ON THE PARA-LINE GRAPHS OF CERTAIN NANOSTRUCTURES BASED ON TOPOLOGICAL INDICES

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Topological indices are valuable in the study of QSAR/QSPR. There are numerous applications of graph theory in the field of structural chemistry. In this paper, we computed generalized Randić, general Zagreb, general sum-connectivity, ABC, GA, ABC_4 and GA_5 indices of the Para-line graph of V-Pantacenic nanotube, H-Pantacenic nanotube and V-Pantacenic nanotorus.

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1. Introduction and Preliminaries

Topological Indices are arithmetical quantities of a graph that are invariant under graph isomorphism. The significance of topological indices is mainly related to their utilizing in quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR). Para-line graphs are very important in structural chemistry, but still in the last few decades they were considered very little in chemical graph theory. To define Para-line graphs we need the following notations.

Let G be a simple graph with vertex set V(G) and edge set E(G). The subdivision graph S(G) is the graph obtained from G by replacing each of its edge by a path of length 2. The line graph L(G) of graph G is the graph whose vertices are the edges of G, two vertices e and f are incident if and only if they have a common end vertex in G. The Para-line graph of G is the line graph of the subdivision graph of G i.e. L(S(G)) which will be denoted by G*. Alternatively, we can construct G* from G as follows:

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(1) Replace each vertex u∈V(G) by K(u); the complete graph on d_u vertices;
(2) There is an edge joining a vertex of $K(u_1)$ and a vertex of $K(u_2)$ in G if and only if there is an edge joining u_1 and u_2 in G;
(3) For each vertex v of K(u), degree of v in G is same as degree of u in G.

A molecular graph is a set of points representing the atoms in the molecule and collection of lines representing the covalent bonds. For example, consider the hydrocarbon C_6H_6, its molecular structure and molecular graph is shown in Fig. 1 (a) and (b). However, there are other ways to attach a graph with molecules, for instance in terms of a minimal set of localized orbitals each taken as a vertex, with edges described the stronger connections between pairs of orbitals. In fact, such a graph was understood in several early quantum chemical mechanisms. The vertices of Para-line graphs of molecular graph correspond to its atomic hybrid orbital, and their edge corresponds to stronger interactions between pairs of such orbital. Para-line graph of molecular graph of hydrocarbon C_6H_6 is shown in Fig. 1 (c).

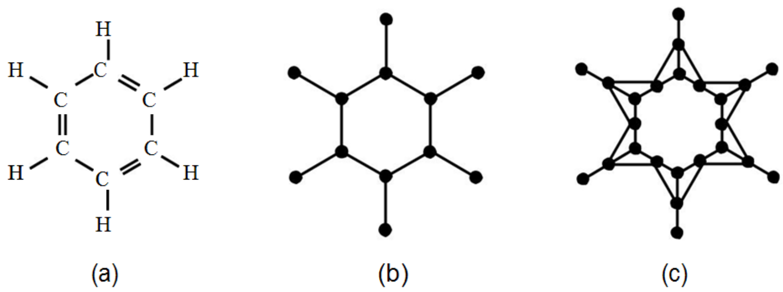

Fig. 1. (a) C_6H_6 (b) Graph of C_6H_6 (c) Para-line graph of C_6H_6

For more details on the para-line graphs and its connection with chemistry, we refer to the article [39].
In [38], Farahani et al. discussed the topological indices of the line graph of H-Pantacenic nanotube. In this article, we study topological indices of the para-line graphs of H-Pantacenic nanotube as well as V-Pantacenic nanotube and V-Pantacenic nanotorus. The 2-D lattice graphs of V-Pantacenic nanotube, H-Pantacenic nanotube and V-Pantacenic nanotorus are shown in Fig. 2, 4 and 6 respectively.
For u ∈ V (G), N_u denotes the set of its neighbors in G, the degree of vertex u is $d_u=|N_u|$ and $S_u = \sum_{v \in N_u} d_v$. In structural chemistry and biology, molecular structure descriptors are utilized for modeling information of molecules, which are known as topological indices. Many topological indices are introduced to explain the physical and chemical properties of molecules. Topological indices

are generally divided into three kinds: degree-based indices [16, 17, 22, 29, 30, 35], distance-based indices [1, 2, 8, 12, 14, 28, 34], and spectrum-based indices [4, 13, 15, 18]. There are also some topological indices based on both degrees and distances (see [5, 7, 11, 32, 33]).

