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COMPUTING GENERAL ZAGREB INDICES OF SOME CARBON NANOTUBES

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Abstract

Chemical graph theory is an important branch of mathematical chemistry which has broad range of applications. In chemical sciences, topological indices or molecular descriptors are used for understanding the physico-chemical properties of molecules. In this communication, we compute the general Zagreb indices for some important Carbon nanotubes.

Keywords: Topological index, General Zagreb Indices, Nanotubes.

2010 AMS Classification: 90C35, 05C07, 05C40.

1. Introduction

In chemistry, a molecular descriptor or topological index is used in isomer discrimination, structural-activity relationships (SAR), structural-property relationships (SPR), chemical documentation and pharmaceutical drug designing etc. A Nanotube is an object of intermediate size between microscopic and molecular structure. It is a product derived through engineering at molecular scale. Carbon nanotube is one of the important class of these materials. Carbon nanotubes are allotrope's of carbon with molecular structure and tubular shape having diameters ranging from a few nanometers and lengths up to several millimeters [1, 6, 17, 21]. Nanotubes are broadly classified as single-walled and multi-walled nanotubes. Carbon nanotubes can be bent, when they are released, they will spring back to their original shape. As individual molecules, nanotubes are hundreds times stronger than steel. Carbon nanotubes have wide range of applications in Nanotechnologies, electronics, optical communications and other fields of material sciences. These are also potentially useful in Infection therapy, Gene therapy, Cancer therapy etc.

In 1991, Iijima [11] discovered carbon nanotubes as multi-walled structures. In this study we compute the general Zagreb indices of some well-known nanotubes such as $TUAC_6$, $TUZC_6$, $TUC_4C_8(R)$, $TUC_4C_8(S)$, $TUHC_5C_7$, $TUSC_5C_7$, $TUHAC_5C_7$ and $TUHAC_5C_6C_7$. For more information on computing topological indices of nanostructures see refs. [4, 6, 10, 12, 13, 19, 20, 23, 24].

Some standard topological indices such as Zagreb indices [8], Randić index [18], Forgotten index [8, 9], Modified second Zagreb indices [2, 3], Reciprocal Randić index [9, 16] are found as special cases of the General Zagreb indices.

The concept of generalization of Zagreb indices is first introduced by Li et al. [14, 15] and is defined as

- First General Zagreb Index

$$M_1^\alpha(G) = \sum_{v\in V(G)} d_G^\alpha(u) = \sum_{uv\in E(G)}[d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)].$$

- Second General Zagreb Index

$$M_2^\alpha(G) = \sum_{uv\in E(G)} d_G^{\alpha-1}(u) d_G^{\alpha-1}(v).$$

Where, α is a real number. More details about the general Zagreb indices may be found in [8, 17, 22].

Topological index	Corresponding General Zagreb index
First Zagreb index, $M_1(G)$	$M_1^2(G)$
Forgotten index, $F(G)$	$M_1^3(G)$
$Randi\acute{c}$ index, $R(G)$	$M_2^{-\frac{1}{2}}(G)$
Reciprocal $Randi\acute{c}$ index, $RR(G)$	$M_2^{\frac{1}{2}}(G)$
Inverse $Randi\acute{c}$ index, R_{-1}	$M_2^{-1}(G)$

Table1: Relationships between General Zagreb-indices and some other Topological indices.

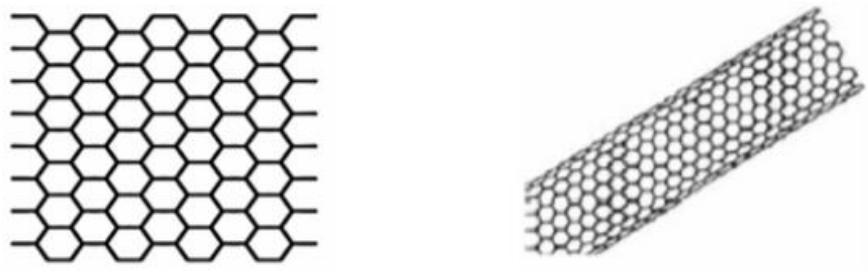
2. Results and Discussion:

In this section we compute the general Zagreb indices of some of the above mentioned carbon nanotubes. Let G be one of the above mentioned nanotubes. It is easy to see that, the degree of each vertex in G either two or three. So we can classify the edge set of G into following ways

$$E_1(G) = \{uv \in E(G): d(u) = 2 \; and \; d(v) = 2\},$$
$$E_2(G) = \{uv \in E(G): d(u) = 2 \; and \; d(v) = 3\},$$
$$E_3(G) = \{uv \in E(G): d(u) = 3 \; and \; d(v) = 3\}.$$

2.1. $\boldsymbol{TUAC_6}$nanotubes:

Let $G = TUAC_6(p,q)$ be an armchair polyhex nanotube, where p is the number of hexagons in each row and q is the number of rows in the molecular graph of G as shown in Figure1, from the molecular graph we have$|E_1(G)| = 2p, |E_2(G)| = 4p, |E_3(G)| = 6pq - 8p$.



