# Chapter 15
# Topological Study of (3,6)– and (4,6)–Fullerenes

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**Abstract** A (3,6)–fullerene is a cubic plane graph whose faces (including the outer face) have sizes 3 or 6. (4,6)–Fullerene graphs are defined analogously by interchanging triangles with quadrangles. (3,6)–Fullerenes have exactly four triangles and (4,6)–fullerenes have exactly 6 quadrangles. The (4,6)–fullerenes are also called boron fullerenes. In this chapter some infinite families of (3,6)–and (4,6)–fullerenes are presented. The modeling of these fullerenes by considering some topological indices is the main part of this chapter. Finally, some open questions are presented.

## 15.1 Introduction and Preliminaries

A *polytope* P is a tessellation of a given manifold M. If M has dimension $n$, then it is convenient to name P as $n$-polytope. A polygon is a 2-polytope and a polyhedron is a 3-polytope. Suppose P is a $d$-dimensional polytope. Then a *Schlegel diagram* of P is a projection of P into $R^{d-1}$. The Schlegel diagrams are an important tool for studying combinatorial and topological properties of polytopes (Goodey 1977).

A *simple graph* is a graph without directed and multiple edges and without loops. If $G$ is such a graph, then the vertex and edge sets of $G$ are represented by $V(G)$ and $E(G)$, respectively. Let $M$ be a molecule. The molecular graph of $M$ is a simple graph in which atoms of $M$ are its vertices and two atoms are adjacent if there is a bond between them.

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A ($k$,6)–fullerene is a cubic plane graph whose faces have sizes $k$ and 6. The only values of k for which a ($k$,6)–fullerene exists are 3, 4, and 5. A (5,6)–fullerene is simply called a fullerene. They are molecules in the form of polyhedral closed cages made up entirely of $n$ carbon atoms that are bonded in a nearly spherically symmetric configuration. The most important fullerene is buckyball. This is a molecule containing 60 carbon atoms, each of which is bonded to three adjacent carbon atoms in a sphere form that's about 1 nm in diameter (Kroto et al. 1985, 1993). The mathematical properties of ordinary fullerenes are studied in Fowler and Manolopoulos (1995) and Kostant (1995).

After successful history of fullerenes, it was natural to consider (3,6)– and (4,6)–fullerenes into account. The (3,6)–fullerenes have received recent attention from chemists due to their similarity to ordinary fullerenes (Yang and Zhang 2012; DeVos et al. 2009). The Euler's formula implies that an $n$–vertex (3,6)–fullerene has exactly four faces of size 3 and $n/2-2$ hexagons. A (3,6)–fullerene is called *ITR* if its triangles have no common edge. Recently some chemists have been attracted to the (4,6)–fullerenes or boron fullerenes (Wang et al. 2010). If six quadrangles of these new types of fullerenes don't have common edge, then we will briefly name them *ISR fullerenes.*

In this chapter, we will describe the mathematical properties of some families of (3,6)– and (4,6)–fullerenes which are built from a given (3,6)– or (4,6)–fullerenes by adding edges in such a way that the resulting graph is cubic. Here, we will show how to construct bigger cages with similar structural characteristics to those found in the smaller one.

Throughout this chapter all graphs considered are simple. Our notation is standard and taken mainly from the standard graph theory textbooks such as (Trinajstić 1992). The aim of this chapter is to investigate (3,6)– and (4,6)–fullerenes under five topological indices, *eccentric connectivity, Szeged, revised Szeged, vertex PI, and Wiener index*, which will be studied with details in Sects. 15.2 and 15.3.

## 15.2 Basic Definitions

Suppose $u$ and $v$ are vertices of a graph $G$. The *distance* $d(u, v)$ is defined as the length of a shortest path connecting them. The *eccentricity* $\varepsilon(u)$ is the largest distance between $u$ and any other vertex $x$ of $G$. The maximum eccentricity over all vertices of $G$ is called the **diameter** of $G$ and denoted by $D(G)$, and the minimum eccentricity among the vertices of $G$ is called *radius* of $G$ and denoted by $R(G)$.

The *Wiener index* is the first distance-based topological index that introduced by chemist Harold Wiener (Wiener 1947). The Wiener defined his index as the sum of all distances between any two carbon atoms in the molecule, in terms of carbon–carbon bonds. The Wiener index is principally defined for trees. It was in 1972 that Hosoya (1971, 1988) described its calculation using the distance matrix and proposed the name "Wiener index."

The *eccentric connectivity index* $\xi^c(G)$ of $G$ is defined as $\xi^c(G) = \Sigma_{u \in V(G)} \deg(u)\, \varepsilon(u)$, where for a given vertex $u$ of $V(G)$, its eccentricity, $\varepsilon(u)$, is the largest distance between $u$ and any other vertex $v$ of $G$ (Sharma et al. 1997). The maximum eccentricity over all vertices of $G$ is called the diameter of $G$ and denoted by $D(G)$. We encourage the reader to consult papers (Dureja and Madan 2007; Kumar et al. 2004; Sardana and Madan 2001; Gupta et al. 2002; Zhou and Du 2010) for more information on mathematical properties and chemical meaning of this topological index and (Ashrafi et al. 2011a, b; Saheli et al. 2010a, b; Ashrafi and Saheli 2010; Saheli and Ashrafi 2010a, b) for some applications in nanoscience.

The *Szeged index* is another distance-based topological index that was introduced by Ivan Gutman (1994). It is defined as $\mathrm{Sz}(G) = \sum_{\mathrm{e}=uv} n_u(e) n_v(e)$, where $n_u(e)$ is the number of vertices closer to $u$ than $v$ and $n_v(e)$ is defined analogously. We encourage the reader to consult paper for more information about Szeged index (Gutman and Dobrynin 1998).

The *vertex PI index* is a recently proposed topological index defined as $\mathrm{PI}_v(G) = \sum_{e=uv} [n_u(e) + n_v(e)]$ (Khalifeh et al. 2008). This topological index was introduced in an attempt to obtain exact expression for the edge version of this index under Cartesian product of graphs. It is worth mentioning that there is an edge version of this topological index proposed by Padmakar Khadikar (2000). In Ashrafi and Loghman (2006a, b, c) this edge version is calculated for some classes of nanostructures.

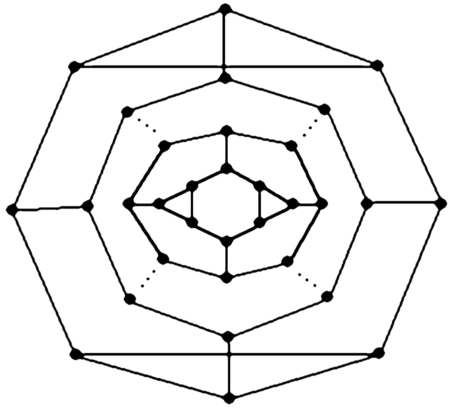
A graph $G$ is called *bipartite* if its vertex set can be partitioned into two subsets $A$ and $B$ such that each edge of $G$ connects a vertex in $A$ to a vertex in $B$. It is well known that a graph $G$ is bipartite if and only if it does not have odd cycle. It is possible to characterize bipartite graphs by vertex PI index. A graph $G$ is bipartite if and only if its vertex PI index is equal to $|V(G)| \times |E(G)|$. So, the vertex PI does not have good correlation with physicochemical properties of chemical compounds, when the molecular graph is bipartite.

The *revised Szeged index* $\mathrm{Sz}^*(G)$ of G is a molecular structure descriptor equal to the sum of products $[n_u(e) + n_0(e)/2] \times [n_v(e) + n_0(e)/2]$ over all edges $\mathrm{e} = uv$ of the molecular graph $G$, where $n_0(e)$ is the number of vertices equidistant from $u$ and $v$. This topological index was introduced by Milan Randić (2002). Nowadays the scientists prefer the name revised Szeged index for this distance-based topological index. It is easy to prove that a graph $G$ is bipartite if and only if the Szeged and revised Szeged indices of $G$ are the same. The interested readers can consult papers (Pisanski and Randić 2010; Pisanski and Žerovnik 2009; Xing and Zhou 2011; Aouchiche and Hansen 2010) for mathematical properties and chemical meaning of this new topological index.

