

# On Multiple Zagreb indices of a family of Hexagonal Nanotubes

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## ABSTRACT

The First and Second Zagreb indices were first introduced by *I. Gutman* and *N. Trinajstić* in 1972. It is reported that these indices are useful in the study of anti-inflammatory activities of certain chemical instances, and in elsewhere. Recently, the First and Second Multiple Zagreb indices of a graph  $G$ , were introduced by *M. Ghorbani* and his co-authors in 2012. In this paper, we computed these new multiple Zagreb topological indices of a family of Hexagonal Nanotubes namely: *Armchair Polyhex Nanotubes*.

**Keywords:** Topological indices, Zagreb indices, Multiple Zagreb indices, Armchair Polyhex Nanotubes.

## 1. INTRODUCTION

Let  $G=(V,E)$  is an arbitrary simple, connected, graph, with the vertex set  $V(G)$  and edge set  $E(G)$ . A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. In chemical graph theory, we have many invariant polynomials and topological indices for a molecular graph. A topological index is a numerical value for correlation of chemical structure with various physical properties, chemical reactivity or biological activity [1-4].

A pair of molecular descriptors (or topological index), known as the *First Zagreb index*  $M_1(G)$  and the *Second Zagreb index*  $M_2(G)$  [4], first appeared in the topological formula for the total  $\pi$ -energy of conjugated molecules that has been derived in 1972 by *I. Gutman* and *N. Trinajstić* [4]. Soon after these indices have been used as branching indices [1-7]. Later the Zagreb indices found applications in QSPR and QSAR studies [4-12].

For a simple molecular graph  $G=(V,E)$  with the vertex\atom and the edge\bond sets  $V(G)$  and  $E(G)$ , the first and second Zagreb indices are given by:

$$M_1(G) = \sum_{v \in V(G)} d_v^2 = \sum_{e=uv \in E(G)} (d_u + d_v)$$
$$M_2(G) = \sum_{e=uv \in E(G)} (d_u \times d_v)$$

respectively, where  $d_v$  denotes the degree (number of first neighbors) of vertex  $v$  in  $G$ .

41 In (2012), *M. Ghorbani* and his co-authors [13] defined the *Multiple Zagreb* topological  
 42 indices of a graph  $G$ , based on degree of vertices of  $G$  as :

43  
 44 
$$PM_1(G) = \prod_{e=uv \in E(G)} (d_u + d_v)$$

45 
$$PM_2(G) = \prod_{e=uv \in E(G)} (d_u \times d_v)$$

46  
 47 Properties of the first and second Zagreb indices and the first and second Multiple Zagreb  
 48 indices may be found in a number of reports [14-40].

49 In this paper, we computed these new multiple Zagreb topological indices of a family of  
 50 Hexagonal Nanotubes namely: *Armchair Polyhex Nanotubes*  $TUAC_6$ . The **3-Dimensional**  
 51 and 2-Dimensional lattices of this family of Hexagonal Nanotubes are shown in Figures 1  
 52 and 2.  
 53



54  
 55 **Fig. 1. The 3-Dimensional Lattice of Armchair Polyhex Nanotubes  $TUAC_6[m,n]$**   
 56  **$(\forall m, n \in \mathbb{N})$ .**

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### 59 3. RESULTS AND DISCUSSION

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61 In this section, we focus on the structure of molecular graph "*Armchair Polyhex Nanotubes*  
 62  $TUAC_6$ " and compute its First and Second Multiple Zagreb indices.

