

On eccentric adjacency index of several infinite classes of fullerenes

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.

MSC(2010): Primary: 05C40, 05C90;

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., $d(u) = |\{v \in V(G) | d(u, v) = 1\}|$. The eccentricity $\varepsilon(u)$ of the vertex u of G is the distance from u to any vertex farthest away from it in G , i.e., $\varepsilon(u) = \max_{v \in V(G)} d(u, v)$. The eccentricity sequence $ec(G)$ of G , is the multi-set of eccentricities of the vertices of G , i.e., $ec(G) = \{\varepsilon(u) | u \in V(G)\}$.

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

33 In this paper, fullerenes are molecules in the form of cage-like polyhedra, con-
 34 sisting solely of carbon atoms, where each carbon atom is chemically bonded to
 35 three other carbon atoms in a nearly spherical configuration. The molecular graph
 36 of a fullerene (fullerene graph) can be viewed as a finite connected trivalent plane
 37 graph, all of its faces are pentagons and hexagons. Consider a fullerene graph with
 38 exactly p, h, n and m pentagons, hexagons, vertices and edges between them, re-
 39 spectively. Since each vertex lies in exactly 3 faces and each edge lies in 2 faces, the
 40 number of vertices is $n = (5p + 6h)/3$, the number of edges is $m = (5p + 6h)/2 =$
 41 $3/2n$ and the number of faces is $f = p + h$. Recall that Euler's formula states that
 42 $n - m + f = 2$. It follows that $(5p + 6h)/3 - (5p + 6h)/2 + p + h = 2$, and therefore
 43 $p = 12, n = 2h + 20$ and $e = 3h + 30$. Therefore the molecular graph of a fullerene
 44 made entirely of n carbon atoms, denoted by C_n , have 12 pentagonal and $(n/2 - 10)$
 45 hexagonal faces, while $n \neq 22$ is an even natural number equal or greater than 20
 46 [10, 21].

47 By IUPAC terminology, a topological index is a numerical value associated
 48 with chemical constitution purporting for correlation of chemical structure with
 49 various physical properties, chemical reactivity or biological activity. The eccen-
 50 tric connectivity index is a topological index which was proposed in [25] and has
 51 been extensively used in molecular chemistry for studies related to structure activ-
 52 ity/property relationships [3, 17, 22]. This index is defined as

$$\xi^c(G) = \sum_{u \in V(G)} d(u)\varepsilon(u).$$

53 Mathematical properties of the eccentric connectivity index was studied in [19, 20,
 54 33]. The connective eccentricity index which is a modification of the eccentric
 55 connectivity index is defined [15, 28, 31, 32] as

$$C^\xi(G) = \sum_{u \in V(G)} \frac{d(u)}{\varepsilon(u)}.$$

56 On can see in the above definition that the reciprocal of the eccentricity is consid-
 57 ered for a vertex, so the contribution of a vertex is non-linear. In the process of
 58 finding an invariant to be better suited to certain tasks than the previous ones, the

eccentric adjacency index was introduced in [16] 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 [4, 5, 6, 8, 24, 29, 30].

Some eccentricity-based invariants of fullerenes were computed already, [1, 7, 11, 12, 13, 14, 24, 26]. 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_{10n} , C_{12n} , C_{24n} , C_{18n+10} , C_{20n+10} , C_{12n+6} and C_{40n+6} .

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 [18, 27].

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_{10n} , C_{12n} , C_{24n} , C_{18n+10} , C_{20n+10} , C_{12n+6} and C_{40n+6} 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}	$3 \times (18/10 + 12/11 + 12/12 + 12/13 + 12/14 + 12/15 + 12/16 + 12/17 + 8/18)$

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

Theorem 2.1.

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

85 *Proof.* Using GAP [9] the eccentricity of these vertices were computed in [14] (see
86 Figure 1). These eccentricities are presented in the following table:

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

87 Now the result follows from the data provided with Table 2 and from the fact that
88 for each $v \in V(C_{12n+2})$, $S(v) = 9$. $\square$

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

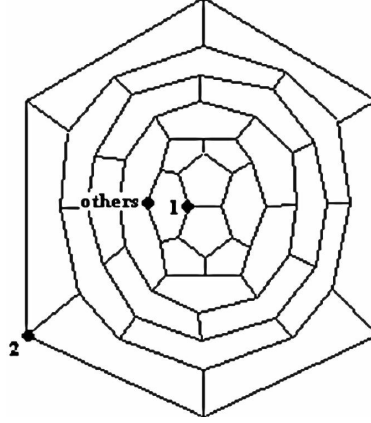


Figure 1: The molecular graph of fullerene C_{12n+2} for $n = 4$

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}	$3(60/25 + 90/16 + 20/17 + 90/18 + 60(1/19 + 1/20 + 1/21 + 1/22 + 1/23 + 1/24 + 1/25) + 30/26 + 30/27)$

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.

