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F -INDICES AND ITS COINDICES OF CHEMICAL GRAPHS

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Abstract. In this paper, we obtain the exact expressions for the F -indices and its coindices of Armchair Polyhex Nanotubes, $TUC4C8[m, n]$ Nanotubes and smart polymer graphs.

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1. Introduction

A chemical graph is a graph whose vertices denote atoms and edges denote bonds between those atoms of any underlying chemical structure. A topological index for a (chemical) graph G is a numerical quantity invariant under automorphisms of G and it does not depend on the labeling or pictorial representation of the graph. Topological indices and graph invariants based on the distances between vertices of a graph or vertex degrees are widely used for characterizing molecular graphs, establishing relationships between structure and properties of molecules, predicting biological activity of chemical compounds and making their chemical applications. These indices may be used to derive quantitative structure-property or structure-activity relationships (QSPR/QSAR).

For a (molecular) graph G, The *first Zagreb index* $M_1(G)$ is the equal to the sum of the squares of the degrees of the vertices, and the *second Zagreb index* $M_2(G)$ is the equal to the sum of the products of the degrees of pairs of adjacent vertices, that is,

$$M_1(G) = \sum_{uv\in E(G)} d_G^2(u) = \sum_{uv\in E(G)} (d_G(u) + d_G(v)),$$
$$M_2(G) = \sum_{uv\in E(G)} d_G(u) d_G(v).$$

The *first and* second *Zagreb coincides were* first introduced by Ashrafi et al. [2]. They are defined as follows:

$$\overline{M}_2(G) = \sum_{uv\in E(G)} (d_G(u) + d_G(v)). \qquad \overline{M}_2(G) = \sum_{uv\in E(G)} d_G(u) d_G(v).$$

The forgotten *topological index* was introduced by Furtula and Gutman [1], and it is defined as

$$F = F(G) = \sum_{u\in V(G)} d_G{}^3(u) = \sum_{uv\in E(G)} (d_G{}^2(u) + d_G{}^2(v)).$$

In this sequence, the *forgotten topological coindex* is defined as

$$\overline{F}(G) = \sum_{uv \notin E(G)} (d_G{}^2(u) + d_G{}^2(v)).$$

Khalifeh et al. [3] obtained the first and second Zagreb indices of the Cartesian, join, composition, disjunction and symmetric difference of two graphs. Ashrafi et al. [2] obtained the first and second Zagreb coindices of the Cartesian, join, composition, disjunction and symmetric difference of two graphs. Furtula and Gutman [1] established a few basic properties of the forgotten topological index and show that can significantly enhance the physico-chemical applicability of the first Zagreb index. Some topological indices of bridge and chain graphs have been computed previously [5, 6, 7]. The properties and several invariants of the transformation graphs are discussed in [8, 9, 10]. In this paper, we obtain the exact expressions for the F -indices and its coindices of Armchair Polyhex Nanotubes, $TUC4C8[m, n]$ Nanotubes and smart polymer graphs.

2. Basic properties

Let G be a graph on n vertices and m edges. The complement of G, denoted by $\overline{G}$, is a simple graph on the same set of vertices of G in which two vertices u and v are adjacent in $\overline{G}$ if and only if they are nonadjacent in G. Obviously,

$$E(G) \cup E(\overline{G}) = E(Kn) \text{ and } \overline{m} = \left|E(\overline{G})\right| = \frac{n(n-1)}{2} - m.$$

The degree of a vertex v in G is denoted by $dG(v)$; the degree of the same vertex in $\overline{G}$ is given by $d_{\overline{G}}(v) = n - 1 - dG(v)$.

Lemma 1. Let Pn and Cn be the path and cycle on n vertices, respectively. Then
(i) $M1(Pn) = 4n - 6$ *and* $M1(Cn) = 4n$.
(ii) $F(Pn) = 8n - 14$ *and* $F(Cn) = 8n$.

