

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 length of a maximal path connecting u to another 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., $ec(G) = \{\varepsilon(u) | u \in V(G)\}$.

The eccentric connectivity index is a graphic invariant which proposed in [24] and has been extensively used in molecular chemistry for studies related to structure activity/property relationships [3, 22, 18]. This index is defined as

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

The connective eccentricity index which is a modification of the eccentric connectivity index was proposed in [16] as

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

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 [17] 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 [5, 6, 7, 9, 23, 27, 28].

Fullerenes, discovered experimentally in 1985, are molecules in the form of cage-like polyhedra, consisting solely of carbon atoms bonded in a nearly spherical configuration. It is well-known fact that fullerenes made entirely of n carbon atoms, have 12 pentagonal and $(n/2 - 10)$ hexagonal faces, while $n \neq 22$ is a natural number equal or greater than 20 [11, 21].

Some eccentricity-based invariants of fullerenes were computed already, [1, 8, 12, 13, 14, 15, 23, 25]. 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, $H_n = 1 + \frac{1}{2} + \frac{1}{3} + \dots + \frac{1}{n} = \sum_{i=1}^n \frac{1}{i}$.

Throughout this paper, our notations are standard and mainly taken from standard books of graph theory such as [19, 26].

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}	$3 \times (18/10 + 12/11 + 12/12 + 12/13 + 12/14 + 12/15 + 12/16 + 12/17 + 8/18)$

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. One can see that there are three types of vertices of fullerene graph C_{12n+2} . These are the vertices of the central and outer pentagons and other vertices of C_{12n+2} , $n \geq 10$. Using GAP [10] the eccentricity of these vertices were computed in [15]. 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

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

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 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. One can see that there are three types of vertices of fullerene graph C_{20n+40} . These are the vertices of the central and outer pentagons and other vertices of C_{20n+40} . Using GAP [10] the eccentricity of these vertices were computed in [15]. 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 1 Vertices	$2n + 5$	10
Other Vertices	$n + 4 + i(0 \leq i \leq n)$	20

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

83 Let us consider C_{12n+4} fullerenes. Note that the molecular graph of C_{12n+4} is
84 cubic with exactly $12n + 4$ vertices and $18n + 6$ edges. In Table 5, the eccentric
85 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}	$\frac{9 \times 24}{9} + \frac{9 \times 12}{10} + \frac{9 \times 12}{11} + \frac{9 \times 12}{12} + \frac{9 \times 12}{13} + \frac{9 \times 12}{14} + \frac{9 \times 4}{15}$

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

Theorem 2.3.

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

88 *Proof.* One can see that there are tow types of vertices of fullerene graph C_{12n+4} .
89 These are the vertices of the central pentagons and other vertices of C_{12n+4} , $n \geq 8$.
90 Using GAP [10] the eccentricity of these vertices were computed in [12]. These
91 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

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

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. The results follow from the fact that the molecular graph of C_{12n+6} is cubic;
and from the eccentricities computed by GAP [10], 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

97

□

Theorem 2.5.

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

Proof. The results follow from the fact that the molecular graph of C_{20n} is cubic;
and from the eccentricities computed by GAP [10], 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

101

□

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. The results follow from the fact that the molecular graph of C_{40n+6} is cubic;
and from the eccentricities computed by GAP [10], 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

