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General Topological Indices of Tetrameric 1,3-Adamantane

Research Article

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Abstract: A topological index is a numerical parameter mathematically derived from the graph structure. In this paper, we compute generalized version of the first Zagreb index, general connectivity index, general sum connectivity index, general reformulated index, forgotten topological index, harmonic index, inverse sum indeg index, atom bond connectivity index, augmented Zagreb index and other topological indices for tetrameric 1,3-adamantane.

MSC: 05C05, 05C12, 05C35

Keywords: Zagreb indices, connectivity indices, inverse sum indeg index, F-index, K-edge index, augmented index, tetrameric 1,3 adamantane.

1. Introduction

A molecular graph of a chemical graph is a simple graph related to the structure of a chemical compound. Each vertex of this graph represents an atom of the molecule and its edges to the bonds between atoms. A topological index is a numerical parameter mathematically derived from the graph structure. In Chemical Science, the physico-chemical properties of chemical compounds are often modelled by means of molecular graph based structure descriptors, which are also referred to as topological indices, see [1]. The graph considered here are finite undirected without loops and multiple edges. Let $G = (V, E)$ be a connected graph. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v. The edge connecting vertices u and v will be denoted by uv. Let $d_G(e)$ denote the degree of an edge e = uv in G, which is defined by $d_G(e) = d_G(u) + d_G(v) - 2$. For all further notation and terminology, we refer to reader to [2]. The degree based graph invariants $M_1(G)$ and $M_2(G)$, called Zagreb indices, were introduced by Gutman et al. in [1] and have been extensively studied. The first and second Zagreb indices of a graph G are defined as $M_1(G) = \sum_{u\in V(G)} d_G(u)^2$ or $M_1(G) = \sum_{uv\in E(G)} [d_G(u) + d_G(v)]$ and $M_2(G) = \sum_{uv\in E(G)} d_G(u)\, d_G(v)$. Followed by the first Zagreb index of a graph G, Furtula et al. [3] introduced the so called forgotten topological index or F-index, defined as

$$F(G) = \sum_{u\in V(G)} d_G(u)^3 .$$

The generalized version of the first Zagreb index [4] of a graph G is defined as

$$ZM_1^{a+1}(G) = \sum_{u\in V(G)} d_G(u)^{a+1} = \sum_{uv\in E(G)} [d_G(u)^a + d_G(v)^a] \tag{1}$$

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where a is a real number. The modified first and second Zagreb indices [5] are respectively defined as

$$^{m}M_1(G)=\sum_{u\in V(G)}\frac{1}{d_G(u)^2},\qquad {}^{m}M_2(G)=\sum_{uv\in E(G)}\frac{1}{d_G(u)+d_G(v)}.$$

These indices were studied by Kulli in [6, 7]. In [8], Shirdel et al. introduced the hyper-Zagreb index of a graph G and defined it as

$$HM_1(G)=\sum_{uv\in E(G)}[d_G(u)+d_G(v)]^2.$$

The sum connectivity index of a graph G was proposed by Zhou et al. in [9] and is defined as

$$X(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_G(u)+d_G(v)}}.$$

The harmonic index of a graph G is defined as

$$H(G)=\sum_{uv\in E(G)}\frac{2}{d_G(u)+d_G(v)}.$$

This index was studied by Favaron et al [10] and Zhong [11]. In [12], Zhou et al. proposed the general sum connectivity index of a graph G and defined it as

$$M_1^a(G)=\sum_{uv\in E(G)}[d_G(u)+d_G(v)]^a. \tag{2}$$

This index was also studied, for example, in [13]. One of the best known and widely used topological index is the product connectivity index or Randić index, introduced by Randić in [14]. The product connectivity index is defined as

$$\chi(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_G(u)\,d_G(v)}}.$$

This index was studied, for example, in [15, 16]. The general product connectivity index [13, 17] is defined as

$$M_2^a(G)=\sum_{uv\in E(G)}[d_G(u)\,d_G(v)]^a. \tag{3}$$

In [18], Miličević et al. proposed the reformulated first Zagreb index of a graph G and defined it as

$$EM_1(G)=\sum_{e\in E(G)}d_G(e)^2.$$

In [19], Kulli introduced the K-edge index of a graph G and defined it as

$$K_e(G)=\sum_{e\in E(G)}d_G(e)^3.$$

This index was also studied, for example, in [20]. The general reformulated Zagreb index [21] of a graph G is defined as

$$EM_1^a(G)=\sum_{e\in E(G)}d_G(e)^a. \tag{4}$$

The inverse sum indeg index is the descriptor that was selected in [21] as a significant predictor of total surface area of octane isomers and for which the extremal graphs obtained with the help of Mathematical Chemistry have a particularly simple and elegant structure. The inverse sum indeg index of a graph G is defined as

$$ISI\,(G) = \sum_{uv \in E(G)} \frac{d_G\,(u)\,d_G\,(v)}{d_G\,(u) + d_G\,(v)}. \tag{5}$$