Lemma 2. Let G be a connected graph with n vertices and m edges. Then

$$F(\overline{G}) = n(n - 1)^3 - F(G) - 6(n - 1)^2m + 3(n - 1)M1(G).$$

Proof.

$$\begin{aligned} F(\overline{G}) &= \sum_{u \in V(\overline{G})} d^3_{\overline{G}}(u) \\ &= \sum_{u \in V(G)} (n-1-d_G(u))^3 \\ &= \sum_{u \in V(G)} ((n-1)^3 - d^3_G(u) - 3(n-1)^2 d_G(u) + 3(n-1) d^2_G(u)) \\ &= n(n-1)^3 - F(G) - 6(n-1)^2 m + 3(n-1) M_1(G). \end{aligned}$$

Lemma 3. Let G be a connected graph with n vertices and m edges. Then

$$\overline{F}(G) = (n - 1)\, M1(G) - F(G).$$

Proof.

$$\overline{F}(G) = \sum_{uv \notin E(G)} (d_G^2(u) + d_G^2(v))$$
$$= \sum_{uv \notin E(G)} ((n-1-d_G(u)-(n-1))^2 + (n-1-d_G(v)-(n-1))^2)$$
$$= \sum_{uv \in E(\overline{G})} (d_{\overline{G}}(u)-(n-1))^2 + (d_{\overline{G}}(v)-(n-1))^2)$$
$$= \sum_{uv \in E(\overline{G})} (d_{\overline{G}}^2(u) + (n-1)^2 - 2(n-1)d_{\overline{G}}(u) + d_{\overline{G}}^2(v) + (n-1)^2 - 2(n-1)d_{\overline{G}}(v))$$
$$= \sum_{uv \in E(\overline{G})} (d_{\overline{G}}^2(u) + d_{\overline{G}}^2(v)) + 2(n-1)^2 \sum_{uv \in E(\overline{G})} (1) - 2(n-1) \sum_{uv \in E(\overline{G})} (d_{\overline{G}}(u) + d_{\overline{G}}(v)$$
$$= F(\overline{G}) - 2(n-1)M1(\overline{G}) + 2(n-1)^2\ \overline{m}.$$

By Lemma 2 and the expression $M1(\overline{G}) = M1(G) + 2(n-1)(\overline{m} - m)$ we obtain:

$$\overline{F}(G) = (n-1)M1(G) - F(G).$$

3. The *TUAC*6[*m*, *n*] Nanotubes

In this section, we compute the forgotten topological indices and coindices of a family of Hexagonal Nanotubes, namely, Armchair polyhex Nanotubes $TUAC6[m, n]$, for every $n,m \in N$. For more study about Armchair polyhex Nanotubes $TUAC6[m, n]$, see [12, 13, 14, 15, 16, 17]. Let $G = TUAC6[m, n]$, for every $n,m \in N$ the Armchair polyhex Nanotubes, see Fig.1. For our convenience, we partition the vertex set of G into two sets, $V1 = \{v \in V(G) | dG(v) = 2\}$ and $V2 = \{v \in V(G) | dG(v) = 3\}$. Thus

$$|V1| = 2(\frac{m}{2}) + 2(\frac{m}{2}) = 2m \text{ and } |V2| = 2mn.$$

Similarly, we partition the edge set of G into three sets,

$$E1 = \{uv \in E(G) | dG(u) = dG(v) = 2\},$$

$E2 = \{uv \in E(G) | dG(u) = 2,\ dG(v) = 3\}$ and $E3 = \{uv \in E(G) | dG(u) = dG(v) = 3\}$. Therefore the size of three edge partitions $E1$, $E2$ and $E3$ of $TUAC6[m, n]$ are equal to m, $2m$ and $3mn - m$, respectively. That is,

$$|E1| = \frac{m}{2} + \frac{m}{2} = \text{m } and\ |E2| = 2\ |E1| = 2m \text{ and } |E2| = 3mn - m.$$

Hence the graph $TUAC6[m, n]$ has $2m(n + 1)$ vertices(atoms) and $3mn + 2m$ edges(bonds).

$$F(TUAC6[m, n]) = \sum_{uv \in E(G)} (d_G^2(u) + d_G^2(v))$$
$$= \sum_{uv \in E_1} (d_G^2(u) + d_G^2(v)) + \sum_{uv \in E_2} (d_G^2(u) + d_G^2(v)) + \sum_{uv \in E_3} (d_G^2(u) + d_G^2(v))$$
$$= \sum_{uv \in E_1} (2^2 + 2^2) + \sum_{uv \in E2} (2^2 + 3^2) + \sum_{uv \in E3} (3^2 + 3^2) = 54\text{mn}+16\text{m}.$$

Using Lemma 3, $F(TUAC6[m, n])$ and $M1(TUAC6[m, n]) = 18mn + 8m$, we obtain the result $\overline{F}(TUAC6[m, n]) = 36m^2n^2 + 52m^2n + 16m^2 - 72mn - 24m$.