(a) (b)

Figure 1: (a) Two dimensional lattice of $TUAC_6$ $(4,8)$ nanotube, (b) $TUAC_6$ nanotubes

Theorem 1. The general Zagreb indices of $G = TUAC_6(p,q)$ nanotubes is given by

- General first Zagreb index

$$M_1^{\alpha}(G) = 2^{\alpha}p - 4(3^{\alpha})(1-q)p.$$

- General Second Zagreb index

$$M_2^{\alpha}(G) = 2^{2\alpha+1}p + 2^{\alpha+1}3^{\alpha}p + (6pq - 8p)3^{2\alpha}.$$

Proof:

$$M_1^{\alpha}(G) = \sum_{uv\in E(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)]$$

$$= \sum_{uv\in E_1(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)] + \sum_{uv\in E_2(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)]$$

$$+ \sum_{uv\in E_3(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)]$$

$$= |E_1(G)|[2^{\alpha-1} + 2^{\alpha-1}] + |E_2(G)|[2^{\alpha-1} + 3^{\alpha-1}] + |E_3(G)|[3^{\alpha-1} + 3^{\alpha-1}]$$

$$= |E_1(G)|2^{\alpha} + |E_2(G)|[2^{\alpha-1} + 3^{\alpha-1}] + |E_3(G)|[3^{\alpha-1} + 3^{\alpha-1}]$$

$$= 2p[2^{\alpha}] + 4p[2^{\alpha-1} + 3^{\alpha-1}] + (6pq - 8p)[3^{\alpha-1} + 3^{\alpha-1}]$$

$$= 2^{\alpha}p - 4(3^{\alpha})(1 - q)p.$$

$$M_2^{\alpha}(G) = \sum_{uv\in E(G)} d_G^{\alpha-1}(u)d_G^{\alpha-1}(v)$$

$$= \sum_{uv\in E_1(G)} d_G^{\alpha-1}(u)d_G^{\alpha-1}(v) + \sum_{uv\in E_2(G)} d_G^{\alpha-1}(u)d_G^{\alpha-1}(v)$$

$$+ \sum_{uv\in E_3(G)} d_G^{\alpha-1}(u)d_G^{\alpha-1}(v)$$

$$= |E_1(G)|[4^{\alpha}] + |E_2(G)|[6^{\alpha}] + |E_3(G)|[3^{2\alpha}]$$

$$=|E_1(G)|[2^{2\alpha}] + |E_2(G)|[2^{\alpha}3^{\alpha}] + |E_3(G)|[3^{2\alpha}]$$

$$=2p[2^{2\alpha}] + 4p[2^{\alpha}3^{\alpha}] + (6pq - 8p)[3^{2\alpha}]$$

$$= 2^{2\alpha+1}p + 2^{\alpha+1}3^{\alpha}p + (6pq - 8p)3^{2\alpha}.$$

For different values of α, we compute some other standard topological indices and the results are found as shown in the following corollary.

Corollary 1. p is the number of hexagons in each row and q is the number of rows in the molecular graph of G. Then

I. $M_1^2(G) = M_1(G) = 4p(9q - 8)$.

II. $M_1^3(G) = F(G) = -100p + 108pq$

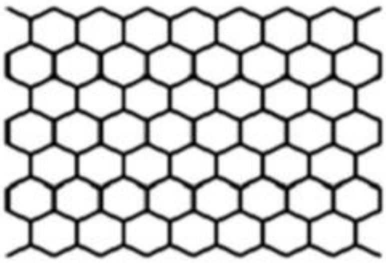
III. $M_2^{-\frac{1}{2}}(G) = R(G) = \left(1 + \sqrt{\frac{2}{3}}\right)p + \frac{6pq-8q}{3}$.

IV. $M_2^{\frac{1}{2}}(G) = RR(G) = 2(\sqrt{6} - 10)p + 18pq$.

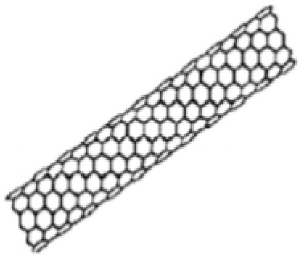
V. $M_2^{-1}(G) = R_{-1}(G) = -\frac{1}{18}p + \frac{2}{3}pq$.

2.2. $TUZC_6$nanotubes:

Let $G = TUZC_6(p, q)$ be an a zigzag polyhex nanotube, where p is the number of hexagons in each row and q is the number of rows in the molecular graph of G as shown in Figure 2, from the molecular graph we have $|E_1(G)| = 0, |E_2(G)| = 4p, |E_3(G)| = 3pq - 5p$.



(a)



(b)

Figure 2: (a) Two dimensional lattice of $TUZC_6(8, 8)$ nanotube, (b) $TUZC_6$ nanotubes

Theorem 2. The general Zagreb indices of $G = TUZC_6(p, q)$ nanotubes is given by

- General first Zagreb index

$$M_1^\alpha(G) = 4(2^{\alpha-1} + 3^{\alpha-1})p + 2(3pq - 5p)3^{\alpha-1}.$$

- General Second Zagreb index

$$M_2^\alpha(G) = 4(6^\alpha)p + (3pq - 5p)3^{2\alpha}.$$

Proof:

$$M_1^\alpha(G) = \sum_{uv\in E(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)]$$

$$= \sum_{uv\in E_1(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)] + \sum_{uv\in E_2(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)] + \sum_{uv\in E_3(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)]$$

$$= |E_1(G)|[2^{\alpha-1} + 2^{\alpha-1}] + |E_2(G)|[2^{\alpha-1} + 3^{\alpha-1}] + |E_3(G)|[3^{\alpha-1} + 3^{\alpha-1}]$$

$$= |E_1(G)|2^{\alpha} + |E_2(G)|[2^{\alpha-1} + 3^{\alpha-1}] + |E_3(G)|[3^{\alpha-1} + 3^{\alpha-1}]$$

$$= 0 \times [2^{\alpha}] + 4p[2^{\alpha-1} + 3^{\alpha-1}] + (3pq - 5p)[3^{\alpha-1} + 3^{\alpha-1}]$$