## 15.3 (3,6)–Fullerenes

The (3,6)–fullerenes that sometimes called (3,6)-cages have received recent attention from chemists due to their similarity to ordinary fullerenes. With the best of our knowledge, there is no classification of these cubic graphs. So, it is natural to

**Fig. 15.1** G[8$n$], $n$ is even



construct more and more (3,6)–fullerenes to find such a classification. In this section seven infinite classes of (3,6)–fullerenes are constructed, and then the eccentric connectivity, Szeged, revised Szeged, vertex PI, and Wiener index of them are computed.

Suppose $F$ is the molecular graph of an arbitrary $n$–vertex (3,6)– or (4,6)–fullerenes. The adjacency matrix of $F$ is an $n \times n$ matrix $A = [a_{ij}]$ defined by $a_{ij} = 1$, if vertices $i$ and $j$ are connected by an edge and $a_{ij} = 0$ otherwise. It is easy to prove the adjacency matrix will determine the fullerene graph up to isomorphism. An $n \times n$ matrix $A = [a_{i,j}]$ is called *symmetric* if $a_{j,\,i} = a_{i\,,j}$ and *centrosymmetric* when its entries satisfy $a_{i,\,j} = a_{n-i+1}a_{n-j-1}$, for $1 \leq i,\, j \leq n$. Recently it is proved that the adjacency matrix of some classes of fullerenes is centrosymmetric. This caused to find exact formula for the Wiener index of these fullerenes in general (Graovac et al. 2011).

The distance matrix $D = [d_{ij}]$ of $F$ is another $n \times n$ matrix in which $d_{ij}$ is the length of a minimal path connecting vertices $i$ and $j$, $i \neq j$, and zero otherwise. Clearly, the summation of all entries in distance matrix of a fullerene $F$ is equal to $2W(F)$. To compute the Szeged, revised Szeged, vertex PI, eccentric connectivity, or Wiener indices of $F$, we first draw $F$ by HyperChem (2002) and then apply TopoCluj software (Diudea et al. 2002) of Diudea and his team to compute the adjacency and distance matrices of this fullerene graph. Finally, we provide a GAP program (Schönert et al. 1995) to calculate these topological indices for $F$.

Our first class of (3,6)–fullerenes is depicted in Figs. 15.1, 15.2, and 15.3. These fullerenes have exactly $8n$ vertices and their Schlegel diagrams show that they are ITR.

Our second class of (3,6)–fullerenes is again ITR with exactly $8n + 4$ vertices depicted in Figs. 15.4 and 15.5.

The third class of (3,6)–fullerenes that is studied in this section is not ITR. The Schlegel diagram of an arbitrary member of this class is depicted in Fig. 15.6. The 3D perception of the first member $I[16]$ of this class, Fig. 15.7, and the algorithm for construction of other members of the class from the first one shows that the elements of this class are different from the first two classes of (3,6)–fullerenes.

**Fig. 15.2** G[8*n*], *n* is odd

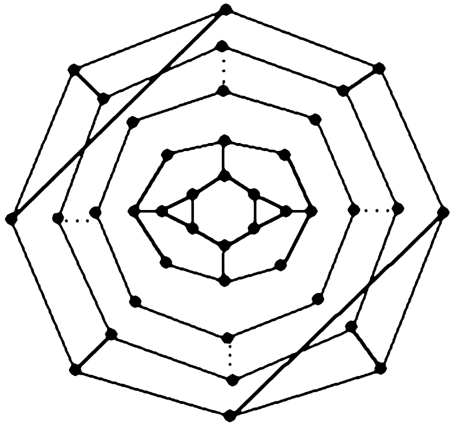


**Fig. 15.3** The 3D perception of $G[16]$

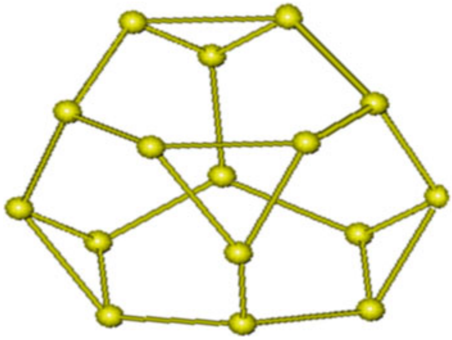
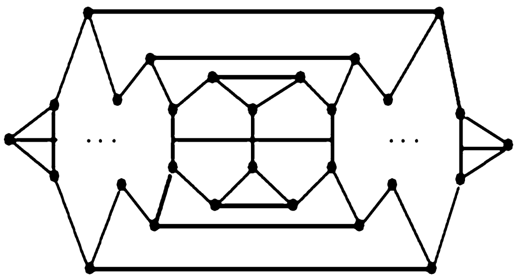


**Fig. 15.4** The Schlegel diagram of $H[8n+4]$



One of the pioneers of fullerene chemistry, P.W. Fowler, believed that a fullerene has to be 3-connected and so $I[16]$ is not a fullerene. Notice that, we don't consider 3-connectivity in our definition for a fullerene.

Our fourth class of (3,6)–fullerenes is not ITR. The Schlegel diagram of an arbitrary element of this class, together with the 3D perception of the first, $J[24]$, is depicted in Figs. 15.8 and 15.9, respectively. It is not so difficult to prove that the members of this class are essentially different from the first three presented classes of (3,6)–fullerenes.

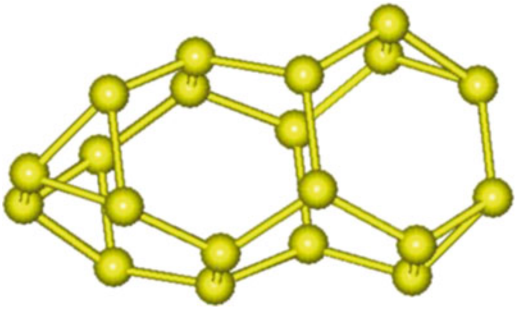


**Fig. 15.5** The 3D perception of $H[20]$

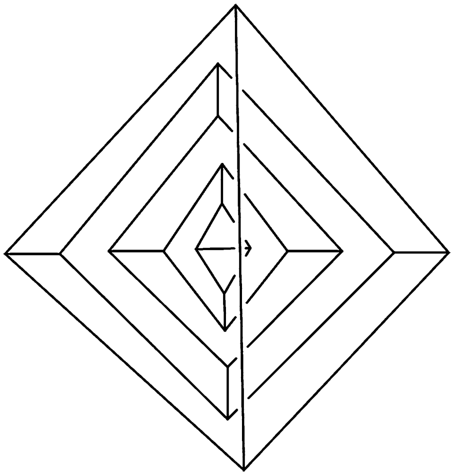


**Fig. 15.6** The Schlegel diagram of $I[4n]$, $n \geq 2$

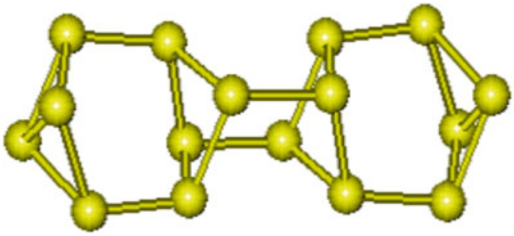


**Fig. 15.7** The 3D perception of $I[16]$

The molecular graph of our fifth class of (3,6)–fullerenes is depicted in Fig. 15.10. These (3,6)–fullerenes have exactly $16n - 32$ vertices and all of them are ITR. In Fig. 15.11, the 3D perception of the first member of this class is depicted.

The sixth class of (3,6)–fullerenes is again ITR which contains $16n + 48$ vertices, $n \geq 1$. The Schlegel diagram and 3D perception of one member of this class are depicted in Figs. 15.12 and 15.13, respectively.

The seventh and our final class of (3,6)–fullerenes has exactly $12n + 4$ vertices, and the molecular graph is ITR; see Figs. 15.14 and 15.15.

Since (3,6)–fullerenes are cubic, it is easy to see that the molecular graphs of $G[8n]$, $H[8n+4]$, $I[4n]$, $J[24n]$, $K[16n-32]$, $L[16n+48]$, and $M[12n+4]$ have exactly $12n$, $12n+6$, $6n$, $36n$, $24n-48$, $24n+72$, and $18n+6$ edges, respectively.

