

Two combinatorial operations and a knot theoretical approach for fullerene polyhedra

Guang HU and Wen-Yuan QIU*

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

Lanzhou University, Lanzhou 730000, P.R. China

E-mail: wyqiu@lzu.edu.cn

(Received April 27, 2009)

Abstract

In this paper, we introduce two combinatorial operations and a knot-theoretical approach for generation and description of fullerene architectures. The ‘Spherical rotating–vertex bifurcation’ operation applied to original fullerene polyhedra can lead to leapfrog fullerenes. However, the ‘Spherical stretching–vertex bifurcation’ operation applied to fullerene generates a family of related polyhedra, which go beyond the scope of fullerenes. These related cages, the cubic tessellations containing not only 5-gons and 6-gons but also 3-gons and 8-gons, are potential candidates in carbon chemistry. By using a simple algorithm based on knot theory, these two homologous series of molecule graphs can be transformed into various polyhedral links. For these interlocked architectures, it is now possible to quantify their properties by knot invariants. By means of this application, we show connections (1) between knot polynomials and fullerene isomers determination, (2) between knot genus and fullerene complexity and (3) between unknotting numbers and fullerene stability. Our results suggest that techniques coming from knot theory have potential applications and offer novel insights in predicting several structural and chemical properties of fullerene polyhedra.

1. Introduction

Fullerenes, a family of ball-shaped carbon allotropes in addition to diamond and graphite, were discovered in 1985^[1]. In mathematical terms, a fullerene graph is a planar, three-regular and three-connected graph, 12 of whose faces are 5-gons and any remaining faces are 6-gons. The interest in these species is rapidly increasing because of not only their activity in chemistry, physics and materials sciences, but also their intriguing and highly symmetric architectures and topologies^[2-6]. For such purposes, it turns out to be useful to look at some mechanisms for fullerene conversion, such as the Stone-Wales (*SW*) rearrangement^[7] for isomerization and the Endo-Kroto C_2 insertion^[8] for growth, which were shown to be two subsets of the more general theoretical framework based on patch replacement^[9, 10]. By extension, research on complex operations^[2, 11], such so-called leapfrog, chamfering and capra operations, are of particular importance and interest.

However, the outcomes of these transformations include not only fullerenes but also some related cages with rings of other sizes. Diudea and coworkers^[12-15] have demonstrated that map operations, as well as *SW* isomerizations, can be used to generate some kinds of nanostructures containing faces of different sizes, such as 4-gons and 8-gons. A different approach, decoration operation, has been used to generate several series of icosahedral fullerooids by Delgado Friedrichs and Deza in 2000^[16]. Perhaps the most famously fullerene-like structures, fullerooids^[17] are the cubic convex polyhedra with faces of size 5 or greater (e.g., 7-gons). Despite these successes, many more hypothetical analogies for carbon-cages remain appealing targets, particularly in theoretical and mathematical chemistry.

A parallel line of investigation involves the use of mathematical techniques to study structural properties of fullerenes, and it is an area ripe for development and deserves special encouragement. In 1995, Fowler and Manolopoulos have made an atlas of fullerenes^[18], from which we can conclude that the mathematics for fullerenes combines techniques in several areas: (1) topology to probe the electronic structure and stability, (2) group theory to capture the symmetry and to distinguish isomers, (3) graph theory to provide several topological indices for coding and nomenclature and (4) geometry for 3-dimensional aspects and

structural formation. For details, we can see more ref. [19-21].

The paper contains two parts. Recently, two types of operations have been proposed for icosahedral fullerenes which are also called Goldberg polyhedra [22-24]. Based on these operations, the first part proposes two combinatorial ways and shows how they can be applied to fullerenes of any symmetry. In addition, a simple method based on knot theory is introduced in the second part, which can easily transform fullerene graphs into corresponding polyhedral links [25-27]. This part also describes how concepts from knot theory for fullerene polyhedral links can be related to other known mathematic tools for fullerene graphs. In particular, we mainly focus on some knot invariants and suggest potential applications in investigating structural and chemical properties of fullerenes. The results also have shed new light to describe the topological properties of a polyhedral molecule.

In particular, there are some important definitions in the paper. We define polyhedra with 3-gons added on fullerenes by (3, 0)-fullerenes, 3-gons and 4-gons added by (3, 4)-fullerenes, and 3-gons and 8-gons added by (3, 8)-fullerenes.

2. Generating leapfrog fullerenes and (3, 8)-fullerenes

This section will show how to combine three basic operations to generate two new combinatorial operations, which can be used to generate leapfrog fullerenes and (3, 8)-fullerenes.