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

Proof. Using GAP [9] the eccentricity of these vertices were computed in [14] (see Figure 2). These eccentricities are presented in the following table:

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

96 Now the result follows from the data provided with Table 4 and from the fact
 97 that for each $v \in V(C_{20n+40})$, $S(v) = 9$. $\square$

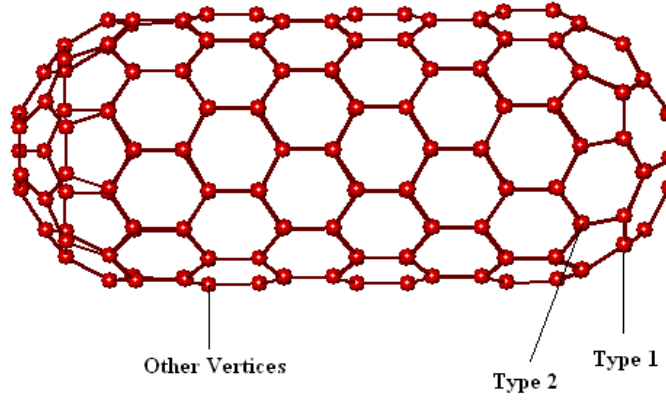


Figure 2: The molecular graph of fullerene C_{20n+40} for $n = 3$

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

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

Fullerene	The eccentric adjacency index
C_{28}	$\frac{9 \times 12}{5} + \frac{9 \times 16}{6}$
C_{40}	$\frac{9 \times 36}{7} + \frac{9 \times 4}{8}$
C_{52}	$\frac{9 \times 12}{7} + \frac{9 \times 32}{8} + \frac{9 \times 8}{9}$
C_{64}	$\frac{9 \times 24}{8} + \frac{9 \times 24}{9} + \frac{9 \times 12}{10} + \frac{9 \times 4}{11}$
C_{76}	$\frac{9 \times 12}{8} + \frac{9 \times 24}{9} + \frac{9 \times 12}{10} + \frac{9 \times 12}{11} + \frac{9 \times 12}{12} + \frac{9 \times 4}{13}$
C_{88}	$\frac{9 \times 24}{9} + \frac{9 \times 12}{10} + \frac{9 \times 12}{11} + \frac{9 \times 12}{12} + \frac{9 \times 12}{13} + \frac{9 \times 12}{14} + \frac{9 \times 4}{15}$

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

Theorem 2.3.

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

103 *Proof.* Using GAP [9] the eccentricity of these vertices were computed in [11] (see
 104 Figure 3). These eccentricities are presented in the following table:

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

105 Now the result follows from the data provided with Table 6 and from the fact that
 106 for each $v \in V(C_{20n+40})$, $S(v) = 9$. $\square$

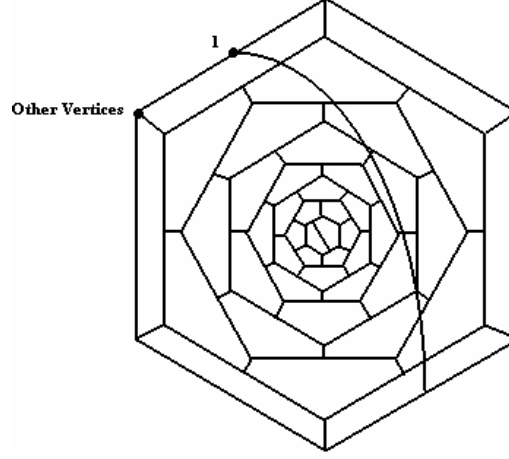


Figure 3: The molecular graph of fullerene C_{12n+4}

Theorem 2.4.

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

107 *Proof.* The results follow from the fact that the molecular graph of C_{12n+6} is cubic;
 108 and from the eccentricities computed by GAP [9], which are presented in Table 7.

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

109

□

Theorem 2.5.

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

110 *Proof.* The results follow from the fact that the molecular graph of C_{20n} is cubic;
 111 and from the eccentricities computed by GAP [9], which are presented in Table 8.

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

112

□

Theorem 2.6.

