Chapter 4
Distance Under Symmetry: (3,6)-Fullerenes

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Abstract A (3,6)-fullerene is a planar 3-connected cubic graph whose faces are triangles and hexagons. In this chapter, the modified Wiener and hyper–Wiener indices of three infinite classes of (3,6)-fullerenes are considered into account. Some open questions are also presented.

4.1 Introduction

Throughout this paper all graphs are assumed to be simple. This means that our graphs don't have multiple edges and loops. A graph G is called *connected* if for each vertex x and y in G, there is path connecting them. The graph G is said to be *3-connected*, if G has more than three vertices and remains connected whenever fewer than three vertices are removed from G. A *chemical graph* is a graph in which the vertices are atoms and edges are the chemical bonds. The *distance* between two vertices of G is defined as the length of the shortest path connecting them. The *distance matrix* $D(G)$ of G is a square matrix of order $n = |V(G)|$, where (i, j) entry is the distance between the ith and jth vertices of G.

A group is a pair $(G, \bullet)$ such that $\bullet: G \times G \rightarrow G$ is a function and the following three axioms are satisfied:

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A.R. Ashrafi, M.V. Diudea (eds.), *Distance, Symmetry, and Topology in Carbon Nanomaterials*, Carbon Materials: Chemistry and Physics 9,
DOI 10.1007/978-3-319-31584-3_4

1. For each $x, y, z \in G$, $x\bullet(y\bullet z) = (x\bullet y)\bullet z$. This equation is called *associative law*.
2. There exists an element $e \in G$ such that for each $x \in G$, $x\bullet e = e\bullet x = x$. The element e is called the *identity* of G.
3. For each element $x \in G$, there exists an element $y \in G$ such that $x\bullet y = y\bullet x = e$. The element y is unique. It is called the *inverse* of x and denoted by x^{-1}.

The concept of group is very useful in explanation of the symmetry properties of molecules. A subgroup of G is a nonempty subset that is closed under taking group product and inverse. A group containing a finite set of elements is said to be finite. Fix an element $x \in G$ and define

$$\langle x \rangle \;=\; \left\{ x^n \,\middle|\, n \text{ is an integer} \right\}.$$

Then $\langle x \rangle$ is called a *cyclic subgroup* of G with *generator* x. G is said to be cyclic, if there exists an element $a \in G$ such that $G = \langle x \rangle$. A cyclic group of order k is denoted by Z_k.

Suppose $X = \{1, \ldots, n\}$ and S_n denote the set of all one to one and onto mapping from X onto X. Then it is easy to see that the set S_n has a group structure under composition of functions. This group is called the *symmetric group* on n symbols. Clearly, the symmetric group on n symbols has order $n!$. The elements of the symmetric group S_n is called a *permutation* on X, and a permutation α on X is said to be *even*, if α can be obtained from an even number of two-element swaps. The set of all even permutations of S_n constitutes a subgroup A_n of order $n!/2$. This subgroup is called the *alternating group* on n symbols. A *dihedral group* is the group of symmetries of a regular polygon containing rotations and reflections. This group can be considered as the rigid motions of the plane preserving a regular n-gon with respect to composition of symmetries. Obviously, this group has order $2n$ denoted by D_{2n}.

Suppose G is a graph and α: $G \to G$ is a function. The mapping α is called an *automorphism*, if α has an inverse and α, α^{-1} preserve adjacency in G. The set of all such mappings is denoted by Aut(G). This set has a group structure under composition of functions and so it is named the *automorphism group* of G. If G is a chemical graph, then the automorphism group of G represents the maximum possible symmetry elements in the molecule under consideration. In some classes of molecules like fullerenes, this group and the symmetry group are the same.

4.2 Distance Under Symmetry for (3,6)-Fullerenes

A cubic graph is a graph in which all vertices have degree 3. A *(3,6)-fullerene graph* ((3,6)-fullerene or fullerene for short) is a planar 3-connected cubic graph whose faces are only triangles and hexagons. A pyramid is a (3,6)-fullerene with the minimum possible number of vertices. It is possible to define (4,6)- and (5,6)-fullerene graphs in a similar way, but by Euler's theorem, there is no (k,6)-fullerene graphs for other values of k. We encourage the interested readers to consult the famous book of Fowler and Manolopoulos (1995). The books (Cataldo et al. 2011; Ashrafi et al. 2013) also contain recent literature reviews on theory and experiment

of fullerenes. We refer also to two important computer packages FuiGui (Myrvold et al. 2007) and Program Fullerene (Schwerdtfeger et al. 2013) for investigating conjectures and constructing and analyzing structures of fullerenes. For the mathematical properties of (3,6)-fullerenes, the interested readers can consult Fowler et al. (2000), John and Sachs (2009), Devos et al. (2009), Yang and Zhang (2012), Ashrafi and Mehranian (2013), and Behmaram et al. (2013).

