

On Multiple Zagreb indices of a family of Hexagonal Nanotubes

Mohammad Reza Farahani^{1*}

¹ Department of Applied Mathematics of Iran University of Science and Technology (IUST),
Narmak, Tehran 16844, Iran.

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 π -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 **$(\forall m, n \in \mathbb{N})$.**
 57
 58

59 3. RESULTS AND DISCUSSION

60
 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 δ and Δ 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 ($|E(TUAC_6[m,n])|$).

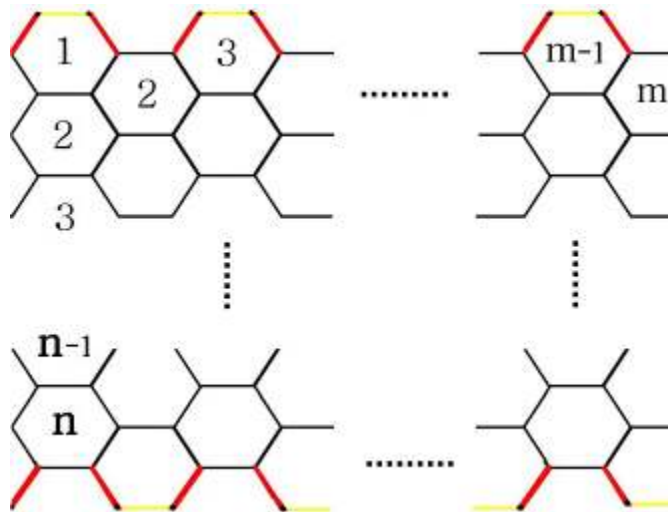


Fig 2. A general form of the Armchair Polyhex Nanotubes $TUAC_6[m,n]$ ($\forall m, n \in \mathbb{N}$) [51].

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
$$PM_1(TUAC_6[m,n]) = \prod_{uv \in E(TUAC_6[m,n])} (d_u + d_v)$$

126
$$= \prod_{uv \in E_4} (d_u + d_v) + \prod_{uv \in E_5} (d_u + d_v) + \prod_{uv \in E_6} (d_u + d_v)$$

127
$$= (2)^{2m} + (5)^{2m} + (6)^{3mn-m}$$

128
129 And the second Multiple Zagreb index is

130
131
$$PM_2(TUAC_6[m,n]) = \prod_{uv \in E(TUAC_6[m,n])} (d_u \times d_v)$$

132
$$= \prod_{uv \in E_4} (d_u \times d_v) + \prod_{uv \in E_5} (d_u \times d_v) + \prod_{uv \in E_6} (d_u \times d_v)$$

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 $TUAC_6[m,n]$ ".

146 147 148 REFERENCES

- 149
150 1. D.B. West. An Introduction to Graph Theory. Prentice-Hall. (1996).
151 2. R. Todeschini and V. Consonni. Handbook of Molecular Descriptors. Wiley, Weinheim.
152 (2000).
153 3. N. Trinajstić. Chemical Graph Theory. CRC Press, Boca Raton, FL. (1992).