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

113 *Proof.* The results follow from the fact that the molecular graph of C_{40n+6} is cubic;
 114 and from the eccentricities computed by GAP [9], which are presented in Table 9.

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

115

□

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

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

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

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

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

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

Fullerene	eccentric adjacency index
C_{82}	$\frac{9 \times 67}{10} + \frac{9 \times 15}{11}$
C_{100}	$\frac{9 \times 18}{10} + \frac{9 \times 50}{11} + \frac{9 \times 22}{12} + \frac{9 \times 10}{13}$
C_{118}	$\frac{9 \times 36}{11} + \frac{9 \times 39}{12} + \frac{9 \times 21}{13} + \frac{9 \times 13}{14} + \frac{9 \times 9}{15}$
C_{136}	$\frac{9 \times 18}{11} + \frac{9 \times 36}{12} + \frac{9 \times 27}{13} + \frac{9 \times 21}{14} + \frac{9 \times 15}{15} + \frac{9 \times 12}{16} + \frac{9 \times 7}{17}$
C_{154}	$\frac{9 \times 36}{12} + \frac{9 \times 27}{13} + \frac{9 \times 21}{14} + \frac{9 \times 18}{15} + \frac{9 \times 21}{16} + \frac{9 \times 15}{17} + \frac{9 \times 9}{18} + \frac{9 \times 7}{19}$
C_{172}	$\frac{9 \times 18}{12} + \frac{9 \times 27}{13} + \frac{9 \times 21}{14} + \frac{9 \times 18}{15} + \frac{9 \times 21}{16} + \frac{9 \times 18}{15} + \frac{9 \times 21}{16} + \frac{9 \times 18}{17} + \frac{9 \times 15}{18} + \frac{9 \times 9}{19} + \frac{9 \times 7}{20} + \frac{9 \times 7}{21}$
C_{190}	$\frac{9 \times 27}{13} + \frac{9 \times 21}{14} + \frac{9 \times 18}{15} + \frac{9 \times 24}{16} + \frac{9 \times 18}{17} + \frac{9 \times 18}{18} + \frac{9 \times 18}{19} + \frac{9 \times 15}{20} + \frac{9 \times 15}{21} + \frac{9 \times 9}{22} + \frac{9 \times 7}{23}$
C_{208}	$\frac{9 \times 9}{13} + \frac{9 \times 21}{14} + \frac{9 \times 18}{15} + \frac{9 \times 24}{16} + \frac{9 \times 18}{17} + \frac{9 \times 18}{18} + \frac{9 \times 18}{19} + \frac{9 \times 18}{20} + \frac{9 \times 18}{21} + \frac{9 \times 18}{22} + \frac{9 \times 18}{23} + \frac{9 \times 15}{24} + \frac{9 \times 9}{25} + \frac{9 \times 7}{26}$
C_{226}	$\frac{9 \times 21}{14} + \frac{9 \times 18}{15} + \frac{9 \times 24}{16} + \frac{9 \times 18}{17} + \frac{9 \times 18}{18} + \frac{9 \times 18}{19} + \frac{9 \times 18}{20} + \frac{9 \times 18}{21} + \frac{9 \times 18}{22} + \frac{9 \times 18}{23} + \frac{9 \times 18}{24} + \frac{9 \times 15}{25} + \frac{9 \times 9}{26} + \frac{9 \times 7}{27}$
C_{244}	$\frac{9 \times 12}{15} + \frac{9 \times 24}{16} + \frac{9 \times 18}{17} + \frac{9 \times 18}{18} + \frac{9 \times 18}{19} + \frac{9 \times 18}{20} + \frac{9 \times 18}{21} + \frac{9 \times 18}{22} + \frac{9 \times 18}{23} + \frac{9 \times 18}{24} + \frac{9 \times 18}{25} + \frac{9 \times 15}{26} + \frac{9 \times 9}{27} + \frac{9 \times 7}{28} + \frac{9 \times 7}{29}$

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 2.1 ([7]). For $n \geq 8$, we have $ec(C_{10n}) = \left\{ \overbrace{n, \dots, n}^{10}, \dots, \overbrace{2n-1, \dots, 2n-1}^{10} \right\}$

and $ec(C_{12n}) = \left\{ \overbrace{n, \dots, n}^{12}, \dots, \overbrace{2n-1, \dots, 2n-1}^{12} \right\}$ if $n \geq 10$.