This chapter is mainly concerned with the symmetry and distance topology of (3,6)-fullerenes. In Ghorbani et al. (2015), it is proved that the order of the automorphism group of a (3,6)-fullerene divides 24. It is merit to state here that Deza et al. (2009) proved that there are five possible symmetry groups for a (3,6)-fullerene. These are $D_2 \cong Z_2 \times Z_2$, $D_{2h} \cong Z_2 \times Z_2 \times Z_2$, $D_{2d} \cong D_8$, $T \cong A_4$, and $T_d \cong S_4$. The 2D and 3D perceptions of (3,6)-fullerenes with these symmetry groups and minimum possible number of vertices are depicted in Figs. 4.1 and 4.2, respectively.

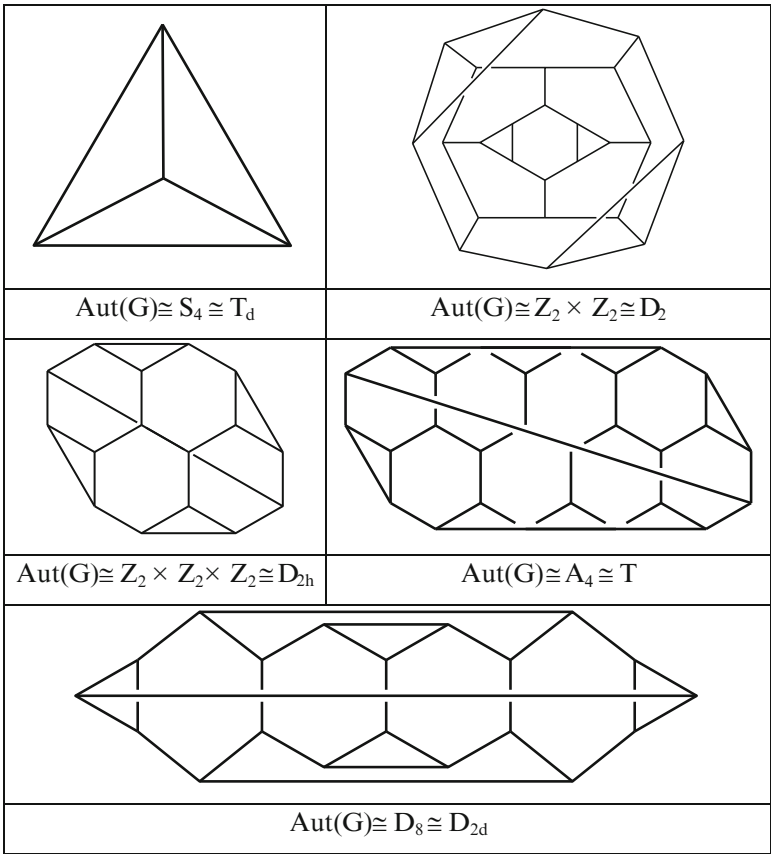

Fig. 4.1 2D perception of (3,6)-fullerenes with five different symmetry groups

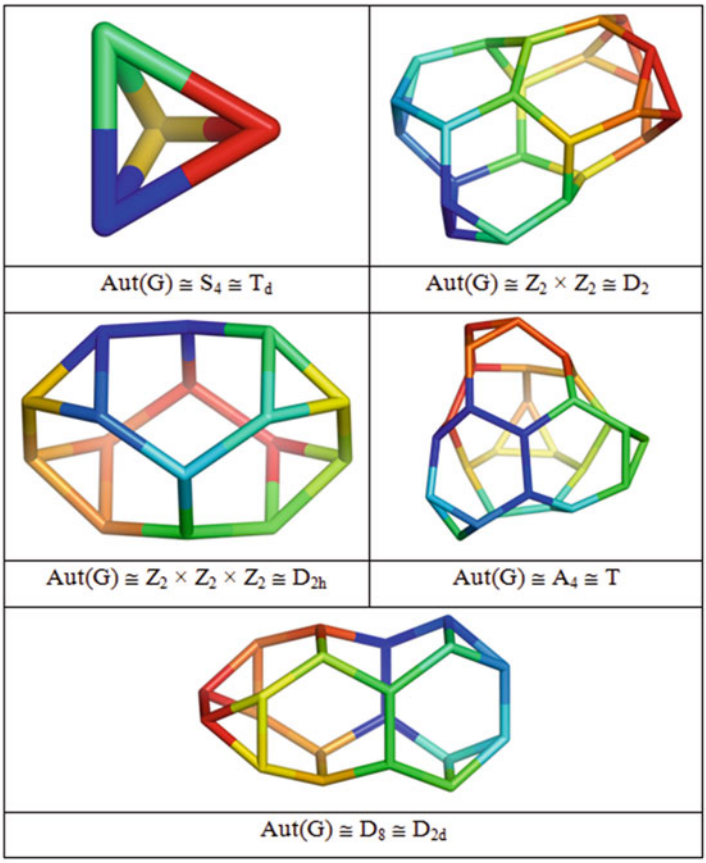

Fig. 4.2 3D perception of (3,6)-fullerenes with five different symmetry groups

The *Wiener index* of G, $W(G)$, is defined as the sum of distances between all pairs of vertices in G (Wiener 1947). This graph invariant has remarkable applications in chemistry and also in computer science. We refer to Gutman and Šoltés (1991) for application of this number in chemistry.

A connected graph G without cycles is said to be an *acyclic graph*. The hyper–Wiener index of acyclic graphs was introduced by Milan Randić, as a generalization of the Wiener index. Then Klein et al. (1995) extended this graph invariant for arbitrary graphs. It is defined as

$$WW(G) = \frac{1}{2}W(G) + \frac{1}{2}\sum_{\{x,y\}} d(x,y)^2.$$

The mathematical properties and chemical meaning of this topological index are reported in Khalifeh et al. (2008) and Gutman et al. (1997). It is merit to mention here that there is a matrix version of the hyper–Wiener index introduced by

