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On Eccentric Adjacency index of Several Infinite Classes of Fullerenes

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Abstract

In theoretical chemistry, molecular structure descriptors are used for modeling physio-chemical, pharmacologic, toxicological, biological and other properties of chemical compound. The eccentric adjacency index of a graph G is defined as

$$\xi^{ad}(G) = \sum_{u \in V(G)} S(u)\varepsilon(u)^{-1},$$

where $S(u)$ denotes sum of degrees of vertices adjacent to the vertex u and $\varepsilon(u)$ is defined as the maximum length of any minimal path connecting u to any other vertex of G. Fullerenes are molecules in the form of cage-like polyhedra, consisting solely of carbon atoms bonded in a nearly spherical configuration. In this paper we calculate the eccentric adjacency index for several infinite classes of fullerenes.

Keywords: Graph; eccentricity; eccentric adjacency index; fullerenes.

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1 Introduction

Let G be any simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$. For two vertices u and v in $V(G)$ their distance $d(u,v)$ is defined as the length of a shortest path connecting u and v in G.

The degree $d(u)$ of the vertex u in G is defined as the number of neighbors of u in G, i.e., $d(u) = |\{v \in V(G) \mid d(u,v) = 1\}|$. The eccentricity $\varepsilon(u)$ of the vertex u of G is the The eccentricity sequence $ec(G)$ of G, is the multi-set of eccentricities of the vertices of G, i.e., $ec(G) = \{\varepsilon(u) \mid u \in V(G)\}$.

Mathematical chemistry is a branch of theoretical chemistry in which with the help of mathematical methods the molecular structure are investigated. Molecular graphs or chemical graphs are models of molecules in which atoms are represented by vertices and chemical bonds by edges. The chemical graph theory is a branch of mathematical chemistry in which the physico-chemical properties of molecules are studied by using their molecular graphs.

In this paper, fullerenes are molecules in the form of cage-like polyhedra, consisting solely of carbon atoms, where each carbon atom is chemically bonded to three other carbon atoms in a nearly spherical configuration. The molecular graph of a fullerene (fullerene graph) can be viewed as a finite connected trivalent plane graph, all of its faces are pentagons and hexagons. Consider a fullerene graph with exactly p, h, n and m pentagons, hexagons, vertices and edges between them, respectively. Since each vertex lies in exactly 3 faces and each edge lies in 2 faces, the number of vertices is $n = (5p + 6h)/3$, the number of edges is $m = (5p + 6h)/2 = 3/2n$ and the number of faces is $f = p + h$. Recall that Euler's formula states that $n - m + f = 2$. It follows that $(5p + 6h)/3 - (5p + 6h)/2 + p + h = 2$, and therefore $p = 12, n = 2h + 20$ and $e = 3h + 30$. Therefore the molecular graph of a fullerene made entirely of n carbon atoms, denoted by C_n, have 12 pentagonal and $(n/2 - 10)$ hexagonal faces, while $n \neq 22$ is an even natural number equal or greater than 20 (see [1] and [2]).

By IUPAC terminology, a topological index is a numerical value associated with chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. The eccentric connectivity index is a topological index which was proposed in [3] and has been extensively used in molecular chemistry for studies related to structure activity/property relationships (see [4], [5] and [6]). This index is defined as $\xi^c(G) = \sum_{u \in V(G)} d(u)\varepsilon(u)$. Mathematical properties of the eccentric connectivity index was studied in [7], [8] and [9]. The connective eccentricity index which is a modification of the eccentric connectivity index is defined as (see [10], [11], [12] and [13]) $C^{\xi}(G) = \sum_{u \in V(G)} d(u)\varepsilon(u)^{-1}$.

On can see in the above definition that the reciprocal of the eccentricity is considered for a vertex, so the contribution of a vertex is non-linear. In the process of finding an invariant to be better suited to certain tasks than the previous ones, the eccentric adjacency index was introduced in [14] as

$$\xi^{ad}(G) = \sum_{u \in V(G)} \frac{S(u)}{\varepsilon(u)},$$

where $S(u)$ denotes the sum of degrees of all neighbors of the vertex u. As it is seen in the definition of $\xi^{ad}(G)$, the degrees are taken over the neighborhoods and then summed and also the reciprocal of the eccentricity is considered for a vertex, so the contribution of a vertex to $\xi^{ad}(G)$ is non-local and non-linear.

It is worth mentioning that the product version of the eccentric adjacency index, termed as augmented eccentric connectivity index, has been proposed by replacing $S(u)$ with the product of degrees of all neighbors of the vertex u (see [15], [16], [17], [18], [19], [20], [21] and [22]).