2.1. Basic operations

First, we recall two basic operations [22] of 'Spherical rotating' and 'Spherical stretching' on polyhedra. The spherical rotating (*SR*) describes the deformation of rotating polygons on a sphere and introduces 3-gons to replace vertices of parent polyhedra, while the spherical stretching (*SS*) depicts the deformation of stretching spaces between polygons on a sphere and introduces 3-gons and 4-gons to replace vertices and edges of parent polyhedra, respectively. The results are hence some four-valent polyhedra and two transformation matrixes M_{SR} and M_{SS} which can be described by three geometrical parameters of vertex (v), face (f) and edge numbers (e) as follows:

$$\begin{pmatrix} v' \\ e' \\ f' \end{pmatrix} = M \begin{pmatrix} v \\ e \\ f \end{pmatrix}, \quad M_{SR} = \begin{pmatrix} 0 & 1 & 0 \\ 3 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix} \quad \text{and} \quad M_{SS} = \begin{pmatrix} 3 & 0 & 0 \\ 3 & 2 & 0 \\ 1 & 1 & 1 \end{pmatrix}.$$

Now, we introduce another basic operation of 'vertex bifurcation', which was proposed by Jablan [28], who utilized bigons to replace vertices of basic planar graphs (all four-valent). In the following, we apply the vertex bifurcation (*VB*) to 4-valent fullerenes which are obtained by two above methods. It can be noted that the replacement of bigons has two choices, which are illustrated in Figure 1. In order to generate new pentagons and hexagons, we add another restriction in which bigons must traverse original pentagons or hexagons. Accordingly, vertices can be inserted into edges, each new edge joined the two new vertices and extra faces are formed. This operation may be chemically realized by the reaction which is similar to C_2 insertion [8], and the transformation matrix M_{VB} is

$$M_{VB} = \begin{pmatrix} 2 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$



Figure 1. Two ways of the operation of vertex bifurcation (bigons are denoted by bold edges).

2.2. Spherical rotating–vertex bifurcation

Spherical rotating–vertex bifurcation (*SRVB*) is a transformation which combines two operations of *SR* and *VB*. First, we apply *SR* operation on fullerene graph, and add trigons at vertices of the parent fullerene graphs G , thus many 4-regular extended (3, 0)-fullerene graphs G' are obtained. Then, by replacing their vertices of G' with bigons, larger fullerene graphs G'' are obtained. For the operation, we can conclude that the transformation matrix M_{SRVB} is

$$M_{SRVB} = M_{VB} M_{SR} = \begin{pmatrix} 0 & 2 & 0 \\ 3 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}.$$

The *SRVB* transformation contains three stages:

(1) Start with an original fullerene graph C_n , whose geometrical parameters are

$$v, e, f = f_5 + f_6,$$

where $f_5=12, f_6=\frac{n}{2}-10$, and f_i denotes the number of i -gonal faces.

(2) Add n trigons at all vertices, a $(3, 0)$ -fullerene graph with $\frac{3n}{2}$ four-valent vertices is obtained. For this intermediate, the number of vertices v' equals to the original edge number e ; the number of edges e' is twice of the original edge number e ; while the number of faces f' equals to the sum of original face number f and the original vertex number v . The transformation geometrical parameters are

$$v'=e, e'=2e, f'=v+f.$$

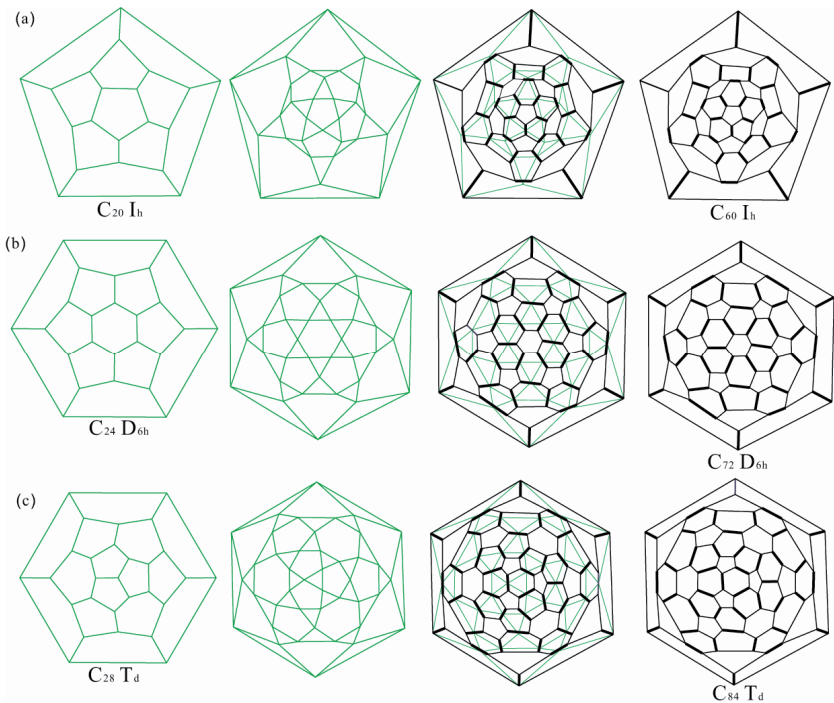


Figure 2. The SRVB operation to C_{20} , C_{24} and C_{28} fullerene graphs.

