version of the Möbius Kantor graph can probably be improved.

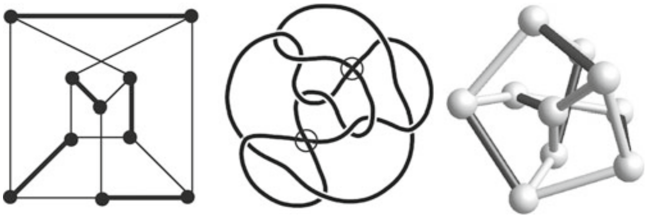

Fig. 6 Petersen graph, its corresponding virtual knot 6*2.2.2 i.2 0.2 0.i, and 3D graph

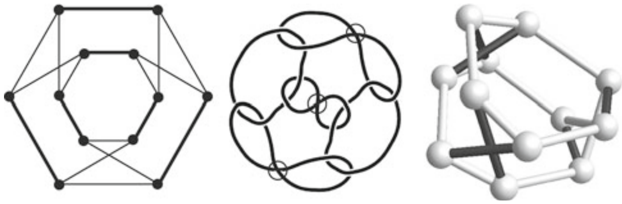

Fig. 7 Franklin graph, its corresponding virtual link (2, i, 2), (2, i, 2), (2, i, 2), and 3D graph

n	Name	Val	k	KL	c
10	“*PetersenGraph*”	3	2	6*2.2.2 i.2 0.2 0.i	1
12	“*FranklinGraph*”	3	3	(2, i, 2), (2, i, 2), (2, i, 2)	5
12	“*TietzeGraph*”	3	3	6* (i, 2) 0.2 0.(i, 2) 0.2 0.(i, 2) 0.2 0	4
12	“*ChvatalGraph*”	4	8	2049773*i : i :: .i.i.i.i :::: i	3
14	“*HeawoodGraph*”	3	3	10**2 0.2 0.i.2 0.2 0.i.2 0.2 0.i.2 0	1
16	“*MoebiusKantorGraph*”	3	4	138*2 0.2 0.i.2 0.i.2 0 : 2.2.(i, 2) 0.i.i	2
18	“*PappusGraph*”	3	5	1413*2.i.i.2.2.2.2.2.i.i.2.2.i.2	1
18	{“*BlanusaSnark*”, {1, 1}}	3	6	15127*i.2.2.2 0.2 0.i.2 0.2 0.i.i.2 0.2 0.2 0.i.i	1
18	{“*BlanusaSnark*”, {1, 2}}	3	4	1312*i.2.2 0.2.2.i.i.i.2.2 0.2 0.2 0.2	2
20	“*DesarguesGraph*”	3	6	1448*2.i.2 0.2 0.(i, 2) 0.(i, 2) 0.i.2.2.i.i.2.2 0.2 0	2
20	“*FlowerSnarkJ5*”	3	5	1599*i.2.2.i.i.2 0.2 0.2 0.2.i.i.2.2 0.2 0.2	6

4 Classes of virtual *KL*s and nonplanar graphs

Applying Theorem 2.3 to different classes of virtual *KL*s: rational, pretzel, and Montesinos *KL*s with positive tangles, we prove the following theorems (Figs. 8, 9):

Theorem 4.1 *All rational virtual KLs have Gauss codes which result in planar graphs.*

Tangle of the form i^k is called a *virtual twist* of the length k.

KL of the form $p_1, p_2, \ldots, p_n$ ($p_i \geq 2$, $i = 1, 2, \ldots, n$, $n \geq 3$) where all p-tangles are positive integer tangles (twists) is an *alternating pretzel KL*.

Theorem 4.2 *Virtual alternating pretzel KL has a Gauss code which represents a nonplanar graph iff it contains an odd number of virtual twists of an odd length, and all other twists contain at least two real crossings.*

Proof Applying reduction rules 1) $i, 1 = 1, i = 1$ (Fig. 3a) and 2) $i^2 = i$ (Fig. 3b) from Theorem 2.3, to pretzel *KL* of the mentioned form reduces it to pretzel *KL* con-