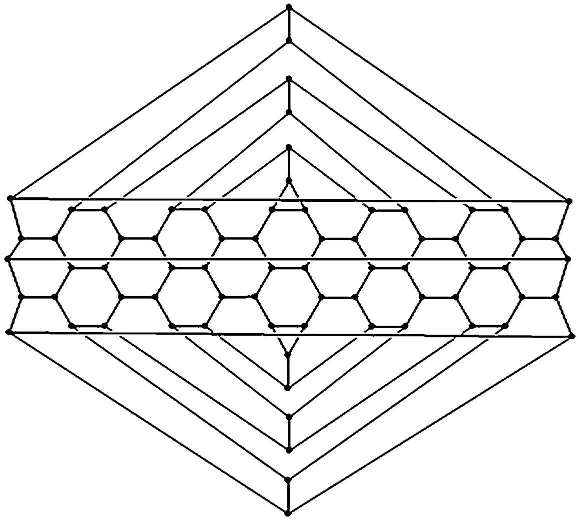


**Fig. 15.8** The Schlegel diagram of $J[24n]$

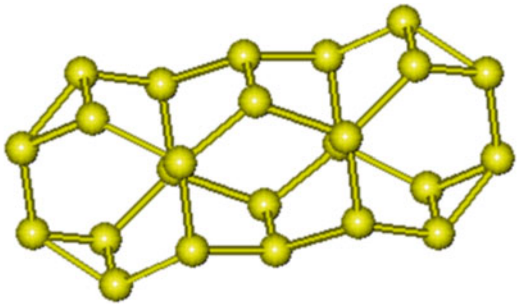


**Fig. 15.9** The 3D perception of $J[24]$

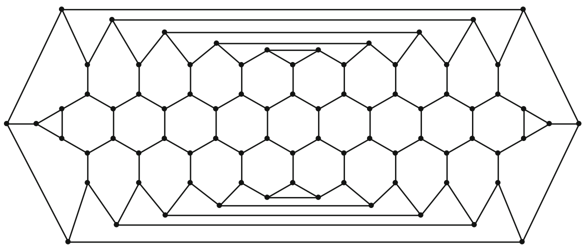


**Fig. 15.10** The Schlegel diagram of $K[16n-32]$, $n \geq 5$

### *15.3.1 Wiener and Eccentric Connectivity Indices of (3,6)–Fullerenes*

In this section the Wiener and eccentric connectivity indices of $G[8n]$, $H[8n+4]$, $I[4n]$, $J[24n]$, $K[16n-32]$, $L[16n+48]$, and $M[12n+4]$ are computed. By an easy calculation, one can see that $W(G[16]) = 294$, $\xi^c(G[16]) = 192$, $\xi^c(G[24]) = 348$,

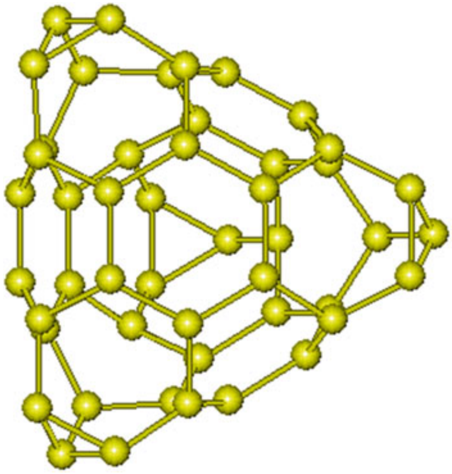


**Fig. 15.11** The 3D perception of $K[48]$

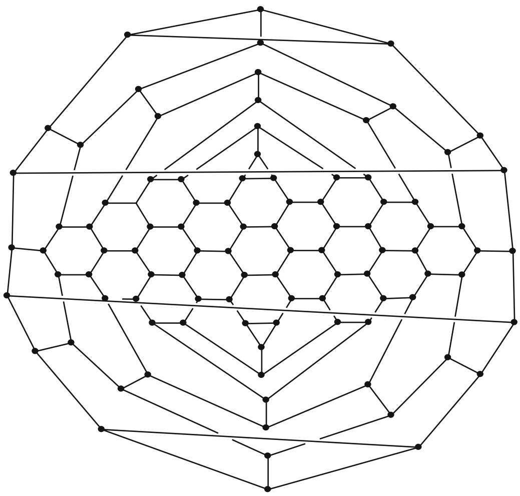


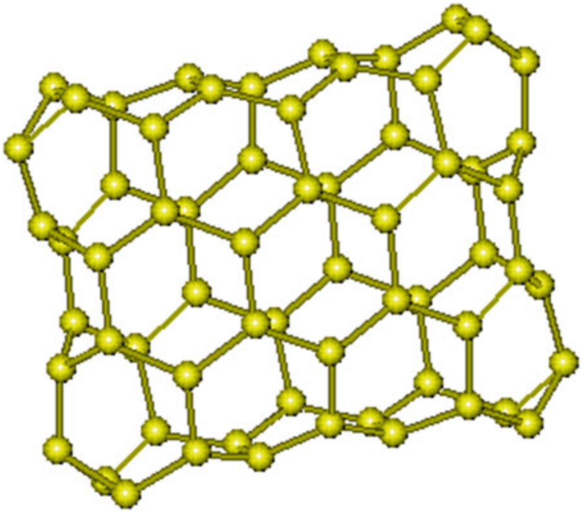
**Fig. 15.12** The Schlegel diagram of $L[16n+48]$, $n \geq 1$

$\xi^c(G[32]) = 600$, $\xi^c(G[40]) = 888$, and $\xi^c(G[48]) = 1{,}248$. On the other hand, for $n \geq 7$, we can partition the vertex set of $G[8n]$ into n parts, each of which contains eight vertices in such a way that the eccentricity of each vertex in the first part is $n$, the eccentricity of each vertex in the second part is $n+1, \ldots,$ and the eccentricity of each vertex in the nth part is equal to $2n-1$. In Fig. 15.16, the black vertices have the maximum eccentricity and red vertices have second maximum eccentricity in $G[8n]$, $n \geq 7$.

Our calculations show the following:

**Result 15.1** For $n \geq 3, W(G[8n]) = (64/3)n^3 + (464/3)n - 206,$ and for $n \geq 7, \xi^c(G[8n]) = 36n^2 - 12n.$

**Fig. 15.13** The 3D perception of $L[64]$



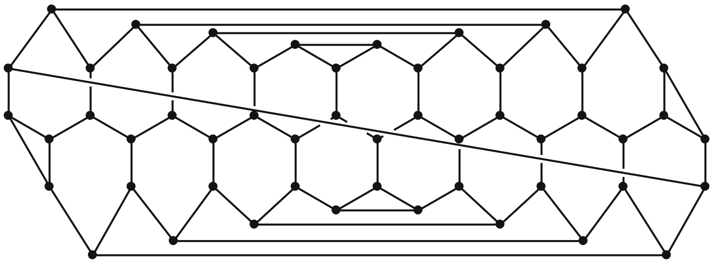
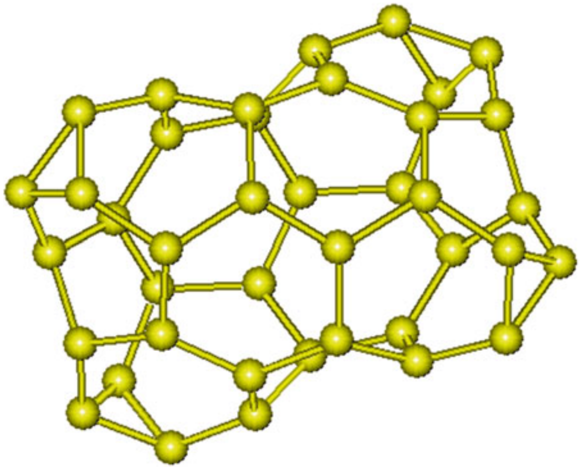