- 154 4. I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. III. Total π -electron energy
155 of alternant hydrocarbons. *Chem. Phys. Lett.* 17, 535-538 (1972).
156 5. I. Gutman, B. Rušćić, N. Trinajstić, C.F. Wilcox, Graph theory and molecular orbitals. XII.
157 Acyclic polyenes. *J. Phys. Chem.* 62, 3399-3405 (1975).
158 6. A.T. Balaban, From Chemical Topology to Three-Dimensional Geometry, Plenum Press,
159 New York, (1997).
160 7. J. Devillers, A.T. Balaban (eds.), Topological Indices and Related Descriptors in QSAR
161 and QSPR (Gordon & Breach, Amsterdam, 1999)
162 8. M.V. Diudea, (Ed.), *QSPR/QSAR Studies by Molecular Descriptors*, NOVA, New York,
163 (2001).
164 9. M.V. Diudea, I. Gutman and L. Jäntschi, *Molecular Topology*, NOVA, New York, (2002).
165 10. M.V. Diudea, M.S. Florescu and P.V. Khadikar, *Molecular Topology and Its Applications*,
166 EFICON, Bucharest, (2006).
167 11. I. Gutman and O.E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer-
168 Verlag, New York, 1986.
169 12. M.A. Johnson and G.M. Maggiora, *Concepts and Applications of Molecular Similarity*,
170 Wiley Interscience, New York, 1990.
171 13. M. Ghorbani and N. Azimi. Note on multiple Zagreb indices. *Iranian Journal of*
172 *Mathematical Chemistry*, 3(2), (2012), 137-143.
173 14. I. Gutman and M. Ghorbani, Some properties of the Narumi-Katayama index, *Appl.*
174 *Math. Lett.* (2012), 25, 1435-1438.
175 15. I. Gutman, K.C. Das, The first Zagreb index 30 years after. *MATCH Commun. Math.*
176 *Comput. Chem.* 50, 83-92 (2004).
177 16. M. Ghorbani, M. Songhori and I. Gutman, Modified Narumi-Katayama index, *Kragujevac*
178 *J. Sci.* (2012), 34, 57-64.
179 17. T. Došlić, On Discriminativity of Zagreb Indices, *Iranian J. Math. Chem.* (2012), 3(1), 25-
180 34.
181 18. A. AstanehAsl and G.H. FathTabar, Computing the first and third Zagreb polynomials of
182 Cartesian product of graphs, *Iranian J. Math. Chem.* (2011), 2(2), 73-78.
183 19. K. Xu, K.Ch. Das. Trees, Unicyclic, and Bicyclic Graphs Extremal with Respect to
184 Multiplicative Sum Zagreb Index. *MATCH Commun. Math. Comput. Chem.* 68 (2012))
185 257-272.
186 20. M. Eliasi, A. Iranmanesh, I. Gutman. Multiplicative Versions of First Zagreb Index.
187 *MATCH Commun. Math. Comput. Chem.* 68 (2012)) 217-230.
188 21. B. Bollobás, P. Erdős, Graphs of extremal weights. *Ars Combin.* 50, 225-233 (1998).
189 22. S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, The Zagreb indices 30 years after.
190 *Croat. Chem. Acta* 76, 113-124 (2003).
191 23. K.C. Das, I. Gutman, Some properties of of the second Zagreb index. *MATCH Commun.*
192 *Math. Comput. Chem.* 52, 103-112 (2004).
193 24. D. Janežič, A. Miličević, S. Nikolić, N. Trinajstić, D. Vukičević, Zagreb indices: extension
194 to weighted graphs representing molecules containing heteroatoms. *Croat. Chem. Acta*
195 80, 541-545 (2007).
196 25. D. Vukičević, S.M. Rajtmajer, N. Trinajstić, Trees with maximal second Zagreb index and
197 prescribed number of vertices of the given degree. *MATCH Commun. Math. Comput.*
198 *Chem.* 60, 65-70 (2008).
199 26. D. Vukičević, S. Nikolić, N. Trinajstić, On the path-Zagrebmatrix. *J.Math. Chem.* 45, 538-
200 543 (2009).
201 27. D. Vukičević, N. Trinajstić, On the discriminatory power of the Zagreb indices for
202 molecular graphs. *MATCH Commun. Math. Comput. Chem.* 53, 111-138 (2005).