The general Randić connectivity index of G is defined as [3]

$$R_\alpha(G) = \sum_{uv\in E(G)} (d_u d_v)^\alpha. \tag{1}$$

where is α a real number. Then $R_{-1/2}(G)$ is known as Randić connectivity index of G. Li and Zhao introduced the first general Zagreb index in [19]:

$$M_\alpha(G) = \sum_{u\in V(G)} (d_u)^\alpha. \tag{2}$$

In 2010, general sum-connectivity index χ_α(G) has been introduced in [36]:

$$\chi_\alpha(G) = \sum_{uv\in E(G)} (d_u + d_v)^\alpha. \tag{3}$$

The atom-bond connectivity (ABC) index, introduced by Estrada et al. in [6]. The ABC index of graph G is defined as

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}. \tag{4}$$

D. Vukicevic and B. Furtula introduced the Geometric arithmetic (GA) index in [27]. The GA index for graph G is defined by

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}. \tag{5}$$

The fourth member of the class of ABC index was introduced by M. Ghorbani et al. in [9] as:

$$ABC_4(G) = \sum_{uv\in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}. \tag{6}$$

The 5th GA index was introduced by Graovac et al. in [10] as

$$GA_5(G) = \sum_{uv\in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}. \tag{7}$$

2. Topological indices of Para-line graphs

The study of the topological indices of Para-line graphs is a popular topic in the inter-disciplinary of chemistry and graph theory (see [37, 38]). In 2011, Ranjini et al. calculated the explicit expressions for the Shultz index of the subdivision graph of the tadpole, wheel, helm and ladder graphs [25]. They also studied the Zagreb indices of the Para-line graph of the tadpole, wheel and ladder in [24]. In 2015, Su and Xu calculate the general sum-connectivity index and co-index of the Para-line graph of the tadpole, wheel and ladder graphs in [26]. In [20], Nadeem et al. computed ABC_4 and GA_5 index of the Para-line graphs of the tadpole, wheel and ladder graphs. They also studied generalized Randić, general Zagreb, general sum-connectivity, ABC, GA, ABC_4 and GA_5 indices of the Para-line graph of 2D lattice, nanotube and nanotorus TUC_4C_8[p,q] in [21].

In this paper, we computed generalized Randić, general Zagreb, general sum-connectivity, ABC, GA, ABC_4 and GA_5 indices of the para-line graphs of V-Pantacenic nanotube, H-Pantacenic nanotube and V-Pantacenic nanotorus.

In order to calculate the number of edges of the line graph, the following lemma is important for us and can be deduced by the definition of the line graph.

Lemma 1. Let G be a graph. Then

$$|E(L(G))| = \sum_{u \in V(G)} \frac{d_u^2}{2} - |E(G)|$$

where L(G) is the line graph of G.

2.1. Topological indices of the Para-line graph of V-Pantacenic nanotube.

The 2-D graph lattice of V-Pantacenic nanotube is shown in Fig. 2 and it is denoted by F [p,q]. There are 22pq vertices and 33pq-5p edges in F [p,q].

Theorem 2. Let G* be the Para-line graph of F [p,q]. Then

$$M_\alpha(G^*) = 5p\,2^{\alpha+2} + 3^{\alpha+1}(22pq - 10p).$$

Proof. The graph G* is shown in Fig. 3. In G* there are total 66pq-10p vertices among which 20p vertices are of degree 2 and 66pq-30p vertices are of degree 3. Hence, we get $M_\alpha(G^*)$ by using formula 2.