105

□

106 The eccentric adjacency index of C_{12n} , for $n \leq 9$, C_{10n} , for $n \leq 7$ and C_{18n+10} ,
 107 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}	$\frac{9 \times 12}{7} + \frac{9 \times 36}{8} = 9 \times 12 \sum_{n=7}^8 \frac{1}{n} + \frac{24}{8}$
C_{60}	$\frac{9 \times 24}{8} + \frac{9 \times 24}{9} + \frac{9 \times 12}{10} = 9 \times 12 \sum_{n=8}^{10} \frac{1}{n} + \frac{12}{8} + \frac{12}{9}$
C_{72}	$\frac{9 \times 12}{8} + \frac{9 \times 24}{9} + \frac{9 \times 24}{10} + \frac{9 \times 12}{11} = 9 \times 12 \sum_{n=8}^{11} \frac{1}{n} + \frac{12}{9} + \frac{12}{10}$
C_{84}	$\frac{9 \times 24}{9} + \frac{9 \times 24}{10} + \frac{9 \times 12}{11} + \frac{9 \times 12}{12} + \frac{9 \times 12}{13} = 9 \times 12 \sum_{n=9}^{13} \frac{1}{n} + \frac{12}{9} + \frac{12}{10}$
C_{96}	$\frac{9 \times 12}{9} + \frac{9 \times 24}{10} + \frac{9 \times 12}{11} + \frac{9 \times 12}{12} + \frac{9 \times 12}{13} + \frac{9 \times 12}{14} + \frac{9 \times 12}{15} = 9 \times 12 \sum_{n=9}^{15} \frac{1}{n} + \frac{12}{10}$
C_{108}	$\frac{9 \times 24}{10} + \frac{9 \times 12}{11} + \frac{9 \times 12}{12} + \frac{9 \times 12}{13} + \frac{9 \times 12}{14} + \frac{9 \times 12}{15} + \frac{9 \times 12}{16} + \frac{9 \times 12}{17} = 9 \times 12 \sum_{n=10}^{17} \frac{1}{n} + \frac{12}{10}$

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}	$\frac{9 \times 10}{6} + \frac{9 \times 20}{7} + \frac{9 \times 10}{8} = 9 \times 10 \sum_{n=6}^8 \frac{1}{n} + \frac{10}{7}$
C_{50}	$\frac{9 \times 10}{8} + \frac{9 \times 20}{9} + \frac{9 \times 10}{10} + \frac{9 \times 10}{11} = 9 \times 10 \sum_{n=8}^{11} \frac{1}{n} + \frac{10}{9}$
C_{60}	$\frac{9 \times 10}{7} + \frac{9 \times 20}{8} + \frac{9 \times 10}{9} + \frac{9 \times 10}{10} + \frac{9 \times 10}{11} = 9 \times 10 \sum_{n=7}^{11} \frac{1}{n} + \frac{10}{8}$
C_{70}	$\frac{9 \times 20}{8} + \frac{9 \times 10}{9} + \frac{9 \times 10}{10} + \frac{9 \times 10}{11} + \frac{9 \times 10}{12} + \frac{9 \times 10}{13} = 9 \times 10 \sum_{n=8}^{13} \frac{1}{n} + \frac{10}{8}$

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}	$\frac{9 \times 18}{12} + \frac{9 \times 27}{13} + \frac{9 \times 21}{14} + \frac{9 \times 18}{15} + \frac{9 \times 21}{16} + \frac{9 \times 18}{15} + \frac{9 \times 21}{16} + \frac{9 \times 18}{17} + \frac{9 \times 15}{18} +$ $\frac{9 \times 15}{19} + \frac{9 \times 9}{20} + \frac{9 \times 7}{21}$
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}	$\frac{9 \times 9}{13} + \frac{9 \times 21}{14} + \frac{9 \times 18}{15} + \frac{9 \times 24}{16} + \frac{9 \times 18}{17} + \frac{9 \times 18}{18} + \frac{9 \times 18}{19} + \frac{9 \times 18}{20} +$ $\frac{9 \times 18}{21} + \frac{9 \times 15}{22} + \frac{9 \times 15}{23} + \frac{9 \times 9}{24} + \frac{9 \times 7}{25}$
C_{226}	$\frac{9 \times 21}{14} + \frac{9 \times 18}{15} + \frac{9 \times 24}{16} + \frac{9 \times 18}{17} + \frac{9 \times 18}{18} + \frac{9 \times 18}{19} + \frac{9 \times 18}{20} + \frac{9 \times 18}{21} + \frac{9 \times 18}{22} +$ $\frac{9 \times 18}{23} + \frac{9 \times 15}{24} + \frac{9 \times 15}{25} + \frac{9 \times 9}{26} + \frac{9 \times 7}{27}$
C_{244}	$\frac{9 \times 12}{15} + \frac{9 \times 24}{16} + \frac{9 \times 18}{17} + \frac{9 \times 18}{18} + \frac{9 \times 18}{19} + \frac{9 \times 18}{20} + \frac{9 \times 18}{21} + \frac{9 \times 18}{22} + \frac{9 \times 18}{23} +$ $\frac{9 \times 18}{24} + \frac{9 \times 18}{25} + \frac{9 \times 15}{26} + \frac{9 \times 15}{27} + \frac{9 \times 9}{28} + \frac{9 \times 7}{29}$