Some eccentricity-based invariants of fullerenes were computed already (see [23], [24], [25], [26], [27], [28], [20] and [29]). In this paper we aim to compute the eccentric adjacency index of the molecular graph of several infinite classes of fullerenes, namely C_{12n+2}, C_{20n+40}, C_{12n+4}, C_{12n+6}, C_{20n}, C_{40n+6} ,C_{10n}, C_{18n+10}, C_{12n} and C_{24n}.

Let us recall that the n-th harmonic number H_n is given as the n-th partial sum of the harmonic series, $H_n = 1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{n} = \sum_{i=1}^{n} \frac{1}{i}$. Throughout this paper, our notations are standard and mainly taken from standard books of graph theory such as [30] and [31].

2 Main Results

In this section, the eccentric adjacency indices of the molecular graph of some infinite classes of fullerenes, namely C_{12n+2}, C_{20n+40}, C_{12n+4}, C_{12n+6}, C_{20n}, C_{40n+6} ,C_{10n}, C_{18n+10}, C_{12n} and C_{24n} are computed.

Let us consider C_{12n+2} fullerenes. Note that the molecular graph of C_{12n+2} is cubic with exactly $12n + 2$ vertices and $18n + 3$ edges. In Table 1, the eccentric adjacency index of C_{12n+2}, $2 \leq n \leq 9$, is computed.

Table 1. The eccentric adjacency index of C_{12n+2}, $2 \leq n \leq 9$.

Fullerenes	eccentric adjacency index
C_{26}	$3 \times (72/5 + 1)$
C_{38}	$3 \times 114/7$
C_{50}	$3 \times 36/7 + 3 \times 102/8 + 3 \times 12/9$
C_{62}	$3 \times 72/8 + 3 \times 72/9 + 3 \times 42/10$
C_{74}	$3 \times 36/8 + 3 \times 72/9 + 3 \times 54/10 + 3 \times 36/11 + 3 \times 24/12$
C_{86}	$3 \times 72/9 + 3 \times 54/10 + 3 \times 36/11 + 3 \times 36/12 + 3 \times 36/13 + 3 \times 24/14$
C_{98}	$3 \times (12/9 + 18/10 + 12/11 + 12/12 + 12/13 + 12/14 + 12/15 + 8/16)$
C_{110}	$3 \times (18/10+12/11+12/12+12/13+12/14+12/15+12/16+12/17+8/18)$

A general formula for the eccentric adjacency index of C_{12n+2}, $n \geq 10$, is obtained as follows:

Theorem 2.1.

$$\xi^{ad}(C_{12n+2}) = \frac{90}{n} + 108(H_{2n-1} - H_n).$$

Proof. Using GAP [32] the eccentricity of the vertices of C_{12n+2} were computed in [28] (see Fig. 1). These eccentricities are presented in Table 2. Now the result follows from the data provided with Table 2 and from the fact that for each $v \in V(C_{12n+2})$, $S(v) = 9$. ☐

Let us consider C_{20n+40} fullerenes. Note that the molecular graph of C_{20n+40} fullerene is cubic with exactly $20n + 40$ vertices and $30n + 60$ edges. In Table 3, the eccentric adjacency index of C_{20n+40} fullerenes are computed for $1 \leq n \leq 10$.

Table 2. The eccentricity of molecular graph C_{12n+2}, for $n \geq 10$.

Type of vertices	eccentricity	Number
The Type 1 Vertices	$2n$	8
The Type 2 Vertices	n	6
Other Vertices	$n + i (1 \leq i \leq n - 1)$	12

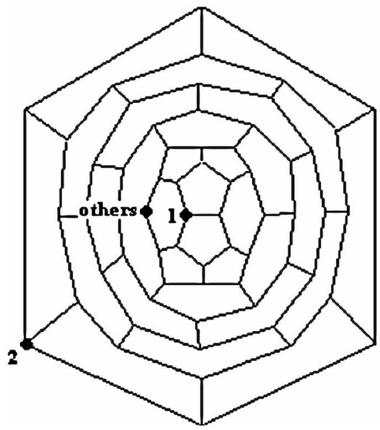

Fig. 1. The molecular graph of fullerene C_{12n+2} for $n = 4$

In the case that $n \geq 11$, a general formula for the eccentric adjacency index of C_{20n+40} is obtained as follows:

Theorem 2.2.

$$\xi^{ad}(C_{20n+40}) = 180(H_{2n+4} - H_{n+3}) + 90(\frac{1}{2n+5} + \frac{1}{2n+6}).$$

Proof. Using GAP [32] the eccentricity of the vertices of C_{20n+40} were computed in [28] (see Fig. 2). These eccentricities are presented in Table 4. Now the result follows from the data provided

Table 3. The eccentric adjacency index of C_{20n+40}, $1 \leq n \leq 10$.