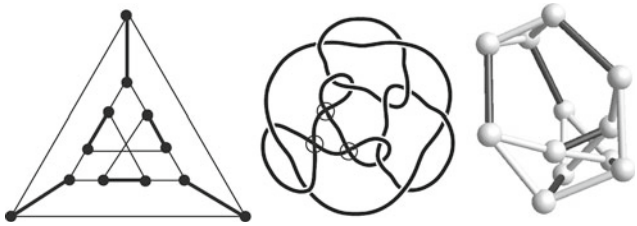

Fig. 8 Tietze graph, $6^{*}(i, 2)\,0.2\,0.(i, 2)\,0.2\,0.(i, 2)\,0.2\,0$ its corresponding virtual link, and 3D graph

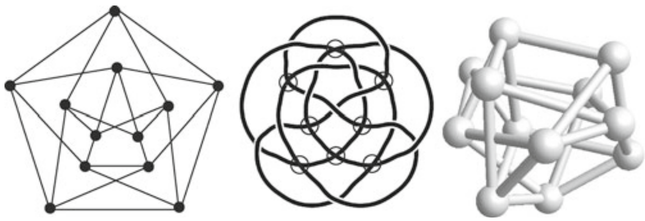

Fig. 9 Chvatal graph, its corresponding virtual link $2049773^{*}i : i :: .i.i.i.i.i :::: i$, and 3D graph

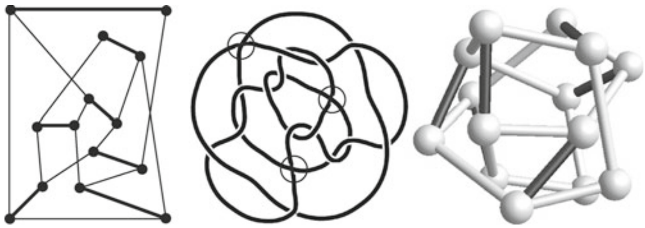

Fig. 10 Heawood graph, its corresponding virtual knot $10^{**}2\,0.2\,0.i.2\,0.2\,0.i.2\,0.2\,0.i.2\,0$, and 3D graph

sisting of n twists with all real crossings, each of them with the length at least 2, and a single virtual crossing obtained by reduction from an odd number of the virtual twists of odd lengths. The obtained *KL* has the Gauss code resulting in Möbius ladders with n twisted rungs. The proof in the opposite way is straightforward. □

For example, virtual pretzel link $(1, i, 1), 3, (1, 1, i, i, i), (i, i, i)$ satisfies the conditions of the preceding theorem and reduces to the virtual link $2, 3, 2, i$. Its Gauss code results in Möbius ladders with three twisted rungs (Figs. 10, 11).

Corollary 4.1 *Only nonplanar graphs that can be obtained from Gauss codes of virtual pretzel KLs are Möbius ladders with twisted rungs.*

KL of the form $r_1, r_2, \ldots, r_n$ $(n \geq 3)$ where all r-tangles are rational tangles not beginning with 1 is called *Montesinos KL*.

Theorem 4.3 *Virtual Montesinos KL has the Gauss code which represents a nonplanar graph iff it contains an odd number of r-tangles ending by virtual twists of odd*

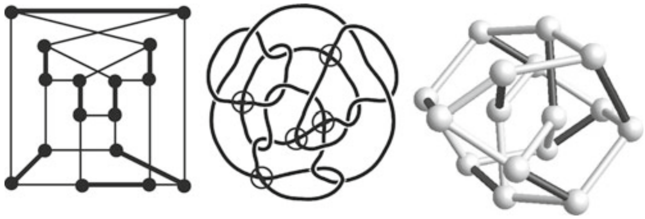

Fig. 11 Möbius Kantor graph, its corresponding virtual link 138*2 0.2 0.i.2 0.i.2 0 : 2.2.(i, 2) 0.i.i, and 3D graph

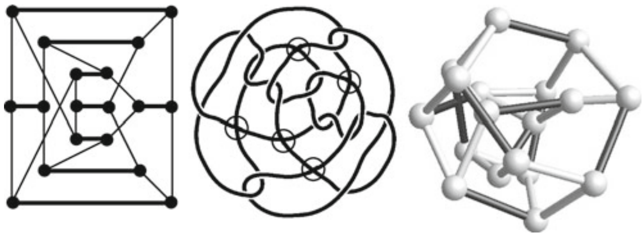

Fig. 12 Pappus graph, its corresponding virtual knot 1413*2.i.i.2.2.2.2.2.i.i.2.2.i.2, and 3D graph

lengths, their preceding twists in the same rational tangles contain at least one real crossing, and each other r-tangle does not end with a virtual twist.