Theorem 3. Let G* be the Para-line graph of F [p,q]. Then

$$R_\alpha(G^*) = 10p.4^\alpha + 20p.6^\alpha + (99pq - 55p)9^\alpha,$$

$$\chi_\alpha(G^*) = 10p.4^\alpha + 20p.5^\alpha + (99pq - 55p)6^\alpha,$$

$$ABC(G^*) = \left(15\sqrt{2} - \frac{110}{3}\right)p + 66pq,$$

$$GA(G^*) = 99pq + \left(8\sqrt{6} - 45\right)p.$$

Proof. The subdivision graph S(F[p,q]) contains 66pq-10p edges and 55pq-5p vertices among which 33pq+5p vertices are of degree 2 and remaining 22pq-10p vertices are of degree 3. Hence by Lemma 1, the total number of edges of G* are 99pq-25p. The edge set E(G*) divides into three edge partitions based on degrees of the end vertices, i.e. $E(G^*)=E_1(G^*)\cup E_2(G^*)\cup E_3(G^*)$. The edge partition $E_1(G^*)$ contains 10p edges uv, where $d_u=d_v=2$, the edge partition $E_2(G^*)$ contains 20p edges uv, where $d_u=2$ and $d_v=3$, and the edge partition $E_3(G)$ contains 99pq-55p edges uv, where $d_u=d_v=3$. From formulas 1, 3, 4 and 5, we obtain the required results.

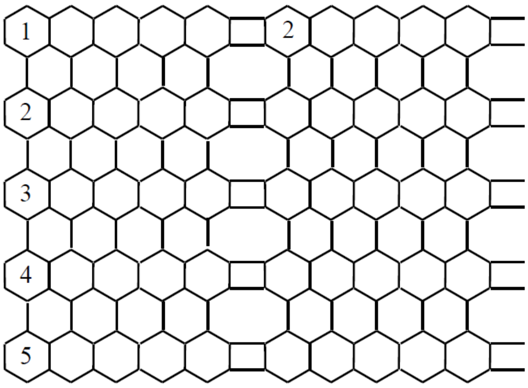

Fig. 2. 2-D graph lattice of V-Pantacenic nanotube

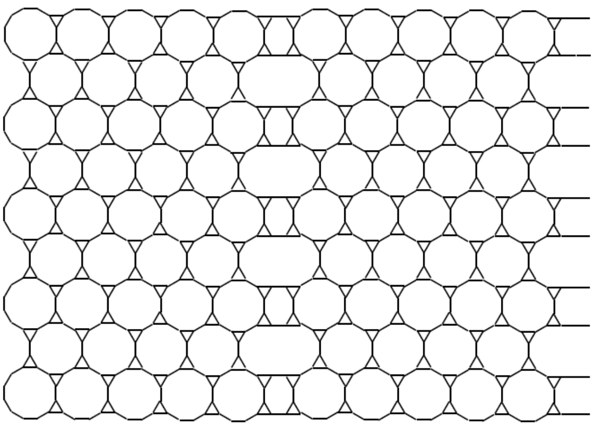
Fig. 3. Para-line graph of 2-D lattice of V-Pantacenic nanotube

Theorem 4. Let G* be the Para-line graph of F [p,q]. Then

$$ABC_4(G^*)=\left(4\sqrt{2}+\sqrt{110}+\sqrt{14}+2\sqrt{30}-\frac{116}{3}\right)p+44pq,$$

$$GA_5(G^*)=\left(-69+\frac{80}{13}\sqrt{10}+\frac{288}{17}\sqrt{2}\right)p+99pq\ .$$

Proof. If we consider an edge partition based on degree sum of neighbors of end vertices then the edge set E(G*) can be divided into five edge partitions $E_i(G^*)$, i=4,5,...,8 i.e. $E(G^*) = \cup_{i=4}^{8} E_i(G^*)$. The edge partition $E_4(G^*)$ contains 10p edges uv, where $S_u=S_v=5$, the edge partition $E_5(G^*)$ contains 20p edges uv, where $S_u=5$ and $S_v=8$, the edge partition $E_6(G^*)$ contains 8p edges uv, where $S_u=S_v=8$, the edge partition $E_7(G^*)$ contains 24p edges uv, where $S_u=8$ and $S_v=9$ and the edge partition $E_8(G^*)$ contains 99pq-87p edges uv, where $S_u=S_v=9$. From formulas 6 and 7, we obtain the required results.

2.2. Topological indices of the Para-line graph of H-Pantacenic nanotube.

The 2-D graph lattice of H-Pantacenic nanotube is shown in Fig. 4 and it is denoted by K[p,q]. There are 22pq vertices and 33pq-2q edges in K[p,q].

Theorem 5. Let G* be the Para-line graph of K[p,q]. Then

$$M_\alpha(G^*) = q.2^{\alpha+3} + 3^{\alpha+1}(22pq - 4q).$$

Proof. The graph G* is shown in Fig. 5. In G* there are total 66pq-4q vertices among which 8q vertices are of degree 2 and 66pq-12q vertices are of degree 3. Hence, we get $M_\alpha(G^*)$ by using formula 2.