63 Let  $TUAC_6[m,n]$  be the Armchair Polyhex Nanotubes and we denote the number of  
 64 hexagons in the first row/column of the **3-Dimensional** and 2-Dimensional lattices of (see  
 65 **Figures 1 and 2**) by  $m$  and  $n$  ( $\forall m, n \in \mathbb{N}$ ), respectively. For more historical details of families of  
 66 Hexagonal Nanotubes and especially Armchair Polyhex Nanotubes  $TUAC_6[m,n]$ , see papers  
 67 [41-51].  
 68

69 **Theorem 1.** [51] Let  $TUAC_6[m,n]$   $\forall m, n \in \mathbb{N}$ , be the Armchair Polyhex Nanotubes. Then:

70

71 • The First Zagreb index of  $TUAC_6[m,n]$  is equal to  
 72  $M_1(TUAC_6[m,n]) = 18mn + 8m$

73

74 • The Second Zagreb index of  $TUAC_6[m,n]$  is equal to  
 75  $M_2(TUAC_6[m,n]) = 27mn + 7m$

76 **Theorem 2.** Let  $TUAC_6[m,n]$   $\forall m, n \in \mathbb{N}$ , be the Armchair Polyhex Nanotubes. Then:

77

• The First Multiple Zagreb index of  $TUAC_6[m,n]$  is equal to

$$PM_1(TUAC_6[m,n]) = (2)^{2m} + (5)^{2m} + (6)^{3mn-m}$$

- The Second Multiple Zagreb index of  $TUAC_6[m,n]$  is equal to  
 $PM_2(TUAC_6[m,n]) = (2)^{2m} + (6)^{2m} + (3)^{2(3mn-m)}$

Before presenting the main results, let us introduce some definitions as:

**Definition 1.** [51] Let  $G$  and  $\forall v \in V(G)$ ,  $d_v$  ( $1 \leq d_v \leq n-1$ ) be a simple connected molecular graph and the vertex degrees of vertices/atom  $v$  in  $G$ . We divide the vertex set  $V(G)$  and edge set  $E(G)$  of  $G$  into several partitions based on  $d_v$  as follows

$$\forall k: \delta \leq k \leq \Delta, V_k = \{v \in V(G) | d_v = k\}$$

$$\forall i: 2\delta \leq i \leq 2\Delta, E_i = \{e = uv \in E(G) | d_u + d_v = i\}$$

$$\forall j: \delta^2 \leq j \leq \Delta^2, E_j^* = \{e = uv \in E(G) | d_u \times d_v = j\}.$$

where  $\delta$  and  $\Delta$  are the minimum and maximum, respectively of  $d_v$  for all  $v \in V(G)$ .

Obviously, in an arbitrary nanostructure  $G$  the degree of a vertex/atom is equal to 1, 2 or 3. Such that Hydrogen atoms in molecular graphs are often omitted. Therefore,

$$V_3 = \{v \in V(G) | d_v = 3\}$$

$$V_2 = \{v \in V(G) | d_v = 2\}$$

$$E_4 = E_4^* = \{e = uv \in E(G) | d_u = d_v = 2\}$$

$$E_5 = E_6^* = \{e = uv \in E(G) | d_u = 2 \text{ \& } d_v = 3\}$$

$$E_6 = E_9^* = \{e = uv \in E(G) | d_u = d_v = 3\}.$$

such that  $V(G) = \bigcup_{i=\delta}^{\Delta} V_i(G)$ ,  $E(G) = \bigcup_i E_i(G) = \bigcup_j E_j^*(G)$

Now, by these preliminaries, we start the proof of *Theorem 2*.

**Proof of Theorem 2.** Consider the Armchair Polyhex Nanotubes  $TUAC_6[m,n]$  ( $\forall m, n \in \mathbb{N}$ ). There are  $2m(n+1)$  vertices/atoms in this Nanotubes. According to Figure 2,

$|V_2| = 2\frac{m}{2} + 2\frac{m}{2} = 2m$  and  $|V_3| = 2mn$ . These imply that for every Armchair Polyhex Nanotubes

$TUAC_6[m,n]$  has  $\frac{1}{2}[2(2m) + 3(2mn)] = 3mn + 2m$  number of edges/bonds ( $|E(TUAC_6[m,n])|$ ).