For example, virtual Montesinos link $3\,(i, i, i), 2\,2, 5\,(1, i, 1, i), 4, 2, 4\,(1, i, i), 2\,3\,i, 2\,i$ satisfies the conditions of the preceding theorem. Applying the reduction rules 1) $i, 1 = 1, i = 1$ and 2) $i^2 = i$ from Theorem 2.3, it reduces to a virtual $KL 3\,i, 2\,2, 5\,2, 4, 2, 4\,1, 2\,3\,i, 2\,i$. Further reduction using rules 9) and 2) gives the virtual link $3, 2\,2, 5\,2, 4, 2, 4\,1, 2\,3, 2, i$ with the Gauss code corresponding to the nonplanar graph.

Corollary 4.2 *Only nonplanar graphs that can be obtained from Gauss codes of virtual pretzel KLs are Möbius ladders with branched and twisted rungs, with the graph crossing number 1.*

Based on the preceding theorems and the reduction rules from Theorem 2.3, we can make conclusions about planarity of graphs obtained from Gauss codes of algebraic virtual *KL*s (Figs. 12, 13). For example, product of two Montesinos tangles yields a nonplanar graph if at least one of them gives a nonplanar graph, i.e., satisfies the conditions of Theorem 4.3. A nice example of the family of nonplanar graphs that can be obtained from algebraic virtual *KL*s are n-crossed prism graphs ($n \geq 3$), beginning with the Franklin graph, obtained from virtual links of the form $(2, i, 2), (2, i, 2), \ldots, (2, i, 2)$, where the tangle $(2, i, 2)$ repeats n times.

A *vertex cut set* of a connected graph G is a set of vertices whose removal renders G disconnected.

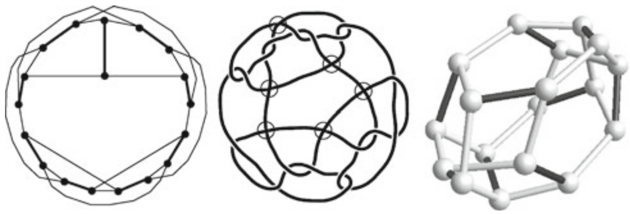

Fig. 13 Blanusa Snark 1, its corresponding virtual knot 15127*i.2.2.2 0.2 0.i.2 0.2 0.i.i.2 0.2 0.2 0.i.i, and 3D graph

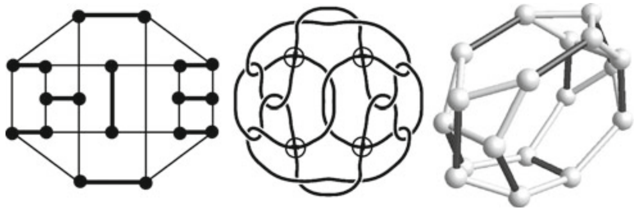

Fig. 14 Blanusa Snark 2, its corresponding virtual link 1312*i.2.2 0.2.2.i.i.i.2.2 0.2 0.2 0.2, and 3D graph

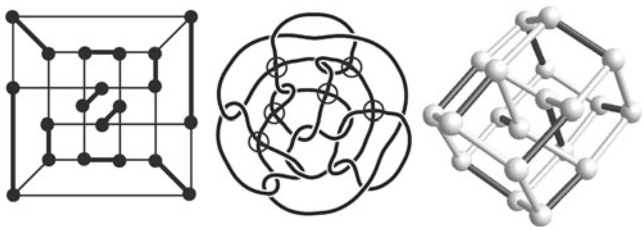

Fig. 15 Desargues graph, its corresponding virtual link 1448*2.i.2 0.2 0.(i, 2) 0.(i, 2) 0.i.2.2.i.i.2.2 0.2 0, and 3D graph

Theorem 4.4 *For virtual KLs with v virtual crossings derived from a basic polyhedron with n crossings the following statements hold:*

- *all virtual KLs obtained from a basic polyhedron that is not 2-vertex connected with* $v = 1$ *have Gauss codes resulting in nonplanar graphs;*
- *all virtual KLs obtained from a 2-vertex connected basic polyhedron with* $v = 1$ *have Gauss codes resulting in planar graphs if the virtual crossing belongs to the cut set of the basic polyhedron, and in nonplanar graphs otherwise;*
- *all virtual KLs obtained from a basic polyhedron that is not 2-vertex connected with* $2 \leq v \leq n - 5$ *have Gauss codes resulting in planar and nonplanar graphs;*
- *all virtual KLs obtained from a basic polyhedron with* $v \geq n - 4$ *have Gauss codes resulting in planar graphs (Figs. 14, 15).*