M.V. Diudea (1996a, b, 1997, Diudea et al. 1997). To explain, we assume that G is a connected graph and $D = D(G)$ is its distance matrix. The Wiener matrix $W = W(G)$ is another $n \times n$ matrix such that its ijth entry is defined as the number of paths containing the (i, j) path. These matrices are basis for calculating W, whereas distance path and Wiener path are basis for the calculation of hyper–Wiener index. We encourage the interested readers to consult the mentioned papers by Diudea and references therein for more information on this topic.

Graovac and Pisanski (1991) in their seminal paper combine distance and symmetry to propose a generalization of the classical Wiener index. To explain, we assume that G is a graph with automorphism group $\Gamma = \mathrm{Aut}(G)$. The modified Wiener index of G is defined as

$$\hat{W}(G) = \frac{|V(G)|}{2|\Gamma|} \sum_{x \in V(G)} \sum_{\alpha \in \Gamma} d(x, \alpha(x)).$$

Firouzian et al. (2014) introduced in a similar way the modified hyper–Wiener index of a graph G as follows:

$$\hat{WW}(G) = \frac{1}{2} \hat{W}(G) + \frac{|V(G)|}{4|\Gamma|} \sum_{u \in V(G),\ \alpha \in \Gamma} d(u, \alpha(u))^2.$$

The aim of this chapter is to compute the modified Wiener and modified hyper–Wiener indices of three classes of fullerene graphs. To compute these graph invariants, we need their symmetry groups. The symmetry group of some classes of ordinary fullerenes ((5,6)-fullerenes) is reported in Djafari et al. (2013) and Koorepazan−Moftakhar and Ashrafi (2013). For symmetry of our three classes of (3,6)-fullerenes, we refer to Koorepazan−Moftakhar and Ashrafi (2014) and Koorepazan−Moftakhar et al. (2014a, b). In our calculations, we use the computer packages HyperChem (HyperChem Package Release 7.5 for Windows 2002), TopoCluj (Diudea et al. 2002), GAP (The GAP Team 1995), and MAGMA (Bosma et al. 1997). We refer the interested readers to consult papers (Ashrafi et al. 2008, 2009; Ashrafi and Sabaghian−Bidgoli 2009) and references therein for more information on topological properties of fullerenes.