$$= 4(2^{\alpha-1} + 3^{\alpha-1})p + 2(3pq - 5p)3^{\alpha-1}.$$

$$M_2^{\alpha}(G) = \sum_{uv \in E(G)} d_G^{\alpha-1}(u) d_G^{\alpha-1}(v)$$

$$= \sum_{uv \in E_1(G)} d_G^{\alpha-1}(u) d_G^{\alpha-1}(v) + \sum_{uv \in E_2(G)} d_G^{\alpha-1}(u) d_G^{\alpha-1}(v)$$

$$+ \sum_{uv \in E_3(G)} d_G^{\alpha-1}(u) d_G^{\alpha-1}(v)$$

$$= |E_1(G)|[4^{\alpha}] + |E_2(G)|[6^{\alpha}] + |E_3(G)|[3^{2\alpha}]$$

$$= |E_1(G)|[2^{2\alpha}] + |E_2(G)|[2^{\alpha}3^{\alpha}] + |E_3(G)|[3^{2\alpha}]$$

$$= 0 \times [2^{2\alpha}] + 4p[2^{\alpha}3^{\alpha}] + (3pq - 5p)[3^{2\alpha}]$$

$$= 4(6^{\alpha})p + (3pq - 5p)3^{2\alpha}.$$

For different values of α, we compute some other standard topological indices and the results are found as shown in the following corollary.

Corollary 2. p is the number of hexagons in each row and q is the number of rows in the molecular graph of G. Then

I. $M_1^2(G) = M_1(G) = 18pq - 10p.$

II. $M_1^3(G) = F(G) = 54pq - 38p.$

III. $M_2^{-\frac{1}{2}}(G) = R(G) = \left(\frac{4}{\sqrt{6}}\right)p + \frac{3pq-5q}{3}.$

IV. $M_2^{\frac{1}{2}}(G) = RR(G) = 4\sqrt{6}p + 3(3pq - 5p)\,.$

V. $M_2^{-1}(G) = R_{-1}(G) = \frac{2}{3}p + \frac{3pq-5q}{9}$.

3. TUC_4C_8 Nanotubes

A C_4C_8net is a trivalent decoration constructed from alternating squares $C_4$and octagons C_8: Two classes of these nanotubes are $\mathrm{TUC_4C_8(R)}$ and $\mathrm{TUC_4C_8(S)}$nanotubes.

3.1. $TUC_4C_8(R)$ Nanotubes

Let $G = TUC_4C_8(R)$ be nanotube which molecular graph is constructed from alternating squares and octagons as shown in Figure 3. In the molecular graph p is the number of squares in each row and q is the number of squares in each column. From the molecular graph we have$|E_1(G)| = 0, |E_2(G)| = 4p, |E_3(G)| = 6pq - 5p$.

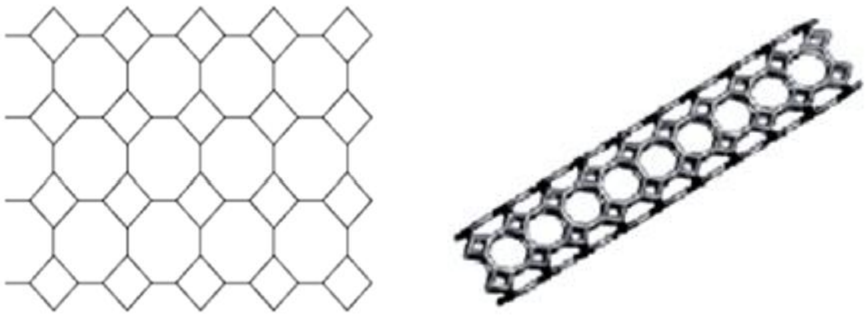
Theorem 3. The general Zagreb indices of $G = TUC_4C_8(R)$ nanotubes is given by

- General first Zagreb index

$$M_1^{\alpha}(G) = 4(2^{\alpha-1} + 3^{\alpha-1})p + 2(6pq - 5p)3^{\alpha-1}.$$

- General Second Zagreb index

$$M_2^{\alpha}(G) = 4(6^{\alpha})p + (6pq - 5p)3^{2\alpha}.$$



(a) (b)

Figure 3: (a) Two dimensional lattice of $\mathrm{TUC_4C_8(R)}$ nanotube with p=5 and q=4, (b) $\mathrm{TUC_4C_8(R)}$ nanotubes.

Proof:

$$M_1^{\alpha}(G) = \sum_{uv\in E(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)]$$

$$= \sum_{uv\in E_1(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)] + \sum_{uv\in E_2(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)]$$

$$+ \sum_{uv\in E_3(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)]$$

$$= |E_1(G)|[2^{\alpha-1} + 2^{\alpha-1}] + |E_2(G)|[2^{\alpha-1} + 3^{\alpha-1}] + |E_3(G)|[3^{\alpha-1} + 3^{\alpha-1}]$$

$$= |E_1(G)|2^{\alpha} + |E_2(G)|[2^{\alpha-1} + 3^{\alpha-1}] + |E_3(G)|[3^{\alpha-1} + 3^{\alpha-1}]$$

$$= 0 \times [2^{\alpha}] + 4p[2^{\alpha-1} + 3^{\alpha-1}] + (6pq - 5p)[3^{\alpha-1} + 3^{\alpha-1}]$$