4. The *TUC*4*C*8[*m*, *n*] Nanotubes

In this section, we compute the exact formulae of F -index and coindex for a family of Nanostructures and molecular graphs with structure consist of cycles $C4$ and $C8$ ($TUC4C8[m, n]$ Nanotubes). M.V. Diudea denoted the number of Octagons C_8 in the first row of G by m and the number of Octagons $C8$ in the first column of G by n, and he denoted $TUC4C8(S)$ Nanotubes by $G = TUC4C8[m, n]$, for every $n,m \in N$. One can see that 2 and 3-Dimensional lattices of $G = TUC4C8[m, n]$ in Fig.2 and more details, see [18, 19, 20, 21, 22].

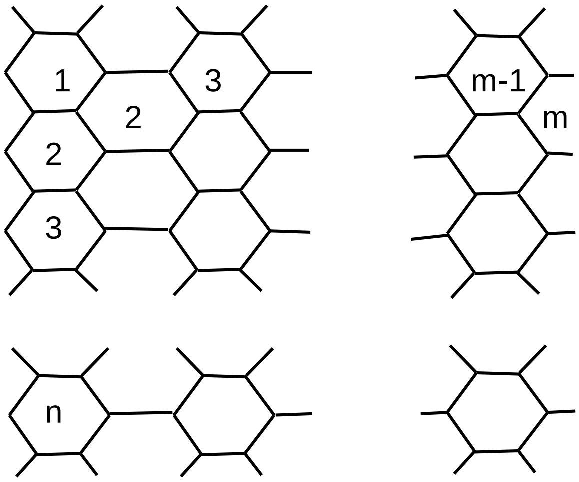

Fig.1. Two dimensional lattice of the Armchair Polyhex Nanotubes $TUAC6[m, n]$

For our convenience, we partition the vertex set of G into two sets, $V1 = \{v \in V(G)|dG(v) = 2\}$ and $V2 = \{v \in V(G)|dG(v) = 3\}$. Thus $|V1| = 2m + 2m = 4m$ and $|V2| = 8mn$. From the structure of $TUC4C8[m, n]$, we partition the edge set of $TUC4C8[m, n]$ into three sets, $E1 = \{uv \in E(G)|dG(u) = dG(v) = 2\}$, $E2 = \{uv \in E(G)|dG(u) = 2, dG(v) = 3\}$ and $E3 = \{uv \in E(G)|dG(u) = dG(v) = 3\}$. Thus we have $|E1| = \frac{1}{2}|V2| = 2m$ and $|E2| = |V2| = 4m$ and $|E2| = 12mn - 2m$. Hence the graph $TUC4C8[m, n]$ has $(8mn + 4m)$ vertices (atoms) and $12mn + 4m$ edges (bonds). A similar argument of previous Section, we have $F(TUC4C8[m, n]) = 216mn + 32m$.

Using Lemma 3, $F(TUC4C8[m, n])$ and $M1(TUC4C8[m, n]) = 72mn + 16m$, we obtain the result $\overline{F}(TUC4C8[m, n]) = 576m^2n^2 + 488m^2n + 64m^2 - 288mn - 48m$.

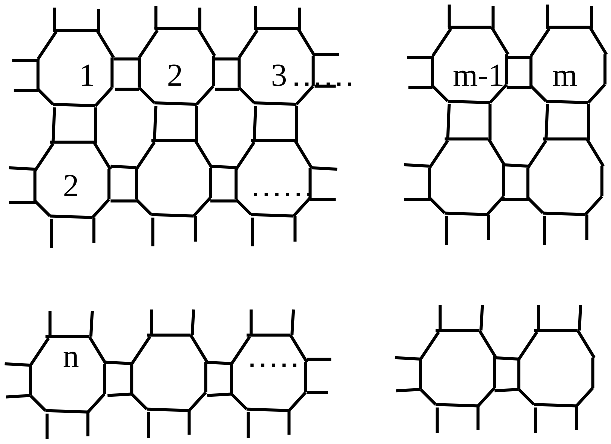

Fig. 2. Two Dimensional lattice of the TUSC4C8(S) Nanotubes.

