International Journal of Engineering and Technology Research
Vol. 3, No. 1, February 2015, pp. 1 - 6, ISSN: 2327- 0349 (Online)
Available online at www.ijeatr.org

Research article

The Hyper-Zagreb Index of $TUSC_4C_8(S)$ Nanotubes

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Abstract

Let G be a simple molecular graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. As usual, the distance between the vertices u and v of G is denoted by $d_G(u,v)$ (or $d(u,v)$ for short) and it is defined as the number of edges in a minimal path connecting vertices u and v. Topological indices are numerical parameters of a graph which characterize its topology. The first and second Zagreb indices of a graph G are defined as $M_1(G)=\sum_{e=uv\in E(G)}(d_v+d_v)$ and $M_2(G)=\sum_{e=uv\in E(G)}(d_v\times d_v)$ where d_u is the degree of the vertex u and d_v is defined analogously. In 2013, *G.H. Shirdel*, *H. RezaPour* and *A.M. Sayadi* [4] introduced a new distance-based of Zagreb indices named "*Hyper-Zagreb index*" as $HM(G)=\sum_{e=uv\in E(G)}(d_v+d_v)^2$. In this, we determine exact formulas of the Hyper-Zagreb index of the $TUSC_4C_8(S)$ Nanotubes.

Keywords: Molecular graphs, Nanotubes, Topological index, Zagreb index, Hyper-Zagreb index.

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Introduction

Let G be a simple molecular graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. As usual, the distance between the vertices u and v of G is denoted by $d_G(u,v)$ (or $d(u,v)$ for short) and it is defined as the number of edges in a minimal path connecting vertices u and v [1, 2].

The first and second Zagreb indices of a graph G are defined as: [3].

$$M_1(G)=\sum_{e=uv\in E(G)} (d_v+d_v)$$

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

where d_u is the degree of the vertex u and d_v is defined analogously.

In 2013, *G.H. Shirdel, H. RezaPour* and *A.M. Sayadi* [4] introduced a new distance-based of Zagreb indices named "*Hyper-Zagreb index*" as

$$HM(G)=\sum_{e=uv\in E(G)} (d_v+d_v)^2.$$

The mathematical properties of these topological indices can be found in some recent papers. We encourage the reader to consult [5-34] for historical background, computational techniques and mathematical properties of Zagreb indices.

In this paper our notation is standard and taken mainly from the standard book of graph theory.

In this paper, we use definition of the *Hyper-Zagreb index HM* and compute exact formulae of this index for a family of Nanostructures and Molecular graphs with structure consist of cycles C_4 and C_8, that named "$TUSC_4C_8(S)$ Nanotubes".

Results and Discussion

The aim of this section Hyper-Zagreb $HM(G)$ index of the $TUSC_4C_8(S)$ Nanotubes are computed. *M.V. Diudea* denoted the number of Octagons C_8 in the first row of G by m and the number of Octagons C_8 in the first column of G by n, and he denoted $TUSC_4C_8(S)$ Nanotubes by $G=TUC_4C_8[m,n]$ $(\forall m,n\in\mathbb{N})$. Reader can see the 3-Dimensional and 2-Dimensional lattices of $G=TUC_4C_8[m,n]$ in Figure 1 and for historical background see references [35-49].

Theorem 1. [48] Let G be the $TUSC_4C_8(S)$ Nanotubes. Then the First and Second Zagreb indices of G are equal to

$$M_1(TUSC_4C_8(S))=72mn+16m$$

$$M_2(TUSC_4C_8(S))=108mn+14m.$$

Theorem 2. $\forall m,n\in\mathbb{N}$, let G be the $TUC_4C_8[m,n]$ Nanotubes. Then the Hyper-Zagreb index of G is equal to

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$$HM(TUC_4C_8[m,n])=12m(36n+5)$$