$$= 4(2^{\alpha-1} + 3^{\alpha-1})p + 2(6pq - 5p)3^{\alpha-1}.$$

$$M_2^{\alpha}(G) = \sum_{uv\in E(G)} d_G^{\alpha-1}(u) d_G^{\alpha-1}(v)$$

$$= \sum_{uv\in E_1(G)} d_G^{\alpha-1}(u) d_G^{\alpha-1}(v) + \sum_{uv\in E_2(G)} d_G^{\alpha-1}(u) d_G^{\alpha-1}(v)$$

$$+ \sum_{uv\in E_3(G)} d_G^{\alpha-1}(u) d_G^{\alpha-1}(v)$$

$$= |E_1(G)|[4^{\alpha}] + |E_2(G)|[6^{\alpha}] + |E_3(G)|[3^{2\alpha}]$$

$$=|E_1(G)|[2^{2\alpha}] + |E_2(G)|[2^{\alpha}3^{\alpha}] + |E_3(G)|[3^{2\alpha}]$$

$$=0 \times [2^{2\alpha}] + 4p[2^{\alpha}3^{\alpha}] + (6pq - 5p)[3^{2\alpha}]$$

$$= 4(6^{\alpha})p + (6pq - 5p)3^{2\alpha}.$$

For different values of α, we compute some other standard topological indices and the results are found as shown in the following corollary.

Corollary 3. p is the number of squares in each row and q is the number of squares in each column of the molecular graph G. Then

I. $M_1^2(G) = M_1(G) = 36pq - 10p$.

II. $M_1^3(G) = F(G) = 2p(54q - 19)$

III. $M_2^{-\frac{1}{2}}(G) = R(G) = \left(\frac{4}{\sqrt{6}}\right)p + \frac{6pq-5q}{3}$.

IV. $M_2^{\frac{1}{2}}(G) = RR(G) = 4\sqrt{6}p + 3(6pq - 5p)$.

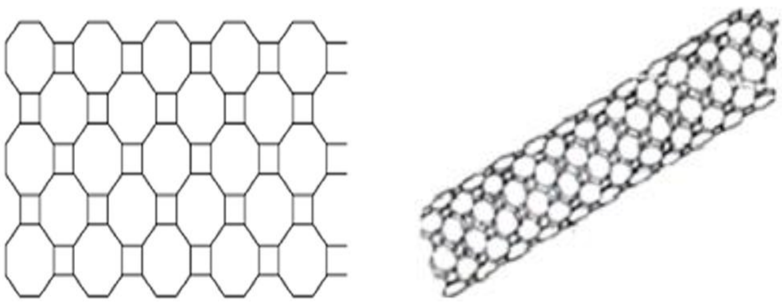
V. $M_2^{-1}(G) = R_{-1}(G) = \frac{2}{3}p + \frac{6pq-5q}{9}$.

3.2 $TUC_4C_8(S)$Nanotubes

Let $G = TUC_4C_8(S)$ be nanotube which molecular graph is constructed from alternating squares and octagons as shown in Figure 4. In the molecular graph p is the number of squares in each row and q is the number of squares in each column. From the molecular graph we have$|E_1(G)| = 2p, |E_2(G)| = 4p, |E_3(G)| = 6pq - 8p$.

Theorem 4. The general Zagreb indices of $G = TUC_4C_8(S)$ nanotubes is given by

- General first Zagreb index
$$M_1^\alpha(G) = p[2^{\alpha+1}] + 4(2^{\alpha-1} + 3^{\alpha-1})p + 2(6pq - 8p)3^{2\alpha}.$$
- General Second Zagreb index
$$M_2^\alpha(G) = 2^{2\alpha+1}p + 4(6^\alpha)p + (6pq - 8p)3^{3\alpha}.$$



(a) (b)

Figure 4: (a) Two dimensional lattice of $\mathrm{TUC_4C_8(S)}$ nanotube with p=5 and q=6, (b)

$TUC_4C_8(S)$ nanotubes.

Proof:

$$M_1^{\alpha}(G) = \sum_{uv \in E(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)]$$

$$= \sum_{uv \in E_1(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)] + \sum_{uv \in E_2(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)] + \sum_{uv \in E_3(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)]$$

$$= |E_1(G)|[2^{\alpha-1} + 2^{\alpha-1}] + |E_2(G)|[2^{\alpha-1} + 3^{\alpha-1}] + |E_3(G)|[3^{\alpha-1} + 3^{\alpha-1}]$$

$$= |E_1(G)|2^{2\alpha} + |E_2(G)|[2^{\alpha-1} + 3^{\alpha-1}] + |E_3(G)|[3^{\alpha-1} + 3^{\alpha-1}]$$

$$= 2p[2^{2\alpha}] + 4p[2^{\alpha-1} + 3^{\alpha-1}] + (6pq - 8p)[3^{\alpha-1} + 3^{\alpha-1}]$$

$$= p[2^{\alpha+1}] + 4(2^{\alpha-1} + 3^{\alpha-1})p + 2(6pq - 8p)3^{\alpha-1}.$$

$$M_2^{\alpha}(G) = \sum_{uv \in E(G)} d_G^{\alpha-1}(u) d_G^{\alpha-1}(v)$$

$$= \sum_{uv \in E_1(G)} d_G^{\alpha-1}(u) d_G^{\alpha-1}(v) + \sum_{uv \in E_2(G)} d_G^{\alpha-1}(u) d_G^{\alpha-1}(v) + \sum_{uv \in E_3(G)} d_G^{\alpha-1}(u) d_G^{\alpha-1}(v)$$

$$= |E_1(G)|[4^{\alpha}] + |E_2(G)|[6^{\alpha}] + |E_3(G)|[3^{2\alpha}]$$

$$= |E_1(G)|[2^{2\alpha}] + |E_2(G)|[2^{\alpha}3^{\alpha}] + |E_3(G)|[3^{2\alpha}]$$

$$= 2p[2^{2\alpha}] + 4p[2^{\alpha}3^{\alpha}] + (6pq - 8p)[3^{2\alpha}]$$

$$= 2^{2\alpha+1}p + 4(6^{\alpha})p + (6pq - 8p)3^{2\alpha}.$$

For different values of α, we compute some other standard topological indices and the results are found as shown in the following corollary.