**Fig. 15.14** The Schlegel diagram of $M[12n+4]$, $n \geq 1$

**Fig. 15.15** The 3D perception of $M[40]$



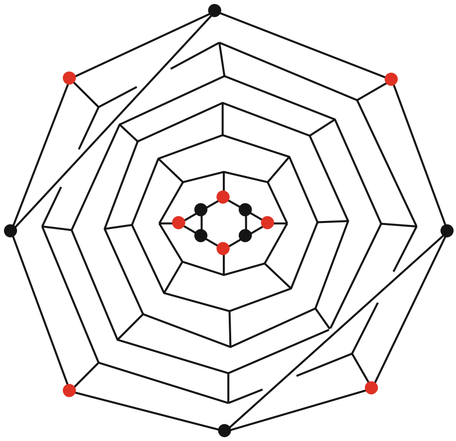


**Fig. 15.16** The maximum (*black*) and second maximum (*red*) eccentricities in $G[n]$

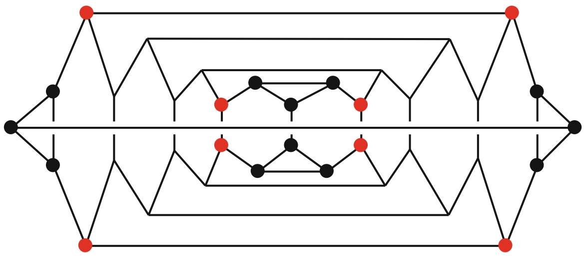


**Fig. 15.17** The maximum (*black*) and second maximum (*red*) eccentricities in $H[8n+4]$

We now consider the class $H[8n+4]$ of (3,6)–fullerenes. We can partition the set of vertices of $H[8n+4]$ into $n-1$ parts in which one of them has size 12 and any other parts having size eight. The eccentricity of the vertices of the first part is $2n+1$, the second part is the set of vertices having eccentricity $n+2$, the third part is the set of all vertices having eccentricity $n+3, \ldots,$ and the $n$th part is the set of vertices having eccentricity $2n$. In Fig. 15.17, the black vertices have the maximum eccentricity and red vertices have the second maximum of eccentricity between vertices of $H[8n+4]$. From these calculations, we have the following result:

**Result 15.2** For $n \geq 1$, $W(H[8n+4]) = (64/3)n^3 + 64n^2 + (152/3)n + 2$ and $\xi^c(H[8n+4]) = 36n^2 + 60n + 12$.

Consider the (3,6)–fullerene $I[4n]$. An easy calculation shows that $\xi^c(I[8]) = 72$. On the other hand, we can partition $V(I[4n])$ into $n$ parts, each of which having size four in such a way that the vertices of the first part have eccentricity $n$, the vertices of the second part have eccentricity $n+1, \ldots,$ and the vertices of the nth part have eccentricity $2n-1$. In Fig. 15.18, the black vertices have the maximum eccentricity and red vertices have the second maximum of eccentricity between vertices of $I[4n]$.

From the calculations given above, one can prove the following:

**Result 15.3** For $n \geq 2$, $W(I[4n]) = (16/3)n^3 + (20/3)n - 6$, and for $n \geq 3$, $\xi^c(I[4n]) = 18n^2 - 6n$.

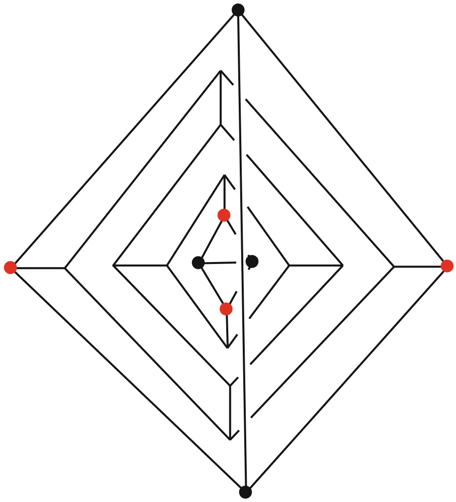


**Fig. 15.18** The maximum (*black*) and second maximum (*red*) eccentricities in $I[4n]$

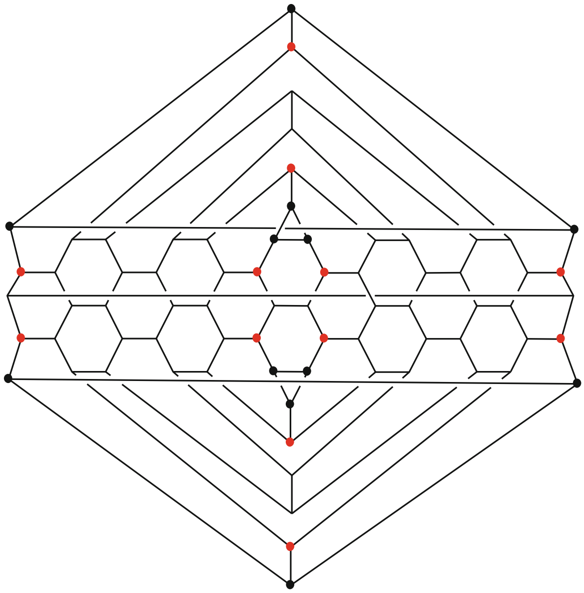


**Fig. 15.19** The maximum (*black*) and second maximum (*red*) eccentricities in $J[24n]$

By an easy calculation, one can see that $W(J[24]) = 864$, $W(J[48]) = 4{,}824$, $\xi^c(J[24]) = 396$, $\xi^c(J[48]) = 1{,}140$, $\xi^c(J[72]) = 2{,}064$, $\xi^c(J[96]) = 3{,}420$, and $\xi^c(J[120]) = 5{,}256$. On the other hand, for $n \geq 6$, we can partition the vertex set of $J[24n]$ into $2n$ parts, each of which contains four vertices in such a way that the eccentricity of each vertex in the first part is $2n$, the eccentricity of each vertex in the second part is $2n+1, \ldots,$ and the eccentricity of each vertex in the $2n$th part is equal to $4n-1$. In Fig. 15.19, the black vertices have the maximum eccentricity and red vertices have second maximum eccentricity in $J[24n]$, $n \geq 6$.

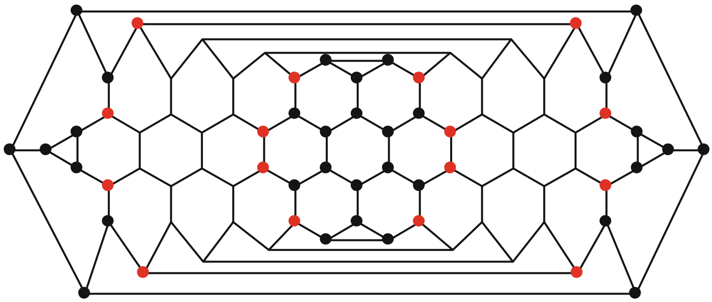


**Fig. 15.20** The maximum (*black*) and second maximum (*red*) eccentricities in $K[16n-32]$

The following result is a direct consequence of our calculations:

**Result 15.4** For $n \geq 3$, $W(J[24n]) = 384n^3 + 1,656n - 1,594$, and for $n \geq 6$, $\xi^c(J[24n]) = 216n^2 - 36n$.

We now consider the (3,6)–fullerene $K[16n-32]$. An easy calculation shows that $\xi^c(K[48]) = 1{,}008$ and $\xi^c(K[64]) = 1{,}632$. On the other hand, we can partition $V(K[16n-32])$ into $n-3$ parts such that one of them have size 32 and any other parts have size 16. Also, the vertices of the part of size 32 have eccentricity $2n-3$, and vertices of other parts have eccentricities $n+1, n+2, \ldots, 2n-4$, respectively. In Fig. 15.20, the black vertices have the maximum eccentricity and red vertices have the second maximum of eccentricity between vertices of $K[16n-32]$.

Our given calculations lead us to the following result:

**Result 15.5** For $n \geq 5$, $W(K[16n-32]) = (256/3)n^3 - 256n^2 + (608/3)n - 492$, and for $n \geq 7$, $\xi^c(K[16n-32]) = 72n^2 - 168n$.

By an easy calculation by our GAP program, we can see that $W(L[64]) = 9{,}968$, $W(L[80]) = 17{,}432$, $W(L[96]) = 27{,}724$, $\xi^c(L[64]) = 1{,}692$, $\xi^c(L[80]) = 2{,}340$, $\xi^c(L[96]) = 3{,}168$, $\xi^c(L[112]) = 3{,}972$, $\xi^c(L[128]) = 4{,}968$, $\xi^c(L[144]) = 6{,}024$, $\xi^c(16n\text{–}32L[160]) = 7{,}260$, $\xi^c(L[176]) = 8{,}652$, $\xi^c(L[192]) = 10{,}224$, $\xi^c(L[208]) = 11{,}952$, $\xi^c(L[224]) = 13{,}824$, $\xi^c(L[240]) = 15{,}840$, $\xi^c(L[256]) = 18{,}048$, and $\xi^c(L[272]) = 22{,}896$.