This index was studied, for example, in [23]. In [24], Estrada et al. defined the atom bond connectivity index which stated as

$$ABC\,(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_G\,(u) + d_G\,(v) - 2}{d_G\,(u)\,d_G\,(v)}}. \tag{6}$$

The following graph invariant has proved to be a valuable predictive index in the study of the heat of formation in octanes and heptanes (see [25]), whose prediction power is better than atom bond connectivity index (see [26]). The augmented Zagreb index of a graph G was introduced by Furtula et al. in [25] and is defined as

$$AZI\,(G) = \sum_{uv \in E(G)} \left(\frac{d_G\,(u)\,d_G\,(v)}{d_G\,(u) + d_G\,(v) - 2}\right)^3. \tag{7}$$

In this paper, we consider the tetrameric 1,3-adamantane and determine several topological indices of tetrameric 1,3-adamantane.

2. Results for Tetrameric 1,3-Adamantane

In chemistry, diamandoids are variants of the carbon cage known as adamantane ($C_{10}H_{16}$), the smallest unit cage structure of the diamond crystal lattice. We focus on the molecular graph structure of the family of Tetrameric 1,3-Adamantane, denoted $TA[n]$. The graph of tetrameric 1,3-adamantane $TA[4]$ is shown in Figure 1, see [27].

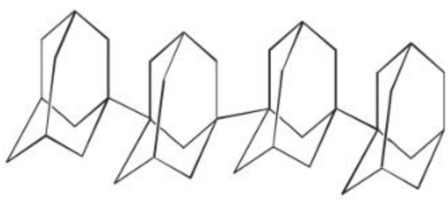

Figure 1. **The graph of tetrameric 1,3-adamantane *TA* [4]**

By algebraic method, we obtain $|V(TA[n])| = 10n$ and $|E(TA[n])| = 13n - 1$. From Figure 1, it is easy to see that there are three partitions of the vertex set of $TA[n]$ as follows: Let G be the graph of $TA[n]$.

$$V_2 = \{u \in V(G) | d_G(u) = 2\}, \ \ |V_2| = 6n.$$

$$V_3 = \{u = V(G) | d_G(u) = 3\}, \ \ |V_3| = 2n + 2.$$

$$V_4 = \{u = V(G) | d_G(u) = 4\}, \ \ |V_4| = 2n - 2.$$

Also by algebraic method, we obtain three edge partitions of G ($=TA[n]$) based on the sum of the degrees of the end vertices of each edge (or the product of the degrees of the end vertices of each edge) as follows:

$$E_5 = E_6^* = \{uv \in E(G) | d_G(u) = 2, d_G(v) = 3\}, \ \ |E_5| = |E_6^*| = 6n + 6.$$

$$E_6 = E_8^* = \{uv \in E(G) | d_G(u) = 2, d_G(v) = 4\}, \ \ |E_6| = |E_8^*| = 6n - 6.$$

$$E_8 = E_{16}^* = \{uv \in E(G) | d_G(u) = d_G(v) = 4\}, \ \ |E_6| = |E_{16}^*| = n - 1.$$

The edge degree partition of G is given in Table 1.

$d_G(u), d_G(v) \backslash uv \in E(G)$	(2, 3)	(2, 4)	(4, 4)
$d_G(e)$,	3	4	6
Number of edges	$6n+6$	$6n-6$	$n-1$

Table 1. **Edge degree partition of** $TA[n]$

Theorem 2.1. *The generalized version of the first Zagreb index of TA[n] is given by*

$$ZM_1^{a+1}(TA[n]) = \left(3 \times 2^{a+1} + 3^{a+1} + 4^{a+1}\right) 2n + \left(3^{a+1} - 4^{a+1}\right) 2. \quad (8)$$

Proof. Let $G = TA[n]$. From equation (1) and by cardinalities of the vertex partition of $TA[n]$, we have

$$\begin{aligned} ZM_1^{a+1}(TA[n]) &= \sum_{u \in V(G)} d_G(u)^{a+1} \\ &= \sum_{u \in V_2} d_G(u)^{a+1} + \sum_{u \in V_3} d_G(u)^{a+1} + \sum_{u \in V_4} d_G(u)^{a+1} \\ &= 2^{a+1} 6n + 3^{a+1}(2n+2) + 4^{a+1}(2n-2) \\ &= \left(3 \times 2^{a+1} + 3^{a+1} + 4^{a+1}\right) 2n + \left(3^{a+1} - 4^{a+1}\right) 2. \end{aligned}$$

□

We obtain the following results by using Theorem 2.1.

Corollary 2.2. *The first Zagreb index of TA[n] is given by* $M_1(TA[n]) = 74n - 14$.