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 ([8]). 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 ([13]). 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

Lemma 2.3 ([14]). The eccentricity of vertices in C_{18n+10} are presented in the following table:

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

As a direct consequence of Lemma 2.1, Lemma 2.2 and 2.3 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 2.7.

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

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

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

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

3 Appendix: A GAP program for computing the eccentric adjacency index of arbitrary graphs

The GAP Groups, Algorithm and Programming is an open source package for computational discrete algebra [10]. The version of GAP used in computations is 4.r.7. To do this, first the molecular graph is drawn by HyperChem software [20] and then the .hin file is loaded into TopoCluj software [4] to obtain adjacency and distance matrices. Second, some GAP codes are utilized for calculating the eccentric adjacency index of the molecular graph by these matrices. Finally, some ordinary interpolation method is applied to find formula for eccentric adjacency index.

A GAP program for computing eccentric adjacency index of arbitrary graphs

```

EAI:=function(A,D) #A is distance matrix      # D is distance matrix
local S,i,t,j,E,f;
S:=[ ];E:=[ ];
for i in D do
    Add(E,1/Maximum(i));

```

```

139         od;
140
141     for i in [1..Size(A)] do
142         t:=0;
143         for j in [1..Size(A)] do
144             if A[i][j]=1 then
145                 t:=t+Sum(A[j]);
146             fi;
147         od;
148
149         Add(S,t);
150     od;
151     f:=E*S;
152     return(f);
153 end;
154
155
156

```

References

- [1] A.R. Ashrafi, M. Ghorbani, Eccentric Connectivity Index of Fullerenes, 2008, In: I. Gutman, B. Furtula, Novel Molecular Structure Descriptors Theory and Applications II, pp. 183–192.
- [2] G. Brinkman, P.W. Fowler, A list of free software for chemical and graph theoretical applications, *MATCH Commun. Math. Comput. Chem.* 58 (2007) 423–430.
- [3] S. Bajaj, S. Sami, A.K. Madan, Topological models for prediction of anti-HIV activity of acylthiocarbamates, *Bioorganic Medicine Chemistry*, 13 (2005) 3263–3268.
- [4] M.V. Diudea, O. Ursu, C.L. Nagy, Topocluj, BabesBolyai Univ., Cluj, 2002.
- [5] T. Došlić and M. Saheli, Augmented eccentric connectivity index of single-defect nanocones, *J. Math. NanoSci.*, 1 (2011) 25–31.
- [6] T. Došlić and M. Saheli, Augmented eccentric connectivity index, *Miskolc Mathematical Notes*, 12 (2) (2011), 149–157.