Theorem 6. Let G* be the Para-line graph of K[p;q]. Then

$$R_\alpha(G^*) = 6q.4^\alpha + 4q.6^\alpha + (99pq - 20q)9^\alpha,$$

$$\chi_\alpha(G^*) = 6q.4^\alpha + 4q.5^\alpha + (99pq - 20q)6^\alpha,$$

$$ABC(G^*) = 5q\sqrt{2} + 66pq - \frac{40}{3}q,$$

$$GA(G^*) = \frac{8}{5}q\sqrt{6} + 99pq - 14q.$$

Proof. The subdivision graph S(K[p,q]) contains 66pq-4q edges and 55pq-2q vertices among which vertices are of degree 2 and remaining vertices are of degree 3. Hence by Lemma 1 the total number of edges of G* are 99pq-10q. The edge set E(G*) divides into three edge partitions based on degrees of the end vertices, i.e. $E(G^*) = E_1(G^*) \cup E_2(G^*) \cup E_3(G^*)$. The edge partition $E_1(G^*)$ contains 6q edges uv, where $d_u=d_v=2$, the edge partition $E_2(G^*)$ contains 4q edges uv, where $d_u=2$ and $d_v=3$, and the edge partition $E_3(G^*)$ contains 99pq-20q edges uv, where $d_u=d_v=3$. From formulas 1, 3, 4 and 5, we obtain the required results.

Theorem 7. Let G* be the Para-line graph of K[p,q]. Then

$$ABC_4(G^*) = 44pq + \left(\frac{2}{5}\sqrt{35} + \frac{1}{5}\sqrt{110} + \frac{1}{3}\sqrt{30} + \frac{1}{2}\sqrt{6} - \frac{32}{3}\right)q,$$

$$GA_5(G^*) = 99pq + \left(\frac{16}{9}\sqrt{5} + \frac{16}{13}\sqrt{10} + \frac{48}{17}\sqrt{2} - 22\right)q \, .$$

Proof. If we consider an edge partition based on degree sum of neighbors of end vertices
then the edge set E(G*) can be divided into five edge partitions $E_i(G^*)$; i=4,5,…,8 i.e. $E(G^*) = \cup_{i=4}^{8} E_i(G^*)$. The edge partition $E_4(G^*)$ contains 2q edges uv, where $S_u=S_v=4$, the edge partition $E_5(G^*)$ contains 4q edges uv, where $S_u=4$ and $S_v=5$, the edge partition $E_6(G^*)$ contains 4q edges uv, where $S_u=5$ and $S_v=8$, the edge partition $E_7(G^*)$ contains 4q edges uv, where $S_u=8$ and $S_v=9$ and the edge partition $E_8(G^*)$ contains 99pq-24q edges uv, where $S_u=S_v=9$. From formulas 6 and 7, we obtain the required results.