Proof. Put $a = 1$ in equation (8), we get the desired result. □

Corollary 2.3. *The F-index of TA[n] is given by* $F(TA[n]) = 230n - 74$.

Proof. Put $a = 2$ in equation (8), we get the desired result. □

Corollary 2.4. *The modified first Zagreb index of* $TA[n]$ *is given by* ${}^mM_1(TA[n]) = \frac{1}{72}(133n + 7)$.

Proof. Put $a = -3$ in equation (8), we get the desired result. □

In the following theorem, we compute the general sum connectivity index of $TA[n]$.

Theorem 2.5. *The general sum connectivity index of TA[n] is given by*

$$M_1^a(TA[n]) = (6 \times 5^a + 6 \times 6^a + 8^a)\, n + (6 \times 5^a - 6 \times 6^a - 8^a). \quad (9)$$

Proof. Let $G = TA[n]$. From equation (2) and by cardinalities of the edge partition of $TA[n]$, we have

$$\begin{aligned} M_1^a(TA[n]) &= \sum_{uv \in E(G)} [d_G(u) + d_G(v)]^a \\ &= \sum_{uv \in E_5} [d_G(u) + d_G(v)]^a + \sum_{uv \in E_6} [d_G(u) + d_G(v)]^a + \sum_{uv \in E_8} [d_G(u) + d_G(v)]^a \\ &= 5^a(6n+6) + 6^a(6n-6) + 8^a(n-1) \\ &= (6 \times 5^a + 6 \times 6^a + 8^a)\, n + (6 \times 5^a - 6 \times 6^a - 8^a). \end{aligned}$$

□

We obtain the following corollaries by using Theorem 2.5.

Corollary 2.6. *The first zegreb index of TA[n] is given by* $M_1(TA[n] = 74n - 14$.

Proof. Put $a = 1$ in equation (9), we get the desired result. □

Corollary 2.7. *The hyper-Zagreb index of TA[n] is given by* $HM_1(TA[n]) = 430n - 130$.

Proof. Put $a = 2$ in equation (9), we get the desired result. □

Corollary 2.8. *The sum connectivity index of TA[n] is given by*

$$X(TA[n]) = \left(\frac{6}{\sqrt{5}} + \frac{6}{\sqrt{6}} + \frac{1}{2\sqrt{2}}\right) n + \left(\frac{6}{\sqrt{5}} - \frac{6}{\sqrt{6}} - \frac{1}{2\sqrt{2}}\right)$$

Proof. Put $a = -\frac{1}{2}$ in equation (9), we get the desired result. □

In the following theorem, we compute the general product connectivity index of $TA[n]$.

Theorem 2.9. *The general product connectivity index of TA[n] is given by*

$$M_2^a\left(TA\left[n\right]\right) = \left(6 \times 6^a + 6 \times 8^a + 16^a\right) n + \left(6 \times 6^a - 6 \times 8^a - 16^a\right). \tag{10}$$

Proof. Let $G = TA[n]$. From equation (3) and by coordinates of the edge partition of $TA[n]$ based on the product degrees of the end vertices of each edge, we have

$$\begin{aligned} M_2^a\left(TA\left[n\right]\right) &= \sum_{uv \in (G)} \left[d_G\left(u\right) d_G\left(v\right)\right]^a \\ &= \sum_{uv \in E_6^*} \left[d_G\left(u\right) d_G\left(v\right)\right]^a + \sum_{uv \in E_8^*} \left[d_G\left(u\right) d_G\left(v\right)\right]^a + \sum_{uv \in E_{16}^*} \left[d_G\left(u\right) d_G\left(v\right)\right]^a \\ &= 6^a\left(6n + 6\right) + 8^a\left(6n - 6\right) + 16^a\left(n - 1\right) \\ &= \left(6 \times 6^a + 6 \times 8^a + 16^a\right) n + \left(6 \times 6^a - 6 \times 8^a - 16^a\right). \end{aligned}$$

□

We now obtain the following corollaries by using Theorem 2.9.

Corollary 2.10. *The second Zagreb index of TA[n] is given by* $M_2(TA[n]) = 100n - 28$.

Proof. Put $a = 1$ in equation (10), we get the desired result. □

Corollary 2.11. *The modified second Zagreb index of TA[n] is given by* ${}^mM_2(TA[n]) = \frac{29}{16}n + \frac{3}{16}$.

Proof. Put $a = -1$ in equation (10), we get the desired result. □

Corollary 2.12. *The product connectivity index of TA[n] is given by*

$$\chi(TA[n]) = \left(\sqrt{6} + \frac{3}{\sqrt{2}} + \frac{1}{4}\right) n + \left(\sqrt{6} - \frac{3}{\sqrt{2}} - \frac{1}{4}\right).$$

Proof. Put $a = -\frac{1}{2}$ in equation (10), we get the desired result. □

In the next theorem, we compute the general first reformulated Zagreb index of $TA[n]$.