(3) Then, use $\frac{3n}{2}$ bigons to cover new four-valent vertices, the original 12 pentagons and f_6 hexagons remain unchanged, while the n trigons are transformed into n benzene structures. These $\frac{3n}{2}$ covering bigons alternatively distribute at n benzene which are obtained from trigons. After this operation, the number of faces does not change, but the number of vertices is increased by twice and edges equals to the sum of vertex number v' and edge number e' of the (3, 0)-fullerene. The transformation geometrical parameters are

$$v'' = 2v', e'' = v' + e', f'' = f'.$$

For examples, Figure 2 shows $C_{60}(I_h)$, $C_{72}(D_{6h})$, and $C_{84}(T_d)$, which are generated from $C_{20}(I_h)$, $C_{24}(D_{6h})$, and $C_{28}(T_d)$, respectively. It is easy to see that the symmetry is remained throughout these operations. Note that the results of *SRVB* are as same as the leapfrog transformation [2], which can be achieved by different combinations of simple operations: truncation of the dual graph or dual of the omnicaapping graph. Thus, the *SRVB* operation applied to fullerenes can lead to leapfrog fullerenes, and the goal of such a transformation is to isolate the pentagons by the appearance of hexagons.

2.3. Spherical stretching–vertex bifurcation

Similar to *SRVB* operation, Spherical stretching–vertex bifurcation (*SSVB*) is a transformation which combines two operations of *SS* and *VB*. First, we apply *SS* on fullerene graph, and add trigons at vertices and tetragons between edges of the parent fullerene graphs G , many 4-regular extended (3, 4)-fullerene graphs G' are obtained. Then by replacing their vertices of G' with bigons, a class of fullerene graphs G'' with novel tilings are obtained. For the operation, the transformation matrix M_{SSVB} is

$$M_{SSVB} = M_{VB}M_{SS} = \begin{pmatrix} 6 & 0 & 0 \\ 6 & 2 & 0 \\ 1 & 1 & 1 \end{pmatrix}.$$

The *SSRB* transformation also contains three stages:

(1) Start with an original fullerene graph C_n , whose geometrical parameters are

$$v, e, f = f_5 + f_6,$$

where $f_5=12, f_6=\frac{n}{2}-10$.

(2) Add n trigons at vertices and $\frac{3n}{2}$ tetragons between edges, a (3, 4)-fullerene graph with $3n$ four-valent vertices is obtained. For this intermediate, the number of vertices v' equals to three times of original; the number of edge e' equals to the twice of original edge number e added to the vertex number v' ; while the number of faces f' equals to the sum of original face number f and the original vertex number v and original edge number e . The transformation geometrical parameters are

