The Generalized Zagreb index of the Armchair Polyhex Nanotubes

TUAC_6[m,n]

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

Abstract
Let G=(V,E) be a simple connected graph with vertices set and edges set V=V(G) and E=E(G), respectively. The First and Second Zagreb indices were first introduced by I. Gutman and N. Trinajstić in 1972 as $M_1(G)=\sum_{v \in V(G)} d_v^2$ and $M_2(G)=\sum_{e \in E(G)} (d_u \times d_v)$, respectively. Recently, the Generalized Zagreb index of a graph G was introduced by A. Iranmanesh and M. Azari as $M_{r,s}(G)=\sum_{e \in E(G)} (d_u^r \times d_v^s + d_u^s \times d_v^r)$. In this paper, we focus on the structure of Nanotube "Armchair Polyhex Nanotubes TUAC_6[m,n]" ($\forall m,n \in \mathbb{N}$) and compute its Generalized Zagreb index.

Indexing terms/Keywords
Molecular graph; Armchair Polyhex Nanotubes, Zagreb indices; Generalized Zagreb

SUBJECT CLASSIFICATION
E.g., Mathematics Subject Classification; Primary 05C05; Secondary 92E10.

INTRODUCTION
Let G=(V,E) be a simple connected graph. The sets of vertices and edges of G are denoted by V=V(G) and E=E(G), respectively. In such a simple molecular graph, vertices represent atoms and edges represent bonds. In chemical graph theory, we have many invariant polynomials and topological indices for a molecular graph. We denote the degree of a vertex v of G by $d_v$, which is defined as the number of edges incident to v and the distance $d(u,v)$ between the vertices u and v of the graph G is equal to the length of (number of edges in) the shortest path that connects u and v. A general reference for the notation in graph theory is [1,2].

A topological index of G is a number related to a graph which is invariant under graph automorphisms. Obviously, every topological index defines a counting polynomial and vice versa.

The First Zagreb index was defined about forty years ago by I. Gutman and N. Trinajstić [2] and is defined as the sum of the squares of the degrees of all vertices of G as

$$M_1(G) = \sum_{v \in V(G)} d_v^2$$

The second Zagreb index of G are denoted by $M_2(G)$ and defined as follows:

$$M_2(G) = \sum_{e \in E(G)} (d_u \times d_v)$$

In 2011, A. Iranmanesh and M. Azari introduced the Generalized Zagreb index of a connected graph G based on degree of vertices of G [4]. The Generalized Zagreb index is defined as

$$M_{r,s}(G) = \sum_{e \in E(G)} (d_u^r \times d_v^s + d_u^s \times d_v^r)$$

where $d_u$ and $d_v$ are the degrees of u and v, respectively and r and s are two non-negative integers ($\forall r,s \in \mathbb{N}$).

For more historical details of Zagreb topological indices see the paper series [5-17].
In this paper, we focus on the structure of Armchair Polyhex Nanotubes TUAC_6 and compute its Generalized Zagreb index.
RESULTS AND DISCUSSION

In this section, we compute a new Zagreb topological index $M_{r,s}(G)$ of a family of Hexagonal Nanotubes namely: Armchair Polyhex Nanotubes $TUAC_6$. M.V. Diudea denoted the number of hexagons in the first row/column of the 3 and 2-Dimensional lattices of (see Figure 1) by $m$ and $n$ ($\forall m,n \in \mathbb{N}$), respectively [18] and denoted Armchair Polyhex Nanotubes by $TUAC_6[m,n]$. The 3 and 2-Dimensional lattices of this family of Hexagonal Nanotubes are shown in Figures 1 and 2.

![Figure 1](image1.png)

**Fig 1.** [5] The 3D Lattice of the Armchair Polyhex Nanotubes $TUAC_6[m,n] (\forall m,n \in \mathbb{N})$.

![Figure 2](image2.png)

**Fig 2.** [5] A general form of the Armchair Polyhex Nanotubes $TUAC_6[m,n], \forall m,n \in \mathbb{N}$.

We refer the reader to [19-27] for more information about families of Hexagonal Nanotubes and especially Armchair Polyhex Nanotubes $TUAC_6$.