Corollary 4. p is the number of squares in each row and q is the number of squares in each column of the molecular graph G. Then

I. $M_1^2(G) = M_1(G) = 36pq - 20p$.

II. $M_1^3(G) = F(G) = 2p(54q - 38)$

III. $M_2^{-\frac{1}{2}}(G) = R(G) = \left(1 + \frac{4}{\sqrt{6}} - \frac{8}{3}\right)p + 2pq$.

IV. $M_2^{\frac{1}{2}}(G) = RR(G) = (4\sqrt{6} - 20)p + 18pq$.

V. $M_2^{-1}(G) = R_{-1}(G) = \frac{5}{8}p + \frac{2}{3}pq$.

4. TUC_5C_7 Nanotubes

A C_5C_7 net is a trivalent decoration constructed from alternating pentagons (C_5) and heptagons (C_7). Three classes of this type of nanotubes are $\mathrm{TUHC_5C_7}$, $\mathrm{TUSC_5C_7}$ & $\mathrm{TUHAC_5C_7}$.

4.1 $\mathrm{TUHC_5C_7}$ Nanotubes:

The molecular graph of the nanotubes $\mathrm{TUHC_5C_7}(p, q)$ as shown in Figure 5 consists of pentagons and heptagons. We denote p is the number of pentagons in each row. In this nanotube, the four first rows of vertices and edges are repeated, alternatively. We denote the number of this repetition by q. The cardinality of the edge sets of the graph are

$|E_1(G)| = 0, |E_2(G)| = 4p, |E_3(G)| = 12pq - 5p$.

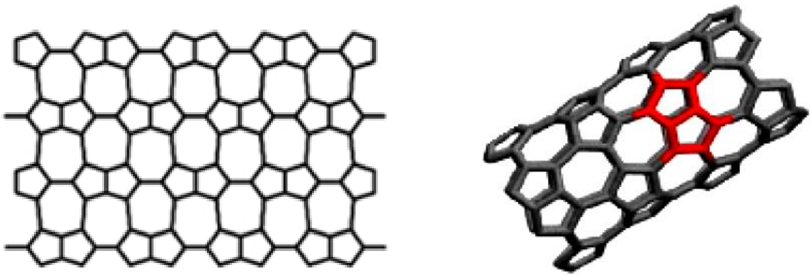
Theorem5. The general Zagreb indices of $G = \mathrm{TUHC_5C_7}(p, q)$ nanotubes is given by

- General first Zagreb index

$$M_1^\alpha(G) = 4(2^{\alpha-1} + 3^{\alpha-1})p + 2(12pq - 5p)3^{\alpha-1}.$$

- General Second Zagreb index

$$M_2^\alpha(G) = 4(6^\alpha)p + (12pq - 5p)3^{2\alpha}.$$



(a) (b)

Figure5: (a) Two dimensional lattice of $TUHC_5C_7(8,2)$ nanotubes, (b) $TUHC_5C_7$nanotubes.

Proof:

$$M_1^{\alpha}(G)=\sum_{uv\in E(G)}[d_G^{\alpha-1}(u)+d_G^{\alpha-1}(v)]$$

$$=\sum_{uv\in E_1(G)}[d_G^{\alpha-1}(u)+d_G^{\alpha-1}(v)]+\sum_{uv\in E_2(G)}[d_G^{\alpha-1}(u)+d_G^{\alpha-1}(v)]$$

$$+\sum_{uv\in E_3(G)}[d_G^{\alpha-1}(u)+d_G^{\alpha-1}(v)]$$

$$=|E_1(G)|[2^{\alpha-1}+2^{\alpha-1}]+|E_2(G)|[2^{\alpha-1}+3^{\alpha-1}]+|E_3(G)|[3^{\alpha-1}+3^{\alpha-1}]$$

$$=|E_1(G)|2^{2\alpha}+|E_2(G)|[2^{\alpha-1}+3^{\alpha-1}]+|E_3(G)|[3^{\alpha-1}+3^{\alpha-1}]$$

$$=0\times[2^{2\alpha}]+4p[2^{\alpha-1}+3^{\alpha-1}]+(12pq-5p)[3^{\alpha-1}+3^{\alpha-1}]$$

$$=4(2^{\alpha-1}+3^{\alpha-1})p+2(12pq-5p)3^{\alpha-1}.$$

$$M_2^{\alpha}(G)=\sum_{uv\in E(G)}d_G^{\alpha-1}(u)d_G^{\alpha-1}(v)$$

$$=\sum_{uv\in E_1(G)}d_G^{\alpha-1}(u)d_G^{\alpha-1}(v)+\sum_{uv\in E_2(G)}d_G^{\alpha-1}(u)d_G^{\alpha-1}(v)$$

$$+\sum_{uv\in E_3(G)}d_G^{\alpha-1}(u)d_G^{\alpha-1}(v)$$

$$= |E_1(G)|[4^{\alpha}] + |E_2(G)|[6^{\alpha}] + |E_3(G)|[3^{2\alpha}]$$

$$=|E_1(G)|[2^{2\alpha}] + |E_2(G)|[2^{\alpha}3^{\alpha}] + |E_3(G)|[3^{2\alpha}]$$

$$=0 \times 2^{2\alpha} + 4p[2^{\alpha}3^{\alpha}] + (12pq - 5p)[3^{2\alpha}]$$

$$= 4(6^{\alpha})p + (12pq - 5p)3^{2\alpha}.$$

For different values of α, we compute some other standard topological indices and the results are found as shown in the following corollary.