5. Smart polymer

In this section, we compute the exact formulae of F -index and coindex for the class of the smart polymer, Dox-loaded micelle comprising PEG-PAsp block copolymer with chemically conjugated Dox $SP[n]$.

Smart polymers are defined as the macromolecules that display a dramatic physiochemical change in response to small changes in their environment such as temperature, pH, light, agnetic field, ionic factors, etc [23]. Smart polymers are also called as stimuli responsive or intelligent or environmentally responsive systems. Smart polymers have various applications in biomedical field as delivery systems like smart polymers with protein or nucleic acid delivery to intracellular targets such as ribosome or nucleus and in tissue engineering [24]. Polymeric micelles are one of the kind of smart polymer, which is used to delivering anti cancer drug. For eg. Dox-conjugated PEG-b-poly (aspartate) (PEG–PAsp) block copolymers [25]. For more details see [26, 27].

Let $G(n) = SP[n]$, where n is step of growth of this type of polymers, be a molecular graph, see Fig.3. Define $E_{ij} = \{uv \in E(G(n)) | d_{G(n)}(u) = i, d_{G(n)}(v) = j\}$. From the structure of the graph $G(n)$, we partition the edge set of $G(n)$ into eight sets, E_{12}, E_{13}, E_{14}, E_{22}, E_{23}, E_{24}, E_{33} and E_{34}. One can conclude that $|E_{12}| = 2n + 1$, $|E_{13}| = 9n + 1$, $|E_{14}| = |E_{34}| = n$, $|E_{22}| = 5n + 4$, $|E_{23}| = 18n - 1$, $|E_{24}| = 2n$ and $|E_{33}| = 16n$. Hence the graph $G(n)$ has $49n + 6$ vertice (atoms) and $54n + 5$ edges (chemical bonds).

$$F(G(n)) = \sum_{uv\in E(G(n))} (d_{G(n)}^2(u) + d_{G(n)}^2(v))$$

$$= \sum_{uv\in E_{12}}(1+4) + \sum_{uv\in E_{13}}(1+9) + \sum_{uv\in E_{24}}(1+16) + \sum_{uv\in E_{22}}(4+4) + \sum_{uv\in E_{23}}(4+9)$$

$$+ \sum_{uv\in E_{24}}(4+16) + \sum_{uv\in E_{33}}(9+9) + \sum_{uv\in E_{34}}(9+16) = 744n+34$$

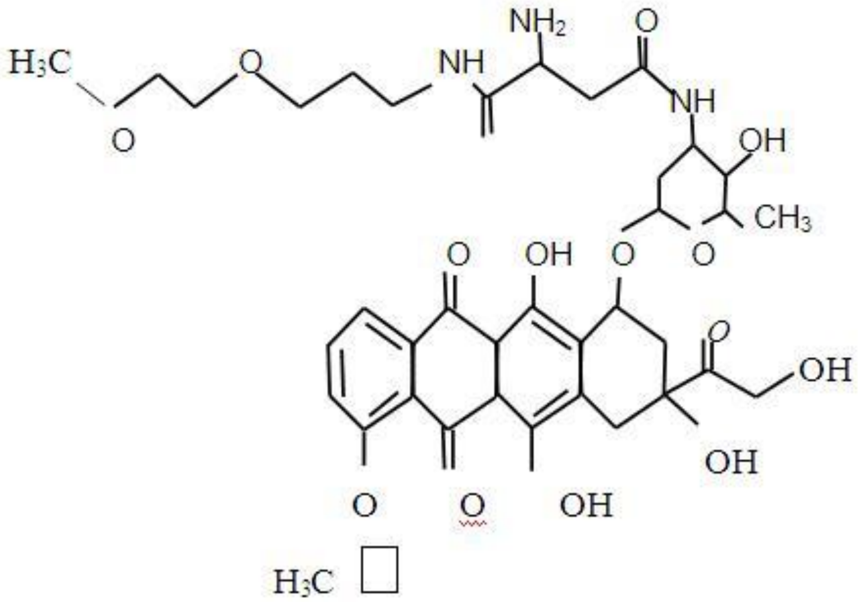

Fig.3. The graph of $G[1]$

Using Lemma 3, $F(G(n))$ and the expression $M1(G(n)) = 272n + 18$, we obtain the result $\overline{F}(G(n)) = 13328n^2 + 2242n + 90$.

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