$$v' = 3v, e' = 3v + 2e, f' = v + e + f.$$

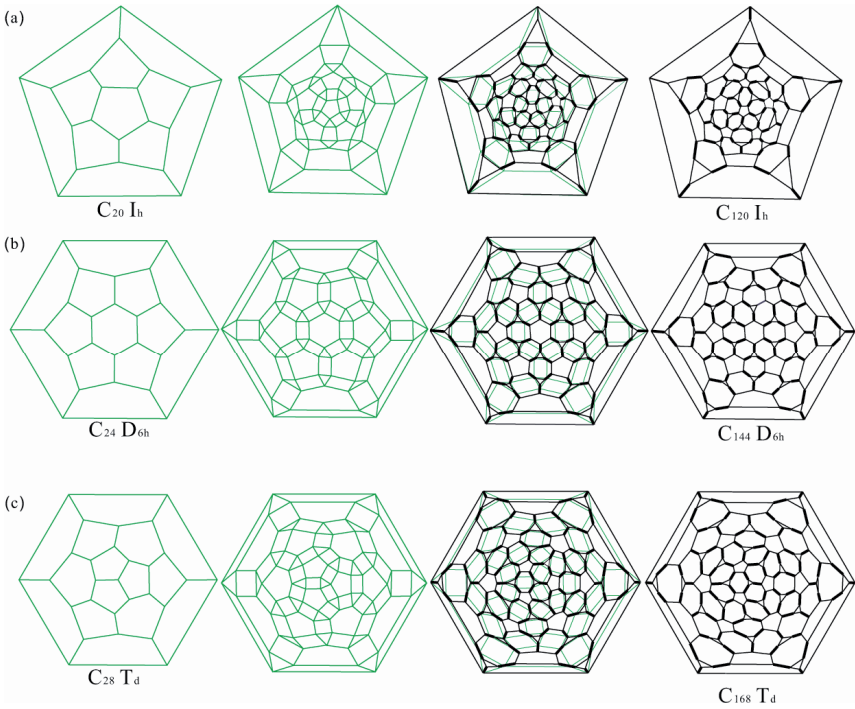


Figure 3. The SSVB operation to C_{20} , C_{24} and C_{28} fullerene graphs.

(3) Then, using $3n$ bigons to cover new coming four-valent vertices, the original 12 pentagons, f_6 hexagons and n trigons remain unchanged, while the $\frac{3n}{2}$ tetragons are transformed into $\frac{3n}{2}$ [8]annulene. These $3n$ covering bigons alternatively distribute at $\frac{3n}{2}$ [8]annulene which are obtained from tetragons. After this operation, the number of faces does not change, but the number of vertices is increased by twice and edges equals to the sum of vertex number v' and edge number e' of the (3, 4)-fullerene. The transformation geometrical parameters are

$$v'' = 2v', e'' = v' + e', f'' = f'.$$

For examples, Figure 2 shows $C_{120} (I_h)$, $C_{144} (D_{6h})$, and $C_{168} (T_d)$, which are generated from $C_{20} (I_h)$, $C_{24} (D_{6h})$, and $C_{28} (T_d)$, respectively. It is clear that the symmetry is still remained throughout these operations. These novel transformations take carbon cages out of the fullerene series and have as yet no direct chemical relevance. Nevertheless, they could be useful in a mathematical context for constructing and counting trivalent polyhedra. We call these related cages as (3, 8)-fullerenes, because they not only contain 5-gons and 6-gons of the original, but also introduce 3-gons and 8-gons. One of the examples is shown in Figure 4.

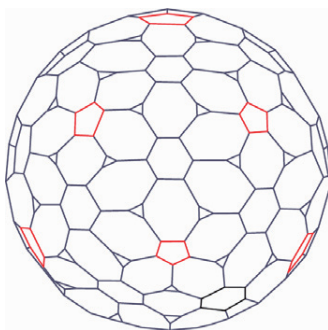


Figure 4. The (3, 8) – fullerene C_{360} which is obtained from C_{60} by the *SSVB* operation

The famous Euler formula is useful in checking the consistence of an assumed structure and yields the following relation:

$$3f_3 + 2f_4 + f_5 = 12(1 - g) + \sum_{i \geq 7} (i - 6)f_i$$

where f_i denotes the number of i -gonal faces of p , and g denotes the genus of a graph. For a (3, 8)-fullerene C_n , it has $f_3 = \frac{n}{6}$, $f_4 = 0$, $f_5 = 12$, $f_8 = \frac{n}{4}$, and $i = 8$, thus we can conclude that $g = 0$, i.e., the (3, 8)-fullerene is a closed sphere. The presence of 3-gonal faces compensates negative curvature leading by 8-gonal faces. These two types of faces may appear by two reasons. One is Buckminster Fuller utilized 3-gons to construct the original geodesic dome; the other is 8-gons preserving the sp^2 -like nature of carbon nets. Despite these feasibilities, the chemical significance and Kekulé count in (3, 8)-fullerenes need further investigating. In particular, molecular graphs for I_h and I symmetry of these novel fullerenes are the architecturally simplest and can be described by the Goldberg vectors (h, k) . The vertex counts are

$$n = 40(h^2 + hk + k^2)$$

where integers $0 \leq k \leq h, h \geq 0$.

3. Knot- theoretical method for fullerene polyhedral links

3.1. The knot algorithm

Mathematically, all normal fullerene and related (3, 8)-fullerene graphs are cubic (3-regular) graphs which can be embedded in the surface of a sphere. But each vertex is connected by a bigon, so they are all 4-valent as chemical entities. In knot theory^[28, 29], each four-valent plane graph can be seen as a projection of an alternating link. Accordingly, a knot algorithm that involves two steps is proposed. First, a bigon is transformed into a double-line, while a set of bigons corresponds to a perfect matching or a Kekulé structure (KS) in chemistry. Second, the related two vertices are transformed into a pair of alternate crossings, where one of them is overcrossing and the other is undercrossing, and *vice versa*. As a result, the vertices of fullerene graphs are changed to crossings, and the edges are changed to the curves supporting the framework of polyhedral links. Although a fullerene graph results in two mirror polyhedral links, only one configuration is counted because KS is insensitive to chirality. Thus, there is a one-to-one correspondence between each KS and a polyhedral link. In order to describe our ideas, some examples are shown in Figure 5, after applying the

algorithm to one of KS s of C_{20} , C_{24} and C_{28} , then a knot, a three-component link and a two-component link are obtained, respectively.