Corollary 5. p is the number of pentagons in each row and q is the number of repetition the first four rows of vertices and edges in G. Then

I. $M_1^2(G) = M_1(G) = 36pq - 20p$.

II. $M_1^3(G) = F(G) = 2p(54q - 38)$.

III. $M_2^{-\frac{1}{2}}(G) = R(G) = \left(\frac{4}{\sqrt{6}} - \frac{5}{3}\right)p + 4pq$.

IV. $M_2^{\frac{1}{2}}(G) = RR(G) = (4\sqrt{6} - 5\sqrt{3})p + 12\sqrt{3}pq$.

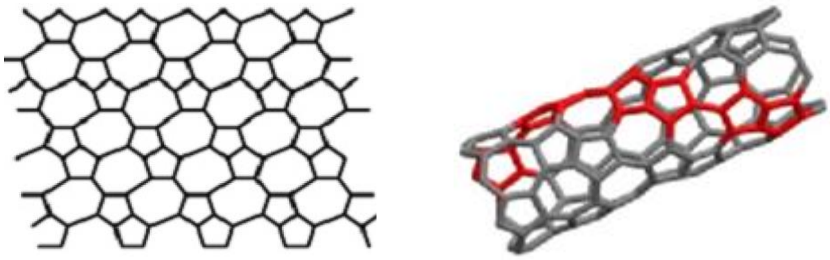
V. $M_2^{-1}(G) = R_{-1}(G) = \frac{1}{9}p + \frac{4}{3}pq$.

4.2 $TUSC_5C_7$ Nanotubes:

The molecular graph of the nanotubes $\mathrm{TUSC_5C_7}(p,q)$ as shown in Figure 6 consists of pentagons and heptagons. We denote p is the number of pentagons in each row. In this nanotube, the two first rows of vertices and edges are repeated, alternatively. We denote the number of this repetition by q. The cardinality of the edge sets of the graph are
$|E_1(G)| = p, |E_2(G)| = 6p, |E_3(G)| = 12pq - 12p$.

Theorem6. The general Zagreb indices of $G = \mathrm{TUHC_5C_7}(p,q)$ nanotubes is given by

- General first Zagreb index
  $M_1^{\alpha}(G) = [(2^{\alpha+2} - 2(3^{\alpha+1})]p + [8(3^{\alpha})]pq$.
- General Second Zagreb index
  $M_2^{\alpha}(G) = [6^{\alpha+1} + 2^{2\alpha} - 4(3^{2\alpha} + 1)]p + 4(3^{2\alpha+1})pq$.



(a) (b)

Figure 6: (a) Two dimensional lattice of $\mathrm{TUSC_5C_7}(4,4)$nanotube, (b) $\mathrm{TUSC_5C_7}$nanotubes.

Proof:

$$M_1^{\alpha}(G) = \sum_{uv\in E(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)]$$

$$= \sum_{uv\in E_1(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)] + \sum_{uv\in E_2(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)] + \sum_{uv\in E_3(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)]$$

$$= |E_1(G)|[2^{\alpha-1} + 2^{\alpha-1}] + |E_2(G)|[2^{\alpha-1} + 3^{\alpha-1}] + |E_3(G)|[3^{\alpha-1} + 3^{\alpha-1}]$$

$$= |E_1(G)|2^{2\alpha} + |E_2(G)|[2^{\alpha-1} + 3^{\alpha-1}] + |E_3(G)|[3^{\alpha-1} + 3^{\alpha-1}]$$

$$= p[2^{2\alpha}] + 6p[2^{\alpha-1} + 3^{\alpha-1}] + (12pq - 12p)[3^{\alpha-1} + 3^{\alpha-1}]$$

$$= [(2^{\alpha+2} - 2(3^{\alpha+1})]p + [8(3^{\alpha})]pq.$$

$$M_2^{\alpha}(G) = \sum_{uv\in E(G)} d_G^{\alpha-1}(u) d_G^{\alpha-1}(v)$$

$$= \sum_{uv\in E_1(G)} d_G^{\alpha-1}(u) d_G^{\alpha-1}(v) + \sum_{uv\in E_2(G)} d_G^{\alpha-1}(u) d_G^{\alpha-1}(v)$$

$$+\sum_{uv\in E_3(G)} d_G^{\alpha-1}(u)d_G^{\alpha-1}(v)$$

$$= |E_1(G)|[4^{\alpha}] + |E_2(G)|[6^{\alpha}] + |E_3(G)|[3^{2\alpha}]$$

$$=|E_1(G)|[2^{2\alpha}] + |E_2(G)|[2^{\alpha}3^{\alpha}] + |E_3(G)|[3^{2\alpha}]$$

$$=p[2^{2\alpha}] + 6p[2^{\alpha}3^{\alpha}] + (12pq - 12p)[3^{2\alpha}]$$

$$= [6^{\alpha+1} + 2^{2\alpha} - 4(3^{2\alpha} + 1)]p + 4(3^{2\alpha+1})pq.$$

For different values of α, we compute some other standard topological indices and the results are found as shown in the following corollary.