Fullerenes	eccentric adjacency index
C_{60}	60
C_{80}	3(240/11)
C_{100}	3(60/11 + 240/12)
C_{120}	3(120/12 + 210/13 + 30/14)
C_{140}	3(60/12 + 120/13 + 180/14 + 30/15 + 30/16)
C_{160}	3(120/13 + 120/14 + 120/15 + 60/16 + 30/17 + 30/18)
C_{180}	3(60/13 + 120/14 + 120/15 + 90/16 + 60/17 + 60/18 + 30/19)
C_{200}	3(60/14 + 120/15 + 90/16 + 60/17 + 90/18 + 60/19 + 60/20 + 60/21 + 30/22 + 30/23)
C_{220}	3(120/15 + 90/16 + 60/17 + 90/18 + 60/19 + 60/20 + 60/21 + 60/22 + 60/23 + 30/24 + 30/25)
C_{240}	3(60/25+90/16+20/17+90/18+60(1/19+1/20+1/21+1/22+1/23+1/24 + 1/25) + 30/26 + 30/27)

with Table 4 and from the fact that for each $v \in V(C_{20n+40})$, $S(v) = 9$. □

Let us consider C_{12n+4} fullerenes. Note that the molecular graph of C_{12n+4} is cubic with exactly $12n+4$ vertices and $18n+6$ edges. In Table 5, the eccentric adjacency index of C_{12n+4} are computed for $2 \leq n \leq 7$.

Table 4. The eccentricity of molecular graph C_{20n+40}, for $n \geq 11$

Type of vertices	eccentricity	Number
The Type 1 Vertices	$2n+6$	10
The Type 2 Vertices	$2n+5$	10
Other Vertices	$n+4+i(0 \leq i \leq n)$	20

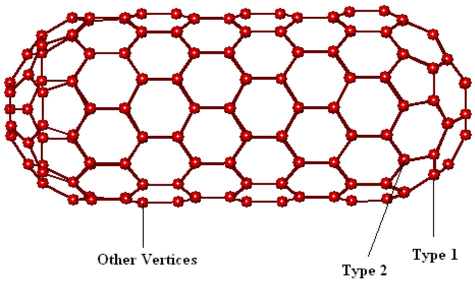

Fig. 2. The molecular graph of fullerene C_{20n+40} for $n=3$

Table 5. The eccentric adjacency index of C_{12n+4}, $2 \leq n \leq 7$.

Fullerene	The eccentric adjacency index
C_{28}	$\frac{9\times12}{5}+\frac{9\times16}{6}$
C_{40}	$\frac{9\times36}{7}+\frac{9\times4}{8}$
C_{52}	$\frac{9\times12}{7}+\frac{9\times32}{8}+\frac{9\times8}{9}$
C_{64}	$\frac{9\times24}{8}+\frac{9\times24}{9}+\frac{9\times12}{10}+\frac{9\times4}{11}$
C_{76}	$\frac{9\times12}{8}+\frac{9\times24}{9}+\frac{9\times12}{10}+\frac{9\times12}{11}+\frac{9\times12}{12}+\frac{9\times4}{13}$
C_{88}	$\frac{9\times24}{9}+\frac{9\times12}{10}+\frac{9\times12}{11}+\frac{9\times12}{12}+\frac{9\times12}{13}+\frac{9\times12}{14}+\frac{9\times4}{15}$

A general formula for the eccentric adjacency index of C_{12n+4}, $n \geq 8$, is obtained as follows:

Theorem 2.3.

$$\xi^{ad}(C_{12n+4}) = \frac{36}{2n+1} + 108(H_{2n} - H_n).$$

Proof. Using GAP [32] the eccentricity of the vertices of C_{12n+4} were computed in [25] (see Fig. 3). These eccentricities are presented in Table 6. Now the result follows from the data provided with Table 6 and from the fact that for each $v \in V(C_{12n+4})$, $S(v) = 9$. □

Theorem 2.4.

$$\xi^{ad}(C_{12n+6}) = \frac{72}{2n+1} + \frac{90}{2n} + 108(H_{2n-1} - H_n), \quad n \geq 9.$$