- 203 28. B. Zhou, Zagreb indices. *MATCH Commun. Math. Comput. Chem.* 52, 113-118 (2004).
- 204 29. B. Zhou, I. Gutman, Further properties of Zagreb indices. *MATCH Commun. Math.*
- 205 *Comput. Chem.* 54, 233-239 (2005).
- 206 30. B. Zhou and N. Trinajstić. Some properties of the reformulated Zagreb indices. *J. Math.*
- 207 *Chem.* 48, (2010), 714-719.
- 208 31. B. Zhou, D. Stevanović, A note on Zagreb indices. *MATCH Commun. Math. Comput.*
- 209 *Chem.* 56, 571-578 (2006).
- 210 32. B. Zhou, Upper bounds for the Zagreb indices and the spectral radius of series-parallel
- 211 graphs. *Int. J. Quantum Chem.* 107, 875-878 (2007).
- 212 33. B. Zhou, Remarks on Zagreb indices. *MATCH Commun. Math. Comput. Chem.* 57, 591-
- 213 596 (2007).
- 214 34. M.R. Farahani. Zagreb index, Zagreb Polynomial of Circumcoronene Series of
- 215 Benzenoid. *Advances in Materials and Corrosion.* 2, (2013), 16-19.
- 216 35. M.R. Farahani and M.P.Vlad. Computing First and Second Zagreb index, First and
- 217 Second Zagreb Polynomial of Capra-designed planar benzenoid series $Ca_n(C_6)$. *Studia*
- 218 *Universitatis Babes-Bolyai Chemia.* 58(2), (2013), 133-142.
- 219 36. M.R. Farahani. The First And Second Zagreb Indices, First And Second Zagreb
- 220 Polynomials Of $HAC_5C_6C_7[p,q]$ And $HAC_5C_7[p,q]$ Nanotubes. *Int. J. Nanosci.*
- 221 *Nanotechnol.* 8(3), Sep. (2012), 175-180.
- 222 37. M.R. Farahani. First and Second Zagreb polynomials of $VC_5C_7[p,q]$ and $HC_5C_7[p,q]$
- 223 nanotubes. *Int. Letters of Chemistry, Physics and Astronomy.* 12, (2014), 56-62.
- 224 38. M.R. Farahani. Zagreb Indices and Zagreb Polynomials of Pent-Heptagon Nanotube
- 225 $VAC_5C_7(S)$ *Chemical Physics Research Journal.* 6(1), (2013), 35-40.
- 226 39. M.R. Farahani. Zagreb Indices and Zagreb Polynomials of Polycyclic Aromatic
- 227 Hydrocarbons PAHs. *Journal of Chemica Acta.* 2, (2013), 70-72.
- 228 40. M.R. Farahani, Some Connectivity index of an infinite class of Dendrimer Nanostars.
- 229 *Romanian Academy Seri B.* 15(3), (2014). In press.
- 230 41. M.V. Diudea, *MATCH, Commun. Math. Comput. Chem.* (2002), 45, 109-122.
- 231 42. A.R. Ashrafi and G.R. Vakili-Nezhaad, Computing the PI index of some chemical graphs
- 232 related to nanostructures, *Journal of Physics: Conference Series*, 29, (2006), 181-184.
- 233 43. A.S. Yousefi, H. Yousefi-Azari, A.R. Ashrafi and M. H. Khalifeh, Computing Wiener and
- 234 Szeged Indices of an Achiral Polyhex Nanotorus. *JSUT*, (2008), 33, 3, 7-11.
- 235 44. A. Iranmanesh and Y. Alizadeh, *Digest. J. Nanomater. Bios*, (2009), 4, 607-611.
- 236 45. H. Shabani and A.R. Ashrafi, *Digest. J. Nanomater. Bios*, (2009), 4, 423-428.
- 237 46. S. Alikhani and M.A. Iranmanesh, Chromatic Polynomials of Some Nanotubes. *Digest. J.*
- 238 *Nanomater. Bios*, (2010), 5, 1-7.
- 239 47. M.R. Farahani. Fifth Geometric-Arithmetic Index of Polyhex Zigzag $TUZC_6[m,n]$
- 240 Nanotube and Nanotori. *Journal of Advances in Physics.* 3(1), (2013), 191-196.
- 241 48. M.R. Farahani. Computing GA_5 Index of Armchair Polyhex Nanotube, *Le Matematiche.*
- 242 69(2), (2014), 69-76.
- 243 49. M.R. Farahani, On the Fourth atom-bond connectivity index of Armchair Polyhex
- 244 Nanotubes. *Proc. Rom. Acad. Series B*, 15(1), (2013), 3-6.
- 245 50. M.R. Farahani. The second-connectivity and second-sum-connectivity indices of
- 246 Armchair Polyhex Nanotubes $TUAC_6[m,n]$. *Int. Letters of Chemistry, Physics and*
- 247 *Astronomy.* 11(1), (2014), 74-80.
- 248 51. M.R. Farahani. Some Connectivity Indices and Zagreb Index of Polyhex Nanotubes.
- 249 *Acta Chim. Slov.* 59, 779-783 (2012).