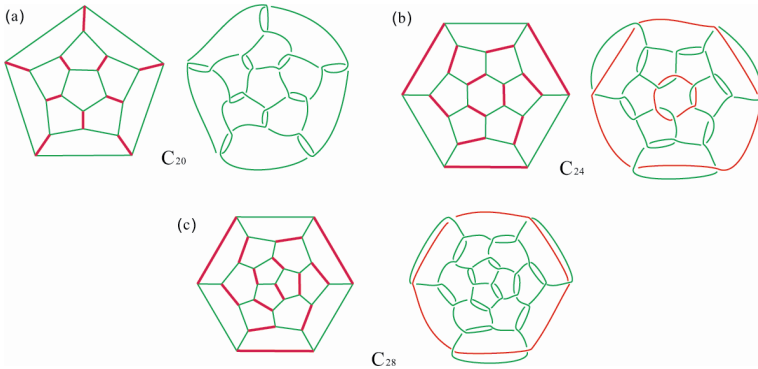


Figure 5. The knot algorithm for one of KS s of C_{20} , C_{24} and C_{28} can lead to (a) a knot, (b) a three-component link and (c) a two-component link.

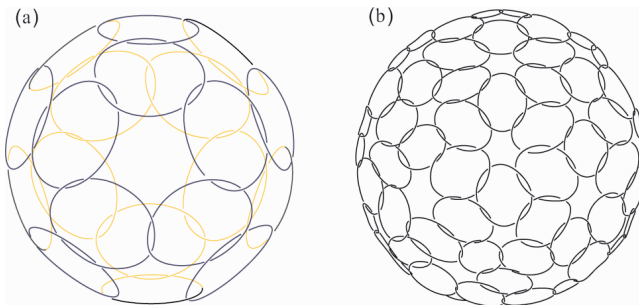


Figure 6. Two fullerene polyhedral links of (a) the least leapfrog fullerene C_{60} and (b) the relating cage of C_{360} .

In addition, we look at what kind of topological structures can be obtained by the application of knot algorithm to leapfrog fullerenes and (3, 8)-fullerenes. A leapfrog fullerene has many notable properties. For instance, it contains at least $2^{v/8}$ different KS [30]. Thus, when a leapfrog fullerene graph is changed to a projection of an alternating polyhedral link, there are at least $2^{v/8}$ polyhedral links for a fullerene graph. By the reason that pentagons in such a series of fullerene having been isolated by hexagons and every bigons are distributed on hexagons, the related links shown in Figure 6(a) are nested by some hexagonal rings, and

such complex forms were found in nature such as kinetoplasts DNA ^[31]. The emergence of alternating bigons in octagons make (3, 8)-fullerenes also have *KS*, so we can also use knot algorithm to generate their corresponding polyhedral links. As a consequence, a (3, 8)-fullerene, with no adjacent 3-gons, 5- and 6-gons, are changed to a network similar to chainmail armor which is regularly catenated by some 8-memberd rings. See Figure 6 (b).

3.2. Some chemical applications

Using the aforementioned connection between alternating link diagrams and 4-regular diagrams of fullerenes, it is now clear that fullerene graphs appear as polyhedral links of interlocked circles that reside in space in a topologically nontrivial way. For such structures, there is hope of using topological methods to gain chemical information. The branch of topology known as knot theory is a powerful tool of quantifying and comparing the various configurations of such nontrivial molecules ^[32-34]. However, since the application of knot-theoretical approaches on fullerenes is a niche research area, which was originally proposed by Jablan (<http://members.tripod.com/~modularity/ful.htm#cont>), there are only two published literatures to our best knowledge ^[35,36].

Now, we only outline a strategy and focus on the application of knot invariants in three aspects preliminarily. These applications are not very clear, thus, our account is informal and needs our own further exploring, and we also hope researchers to pay more attention to this new line of research. Furthermore, a few examples are potential to make these comments clearer. Figure 7 shows two knots corresponding to two different *KSs* of the dodecahedron of C_{20} . To compute knot invariants for links, we put the same orientation to each component.