Theorem 4.5 *A 2-vertex connected basic polyhedron with two virtual crossings, where one coincides with a cut vertex, gives virtual KL with Gauss code resulting in a nonplanar graph iff the other virtual crossing does not coincide with the other cut vertex, and a planar graph otherwise.*

Fig. 16 Flower Snark J5, its corresponding virtual link $1599^*i.2.2.i.i.2\,0.2\,0.2\,0.2.i.i.2.2\,0.2\,0.2$, and 3D graph

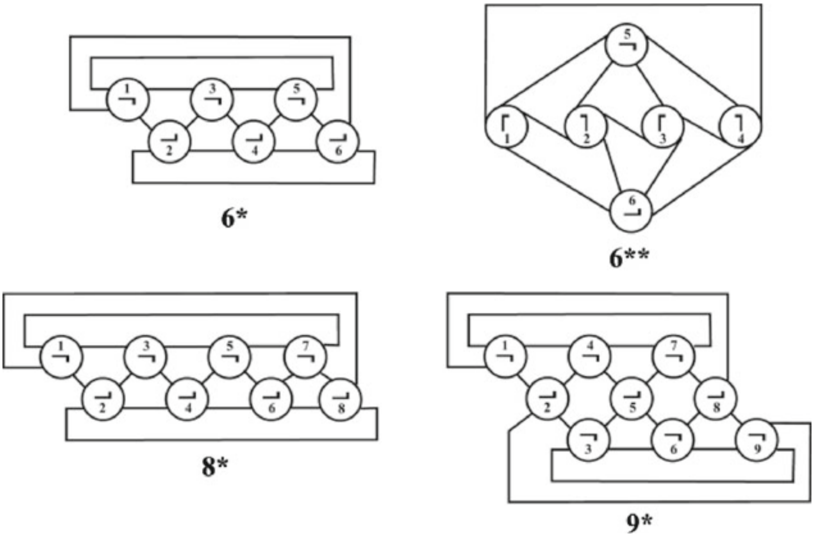

Fig. 17 The basic polyhedra 6^*, 8^*, and 9^*

Theorem 4.5 can be generalized if the virtual crossings are replaced by arbitrary virtual rational, pretzel, or Montesinos tangles (Fig. 16).

As the next step, we derived all virtual *KL*s which have Gauss codes resulting in nonplanar graphs from basic polyhedra with $n \leq 12$ crossings [7]. The basic polyhedra up to 12 crossings are illustrated in Figs. 17, 18, 19, 20 and 21. All computations are made in the *Mathematica* based program *LinKnot* written by Jablan and Sazdanović [7].

From the basic polyhedra with $n \leq 12$ crossings we derived 593 virtual *KL*s with this property. Among them 279 virtual *KL*s correspond to nonplanar graphs obtained from Gauss codes have no double bonds, since such graphs can be obtained from *KL*s with a smaller number of crossings. For example, the nonplanar graph obtained from the Gauss code of the virtual knot $8^*i.i$ with $n = 8$ crossings can be obtained from the virtual link $6^*2.i$ with $n = 7$ crossings. From the remaining virtual *KL*s we selected 94 virtual *KL*s giving different nonplanar graphs. Their list is given in the following