Proof. Using GAP [32] the eccentricity of the vertices of C_{12n+6} were computed in [33]. These eccentricities are presented in Table 7. Now the result follows from the data provided with Table 7 and from the fact that for each $v \in V(C_{12n+6})$, $S(v) = 9$. □

Table 6. The eccentricity of molecular graph C_{12n+4}, for $n \geq 8$

Type of vertices	eccentricity	Number
The Type 1 Vertices	$2n+1$	4
Other Vertices	$n+i$ $(1 \leq i \leq n)$	12

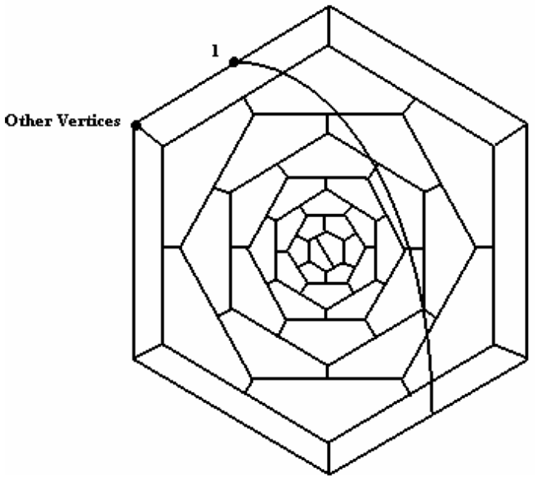

Fig. 3. The molecular graph of fullerene C_{12n+4}

Table 7. The eccentricity of molecular graph C_{12n+6}, for $n \geq 9$

Type of vertices	eccentricity	Number
The Type 1 Vertices	$2n+1$	8
The Type 2 Vertices	$2n$	10
Other Vertices	$2n+1-i$ $(2 \leq i \leq n)$	12

Theorem 2.5.

$$\xi^{ad}(C_{20n}) = 180(H_{2n+3} - H_{n+3}), \quad n \geq 6.$$

Proof. Using GAP [32] the eccentricity of the vertices of C_{20n} were computed in [33]. These eccentricities are presented in Table 8. Now the result follows from the data provided with Table 8 and from the fact that for each $v \in V(C_{20n})$, $S(v) = 9$. □

Theorem 2.6.

$$\xi^{ad}(C_{40n+6}) = \frac{72}{4n+2} + \frac{108}{4n+1} + \frac{144}{4n} + \frac{90}{2n+1} + 180(H_{4n-1} - H_{2n+1}), \quad n \geq 9.$$

Proof. Using GAP [32] the eccentricity of the vertices of C_{40n+6} were computed in [33]. These eccentricities are presented in Table 9. Now the result follows from the data provided with Table 9 and from the fact that for each $v \in V(C_{40n+6})$, $S(v) = 9$. □

The eccentric adjacency index of C_{12n}, for $n \leq 9$, C_{10n}, for $n \leq 7$ and C_{18n+10}, for $4 \leq n \leq 13$ are computed in Table 10, Table 11 and Table 12, respectively.

Table 8. The eccentricity of molecular graph C_{20n}, for $n \geq 6$

Type of vertices	eccentricity	Number
All Vertices	$2n+3-i\ (0 \leq i \leq n-1)$	20

Table 9. The eccentricity of molecular graph C_{40n+6}, for $n \geq 9$

Type of vertices	eccentricity	Number
The Type 1 Vertices	$4n+1$	8
The Type 2 Vertices	$4n+1$	12
The Type 3 Vertices	$4n$	16
The Type 4 Vertices	$4n+2-i\ (3 \leq i \leq 2n)$	20
The Type 5 Vertices	$2n+1$	10

By the means of group actions, the eccentricity of vertices of C_{10n}, C_{12n}, C_{24n} and C_{18n+10} were computed. Let us summarize them in the following lemmas:

Lemma 2.7 ([24]). *For $n \geq 8$, we have* $ec(C_{10n}) = \left\{ \overbrace{n, \cdots, n}^{10}, \cdots, \overbrace{2n-1, \cdots, 2n-1}^{10} \right\}$ *and* $ec(C_{12n}) = \left\{ \overbrace{n, \cdots, n}^{12}, \cdots, \overbrace{2n-1, \cdots, 2n-1}^{12} \right\}$ *if $n \geq 10$.*