On the other hand, for $n \geq 15$, we can partition the vertex set of $L[16n+48]$ into $n+3$ parts, each of which contains 16 vertices in such a way that the eccentricity of each vertex in the first part is $n+3$, the eccentricity of each vertex in the second part is $n+4, \ldots$, and the eccentricity of each vertex in the $(n+3)$th part is equal to $2n+5$. In Fig. 15.21, the black vertices have the maximum eccentricity and red vertices have second maximum eccentricity in $L[16n+48]$, $n \geq 15$. These calculations suggest the following result:

**Result 15.6** For $n \geq 4$, $W(L[16n+48]) = (256/3)n^3 + 768n^2 + (14{,}912/3)n + 5{,}340$, and for $n \geq 15$, $\xi^c(L[16n+48]) = 72n^2 + 408n + 576$.

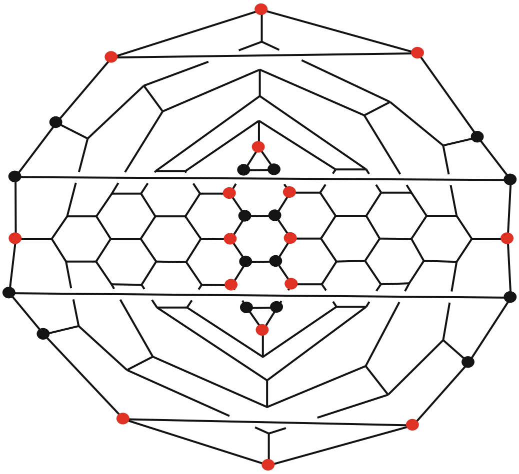


**Fig. 15.21** The maximum (*black*) and second maximum (*red*) eccentricities in $L[16n+48]$

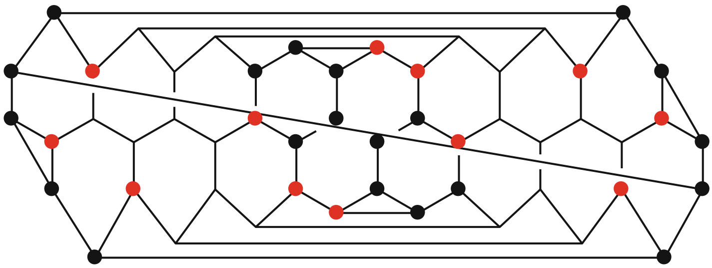


**Fig. 15.22** The maximum (*black*) and second maximum (*red*) eccentricities in $M[12n+4]$

In the end of this section, the Wiener and eccentric connectivity indices of (3,6)–fullerene $M[12n+4]$ is computed. Using our GAP program, we can see that $W(M[16]) = 296$, $\xi^c(M[16]) = 204$, $\xi^c(M[28]) = 420$, $\xi^c(M[40]) = 804$, and $\xi^c(M[52]) = 1{,}248$. On the other hand, we can partition $V(M[12n+4])$ into n parts such that one of them has size eight, another of size 20, and any other parts have size 12 in such a way that the elements of these classes have the same eccentricity. The eccentricities of a representative of the first two classes are $n+2$ and $2n+1$, respectively. On the other hand, the representatives of other parts have eccentricities $n+3$, $n+4, \ldots, 2n$, respectively. In Fig. 15.22, the black vertices have the maximum eccentricity and red vertices have the second maximum of eccentricity between vertices of $M[12n+4]$.

From these calculations, we have the following:

**Result 15.7** For $n \geq 2$, $W(M[12n+4]) = 48n^3 + 144n^2 + 192n - 126$, and for $n \geq 5, \xi^c(M[12n+4]) = 54n^2 + 90n$.

**Table 15.1** The values of $n_u(e)$, $n_v(e)$, and $n_0(e)$ for a given edge e = $uv$ in $G[8n]$

| Edges | The values of $n_u(e)$, $n_v(e)$, and $n_0(e)$ | No |
|---|---|---|
| 1 | 6, 6, $8n-12$ | 4 |
| 2 | $8n-9$, 8, 1 | 4 |
| 3 | $8n-8$, 8, 0 | 4 |
| 4 | $8n-16$, 10, 6 | 8 |
| 5 | $8n-12$, 10, 2 | 8 |
| 6 | $8n-16$, 16, 0 | 8 |
| 7 | $8n-17$, 15, 2 | 8 |
| 8 | $8n-15$, 14, 1 | 8 |
| 9 | $8n-22$, 21, 1 | 16 |
| 10 | $8n-24-4i$, $24+4i$, 0; $n=6+i$, $i=0, 2, 4, \ldots$ | 4 |
| | $8n-24-4i$, $24+4i$, 0; $n=6+i$, $i=1, 3, 5, \ldots$ | 8 |
| 11 | $8n-24-4i$, $24+4i$, 0; $n\geq 7+i$, $i=0, 2, 4, \ldots$ | 8 |
| | $8n-24-4i$, $24+4$i, 0; $n\geq 7+i$, $i=1, 3, 5, \ldots$ | 16 |

## 15.3.2 Vertex PI, Szeged, and Revised Szeged Indices of (3,6)–Fullerenes

Consider the (3,6)–fullerene $G[8n]$ depicted in Figs. 15.1 and 15.2. Apply our method described in the third paragraph of this section for some small numbers of $n$. Using our program we obtain four exceptional cases that $n=2$, 3, 4, and 5. Then an easy calculation shows that PI($G$[16]) = 300, Sz($G$[16]) = 972, Sz($G$[24]) = 3,418, Sz($G$[32]) = 8,944, Sz($G$[40]) = 17,840, Sz*($G$[16]) = 1,533, Sz*($G$[24]) = 5,010, Sz*($G$[32]) = 11,445, Sz*($G$[40]) = 21,357.

From calculations given in Table 15.1 and Figs. 15.23 and 15.24, we have the following result:

**Result 15.8** For $n \geq 6$, $\mathrm{Sz}^*(G[8n]) = 128n^3 + 64n^2 + 1648n - 4,519$, $\mathrm{Sz}(G[8n]) = 128n^3 + 1,216n - 4,280$, and for $n \geq 3$, $\mathrm{PI}_v(G[8n]) = 96n^2 - 32n - 60$.

We now consider our second class $H[8n+4]$ of (3,6)–fullerenes. An easy calculation by our program shows that Sz($H$[12]) = 34 and Sz*($H$[12]) = 648.

By our calculations given in Table 15.2 and Figs. 15.25 and 15.26, we have the following result:

**Result 15.9** For $n \geq 2$, $Sz^*(H[8n+4]) = (448/3)n^3 + 320n^2 + (656/3)n - 42$, $Sz(H[8n+4]) = (448/3)n^3 + 192n^2 + (188/3)n - 66$, and for $n \geq 1$, $PI_v(H[8n+4]) = 96n^2 + 56n + 4$.