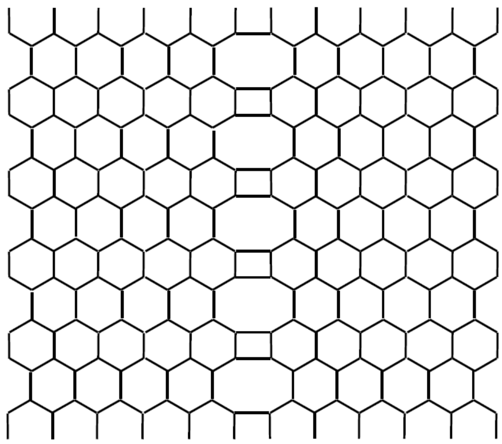

Fig. 4. 2-D graph lattice of H-Pantacenic nanotube

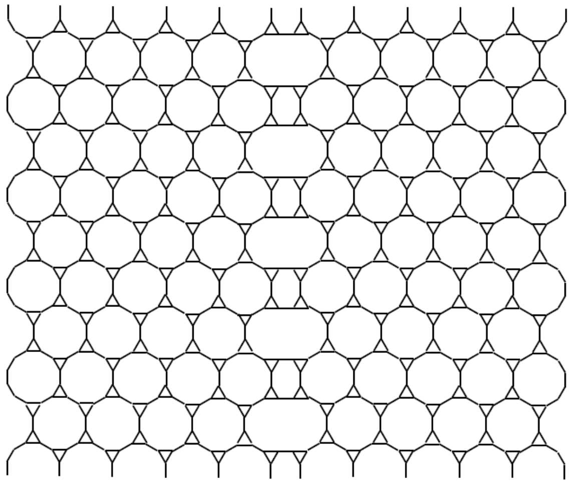

Fig. 5. Para-line graph 2-D lattice of H-Pantacenic nanotube

2.3. Topological indices of the Para-line graph of V-Pantacenic nanotorus.

The 2-D graph lattice of V-Pantacenic nanotorus is shown in Fig. 6 and it is denoted by L[p,q]. There are 22pq vertices and 33pq edges in L[p,q].

Theorem 8. Let G* be the Para-line graph of L[p,q]. Then $M_{\alpha}(G^{*}) = 22pq.3^{\alpha+1}$.

Proof. The graph G* is shown in Fig. 7. In G there are total 66pq vertices and all of them are of degree 3. Hence, we get $M_{\alpha}(G^*)$ by using formula 2.

Theorem 9. Let G* be the Para-line graph of L[p,q]. Then
$R_{\alpha}(G^{*}) = 99pq.9^{\alpha}$,
$\chi_{\alpha}(G^{*}) = 99pq.6^{\alpha}$,
$ABC(G^{*}) = 66pq$,
$GA(G^{*}) = 99pq$.

Proof. The subdivision graph S(L[p,q]) contains 66pq edges and 55pq vertices among which 33pq vertices are of degree 2 and remaining 22pq vertices are of degree 3. Hence by Lemma 1 the total number of edges of G is 99pq. All the edges uv in G have d_u=d_v=3. From formulas 1, 3, 4 and 5, we obtain the required results.

Theorem 10. Let G* be the Para-line graph of L[p,q]. Then

$$ABC_4(G^*) = \frac{33}{2}\sqrt{6}pq,$$

$$GA_5(G^*) = 66pq$$

Proof. If we consider an edge partition based on degree sum of neighbors of end vertices then all 99pq edges uv in G have $S_u=S_v=9$. From formulas 6 and 7, we obtain the required results.

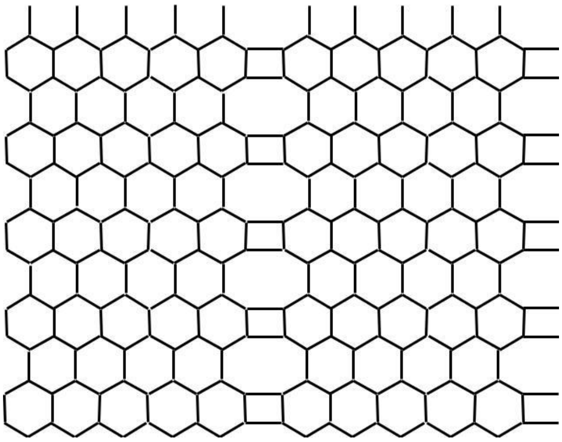

Fig. 6. 2-D graph lattice of V-Pantacenic nanotorus

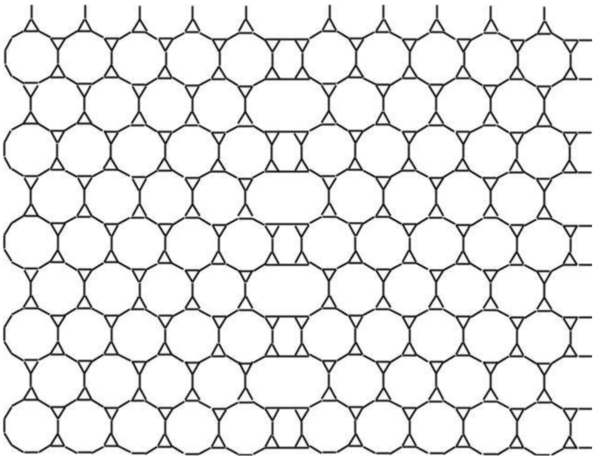

Fig. 7. Para-line graph of 2-D lattice of V-Pantacenic nanotorus

3. Conclusion

To study chemical graphs in the framework of para-line operator is a new direction in the field of structural chemistry. In this paper, we paid attention to the para-line graph of nanostructures and study their topological indices which are practically helpful to identify their underlying topologies.

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