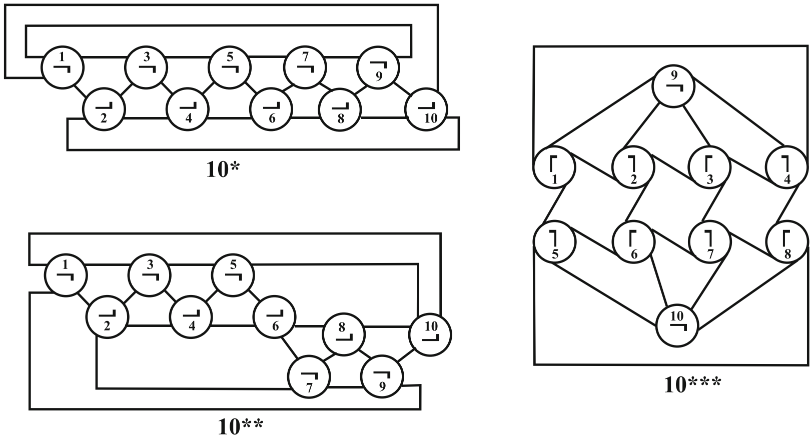

Fig. 18 The basic polyhedra 10^{*}, 10^{**}, and 10^{***}

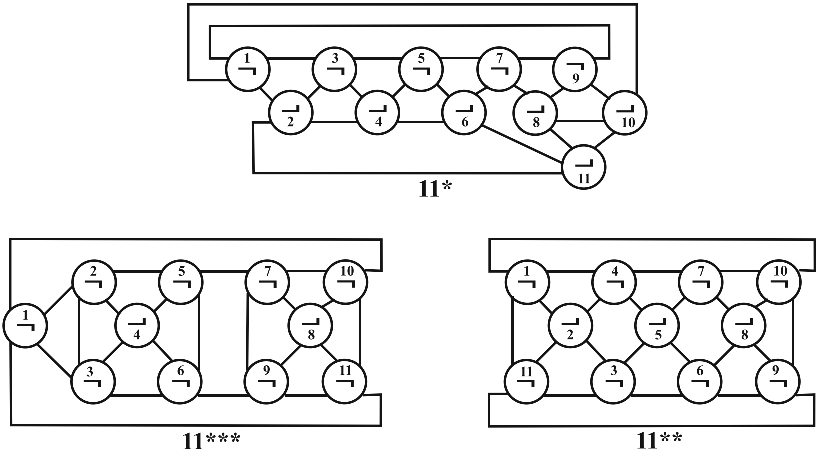

Fig. 19 The basic polyhedra 11^{*}, 11^{**}, and 11^{***}

table. The order of crossings corresponds to the labeled images of the basic polyhedra shown in Figs. 17 and 18. In the following table the basic polyhedra are denoted as 101^{*}–103^{*} instead of 10^{*}–10^{***}, 111^{*}–113^{*} instead of 11^{*}–11^{***}, and 121^{*}–1212^{*} instead of 12A–12L [7].

5 Conclusion

It is well known that one of the main properties of the virtual knot theory is the possibility to represent nonplanar graphs, i.e. graphs embedded on surfaces different from a plane or sphere. From the mathematical point of view, it is interesting to notice that