Table 10. The eccentric adjacency index of C_{12n}, for $n \leq 9$

Fullerene	Eccentric adjacency index
C_{24}	$\frac{9\times24}{5}$
C_{36}	$\frac{9\times36}{7}$
C_{48}	$\frac{9\times12}{7}+\frac{9\times36}{8}$
C_{60}	$\frac{9\times24}{8}+\frac{9\times24}{9}+\frac{9\times12}{10}$
C_{72}	$\frac{9\times12}{8}+\frac{9\times24}{9}+\frac{9\times24}{10}+\frac{9\times12}{11}$
C_{84}	$\frac{9\times24}{9}+\frac{9\times24}{10}+\frac{9\times12}{11}+\frac{9\times12}{12}+\frac{9\times12}{13}$
C_{96}	$\frac{9\times12}{9}+\frac{9\times24}{10}+\frac{9\times12}{11}+\frac{9\times12}{12}+\frac{9\times12}{13}+\frac{9\times12}{14}+\frac{9\times12}{15}$
C_{108}	$\frac{9\times24}{10}+\frac{9\times12}{11}+\frac{9\times12}{12}+\frac{9\times12}{13}+\frac{9\times12}{14}+\frac{9\times12}{15}+\frac{9\times12}{16}+\frac{9\times12}{17}$

Table 11. The eccentric adjacency index of C_{10n}, for $2 \leq n \leq 7$

Fullerene	Eccentric adjacency index
C_{20}	$\frac{9\times20}{5}$
C_{30}	$\frac{9\times30}{6}$
C_{40}	$\frac{9\times10}{6}+\frac{9\times20}{7}+\frac{9\times10}{8}$
C_{50}	$\frac{9\times10}{8}+\frac{9\times20}{9}+\frac{9\times10}{10}+\frac{9\times10}{11}$
C_{60}	$\frac{9\times10}{7}+\frac{9\times20}{8}+\frac{9\times10}{9}+\frac{9\times10}{10}+\frac{9\times10}{11}$
C_{70}	$\frac{9\times20}{8}+\frac{9\times10}{9}+\frac{9\times10}{10}+\frac{9\times10}{11}+\frac{9\times10}{12}+\frac{9\times10}{13}$

Table 12. The eccentric adjacency index of C_{18n+10}, for $4 \le n \le 13$

Fullerene	eccentric adjacency index
C_{82}	$\frac{9\times67}{10}+\frac{9\times15}{11}$
C_{100}	$\frac{9\times18}{10}+\frac{9\times50}{11}+\frac{9\times22}{12}+\frac{9\times10}{13}$
C_{118}	$\frac{9\times36}{11}+\frac{9\times39}{12}+\frac{9\times21}{13}+\frac{9\times13}{14}+\frac{9\times9}{15}$
C_{136}	$\frac{9\times18}{11}+\frac{9\times36}{12}+\frac{9\times27}{13}+\frac{9\times21}{14}+\frac{9\times15}{15}+\frac{9\times12}{16}+\frac{9\times7}{17}$
C_{154}	$\frac{9\times36}{12}+\frac{9\times27}{13}+\frac{9\times21}{14}+\frac{9\times18}{15}+\frac{9\times21}{16}+\frac{9\times15}{17}+\frac{9\times9}{18}+\frac{9\times7}{19}$
C_{172}	$\frac{9\times18}{12}+\frac{9\times27}{13}+\frac{9\times21}{14}+\frac{9\times18}{15}+\frac{9\times21}{16}+\frac{9\times18}{15}+\frac{9\times21}{16}+\frac{9\times18}{17}+\frac{9\times15}{18}+$ $\frac{9\times15}{19}+\frac{9\times9}{20}+\frac{9\times7}{21}$
C_{190}	$\frac{9\times27}{13}+\frac{9\times21}{14}+\frac{9\times18}{15}+\frac{9\times24}{16}+\frac{9\times18}{17}+\frac{9\times18}{18}+\frac{9\times18}{19}+\frac{9\times15}{20}+$ $\frac{9\times15}{21}+\frac{9\times9}{22}+\frac{9\times7}{23}$
C_{208}	$\frac{9\times9}{13}+\frac{9\times21}{14}+\frac{9\times18}{15}+\frac{9\times24}{16}+\frac{9\times18}{17}+\frac{9\times18}{18}+\frac{9\times18}{19}+\frac{9\times18}{20}+$ $\frac{9\times18}{21}+\frac{9\times15}{22}+\frac{9\times15}{23}+\frac{9\times9}{24}+\frac{9\times7}{25}$
C_{226}	$\frac{9\times21}{14}+\frac{9\times18}{15}+\frac{9\times24}{16}+\frac{9\times18}{17}+\frac{9\times18}{18}+\frac{9\times18}{19}+\frac{9\times18}{20}+\frac{9\times18}{21}+\frac{9\times18}{22}+$ $\frac{9\times18}{23}+\frac{9\times15}{24}+\frac{9\times15}{25}+\frac{9\times9}{26}+\frac{9\times7}{27}$
C_{244}	$\frac{9\times12}{15}+\frac{9\times24}{16}+\frac{9\times18}{17}+\frac{9\times18}{18}+\frac{9\times18}{19}+\frac{9\times18}{20}+\frac{9\times18}{21}+\frac{9\times18}{22}+\frac{9\times18}{23}+$ $\frac{9\times18}{24}+\frac{9\times18}{25}+\frac{9\times15}{26}+\frac{9\times15}{27}+\frac{9\times9}{28}+\frac{9\times7}{29}$