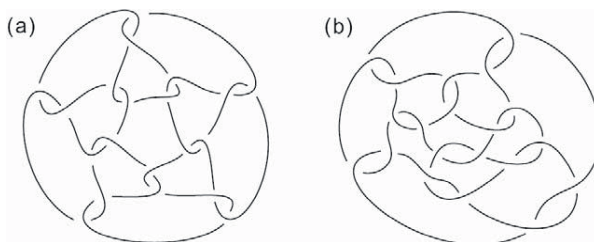


Figure 7. Two knots corresponding to two different *KSs* of the dodecahedron of C_{20} .

(1) The determination of fullerene isomers. To enumerate all isomers of a fullerene is a complicated mathematical problem that has still not been solved completely; even through some methods such as the *SW* rearrangement ^[18]. If we transform fullerene graphs into polyhedral links, it corresponds to a fundamental problem in knot theory: recognition of links. To address the problem, mathematicians have developed a number of elegant and powerful knot polynomials ^[29]. For instance, the HOMFLY polynomial, the Alexander polynomial and the Jones polynomial are able to distinguish between various links and indicate the structure of related fullerenes. These polynomials are powerful tools as invariants because they are the same if one oriented link is ambient isotopic to another. In fact, some of the earlier works can be found in ref. ^[28]. So far, there are a number of excellent computer programs that can compute all of the link polynomials.

To distinguish knots in Figure 7, we use the Program "KNOT" made by Kodama to calculate the one-variable HOMFLY polynomial because of its computational feasibility. For each link, we associate a polynomial. By calculation, the corresponding HOMFLY polynomial of the knot of Figure 7 (a) is

$$v^{-10} - 5v^{-6} + 10v^{-4} - 10v^{-2} + 9 - 10v^4 - 5v^6 + v^{10} ,$$

while the HOMFLY polynomial of the knot of Figure. 7 (b) is

$$v^{-10} - 4v^{-6} + 6v^{-4} - 2v^{-2} - 1 - 2v^2 + 6v^4 - 4v^6 + v^{10} .$$

Thus, they are topologically distinct.

(2) The complexity of fullerenes. On this topic, several graph invariants have been successfully defined to describe the complexity of fullerene graphs ^[37]. Similarly, a number of knot invariants are examined to evaluate the complexity of fullerene polyhedral links. Knot genus is the least genus of any Seifert surface for a given knot, whose value quantifies the complexity of links. In Figure 8, applying Seifert's algorithm D_0 to a projection of an alternating knot or link, the crossing has been eliminated to yield a Seifert surface of minimal genus. For example, the genus of unknot is zero. Except for the knot genus, other measures of link complexity include the crossing number, the bridge index, the stick number and span of any knot polynomial, *etc.*

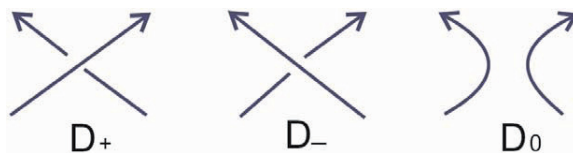


Figure 8. Three digrams of (+), (-), and (0) crossings. The arrows indicate the orientation of curves.

For the cases in Figure 7, we apply Seifert's algorithm to get their Seifert surfaces with maximum Seifert circles, and then use the following equation to obtain the genus:

$$2g(F) = [1 - s(L(G)) + c(L(G))] + [1 - \mu(L(G))]$$

where s is the number of Seifert circles, c is the crossing number and μ is component number. For the knot in Figure 7 (a), $s = 13$, then the genus $g = 4$; and for the knot in Figure 7 (b), $s = 11$, then the genus $g' = 5$. Accordingly, we conjecture that the knot of Figure 7 (b) is more complex.

(3) The stability of fullerenes. As far as we know, besides some graph invariants^[38], there are some operations and criterions to yield and to estimate stable isomers, such as leapfrog transformation in geometry, Clar type in graph theory and steric strain in topology^[18, 39]. For fullerene polyhedral links, a different approach using the calculation of the unknotting or unlinking numbers is selected for our potential idea^[40]. It can be assumed that the most stable isomer corresponds to a knot or link with the largest unknotting or unlinking number. Our reason is that we can use these two invariants to estimate how hard a fullerene link is turned into a knot or a trivial link. These two numbers are related to the simple operation of crossing changes, which can be found from a sequence determined by particular diagrams from D_+ to D_- or from D_- to D_+ , as shown in Figure 8.

To compute unlinking numbers, we have to encode a knot or link with DT notation or Conway notation. Then, using the program LinKnot^[28], we can obtain the estimated values of unknotting numbers of the knot or link according to Bernhard-Jablan Conjecture. However, LinKnot can only be used for alternating knots and links up to 12 crossings. Thus, we cannot compare the stability by this invariant for the examples in Figure 7, and it is still an area full of open questions which needs developing a more effective measure in the future works.