Lemma 2.2 ([12]). 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	$2n + 3i \ (1 \leq i \leq n - 2)$	24

124 **Lemma 2.3** ([13]). *The eccentricity of vertices in C_{18n+10} are presented in the*
 125 *following table (see Figure 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	$n + i \ (2 \leq i \leq n - 1)$	18

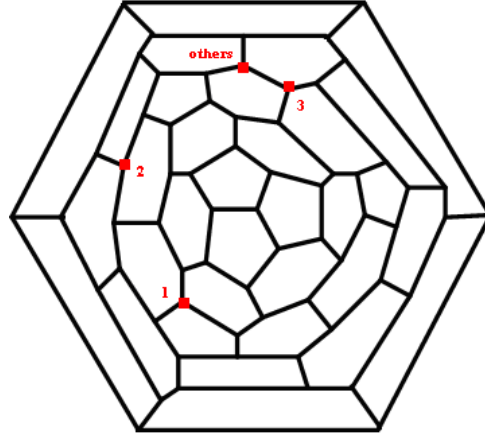


Figure 4: The molecular graph of fullerene C_{18n+10}

126 As a direct consequence of Lemma 2.1, Lemma 2.2 and 2.3 the eccentric adja-
 127 cency 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
 128 computed.

Theorem 2.7.

$$\xi^{ad}(C_{10n}) = 90(H_{2n-1} - H_{n-1}),$$

$$\xi^{ad}(C_{12n}) = 108(H_{2n-1} - H_{n-1}),$$

130

$$\xi^{ad}(C_{24n}) = \frac{432}{2n+3} + 216 \sum_{i=1}^{n-2} \frac{1}{2n+3i},$$

131

$$\xi^{ad}(C_{18n+10}) = \frac{63}{2n+3} + \frac{81}{2n+2} + \frac{135}{2n+1} + \frac{135}{2n} + 162(H_{2n-1} - H_{n+1}).$$

132 **Acknowledgements** The authors would like to expressly thank M. Ghorbani and
 133 F. Koorepazan-Moftakhar for consulting about the GAP programming.

134 References

- 135 [1] A.R. Ashrafi, M. Ghorbani, Eccentric Connectivity Index of Fullerenes, 2008,
 136 In: I. Gutman, B. Furtula, Novel Molecular Structure Descriptors Theory and
 137 Applications II, pp. 183–192.
- 138 [2] G. Brinkman, P.W. Fowler, A list of free software for chemical and graph
 139 theoretical applications, *MATCH Commun. Math. Comput. Chem.* 58 (2007)
 140 423–430.
- 141 [3] S. Bajaj, S. Sami, A.K. Madan, Topological models for prediction of anti-
 142 HIV activity of acylthiocarbamates, *Bioorganic Medicine Chemistry*, 13
 143 (2005) 3263–3268.
- 144 [4] T. Došlić and M. Saheli, Augmented eccentric connectivity index of single-
 145 defect nanocones, *J. Math. NanoSci.*, 1 (2011) 25–31.
- 146 [5] T. Došlić and M. Saheli, Augmented eccentric connectivity index, *Miskolc*
 147 *Mathematical Notes*, 12 (2) (2011), 149–157.
- 148 [6] H. Dureja and A.K. Madan, Superaugmented eccentric connectivity in-
 149 dices: new-generation highly discriminating topological descriptors for
 150 QSAR/QSPR modeling, *Med. Chem. Res.*, 16 (2007), 331–341.
- 151 [7] S. Djafari, F. Koorepazan-Moftakhar, A.R. Ashrafi, Eccentric Sequences of
 152 Two Infinite Classes of Fullerenes, *Journal of Computational and Theoretical*
 153 *Nanoscience*, 10(11) (2013) 2636–2638.
- 154 [8] S. Ediz, The augmented eccentric connectivity index of nanotubes and nan-
 155 otori, *J. Math. Nanosci.*, 2(1)(2012) 1–8.
- 156 [9] The GAP Team: GAP Groups, Algorithms and Programming, RWTH,
 157 Aachen, 1995.