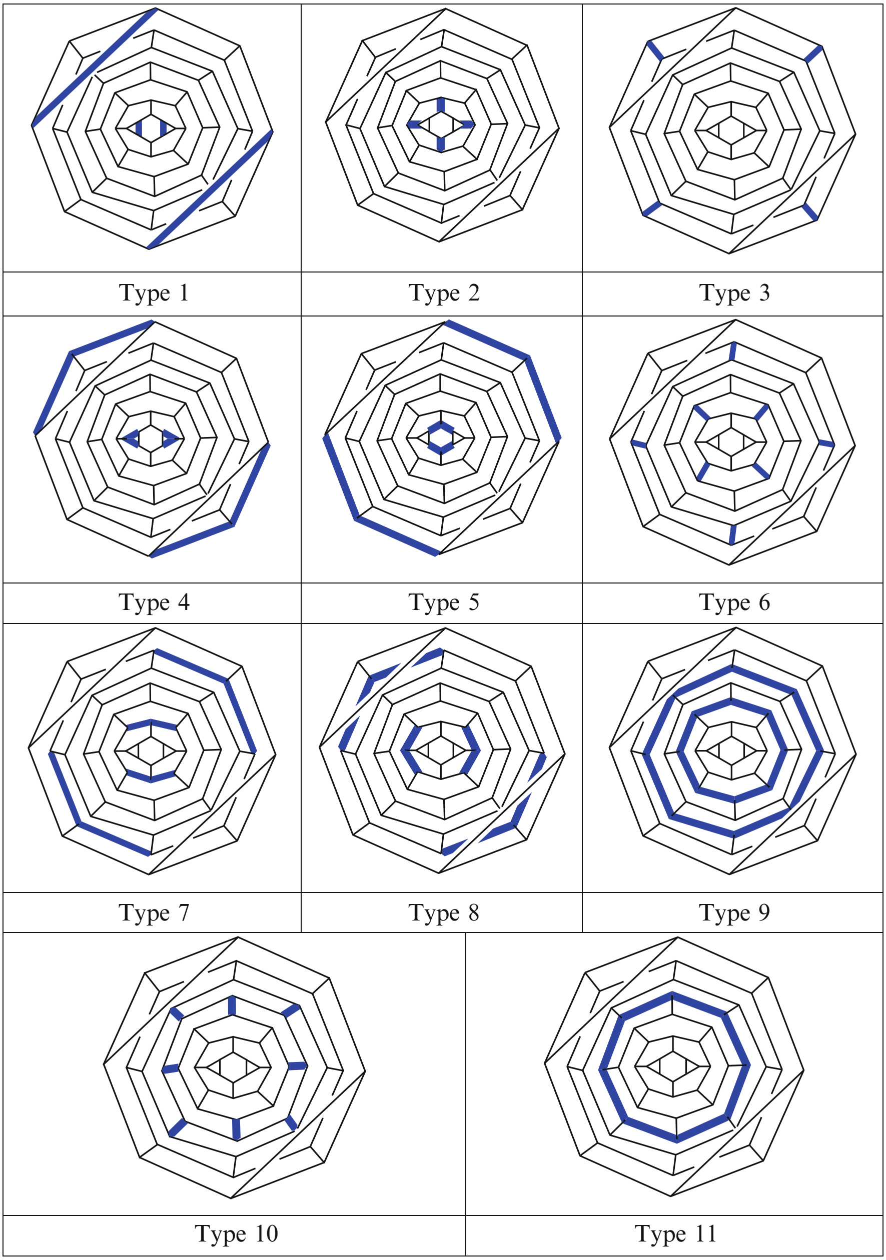



**Fig. 15.23** The 11 types of edges in $G[8n]$

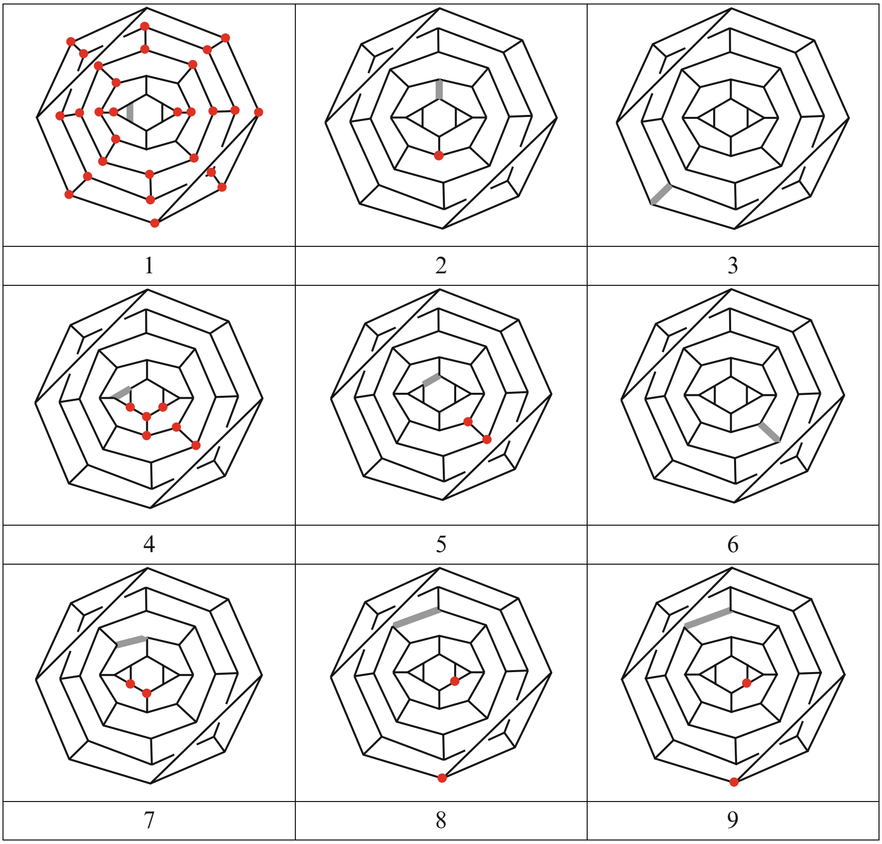



**Fig. 15.24** The vertices equidistant from $u$ to $v$

**Table 15.2** The values of $n_u(e)$, $n_v(e)$, and $n_0(e)$ for a given edge $e = \text{uv}$ in $H[8n+4]$

| Edges | The values of $n_u$(e), $n_v(e)$, and $n_0(e)$ | No |
|---|---|---|
| 1 | $4n$, 4, $4n$ | 8 |
| 2 | $4n$, $4n$, 4 | 4 |
| 3 | $8n-3$, 6, 1 | 8 |
| 4 | $4n+2$, $4n+2$, 0 | 4 |
| 5 | $4n+1$, $4n+1$, 2 | 4n − 2 |
| 6 | $8n-6-4i$, $10+4i$, 0; $n \geq 3+i$, $i = 0, 1, 2, \ldots$ | 8 |

## 15.4 (4,6)–Fullerenes

In this section two infinite families $A[8n]$ and $B[12n+6]$ of (4,6)–fullerenes are constructed, Figs. 15.27, 15.28, 15.29, and 15.30. Since $A[8n]$ and $B[12n+6]$ are bipartite, $\mathrm{Sz}(A[8n]) = \mathrm{Sz}^*(A[8n])$, $\mathrm{Sz}(B[12n+6]) = \mathrm{Sz}^*(B[12n+6])$, $\mathrm{PI}_v(A[8n]) =$