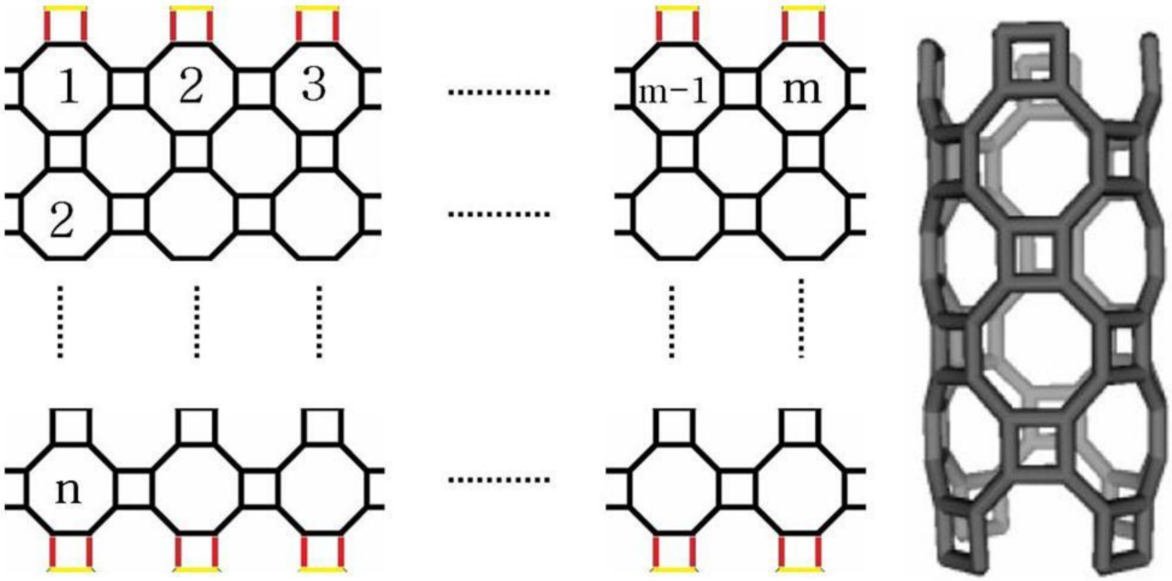

Figure 1. -Dimensional and 2-Dimensional lattices of the $TUSC_4C_8(S)$ Nanotubes [43-48].

Proof of Theorem 2. $\forall m,n\in\mathbb{N}$, consider the $TUC_4C_8[m,n]$ Nanotubes with $8mn+4m$ vertices/atoms and $12mn+4m$ edges\bonds [43-48]. By according to Figure 1, one can see that the degree of a vertex/atom of all Nanotubes is equal to 1 or 2 or 3 and there are two partitions of vertex/atom set $V(TUC_4C_8[m,n])$ are equal to

$$V_2=\{v\in V(TUC_4C_8[m,n])|\ d_v=2\}\rightarrow|V_2|=2m+2m$$

$$V_3=\{v\in V(TUC_4C_8[m,n])|\ d_v=3\}\rightarrow|V_3|=8mn$$

Also, there are $|E(TUC_4C_8[m,n])|=½(2(4m)+4(8mn))=12mn+4m$ edges\bonds in this Nanotubes. From the structure of $TUC_4C_8[m,n]$ in Figure 1, we see that there are three partitions of edge\bond set $E(TUC_4C_8[m,n])$ with their size are as follows:

$$E_{\{2,2\}}=\{e=uv\in E(TUC_4C_8[m,n])|\ d_u=d_v=2\}\rightarrow|\ E_4|=e_4=½|V_2|=2m$$

$$E_{\{2,3\}}=\{e=uv\in E(TUC_4C_8[m,n])|\ d_u=3\ \&d_v=2\}\rightarrow|\ E_5|=e_5=|V_2|=4m$$

$$E_{\{3,3\}}=\{e=uv\in E(TUC_4C_8[m,n]])|\ d_u=d_v=3\}\rightarrow|\ E_6|=e_6=12mn-2m$$

In Figure 1, we marked all members of these edgs partitions of $TUC_4C_8[m,n]$ ($E_{\{2,2\}}, E_{\{2,3\}}$ and $E_{\{3,3\}}$) br yellow, red and black colors, respectively.

We now compute the Hyper-Zagreb index of $TUC_4C_8[m,n]$ Nanotubes $\forall m,n \in \mathbb{N}$.

$$HM(TUC_4C_8[m,n])=\sum_{e=uv\in E(TUC_4C_8[m,n])}(d_v+d_v)^2$$

$$=\sum_{uv\in E_{\{2,2\}}}(d_v+d_v)^2+\sum_{uv\in E_{\{2,3\}}}(d_v+d_v)^2+\sum_{uv\in E_{\{3,3\}}}(d_v+d_v)^2$$

$$=\sum_{i=4}^{6} e_i \times (i)^2 = e_4\times(4)^2+ e_5\times(5)^2+ e_6\times(6)^2$$

$$=(2m)(4)^2+ (4m)(5)^2+ (12mn-2m)(6)^2$$

Thus the Hyper-Zagreb index $HM(TUC_4C_8[m,n])=12m(36n+5)$

And this completed the proof of Theorem 2. ■

Conclusion

In this paper, I was counting new Zagreb topological index for a family of Carbon Nanotubes namely: $TUSC_4C_8(S)$ Nanotubes. The Hyper-Zagreb index was introduced recently by *G.H. Shirdel, H. RezaPour* and *A.M. Sayadi* in 2013.

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