We are now ready to construct the first (3,6)-fullerene series $B[n]$ of order $8n$, $n \geq 2$. The ninth term of the fullerene sequence $B[n]$ is depicted in Fig. 4.3. This sequence can be constructed by an inductive argument. To explain, we assume that

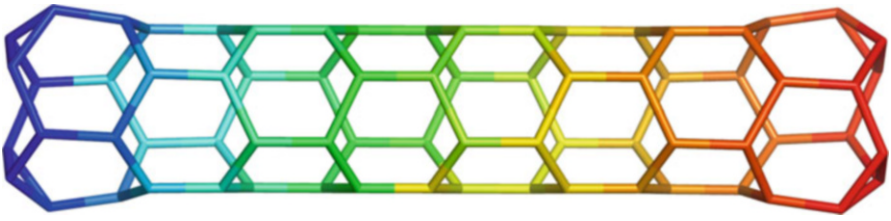

Fig. 4.3 The fullerene B[9]

the term $B[n]$ is constructed. To obtain $B[n+1]$, we add eight new vertices to the tube-shaped part of $B[n]$ and connect them to their corresponding vertices in $B[n]$. By a result in Koorepazan−Moftakhar et al. (2014a, b),

$$Aut(B[n]) = \begin{cases} S_4 & n = 2 \\ D_8 & n \geq 4 \text{ is even} \\ Z_2 \times Z_2 & n \geq 3 \text{ is odd} \end{cases}.$$

We first notice that $W(B[1]) = 294$ and $WW(B[2]) = 981$. The Wiener index of $B[n]$ is computed in general in Ashrafi and Mehranian (2013). In this paper, the authors proved that if $n \geq 3$, then

$$W(B[n]) = \frac{64}{3}n^3 + \frac{464}{3}n - 206.$$

Using a similar argument given the mentioned paper, it is possible to prove

$$WW(B[n]) = \frac{64}{3}n^4 + \frac{32}{3}n^3 - \frac{16}{3}n^2 + \frac{3112}{3}n - 1729.$$

In Koorepazan–Moftakhar and Ashrafi (2015), a representation theory method for computing the modified Wiener index of graphs is presented. Applying this method and the general form of the automorphism group of this fullerene series, we have:

Result 4.1 The modified Wiener and hyper–Wiener indices of $B[n]$ can be computed as follows:

$$\widehat{W}(B[n]) = \begin{cases} 16n^3 + 32n^2 + 20n & n \not\equiv 2 \pmod 4 \\ 16n^3 + 32n^2 + 36n & n \equiv 2 \pmod 4 \end{cases}.$$

$$\overset{\wedge}{WW}(B[n]) = \begin{cases} \frac{32}{3}n^4 + 8n^3 + \frac{232}{3}n^2 + 64n & n \equiv 1,\ 3 \pmod 4 \\ \frac{32}{3}n^4 + 8n^3 + \frac{208}{3}n^2 + 56n & n \equiv 4 \pmod 4 \\ \frac{32}{3}n^4 + 8n^3 + \frac{208}{3}n^2 + 128n & n \equiv 2 \pmod 4 \end{cases}.$$

We now continue our calculations to obtain the same invariant for another sequence of fullerenes, $C[n]$. The general term of this sequence is a fullerene with exactly $8n+4$ carbon atoms. Again, by a result in Koorepazan−Moftakhar et al. (2014a, b) (Fig. 4.4),

$$Aut(C[n]) = \begin{cases} S_4 & n = 1 \\ D_8 & n > 1 \end{cases}.$$

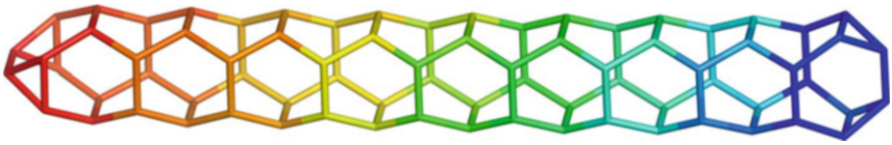

Fig. 4.4 The fullerene C[9]

In a similar way as $B[n]$, the general term of $C[n]$ can be constructed by an inductive argument. A result in Ashrafi and Mehranian (2013) states that *for* $n \geq 1$, we have

$$W(C[n]) = \frac{64}{3}n^3 + 64n^2 + \frac{152}{3}n + 2.$$

Again, we use calculations given this paper to show that

$$WW(C[n]) = \frac{64}{3}n^4 + 96n^3 + \frac{464}{3}n^2 + 148n - 21.$$

Result 4.2 The modified Wiener and hyper–Wiener indices of the fullerene sequence $C[n]$ can be computed as follows:

$$\hat{W}(C[1]) = 138 \text{ and } \hat{W}(C[n]) = 16n^3 + 72n^2 + 40n + 4 (n \geq 2).$$
$$\hat{WW}(C[n]) = \frac{32}{3}n^4 + \frac{136}{3}n^3 + \frac{388}{3}n^2 + \frac{152}{3}n - 2 (n \geq 1).$$