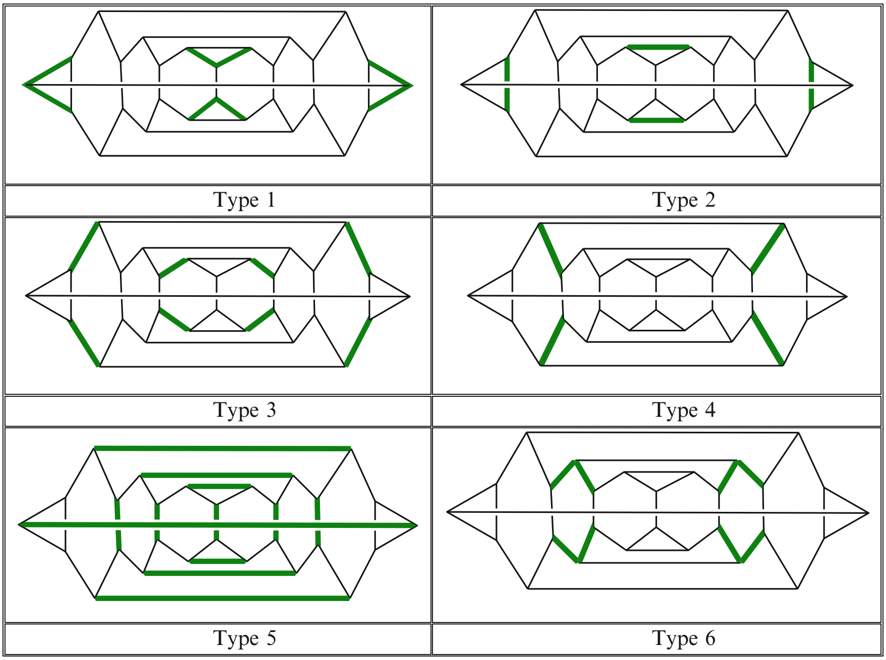



**Fig. 15.25** The six types of edges in $H[8n+4]$

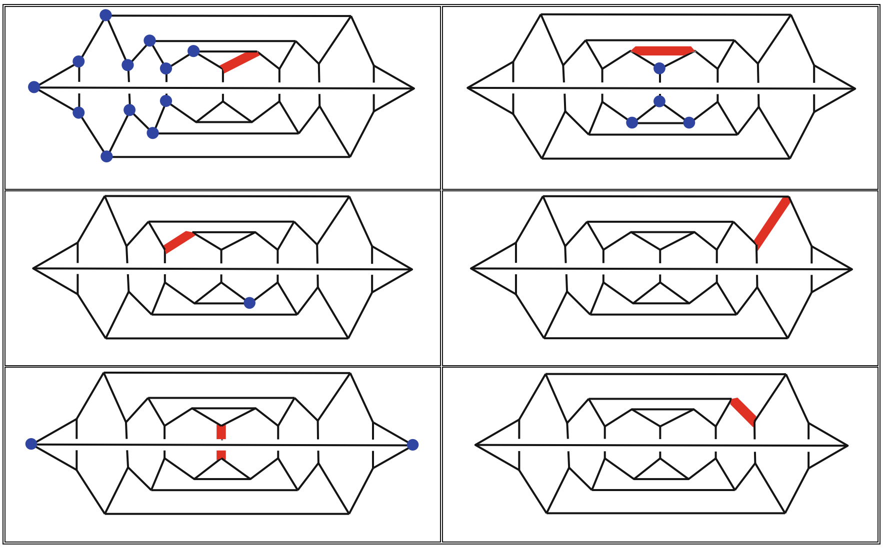


**Fig. 15.26** The vertices equidistant from $u$ to $v$

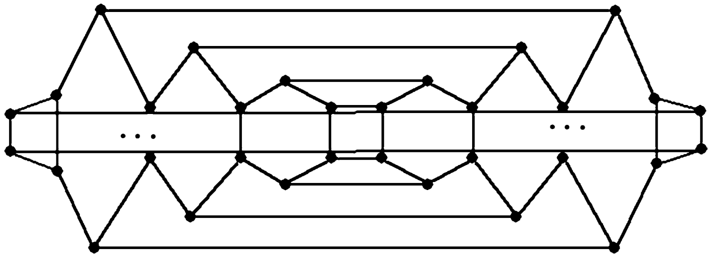


**Fig. 15.27** The Schlegel diagram of the (4,6)–fullerene $A[8n]$, $n \geq 2$

**Fig. 15.28** The 3D perception of $A[24]$

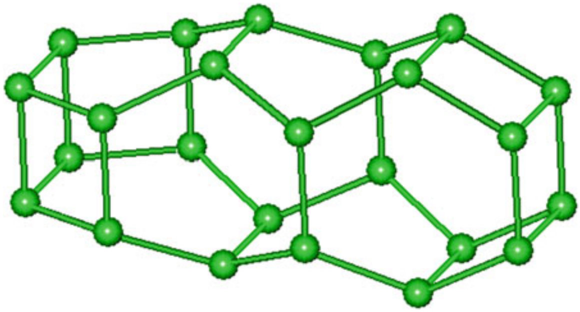
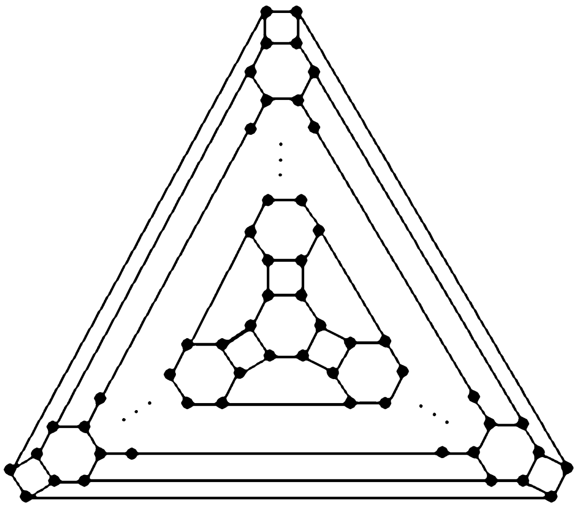


**Fig. 15.29** The Schlegel diagram of the (4,6)–fullerene $B[12n+6]$, $n \geq 2$



$8n \times 12n = 96n^2$, and $\mathrm{PI}_v(B[12n+6]) = (12n+6)\times(18n+9) = 216n^2 + 216n + 54$. So, it is enough to compute the Wiener, eccentric connectivity, and Szeged indices of these families of fullerenes. We begin by computing these quantities for (4,6)–fullerene A[$8n$].

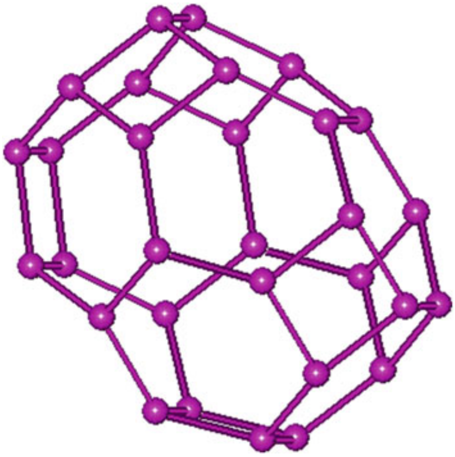


**Fig. 15.30** The 3D perception of $B[30]$

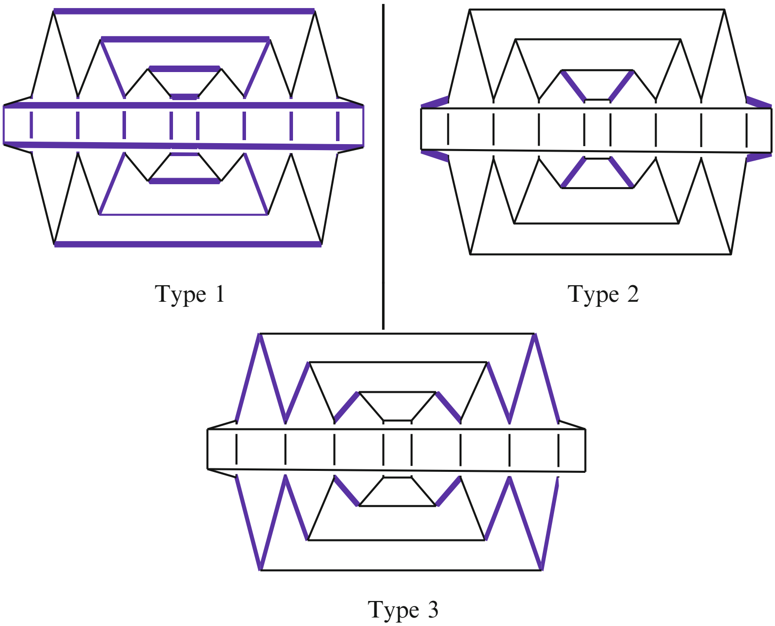



**Fig. 15.31** The three types of edges in $A[8n]$

From Fig. 15.31, one can see that there are three types of edges in $A[8n]$. These together with quantities $n_u$ and $n_v$ are recorded in Table 15.3.

We can partition $V(A[8n])$ into n parts such that each part has size eight in such a way that the elements of each part have the same eccentricity. Also, a representative of distinct parts has eccentricities $n+2$, $n+3, \ldots, 2n+1$, respectively. In Fig. 15.32, the black vertices have the maximum eccentricity and red vertices have the second maximum of eccentricity between vertices of $A[8n]$.