4. Conclusion

Polyhedra are higher forms of molecular organisms, thus, they are very useful for theoretical speculation on diverse chemical structures. In the paper, combinations of the spherical rotating and the spherical stretching with vertex bifurcation can be used to define two symmetry transformations as *SRVB* and *SSVB*, respectively. The *SRVB* applied to fullerenes can generate leapfrog fullerenes, and the *SSVB* generates a family of novel polyhedra named (3, 8)-fullerenes. Except for 5-gonal and 6-gonal faces, (3, 8)-fullerenes also contain 3-gonal and 8-gonal faces. These exotic faces lead very little mechanical strain, so we hypothesize these structures may be stable. These polyhedra are all 3-regular but 4-valent, thus, may be promising as candidates for carbon solids. It is very interesting that the construction of their duals, in which all faces are 3-gons, are of a special important type and may be used to model virus capsids. Additionally, two transformation matrixes offer a systematic way of predicting the shapes.

Furthermore, the knot algorithm has been proposed to transform fullerene graphs into polyhedral links. These carbon chain mails, such as regular networks of topological interlocked with hexagonal or octagonal carbon-carbon rings imply a new method. In contrast with commonly used mathematical tools, the knot-theoretical method can find their applications in describing such topological nontrivial structures. In general, we can use knot polynomials to distinguish fullerene isomers, knot genus to predict the complexity of fullerenes, and unknotting numbers to estimate the stability of fullerenes. Although the method has some inherent restrictions limited by the development of knot theory itself, we expect this work to create more opportunities to show how knot invariants are related to polyhedral molecules, most significantly, fullerene graphs.

Acknowledgements

This work was supported by grants from The National Natural Science Foundation of China (No.90203012 and No.10831001) and Specialized Research Fund for the Doctoral Program of Higher Education of China (No. 20020730006).

References

- [1] W. Kroto, J. Heath, S. O'Brien, R. Curl, R. Smalley, C₆₀ Buckminsterfullerene, *Nature* **318** (1985) 162-163.
- [2] P. W. Fowler, D. B. Redmond, Symmetry aspects of bonding in carbon clusters: the leapfrog transformation. *Theor. Chim. Acta* **83** (1992) 367-375.
- [3] T. Pisanski, M. Randić, Bridges between Geometry and Graph Theory, in: C. A. Gorini (Eds.), *Geometry at Work: A Collection of Papers Showing Applications of Geometry*, Math. Assoc. Amer., Washington, 2000, Vol. 53, pp. 174-194.
- [4] E. C. Kirby, On the partially random generation of fullerenes, *Croat. Chem. Acta.* **73** (2000) 983-991.
- [5] M. Hasheminezhad, H. Fleischner, B. D. McKay, A universal set of growth operations for fullerenes, *Chem. Phys. Lett.* **464** (2008) 118-121.
- [6] S. Schein, T. Friedrich, A geometric constraint, the head-to-tail exclusion rule, may be the basis for the isolated-pentagon rule in fullerenes with more than 60 vertices, *Proc. Natl. Acad. Sci. U. S. A.* **105** (2008) 19142-19147.
- [7] A. J. Stone, D. J. Wales, Theoretical studies of icosahedral C₆₀ and some related species, *Chem. Phys. Lett.* **128** (1986) 501-503.
- [8] M. Endo, H. W. Kroto, Formation of carbon nanofibers, *J. Phys. Chem.* **96** (1992) 6941-6944.
- [9] G. Brinkmann, P. W. Fowler, A catalogue of growth transformations of fullerene polyhedra, *J. Chem. Inf. Comput. Sci.* **43** (2003) 1837-1843.
- [10] G. Brinkmann, P. W. Fowler, C. Justus, A catalogue of isomerization transformations of fullerene polyhedra, *J. Chem. Inf. Comput. Sci.* **43** (2003) 917-927.
- [11] R. B. King, M. V. Diudea, The chirality of icosahedral fullerenes: a comparison of the tripling (leapfrog), quadrupling (chamfering), and septupling (capra) transformations, *J. Math. Chem.* **39** (2006) 597-604.
- [12] M. V. Diudea, P. E. John, Covering polyhedral tori, *MATCH Commun. Math. Comput. Chem.* **44** (2001) 103-116.
- [13] M. V. Diudea, Corannulene and corazulene tiling of nanostructures, *Phys. Chem. Chem. Phys.* **7** (2005) 3626-3633.
- [14] M. V. Diudea, Nanoporous carbon allotropes by septupling map operations, *J. Chem. Inf. Comput. Sci.* **45** (2005) 1002-1009.
- [15] M. V. Diudea, Retro-leapfrog and structure elucidation, *J. Math. Chem.* **45** (2009) 354-363.
- [16] O. Delgado Friedrichs, M. Deza, Icosahedral fulleroids, in: P. Hausen, P. W. Fowler, M. Zheng (Eds.), *DIMACS Series in Discrete Mathematics and Theoretical Computer Science*, 2000, Vol. 51, pp. 97-115.
- [17] A. Dress, G. Brinkmann, Phantasmagorical fulleroids, *MATCH Commun. Math. Comput. Chem.* **33** (1996) 87-100.
- [18] P. W. Fowler, D. E. Manolopoulos, *An Atlas of Fullerenes*, Oxford University Press, Oxford, 1995.
- [19] F. Chung, S. Sternberg, Mathematics and the buckyball. *Am. Sci.* **81** (1993) 56-71.
- [20] A. T. Balaban, X. Liu, D. J. Klein, D. Babic, T. G. Schmalz, W. A. Seitz, M. Randic, Graph invariants for fullerenes, *J. Chem. Inf. Comput. Sci.* **35**(1995) 396-404.