Lemma 2.8 ([26]). The eccentricity of vertices in C_{24n} are presented in the following table:

Table 13. The eccentricity of vertices in C_{24n}

Type of vertices	eccentricity	Number
The Type 1 Vertices	$2n+3$	48
The type 2 vertices	$2n+3i\ (1 \le i \le n-2)$	24

Lemma 2.9 ([27]). The eccentricity of vertices in C_{18n+10} are presented in the following table (see Fig. 4):

Table 14. The eccentricity of vertices in C_{18n+10}

Type of vertices	eccentricity	Number
Type 1 Vertices	$2n+3$	7
Type 2 Vertices	$2n+2$	9
Type 3 Vertices	$2n, 2n+1$	15
Type 4 Vertices	$n+i\ (2 \le i \le n-1)$	18

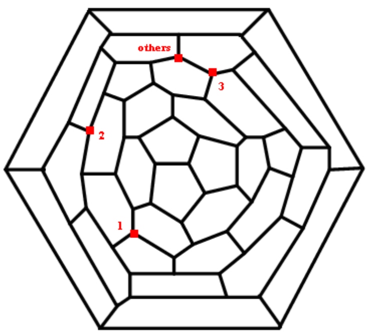

Fig. 4. The molecular graph of fullerene C_{18n+10}

As a direct consequence of Lemma 2.7, Lemma 2.8 and 2.9 the eccentric adjacency index of C_{10n}, for $n \geq 8$, C_{12n}, for $n \geq 10$, C_{24n} and C_{18n+10}, for $n \geq 14$ are computed.

Theorem 2.10.

$$\xi^{ad}(C_{10n}) = 90(H_{2n-1} - H_{n-1}),$$
$$\xi^{ad}(C_{12n}) = 108(H_{2n-1} - H_{n-1}),$$
$$\xi^{ad}(C_{24n}) = \frac{432}{2n+3} + 216\sum_{i=1}^{n-2}\frac{1}{2n+3i},$$
$$\xi^{ad}(C_{18n+10}) = \frac{63}{2n+3} + \frac{81}{2n+2} + \frac{135}{2n+1} + \frac{135}{2n} + 162(H_{2n-1} - H_{n+1}).$$

3 Concluding Remarks

In this paper we have computed the eccentric adjacency index of several infinite class of fullerenes, namely C_{12n+2}, C_{20n+40}, C_{12n+4}, C_{12n+6}, C_{20n}, C_{40n+6} ,C_{10n}, C_{18n+10}, C_{12n} and C_{24n}. However, some fullerenes have been left out. For example, we have not considered C_{60+12n}, C_{50+10n}, $C_{12(2n+1)}$ and $C_{12(2n+8)}$. A fullerene is a cubic 3-connected planar graphs with faces of size r and s. In this paper we have only considered fullerenes with pentagonal and hexagonal faces. However one can construct fullerenes with faces triangles and hexagons (see [34]), fullerenes with faces quadrangles and hexagons (see [29] and Fig. 5) and even fullerenes with pentagonal and heptagonal faces.

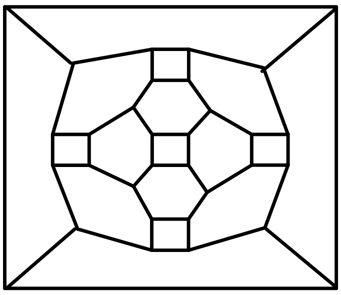

Fig. 5. 2-D graph of fullerene C_{8n^2} for n=2 (with faces of size 4 and 6)

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Competing Interests

The authors declare that no competing interests exist.

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