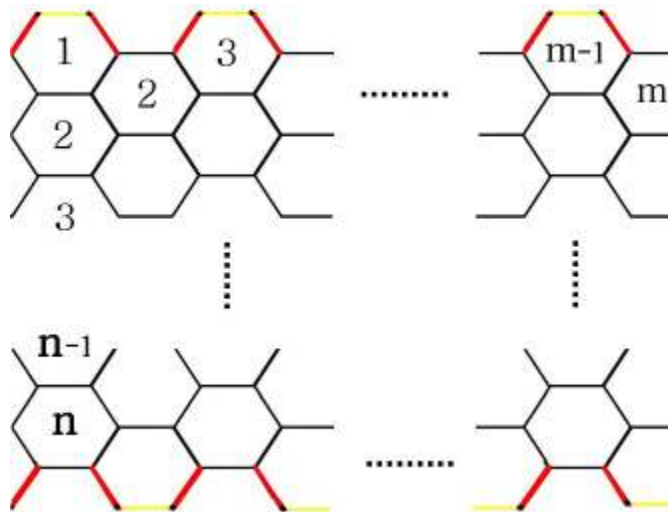


**Fig 2. A general form of the Armchair Polyhex Nanotubes  $TUAC_6[m,n]$  ( $\forall m, n \in \mathbb{N}$ ) [51].**

112  
113 By according to Definition 1, we mark the general **2-Dimensional** lattice form of the Armchair  
114 Polyhex Nanotubes  $TUAC_6[m,n]$  as follow:

115  
116 All members of  $E_4, E_4^*$  by yellow color, all members of  $E_5, E_6^*$  by red color and all members of  
117  $E_6, E_9^*$  by black color. Thus from Figure 2, the size of these six edge sets are equal to

118 
$$|E_4|=|E_4^*|=\frac{m}{2}+\frac{m}{2}=m$$

119  $|E_5|=|E_6^*|=2|E_4|=2m$

120 and  $|E_6|=|E_9^*|=3mn-m.$

121  
122 Therefore, the first Multiple Zagreb indices of the Armchair Polyhex Nanotubes  $TUAC_6[m,n]$   
123 ( $\forall m,n \in \mathbb{N}$ ) are equal to:

124  
125 
$$PM_1(TUAC_6[m,n]) = \prod_{uv \in E(TUAC_6[m,n])} (d_v + d_v)$$
  
126 
$$= \prod_{uv \in E_4} (d_v + d_v) + \prod_{uv \in E_5} (d_v + d_v) + \prod_{uv \in E_6} (d_v + d_v)$$
  
127 
$$= (2)^{2m} + (5)^{2m} + (6)^{3mn-m}$$

128  
129 And the second Multiple Zagreb index is

130  
131 
$$PM_2(TUAC_6[m,n]) = \prod_{uv \in E(TUAC_6[m,n])} (d_v \times d_v)$$
  
132 
$$= \prod_{uv \in E_4} (d_v \times d_v) + \prod_{uv \in E_5} (d_v \times d_v) + \prod_{uv \in E_6} (d_v \times d_v)$$
  
133 
$$= (2)^{2m} + (6)^{2m} + (3)^{2(3mn-m)}$$

134  
135 Here, the proof of Theorem 2 be completed. ■

#### 136 137 138 4. CONCLUSION

139  
140 In this report, we study some properties of new Zagreb indices of (molecular) graphs that  
141 called the Multiple Zagreb indices. The *Multiple Zagreb* topological indices was proposed by  
142 M. Ghorbani and his co-authors [13] in 2012, and was defined as  $PM_1(G) = \prod_{e=uv \in E(G)} (d_u + d_v)$

143 and  $PM_2(G) = \prod_{e=uv \in E(G)} (d_u \times d_v)$ , where  $d_v$  denotes the degree (number of first neighbors) of

144 vertex  $v$  in  $G$ . In continue, closed analytical formulas for  $PM_1$  and  $PM_2$  indices of a physico  
145 chemical structure "Armchair Polyhex Nanotubes  $TUAC_6[m,n]$ ".

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