- [21] N. Trinajstić, M. Randić, D. J. Klein, D. Babić, Z. Mihaljčić, On mathematical properties of buckminsterfullerene, *Croat. Chem. Acta.* **68** (1995) 241-267.
- [22] G. Hu, W.-Y. Qiu, Extended Goldberg polyhedra, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 585-594.
- [23] G. Hu, W.-Y. Qiu, Extended Goldberg polyhedral links with even tangles, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 737-752.
- [24] G. Hu, W.-Y. Qiu, Extended Goldberg polyhedral links with odd tangles, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 753-766.
- [25] W.-Y. Qiu, X.-D. Zhai, Molecular design of Goldberg polyhedral links, *J. Mol. Struct. THEOCHEM* **756** (2005) 163-166.
- [26] W.-Y. Qiu, X.-D. Zhai, Y.-Y. Qiu, Architecture of Platonic and Archimedean polyhedral links, *Sci. China Ser. B-Chem.* **51** (2008) 13-18.
- [27] G. Hu, X.-D. Zhai, D. Lu, W.-Y. Qiu, The architecture of Platonic polyhedral links, *J. Math. Chem.* 2008, DOI:10.1007/s10910-008-9487-z
- [28] S. Jablan, R. Sazdanović, *LinKnot- Knot Theory by Computer*, World Scientific, Singapore, 2007.
- [29] C. C. Adams, *The Knot Book: An Elementary Introduction to the Mathematical Theory of Knots*, W. H. Freeman, New York, 2000.
- [30] T. Doslić, Leapfrog fullerenes have many perfect matchings, *J. Math. Chem.* **44** (2008) 1-4.
- [31] J. H. Chen, C. A. Rauch, J. H. White, P. T. Englund, N. R. Cozzarelli, The topology of the kinetoplast DNA network, *Cell* **80** (1995) 61-69.
- [32] P. G. Mezey, Tying knots around chiral centers: chirality polynomials and conformational invariants for molecules, *J. Am. Chem. Soc.* **108** (1986) 3976-3984.
- [33] D. W. Sumners, The knot theory of molecules, *J. Math. Chem.* **1** (1987) 1-14.
- [34] W.-Y. Qiu, Knot theory, DNA topology, and molecular symmetry breaking, in: D. Bonchev, D. H. Rouvray (Eds.), *Chemical Topology—Applications and Techniques, Mathematical Chemistry Series*, Vol. 6, Gordon and Breach Science Publishers, Amsterdam, 2000, pp. 175–237.
- [35] M. Deza, M. Dutour, P. W. Fowler, Zigzags, railroads, and knots in fullerenes, *J. Chem. Inf. Comput. Sci.* **44** (2004) 1282-1293.
- [36] Y.-M. Yang, W.-Y. Qiu, Molecular design and mathematical analysis of carbon nanotube links, *MATCH Commun. Math. Comput. Chem.* **58** (2007) 635-646.
- [37] M. Randić, X. F. Guo, D. Plavšić, A. T. Balaban, On the Complexity of Fullerenes and Nanotubes, in: D. Bonchev, D. H. Rouvray (Eds.), *Complexity in Chemistry, Biology, and Ecology*, Springer US, New York, 2005, pp 1- 48.
- [38] S. Fajtlowicz, C. E. Larson, Graph-theoretic independence as a predictor of fullerene stability, *Chem. Phys. Lett.* **377** (2003) 485-490.
- [39] P. W. Fowler, T. Pisanski, Leapfrog transformations and polyhedra of Clar type, *J. Chem. Soc. Farad. Trans.* **90** (1994) 2865-2871.
- [40] S. Jablan, R. Sazdanović, Unlinking number and unlinking gap, *J. Knot. Theor. Ramif.* **16** (2007) 1331-1355.