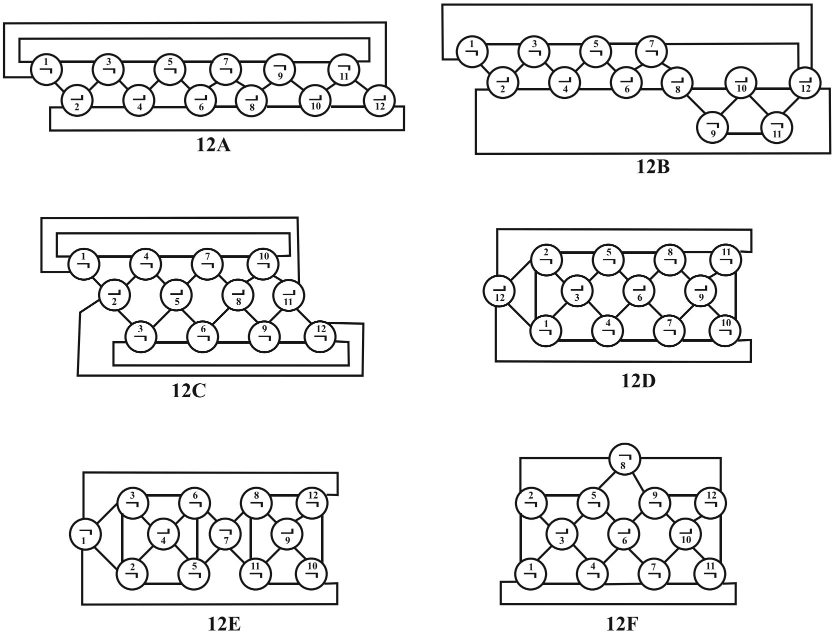

Fig. 20 The basic polyhedra 12A–12F

6*i	8*i	9*.i	9*i	9*i : i	101*i
102*.i	102*i	102*i :: .i	103*i	103*i :: i	103*i.i.i : i
112* :: i	112* : i	112* : i :: i	112*i	112*i ::: .i	112*i :: .i
111* ::::: i	111* ::: .i	111*.i	111*i	111*i ::::: i	111*i ::: i
113*.i	113*.i :: .i	113*.i : .i.i.i	113*i	121*i	122* :::: i
122*.i	122*i	122*i ::: .i	123*i	123*i ::: i	123*i :: .i
123*i : i	123*i : i :: .i	123*i : i :: i	123*i : i :: i : i	123*i.i	123*i.i :::: .i
123*i.i : i	124* ::::: .i	124* :: .i	124* : .i	124* : .i :::: i	124* : .i :: i
124* : .i : .i	124*i	124*i :::: i	124*i ::: i	124*i :: .i	124*i :: .i : .i
125*.i	125*.i ::: i	126* ::: .i	126* :: .i	126* :: .i : i	126* : .i
126* : .i :: i	126*i	127*.i	127*.i :: i	127*.i : i	127*i
127*i :: .i	128* :: .i	128* :: i	128*.i	128*.i ::: .i	128*.i ::: i
128*i	128*i :::: i	128*i ::: .i	129* ::: .i	129*.i	129*i
129*i ::: .i	129*i ::: .i.i : .i	129*i ::: .i.i : i	1210*.i	1210*.i ::: i	1210*.i : .i.i : i
1210*i	1210*i ::: .i	1210*i ::: .i.i : i.	1211*.i	1211*i	1211*i ::::: .i
1212*.i	1212*i	1212*i :::: i	1212*i ::: i		

a large portion of virtual *KL*s, e.g., all rational virtual *KL*s result in graphs obtained from their Gauss codes which are planar. In fact, in this way we can assign graphs to every class of *KL*s and one of the goals of this research was to establish the criteria for planarity of graphs we obtained. In chemistry, the first molecules synthesized in attempt to produce molecular knots and links were various kinds of Möbius ladders, which are nonplanar graphs. However, the detailed planarity test of molecular graphs presented in the paper [25] testifies that nonplanar graphs represent a very small portion of analyzed organic compounds. The authors concluded with the impression that "Nature does not like to produce graph-theoretically nonplanar compounds" and

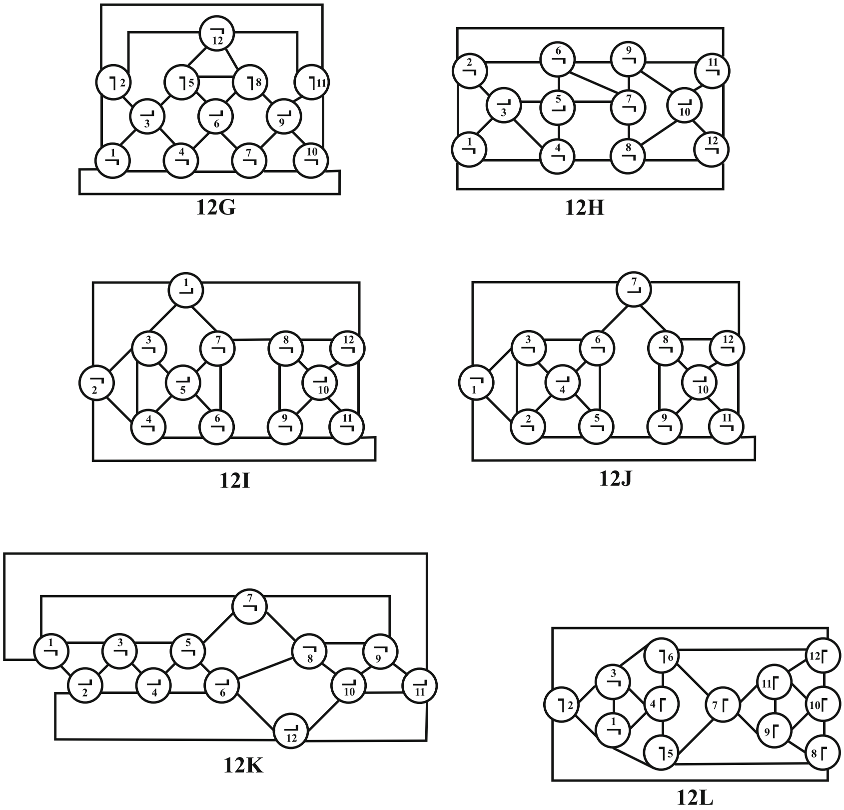

Fig. 21 The basic polyhedra 12G–12L

that synthesis of nonplanar compounds seems to be inherently difficult. However, we hope that some of the ideas proposed in this paper and application of the virtual knot theory to the analysis of chemical nonplanar compounds establishes a new common ground for knot theory and chemistry.