- 158 [10] M. Ge and K. Sattler, Observation of fullerene cones, *Chem. Phys. Lett.*, 220
159 (1994), 192–196.
- 160 [11] M. Ghorbani, Eccentric connectivity polynomial of C_{12n+4} Fullerenes, *Digest*
161 *Journal of Nanomaterials and Biostructures*, 4(3)(2009), 545–547.
- 162 [12] M. Ghorbani, Kh. Malekjani, A new method for computing the eccentric con-
163 nectivity index of fullerenes, *Serdica J. Comput.*, 6 (2012), 299–308.
- 164 [13] M. Ghorbani, A.R. Ashrafi, and M. Hemmasi, Connective eccentric index of
165 C_{18n+10} fullerenes, *Bulgarian Chem. Comm.*, 45(1)(2013), 5–8.
- 166 [14] M. Ghorbani, Connective eccentric index of fullerenes, *J. Math. Nanosci.*
167 1(2011) 43–50.
- 168 [15] S. Gupta, M. Singh, A.K. Madan, Connective eccentricity Index: A novel
169 topological descriptor for predicting biological activity, *J. Mol. Graph.*
170 *Model.*, 18 (2000), 18–25.
- 171 [16] S. Gupta, M. Singh, A.K. Madan, Predicting anti-HIV activity: computa-
172 tional approach using a novel topological descriptor, *J. Comput. Aided. Mol.*
173 *Des.*, 15(7) (2001), 671–678.
- 174 [17] S. Gupta, M. Singh, and A. K. Madan, Application of graph theory: re-
175 lationship of eccentric connectivity index and Wiener's index with anti-
176 inflammatory activity, *J. Math. Anal. Appl.*, 266(2)(2002), 259–268.
- 177 [18] I. Gutman, O. E. Polansky, Mathematical Concepts in Organic Chemistry,
178 Springer–Verlag, Berlin, 1986.
- 179 [19] A. Ilić, I. Gutman, Eccentric Connectivity Index of Chemical Trees, *MATCH*
180 *Commun. Math. Comput. Chem.* 65 (2011) 731–744.
- 181 [20] A. Ilić, Eccentric connectivity index, in: I. Gutman, B. Furtula, Novel Molec-
182 ular Structure Descriptors - Theory and Applications II, MCM Vol. 9, Uni-
183 versity of Kragujevac, Kragujevac, 2010, pp. 139–168.
- 184 [21] H. W. Kroto, J. R. Heath, S. C. Ó'Brien, R. F. Curl and R. E. Smalley, C_{60} :
185 Buckminsterfullerene, *Nature*, 318 (1985), 162–163.
- 186 [22] S. Sardana and A. K. Madan, Application of graph theory: relationship of
187 molecular connectivity index, Wiener's index and eccentric connectivity index
188 with diuretic activity, *MATCH Commun. Math. Comput. Chem.*, 43 (2001),
189 85–98.

- 190 [23] J. Sedlar, On augmented eccentric connectivity index of graphs and trees,
191 *MATCH Commun. Math. Comput. Chem.*, 68 (2012) 325–342.
- 192 [24] R. Sharafadini, Augmented eccentric connectivity index of Fullerenes, *J.*
193 *Math. Nanosci.* 4(1) (2014), 13–18.
- 194 [25] V. Sharma, R. Goswami, and A.K. Madan, Eccentric connectivity index: A
195 novel highly discriminating topological descriptor for structure-property and
196 structure-activity studies, *J. Chem. Inf. Comput. Sci.*, 37 (1997), 273–282.
- 197 [26] M. Songhori, Eccentric connectivity index of fullerene graphs, *J. Math.*
198 *Nanosci.* 2(1), 2012, 21–27.
- 199 [27] D.B. West, Introduction to graph theory, Upper Saddle River, NJ: Prentice
200 Hall, Inc., 1996.
- 201 [28] K. Xu, K. C. Das, H. Liu, Some extremal results on the connective eccentric-
202 ity index of graphs, *J. Math. Anal. Appl.*, in press.
- 203 [29] Z. Yarahmadi, A.R. Ashrafi, S. Moradi, Extremal values of augmented eccen-
204 tric connectivity index of V-phenylenic nanotorus, *Journal of Applied Math-*
205 *ematics and Computing*, 45 (2014), 35–42.
- 206 [30] Z. Yarahmadi, Eccentric connectivity and augmented eccentric connectiv-
207 ity indices of N-branched phenylacetylenes nanostar dendrimers, *Iranian J.*
208 *Math. Chem.*, 1 (2)(2010), 105–110.
- 209 [31] G. Yu, H. Qu, L. Tang, L. Feng, On the connective eccentricity index of trees
210 and unicyclic graphs with given diameter, *J. Math. Anal. Appl.*, 420(2)(2014)
211 1776–1786.
- 212 [32] G. Yu and L. Feng, On connective eccentricity index of graphs, *MATCH Com-*
213 *mun. Math. Comput. Chem.*, 69 (2013) 611–628.
- 214 [33] B. Zhou, Z. Du, On eccentric connectivity index, *MATCH Commun. Math.*
215 *Comput. Chem.*, 63 (2010) 181–198.