**Theorem 1.** Let $G$ be the Armchair Polyhex Nanotubes $TUAC_6[m,n] (\forall m,n \in \mathbb{N})$. Then, the generalized Zagreb index of $TUAC_6[m,n]$ is equal to

$$M_{r,s}(TUAC_6[m,n]) = m[2^{r+s+2} + 3'2^{s-1} + 3'2^{n-1} + 2(3n-1)(3's)]$$

**Proof of Theorem 1.** $\forall m,n \in \mathbb{N}$, consider the Armchair Polyhex Nanotubes $TUAC_6[m,n]$. By according to Figure 2, one can see that there are $2m(n+1)$ vertices/atoms in this Nanotubes and two partitions of vertex set $V(TUAC_6[m,n])$ are equal to

$$V = \{v \in V(TUAC_6[m,n]) | d_v=2\} \rightarrow |V_2|= \frac{2m}{2} + \frac{2m}{2} = 2m$$

$$V = \{v \in V(TUAC_6[m,n]) | d_v=3\} \rightarrow |V_3|=2mn$$
Thus, there are \( \frac{1}{2} [2(2m) + 3(2m)] = 3mn + 2m \) edges in Armchair Polyhex Nanotubes. From the structure of \( TUAC_6[m,n] \), three partitions of edges set \( E(TUAC_6[m,n]) \) are equal to

\[
E_{(2,2)} = \{ e = uv \in E(TUAC_6[m,n]) \} | d_u = d_v = 2 \to |E_d| = \frac{1}{2}m + \frac{1}{2}m = m
\]

\[
E_{(2,3)} = \{ e = uv \in E(TUAC_6[m,n]) \} | d_u = 3 \& d_v = 2 \to |E_d| = 2|E_d| = 2m
\]

\[
E_{(3,3)} = \{ e = uv \in E(TUAC_6[m,n]) \} | d_u = d_v = 3 \to |E_d| = 3mn - m.
\]

We colored All members of \( E_{(2,2)}, E_{(2,3)} \) and \( E_{(3,3)} \) br yellow, red and black colors, respectively in Figure 2. Thus, we have following computations for the generalized Zagreb index of Armchair Polyhex Nanotubes \( TUAC_6[m,n] \):

\[
M_{r,s}(TUAC_6[m,n]) = \sum_{e = uv \in E(TUAC_6[m,n])} (d_u^r + d_v^r + d_u^s + d_v^s)
\]

\[
= \sum_{e = uv \in E_{(2,2)}} (2^r2^s + 2^r2'2'^s + 2^{r+1}s + 2^{r+s}) + \sum_{e = uv \in E_{(2,3)}} (3^r2^s + 3^r2'2'^s + 3^{r+s})
\]

\[
= 2(2^r2^s + 2^{r+1}s) + \sum_{e = uv \in E_{(2,3)}} (3^r2^s + 3^r2'2'^s + 3^{r+s}) + 2(3^r s)
\]

\[
= 2m \times 2(2^r2^s + 2^{r+1}s) + 2m \times (3^r2^s + 3^r2'2'^s + 3^{r+s}) + (3mn - m) \times 2(3^r s)
\]

Thus \( M_{r,s}(TUAC_6[m,n]) = m[2^{2r+s} + 3^r2^s + 3^{r+1}s + (3mn - m) \times 2(3^r s)] \)

And the proof of Theorem 1 be completed.

**Lemma 1.** From above theorem, we have following results for the generalized Zagreb index of Armchair Polyhex Nanotubes \( TUAC_6[m,n] \) \( \forall m, n \in \mathbb{N} \):

\[
\frac{1}{2} M_{0,0}(TUAC_6[m,n]) = 3mn + 2m = |E(TUAC_6[m,n])|
\]

\[
M_{1,0}(TUAC_6[m,n]) = 18mn + 8m = M(TUAC_6[m,n])
\]

\[
\frac{1}{2} M_{1,1}(TUAC_6[m,n]) = 27mn + 7m = M_2(TUAC_6[m,n])
\]

**REFERENCES**