Theorem 2.13. *The general first reformulated Zagreb index of TA[n] is given by*

$$EM_1^a(TA[n]) = (6\times 3^a + 6\times 4^a + 6^a)\,n + (6\times 3^a - 6\times 4^a - 6^a). \tag{11}$$

Proof. Let $G = TA[n]$. From equation (4) and by cardinalities of the edge partition of $TA[n]$, we have

$$\begin{aligned} EM_1^a(TA[n]) &= \sum_{e\in E(G)} d_G(e)^a \\ &= \sum_{e\in E_5} d_G(e)^a + \sum_{e\in E_6} d_G(e)^a + \sum_{e\in E_8} d_G(e)^a \\ &= 3^a(6n+6) + 4^a(6n-6) + 6^a(n-1) \\ &= (6\times 3^a + 6\times 4^a + 6^a)\,n + (6\times 3^a - 6\times 4^a - 6^a). \end{aligned}$$

□

We obtain the following results by using Theorem 2.13.

Corollary 2.14. *The first reformulated Zagreb index of TA[n] is given by* $EM_1(TA[n]) = 186n - 78$.

Proof. Put $a = 2$ in equation (11), we get the desired result. □

Corollary 2.15. *The K-edge index of TA[n] is given by* $K_e(TA[n]) = 762n - 438$.

Proof. Put $a = 3$ in equation (11), we get the desired result. □

Theorem 2.16. *The harmonic index of TA[n] is given by* $H(G) = \frac{113}{20}n - \frac{17}{20}$.

Proof. Let $G = TA[n]$. By definition and by cardinalities of the edge partition of $TA[n]$, we have

$$\begin{aligned} H(G) &= \sum_{uv\in E(G)} \frac{2}{d_G(u)+d_G(v)} \\ &= (6n+6)\left(\frac{2}{2+3}\right) + (6n-6)\left(\frac{2}{2+4}\right) + (n-1)\left(\frac{2}{4+4}\right) = \frac{113}{20}n - \frac{17}{20}. \end{aligned}$$

□

Theorem 2.17. *The inverse sum indeg index of TA[n] is given by* $ISI(TA[n]) = \frac{86}{5}n - \frac{14}{5}$.

Proof. Let $G = TA[n]$. From equation (5) and by cardinalities of the edge partition of $TA[n]$, we have

$$\begin{aligned} ISI(TA[n]) &= \sum_{uv\in E(G)} \frac{d_G(u)\,d_G(v)}{d_G(u)+d_G(v)} \\ &= (6n+6)\left(\frac{2\times 3}{2+3}\right) + (6n-6)\left(\frac{2\times 4}{2+4}\right) + (n-1)\left(\frac{4\times 4}{4+4}\right) \\ &= \frac{86}{5}n - \frac{14}{5}. \end{aligned}$$

□

Theorem 2.18. *The atom bond connectivity index of TA[n] is given by*

$$ABC(TA[n]) = \left(\frac{12}{\sqrt{2}} + \frac{3}{2\sqrt{2}}\right)n - \frac{\sqrt{3}}{2\sqrt{2}}.$$

Proof. Let $G = TA[n]$. From equation (6) and by cardinalities of the edge partition of $TA[n]$, we have

$$\begin{aligned} ABC(TA[n]) &= \sum_{uv \in E(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u) d_G(v)}} \\ &= (6n+6)\sqrt{\frac{2+3-2}{2\times 3}} + (6n-6)\sqrt{\frac{2+4-2}{2\times 4}} + (n-1)\sqrt{\frac{4+4-2}{4\times 4}} \\ &= \left(\frac{12}{\sqrt{2}} + \frac{\sqrt{3}}{2\sqrt{2}}\right)n - \frac{\sqrt{3}}{2\sqrt{2}}. \end{aligned}$$

□

Theorem 2.19. *The augmented Zagreb index of TA[n] is given by*

$$AZI(TA[n]) = \left(96 + \frac{512}{27}\right)n - \frac{512}{27}.$$

Proof. Let $G = TA[n]$. From equation (7) and by cardinalities of the edge partition of $TA[n]$, we have

$$\begin{aligned} AZI(TA[n]) &= \sum_{uv \in E(G)} \left(\frac{d_G(u) d_G(v)}{d_G(u) + d_G(v) - 2}\right)^3 \\ &= (6n+6)\left(\frac{2\times 3}{2+3-2}\right)^3 + (6n-6)\left(\frac{2\times 4}{2+4-2}\right)^3 + (n-1)\left(\frac{4\times 4}{4+4-2}\right)^3 \\ &= \left(96 + \frac{512}{27}\right)n - \frac{512}{27}. \end{aligned}$$

□

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