Corollary 6.p is the number of pentagons in each row and q is the number of repetition the first two rows of vertices and edges in G. Then

I. $M_1^2(G) = M_1(G) = 72pq - 38p$.

II. $M_1^3(G) = F(G) = 216pq - 130p$.

III. $M_2^{-\frac{1}{2}}(G) = R(G) = \left(\frac{2\sqrt{6}-7}{2}\right)p + 4pq$.

IV. $M_2^{\frac{1}{2}}(G) = RR(G) = (6\sqrt{6} - 34)p + 36pq$.

V. $M_2^{-1}(G) = R_{-1}(G) = \frac{31}{12}p + \frac{4}{3}pq$.

4.3 TUHAC$_5$C$_7$ Nanotubes:

The molecular graph of the nanotubes TUHAC$_5$C$_7(p, q)$ as shown in Figure 7 consists of pentagons and heptagons. We denote p is the number of pentagons in each row. In this nanotube, the three first rows of vertices and edges are repeated, alternatively. We denote the number of this repetition by q. The cardinality of the edge sets of the graph are

$|E_1(G)| = 0, |E_2(G)| = 4p, |E_3(G)| = 12pq - 5p.$

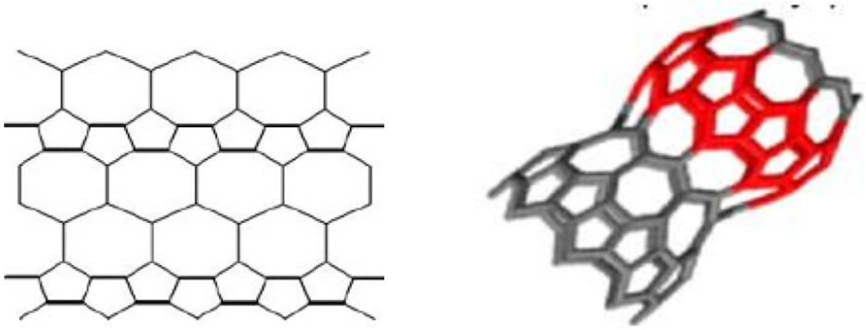
Theorem7. The general Zagreb indices of $G = \text{TUHAC}_5\text{C}_7(p, q)$ nanotubes is given by

- General first Zagreb index

$$M_1^{\alpha}(G) = 4(2^{\alpha-1} + 3^{\alpha-1})p + 2(12pq - 5p)3^{\alpha-1}.$$

- General Second Zagreb index

$$M_2^{\alpha}(G) = 4(6^{\alpha})p + (12pq - 5p)3^{2\alpha}.$$



(a) (b)

Figure 7: (a) Two dimensional lattice of $TUHAC_5C_7(4,2)$ nanotube, (b) $TUHAC_5C_7$nanotube.

Proof:

$$M_1^{\alpha}(G) = \sum_{uv \in E(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)]$$

$$= \sum_{uv \in E_1(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)] + \sum_{uv \in E_2(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)] + \sum_{uv \in E_3(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)]$$

$$= |E_1(G)|[2^{\alpha-1} + 2^{\alpha-1}] + |E_2(G)|[2^{\alpha-1} + 3^{\alpha-1}] + |E_3(G)|[3^{\alpha-1} + 3^{\alpha-1}]$$

$$= |E_1(G)|2^{2\alpha} + |E_2(G)|[2^{\alpha-1} + 3^{\alpha-1}] + |E_3(G)|[3^{\alpha-1} + 3^{\alpha-1}]$$

$$= 0 \times [2^{2\alpha}] + 4p[2^{\alpha-1} + 3^{\alpha-1}] + (12pq - 5p)[3^{\alpha-1} + 3^{\alpha-1}]$$

$$= 4(2^{\alpha-1} + 3^{\alpha-1})p + 2(12pq - 5p)3^{\alpha-1}.$$

$$M_2^{\alpha}(G) = \sum_{uv \in E(G)} d_G^{\alpha-1}(u) d_G^{\alpha-1}(v)$$

$$= \sum_{uv\in E_1(G)} d_G^{\alpha-1}(u)d_G^{\alpha-1}(v) + \sum_{uv\in E_2(G)} d_G^{\alpha-1}(u)d_G^{\alpha-1}(v) + \sum_{uv\in E_3(G)} d_G^{\alpha-1}(u)d_G^{\alpha-1}(v)$$

$$= |E_1(G)|[4^{\alpha}] + |E_2(G)|[6^{\alpha}] + |E_3(G)|[3^{2\alpha}]$$

$$=|E_1(G)|[2^{2\alpha}] + |E_2(G)|[2^{\alpha}3^{\alpha}] + |E_3(G)|[3^{2\alpha}]$$

$$=0 \times 2^{2\alpha} + 4p[2^{\alpha}3^{\alpha}] + (12pq - 5p)[3^{2\alpha}]$$

$$= 4(6^{\alpha})p + (12pq - 5p)3^{2\alpha}.$$

For different values of α, we compute some other standard topological indices and the results are found as shown in the following corollary.