- 172 [7] H. Dureja and A.K. Madan, Superaugmented eccentric connectivity in-
173 dices: new-generation highly discriminating topological descriptors for
174 QSAR/QSPR modeling, *Med. Chem. Res.*, 16 (2007), 331–341.
- 175 [8] S. Djafari, F. Koorepazan-Moftakhar, A.R. Ashrafi, Eccentric Sequences of
176 Two Infinite Classes of Fullerenes, *Journal of Computational and Theoretical*
177 *Nanoscience*, 10(11) (2013) 2636–2638.
- 178 [9] S. Ediz, The augmented eccentric connectivity index of nanotubes and nan-
179 otori, *J. Math. Nanosci.*, 2(1)(2012) 1–8.
- 180 [10] The GAP Team: GAP Groups, Algorithms and Programming, RWTH,
181 Aachen, 1995.
- 182 [11] M. Ge and K. Sattler, Observation of fullerene cones, *Chem. Phys. Lett.*, 220
183 (1994), 192–196.
- 184 [12] M. Ghorbani, Eccentric connectivity polynomial of C_{12n+4} Fullerenes, *Digest*
185 *Journal of Nanomaterials and Biostructures*, 4(3)(2009), 545–547.
- 186 [13] M. Ghorbani, Kh. Malekjani, A new method for computing the eccentric con-
187 nectivity index of fullerenes, *Serdica J. Comput.*, 6 (2012), 299–308.
- 188 [14] M. Ghorbani, A.R. Ashrafi, and M. Hemmasi, Connective eccentric index of
189 C_{18n+10} fullerenes, *Bulgarian Chem. Comm.*, 45(1)(2013), 5–8.
- 190 [15] M. Ghorbani, Connective eccentric index of fullerenes, *J. Math. Nanosci.*
191 1(2011) 43–50.
- 192 [16] S. Gupta, M. Singh, A.K. Madan, Connective eccentricity Index: A novel
193 topological descriptor for predicting biological activity, *J. Mol. Graph.*
194 *Model.*, 18 (2000), 18–25.
- 195 [17] S. Gupta, M. Singh, A.K. Madan, Predicting anti-HIV activity: computa-
196 tional approach using a novel topological descriptor, *J. Comput. Aided. Mol.*
197 *Des.*, 15(7) (2001), 671–678.
- 198 [18] S. Gupta, M. Singh, and A. K. Madan, Application of graph theory: re-
199 lationship of eccentric connectivity index and Wieners index with anti-
200 inflammatory activity, *J. Math. Anal. Appl.*, 266(2)(2002), 259–268.
- 201 [19] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*,
202 Springer–Verlag, Berlin, 1986.

- 203 [20] HyperChem package Release 7.5 for Windows, Hypercube Inc., 1115 NW
204 4th Street, Gainesville, Florida 32601, USA, 2002.
- 205 [21] H. W. Kroto, J. R. Heath, S. C. ÓBrien, R. F. Curl and R. E. Smalley, C_{60} :
206 Buckminsterfullerene, *Nature*, 318 (1985), 162–163.
- 207 [22] S. Sardana and A. K. Madan, Application of graph theory: relationship of
208 molecular connectivity index, Wiener's index and eccentric connectivity index
209 with diuretic activity, *MATCH Commun. Math. Comput. Chem.*, 43 (2001),
210 85–98.
- 211 [23] R. Sharafadini, Augmented eccentric connectivity index of Fullerenes, *J.*
212 *Math. Nanosci.* 4(1) (2014), 13–18.
- 213 [24] V. Sharma, R. Goswami, and A.K. Madan, Eccentric connectivity index: A
214 novel highly discriminating topological descriptor for structure-property and
215 structure-activity studies, *J. Chem. Inf. Comput. Sci.*, 37 (1997), 273–282.
- 216 [25] M. Songhori, Eccentric connectivity index of fullerene graphs, *J. Math.*
217 *Nanosci.* 2(1), 2012, 21–27.
- 218 [26] D.B. West, Introduction to graph theory, Upper Saddle River, NJ: Prentice
219 Hall, Inc., 1996.
- 220 [27] Z. Yarahmadi, A.R. Ashrafi, S. Moradi, Extremal values of augmented eccen-
221 tric connectivity index of V-phenylenic nanotorus, *Journal of Applied Math-*
222 *ematics and Computing*, 45 (2014), 35–42.
- 223 [28] Z. Yarahmadi, Eccentric connectivity and augmented eccentric connectiv-
224 ity indices of N-branched phenylacetylenes nanostar dendrimers, *Iranian J.*
225 *Math. Chem.*, 1 (2)(2010), 105–110.