**Table 15.3** The values of $n_u(e)$ and $n_v(e)$ for a given edge $e = uv$ in $A[8n]$

| Edges | The values of $n_u(e)$ and $n_v(e)$ in $A[8n]$ | No |
|---|---|---|
| 1 | $4n, 4n$ | $4n + 8$ |
| 2 | $8n - 6, 6$ | 8 |
| 3 | $8n - 4i + 4, 4i - 4, n \geq i, i = 3, 4, \ldots$ | 8 |

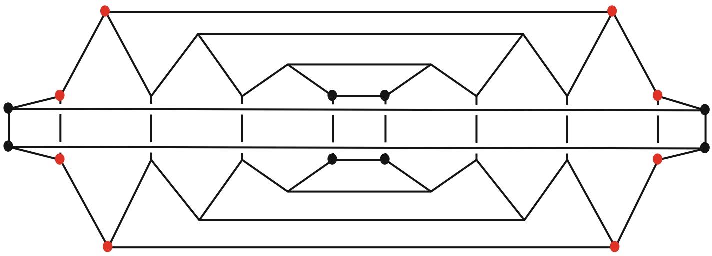


**Fig. 15.32** The maximum (*black*) and second maximum (*red*) eccentricities in $A[8n]$

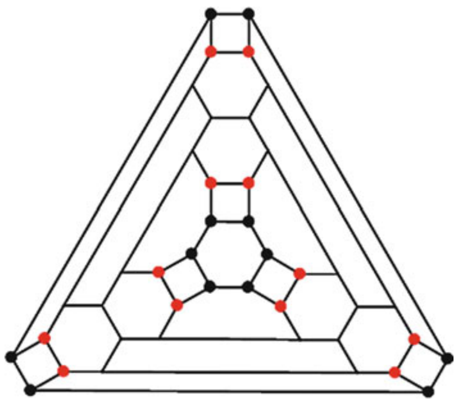


**Fig. 15.33** The maximum (*black*) and second maximum (*red*) eccentricities in $B[12n + 6]$

By above calculations and our calculations given in Table 15.3, we have the following result:

**Result 15.10** For $n \geq 2$, $W(A[8n]) = (64/3)n^3 + 32n^2 + (32/3)n - 16$, $\mathrm{Sz}(A[8n]) = \mathrm{Sz}^*(A[8n]) = (448/3)n^3 + 64n^2 + (320/3)n - 160$, and $\xi^c(A[8n]) = 36n^2 + 36n$.

In the end of this section, we consider the (4,6)–fullerene graph $B[12n + 6]$ into account. It is clear that $\xi^c(B[30]) = 576$. We partition again $V(B[12n + 6])$, $n \geq 3$, into $n + 1$ parts such that one of these parts has size six and any other parts have size 12. The vertices of each part have the same eccentricity, and a representative of the part of size six has eccentricity $n + 3$. The eccentricities of a representative of other parts are $n + 4$, $n + 5, \ldots, 2n + 3$, respectively. In Fig. 15.32, the black vertices have the maximum eccentricity and red vertices have the second maximum of eccentricity between vertices of $B[12n + 6]$ (Figs. 15.33 and 15.34).

From our discussion and calculations given in Table 15.4, one can prove the following result:

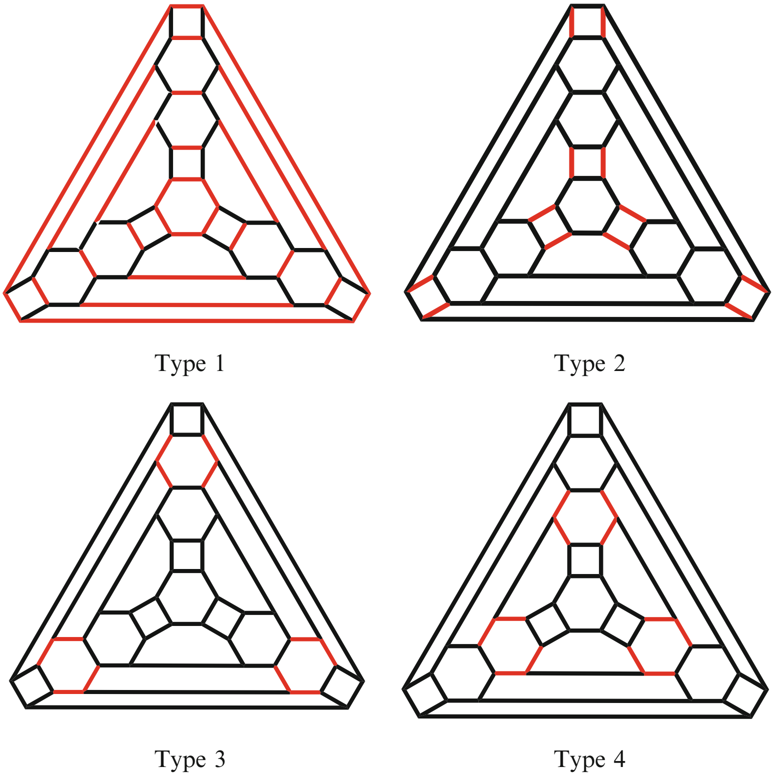



**Fig. 15.34** The four types of edges in $B[12n+6]$

**Table 15.4** The values of $n_u(e)$ and $n_v(e)$ for a given edge $e = uv$ in $B[12n+6]$

| Edges | The values of $nu(e)$ and $nv(e)$ in $B[12n+6]$ | No |
|---|---|---|
| 1 | $6n+3$, $6n+3$ | $6n+9$ |
| 2 | $12n-6$, 12 | 12 |
| 3 | $12n-8$, 14 | 12 |
| 4 | $12n-6i+6$, $6i$, $n \geq i$, $i = 3, 4, \ldots$ | 12 |

**Result 15.11** For $n \geq 2$, $W(B[12n+6]) = 48n^3 + 180n^2 + 228n - 45$, $\mathrm{Sz}(B[12n+6]) = \mathrm{Sz}^*(B[12n+6]) = 504n^3 + 972n^2 + 1{,}674n - 1{,}263$, and for $n \geq 3$, $\xi^c(B[12n+6]) = 54n^2 + 144n + 54$.

## 15.5 Concluding Remarks

Since there are no classification of (3,6)– and (4,6)–fullerenes, it is natural to construct more and more of such molecular graphs. In this chapter, some constructions of these fullerene graphs are presented, and our calculations suggest the following conjectures:

*Conjecture* 1: The Wiener, Szeged, and revised Szeged indices of a ($k$,6)–fullerene with exactly n carbon atoms are a polynomial of degree 3.

*Conjecture* 2: The vertex PI and eccentric connectivity indices of a ($k$,6)–fullerene with exactly n carbon atoms are a polynomial of degree 2.

## Appendix 1 Some GAP Programs

Here, two GAP programs are presented which is useful for calculations presented in this chapter. The first program is for computing Wiener index and the second is for eccentric connectivity index. Notice that these GAP programs have to combine with calculations by TopoCluj described in the Sect. 15.1.

**A Gap Program for Computing Wiener Index of Fullerenes**

```
f:=function(M)
local l,i,j,id,k,t,max,a,s,w,d,g;
l:=Length(M);id:=0;t:=[];s:=[];w:=0;d:=[];g:=0;
        for k in [1..l]do
          id:=1;
               for i in [1..l-1]do
                      for j in [i+1..l] do
                        if M[k][j]>M[k][id] then
                          id:=j;
                        fi;
                      od;
               od;
               Add(t,M[k][id]);
        od;
max:=t[1];
        for a in [2..Length(t)] do
          if t[a] > max then
            max:=t[a];
          fi;
        od;
        for a in [1..max] do
              for i in [2..l] do
                     for j in [1..i-1] do
                       if M[i][j]=a then
                       g:=g+1;
                       fi;
                     od;
              od;
        Add(d,g);
        g:=0;
```

```
          od;
for i in [2..l] do
          for j in [1..i-1] do
             w:=w+M[i][j];
          od;
od;
Print("Distans=",d,"\n");
Print("Wiener index=",w,"\n");
Print("***************","\n");
end;
```

**A Gap Program for Computing Eccentric Connectivity Index of Fullerenes**

```
f:=function(M)
local l,i,j,k,t,id,ii,jj,s,a,iii,w,ww;
t:=[];l:=Length(M);id:=0;s:=0;a:=[];w:=0;ww:=0;
for k in [1..l]do
 id:=1;
 for i in [1..l-1]do
    for j in [i+1..l] do
      if M[k][j]>M[k][id] then
       id:=j;
      fi;
    od;
 od;
Add(t,M[k][id]);
od; ####ecentricity vertices of G
for ii in [1..l]do
   for jj in [1..l]do
     if M[ii][jj]=1 then
        s:=s+1;
     fi;
   od;
   Add(a,s);
   s:=0;
od;####degree vertices of G
for iii in [1..Length(t)] do
   w:=t[iii]*a[iii];
   ww:=ww+w;
   w:=0;
od;######ecentricity connectivity index of G
Print("ecentricity=",t,"\n");
   Print("degree=",a,"\n");
       Print("ecentricity connectivity index=",ww,"\n");
           Print("********************","\n");
end;
```

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