Our final fullerene sequence is $D[n]$ of order $16n + 48$. The general term of this fullerene series can be constructed inductively from $D[16]$. The automorphism groups of these fullerenes were reported in Koorepazan−Moftakhar et al. (2014a, b), and its Wiener index can be found in Ashrafi and Mehranian (2013) (Fig 4.5):

$$Aut(D[n]) = \begin{cases} Z_2 \times Z_2 & n \text{ is even} \\ Z_2 \times Z_2 \times Z_2 & n \text{ is odd} \end{cases}.$$

The reported Wiener index of this fullerene series is not correct. Its correct value is

$$W(D[n]) = \frac{256}{3}n^3 + 768n^2 + \frac{14912}{3}n + 3540 \ (n \geq 4).$$

In the exceptional cases that $n = 1, 2, 3$, we have $W(D[1]) = 9968$, $W(D[2]) = 17432$ and $W(D[3]) = 27714$. The hyper–Wiener index of D[n] in some special

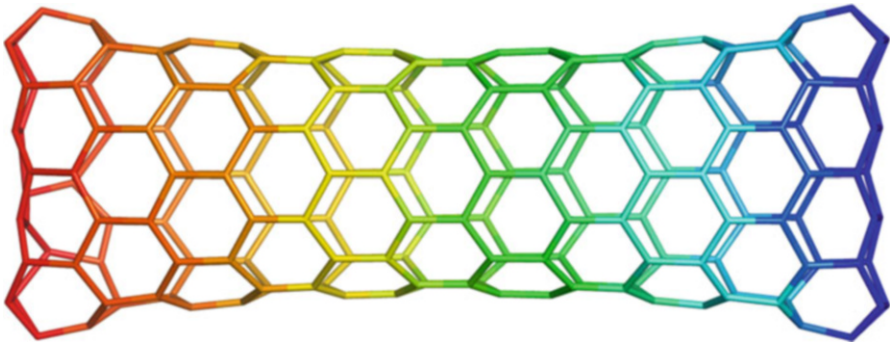

Fig. 4.5 The fullerene D[9]

cases can be computed as $WW(D[1]) = 62872$, $WW(D[2]) = 121392$, and $WW(D[3]) = 212167$. In general, if $n \geq 4$,

$$WW(D[n]) = \frac{256}{3}n^4 + \frac{3200}{3}n^3 + \frac{14912}{3}n^2 + \frac{131488}{3}n - 1022.$$

Our calculation shows that:

Result 4.3 The Wiener and hyper–Wiener indices of $D[n]$ can be computed as follows:

$$\hat{W}(D[1]) = 9728,\ \hat{W}(D[2]) = 16160,\ \hat{W}(D[3]) = 26400,\ \hat{WW}(D[2]) = 69080.$$

$$\hat{W}(D[n]) = \begin{cases} 64n^3 + 832n^2 + 3664n + 5232 & n \equiv 0,\ 2 \pmod 4 \\ 49n^3 + 1237n^2 + 547n + 14871 & n \equiv 1 \pmod 4 \\ 64n^3 + 832n^2 + 3888n + 5904 & n \equiv 3 \pmod 4 \end{cases} \qquad n \geq 4.$$

$$\hat{WW}(D[n]) = \frac{128}{3}n^4 + 544n^3 + \frac{11200}{3}n^2 + 14872n + 22248,\ \ n \text{ is even.}$$

4.3 Conclusions

In this chapter, the modified Wiener and hyper–Wiener indices of three fullerene series are considered into account. In each case, exact formulas for computing these invariants are presented. Our calculations show that in computing the modified hyper–Wiener index of $D[n]$, when n is odd, there is no regularity. We end this chapter by the following open questions:

Open Question 4.4 Find a general formula for the modified hyper–Wiener of $D[16n + 48]$ in odd case.

Open Question 4.5 Is it true that the modified Wiener and hyper–Wiener indices of (3,6)-fullerenes can be evaluated by polynomials of degrees 3 and 4, respectively?

Acknowledgment The first and second authors are partially supported by the University of Kashan under Grant No. 464092/20.

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