Corollary 7. p is the number of pentagons in each row and q is the number of repetition the first three rows of vertices and edges in G. Then

I. $M_1^2(G) = M_1(G) = 36pq - 20p.$

II. $M_1^3(G) = F(G) = 2p(54q - 38)$

III. $M_2^{-\frac{1}{2}}(G) = R(G) = \left(\frac{4}{\sqrt{6}} - \frac{5}{3}\right)p + 4pq.$

IV. $M_2^{\frac{1}{2}}(G) = RR(G) = (4\sqrt{6} - 5\sqrt{3})p + 12\sqrt{3}pq$.

V. $M_2^{-1}(G) = R_{-1}(G) = \frac{1}{9}p + \frac{4}{3}pq.$

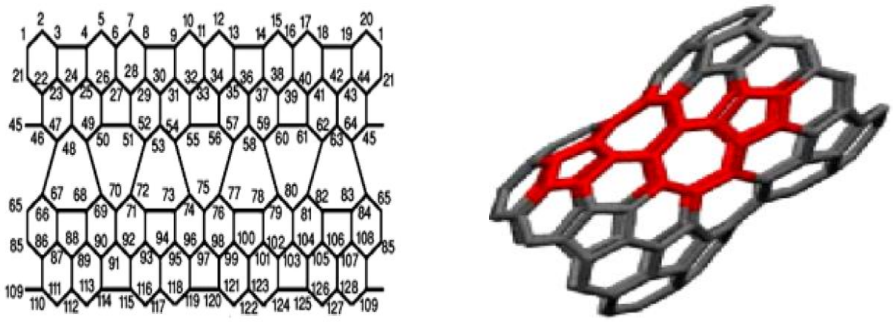
4.4 TUHA$C_5C_6C_7$ Nanotubes:

The molecular graph of the nanotubes TUHA$C_5C_6C_7(p,q)$ as shown in Figure 8 consists of pentagons, hexagons, and heptagons. We denote p is the number of pentagons in each row. In this nanotube, the three first rows of vertices and edges are repeated, alternatively. We denote the number of this repetition by q. The cardinality of the edge sets of the graph are

$|E_1(G)| = 0, |E_2(G)| = 8p, |E_3(G)| = 24pq - 10p.$

Theorem 8. The general Zagreb indices of $G = \mathrm{TUHAC_5C_6C_7}(p,q)$ nanotubes is given by

- General first Zagreb index
  $M_1^{\alpha}(G) = 8p[2^{\alpha-1} + 3^{\alpha-1}] + (24pq - 10p)[3^{\alpha-1} + 3^{\alpha-1}]$.
- General Second Zagreb index
  $M_2^{\alpha}(G) = 8p[2^{\alpha}3^{\alpha}] + (24pq - 10p)[3^{2\alpha}]$.



(a) (b)

Figure 8: (a) Two dimensional lattice of $\mathrm{TUHAC_5C_6C_7}(4,2)$ nanotube, (b) $\mathrm{TUHAC_5C_6C_7}$nanotube.

Proof:

$$M_1^{\alpha}(G) = \sum_{uv\in E(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)]$$

$$= \sum_{uv\in E_1(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)] + \sum_{uv\in E_2(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)] + \sum_{uv\in E_3(G)} [d_G^{\alpha-1}(u) + d_G^{\alpha-1}(v)]$$

$$= |E_1(G)|[2^{\alpha-1} + 2^{\alpha-1}] + |E_2(G)|[2^{\alpha-1} + 3^{\alpha-1}] + |E_3(G)|[3^{\alpha-1} + 3^{\alpha-1}]$$

$$= |E_1(G)|2^{\alpha} + |E_2(G)|[2^{\alpha-1} + 3^{\alpha-1}] + |E_3(G)|[3^{\alpha-1} + 3^{\alpha-1}]$$

$$= 0 \times [2^{\alpha}] + 8p[2^{\alpha-1} + 3^{\alpha-1}] + (24pq - 10p)[3^{\alpha-1} + 3^{\alpha-1}]$$

$$= 8p[2^{\alpha-1} + 3^{\alpha-1}] + (24pq - 10p)[3^{\alpha-1} + 3^{\alpha-1}].$$

$$M_2^{\alpha}(G) = \sum_{uv\in E(G)} d_G^{\alpha-1}(u) d_G^{\alpha-1}(v)$$

$$= \sum_{uv\in E_1(G)} d_G^{\alpha-1}(u) d_G^{\alpha-1}(v) + \sum_{uv\in E_2(G)} d_G^{\alpha-1}(u) d_G^{\alpha-1}(v)$$

$$+ \sum_{uv\in E_3(G)} d_G^{\alpha-1}(u) d_G^{\alpha-1}(v)$$

$$= |E_1(G)|[4^{\alpha}] + |E_2(G)|[6^{\alpha}] + |E_3(G)|[3^{2\alpha}]$$

$$=|E_1(G)|[2^{2\alpha}] + |E_2(G)|[2^{\alpha}3^{\alpha}] + |E_3(G)|[3^{2\alpha}]$$

$$=0 \times 2^{2\alpha} + 8p[2^{\alpha}3^{\alpha}] + (24pq - 10p)[3^{2\alpha}]$$

$$= 8p[2^{\alpha}3^{\alpha}] + (24pq - 10p)[3^{2\alpha}].$$

For different values of α, we compute some other standard topological indices and the results are found as shown in the following corollary.

Corollary 8. p is the number of pentagons in each row and q is the number of repetition the first three rows of vertices and edges in G. Then

I. $M_1^2(G) = M_1(G) = 144pq - 20p$.

II. $M_1^3(G) = F(G) = 432pq - 76p$

III. $M_2^{-\frac{1}{2}}(G) = R(G) = \left(\frac{8}{\sqrt{6}} - \frac{10}{3}\right)p + 8pq$.

IV. $M_2^{\frac{1}{2}}(G) = RR(G) = 72pq + (8\sqrt{6} - 30)p$.

V. $M_2^{-1}(G) = R_{-1}(G) = (\frac{2}{9})p + \frac{8}{3}pq$.

5. Conclusion

In this study, we obtain some closed expressions of the General Zagreb indices and some standard degree based topological indices as special cases of this index for some Carbon nanotubes. The computation of these general indices for some other chemical compounds can be a challenging topic for further study.

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