Acknowledgments The authors express gratitude to the Ministry of Science and Technological Development of Serbia for providing partial support for this project (Grant No. 174012).

References

1. L.H. Kauffman, Virtual knots, Talks at MSRI Meeting, January 1997 and AMS Meeting, at University of Maryland, College Park, March (1997)
2. L.H. Kauffman, Virtual knot theory. Eur. J. Comb. **20**, 663–691 (1999)
3. L.H. Kauffman, A Survey of Virtual Knot Theory, Knots in Hellas '98, *Proceedings of the International Conference on Knot Theory and its Ramifications* (Eds. C.McA. Gordon, V.F.R. Jones, L.H. Kauffman, S. Lambropoulou, J.H. Przytycki), World Scientific, Singapore, pp. 143–202 (2000)
4. V.O. Manturov, *Knot Theory* (Chapman and Hall/CRC, Boca Raton, 2004)

5. H. Dye, Detection and Characterization of Virtual Knot Diagrams, PhD. Thesis, University of Illinois at Chicago (2003)
6. S. Nelson, Unknotting virtual knots with Gauss diagram forbidden moves. J. Knot Theory Ramifi. **10**(6), 931–935 (2001)
7. S.V. Jablan, R. Sazdanović, *LinKnot—Knot Theory by Computer* (World Scientific, New Jersey, 2007). http://math.ict.edu.rs/, http://www.mi.sanu.ac.rs/vismath/linknot/index.html
8. J. Conway, An enumeration of knots and links and some of their related properties, in *Computational Problems in Abstract Algebra*, ed. by J. Leech, Proc. Conf. Oxford 1967 (Pergamon Press, New York, 1970), pp. 329–358
9. A. Caudron, *Classification des nøe uds et des enlancements*, Public. Math. d'Orsay 82. Univ. Paris Sud, Dept. Math., Orsay (1982)
10. J. Green, A table of virtual knots. http://www.math.toronto.edu/~drorbn/Students/GreenJ/
11. P. Cromwell, *Knots and Links* (Cambridge University Press, Cambridge, 2004)
12. K. Kuratowski, Sur le problème des courbes gauches en topologie. Fund. Math. **15**, 271–283 (1930)
13. Y. Makarychev, A short proof of Kuratowski's graph planarity criterion. J. Graph Theory **25**, 129–131 (1997)
14. B. Mohar, C. Thomassen, *Graphs on Surfaces* (Johns Hopkins University Press, Baltimore, 2001)
15. A. Bogomolny, Crossing Number of a Graph. http://www.cut-the-knot.org/do_you_know/CrossingNumber.shtml, http://www.math.uic.edu/~kauffman/CrossingNumber.pdf
16. E. Pegg Jr, G. Exoo, Crossing number graphs. Math. J. **11**(2), 161–170 (2009)
17. WolframMathWorld. http://mathworld.wolfram.com/Girth.html
18. H.E. Simmons, J.E. Maggio, Synthesis of the first topologically nonplanar molecule. Tetrahedron Lett. **22**, 287–290 (1981)
19. E. Flapan, *When Topology Meets Chemistry: A Look at Molecular Chemistry* (Cambridge University Press, Cambridge, 2000)
20. L.A. Paquette, M. Vazeux, Threefold transannular epoxide cyclization synthesis of a heterocyclic C_{17}-hexaquinane. Tetrahedron Lett. **22**, 291–294 (1981)
21. D. Walba, R. Richards, R.C. Haltiwanger, Total synthesis of the first milecular Möbius strip. J. Am. Chem. Soc. **104**, 3219–3221 (1982)
22. D.M. Walba, Q.Y. Zheng, K. Schilling, Topological Stereochemistry. 8. Experimental studies on the hook and ladder approach to molecular knots: synthesis of a topologically chiral cyclized hook and ladder. J. Am. Chem. Soc. **114**, 6259–6260 (1992)
23. N. Sloane, *The On-line Encyclopedia of Integer Sequences*. http://www2.research.att.com/~njas/sequences/
24. *Mathematica 7.0*, Wolfram Mathematica. http://www.wolfram.com/
25. C. Rücker, M. Meringer, How many organic compounds are graph theoretically nonplanar?. MATCH Commun. Math. Comput. Chem. **45**, 153–172 (2002)