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Topological Indices of Para-line Graphs of V-Phenylenic Nanostructures

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Abstract: The degree-based topological indices are numerical graph invariants which are used to correlate the physical and chemical properties of a molecule with its structure. Para-line graphs are used to represent the structures of molecules in another way and these representations are important in structural chemistry. In this article, we study certain well-known degree-based topological indices for the para-line graphs of V-Phenylenic $2D$ lattice, V-Phenylenic nanotube and nanotorus by using the symmetries of their molecular graphs.

Keywords: para-line graph; nanostructure; topological index

MSC: 05C90; 92E10

1 Introduction

Chemical graph theory is a field of mathematical chemistry in which we implement the tools from graph theory to model chemical aspects mathematically. It is recorded in [1, 2] that the structure of a molecule is strongly related to its chemical properties such as strain energy, boiling point and heat of formation. Molecular graphs can be used to model the molecules and molecular compounds by considering atoms as vertices and the chemical bonds between the atoms as edges. Topological index (TI) is a kind of numerical graph invariant which is used to correlate the physical and chemical properties of a molecular graph. In this sense, topological indices perform a significant role in chemical graph theory.

Consider the molecular graph G having vertex set V_G and edge set E_G. Let I_{G_p} be the set of edges of G that are incident with a vertex $p \in V_G$, then the degree, d_p, of p is defined as the cardinality of set I_{G_p} and $S_p = \sum_{q \in N_p} d_q$, where d_q is the degree of vertex q and the set N_p consists of all neighbor vertices of p i.e. $N_p = \{q \in V_G | pq \in E_G\}$. For any natural number t, we define $V_t = \{p \in V_G \mid S_p = t\}$. The subdivided graph of G is denoted by $S(G)$ and defined by replacing each of its edge with the path having length 2. The line graph of G is symbolized by $L(G)$. This graph is constructed by taking the vertex set $V_{L(G)} = E_G$ and the edge set $E_{L(G)}$ which has the property that for two vertices $p, q \in V_{L(G)}$, $pq \in E_{L(G)} \iff p, q \in E_G$ have a common vertex. The line graph of subdivided graph $L(S(G))$ is termed as the para-line graph of G.

Para-line graphs are used to understand the structure of a molecular graph and in this sense they receive much attention in structural chemistry. The atomic hybrid orbitals in a molecular graph corresponds to the vertices of its para-line graph and the strong links between the pairs of these orbitals correspond to the edges of its para-line graph. Klein et al. [3] presented some applications and basic properties of the para-line graphs

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in chemical graph theory.

Generally, topological indices can be categorized in three classes: degree-based, distance-based and spectrum-based indices. Among them, degree-based indices have great applications in chemical graph theory [4, 5] and they can be defined in two ways as

$$TI(G) = \sum_{pq \in E(G)} F(d_p, d_q) \tag{1}$$

$$TI(G) = \sum_{pq \in E(G)} F(S_p, S_q) \tag{2}$$

where the sum runs over all pairs of adjacent vertices of G and $F = F(x, y)$ is a suitably selected function.

Milan Randić proposed in 1975 a structural descriptor called the branching index [6] which is applicable for rating the degree of branching of the carbon-atom skeleton of saturated hydrocarbons. This index was renamed as the Randić connectivity index, which is defined as the sum of the Randić weights $(d_p d_q)^{-\frac{1}{2}}$ for all edges. The generalization of the Randić index for any real number α, is termed as the general Randić connectivity index and is defined by taking $F = (d_p d_q)^{\alpha}$ in equation (1). Li and Zhao presented the first general Zagreb index in [7], which is defined as $M_{\alpha}(G) = \sum_{p \in V(G)} (d_p)^{\alpha}$. The sum-connectivity index was presented in [8] and was modified to the general sum-connectivity index in [9], which is formulated by selecting $F = (d_p + d_q)^{\alpha}$ in equation (1). It is recorded in [10] that the general Randić connectivity and sum-connectivity indices correlate greatly with the π-electron energy of benzenoid hydrocarbons. Estrada et al. [11] presented the atom bond connectivity index (ABC). This index is defined by choosing $F = \sqrt{(d_p + d_q - 2)/d_p d_q}$ in equation (1). D. Vukičević and B. Furtula [12] proposed the geometric-arithmetic (GA) index that is defined by setting $F = 2\sqrt{d_p d_q}/(d_p + d_q)$ in equation (1). The fourth ABC index was presented by Ghorbani and Hosseinzadeh [13] and is defined by choosing $F = \sqrt{(S_p + S_q - 2)/S_p S_q}$ in equation (2). The fifth GA index (GA_5) was presented by Graovac et al. [14] which is defined by setting $F = 2\sqrt{S_p S_q}/(S_p + S_q)$ in equation (2). The explicit expressions of Zagreb indices for the para-line graphs of ladder, tadpole and wheel graphs, was presented by Ranjini et al. [15]. Su and Xu [16] studied general sum-connectivity indices for these para-line graphs. Nadeem et al. [17] presented the ABC_4 and GA_5 indices for these para-line graphs. In [18], they also studied ABC, ABC_4, GA, GA_5, general Zagreb, generalized Randić and general sum-connectivity indices for the para-line graphs of $2D$-lattice $TUC_4C_8(R)$, $TUC_4C_8(R)$ nanotube and $TUC_4C_8(R)$ nanotorus.

Recently, Akhter et al. [19] and Mufti et al. [20] computed ABC, ABC_4, GA, GA_5, first general Zagreb, general sum-connectivity and general Randić connectivity indices for the para-line graphs of certain benzenoid structures. In this paper, we present these indices for the para-line graphs of V-phenylenic $2D$-lattice, V-phenylenic nanotube and nanotorus.

2 V-Phenylenic Nanostructures

The Phenylenes belong to the family of polycyclic non-benzenoid alternate conjugated hydrocarbons in which the carbon atoms form hexagons and squares. Each square is adjacent to two detached hexagons. From this, some larger compounds can be formed such as V-phenylenic $2D$ lattice, V-Phenylenic nanotube and nanotorus.

Let $TUC_4C_6C_8[m, n]$ represents the V-phenylenic nanostructures where m denotes the number of hexagons in a row and n denotes the number of rows of hexagons in V-Phenylenic $2D$-lattice, V-Phenylenic nanotube and nanotorus as presented respectively in Figure 1 (a), (b) and (c). The order and size of these nanostructures are given in Table 1.

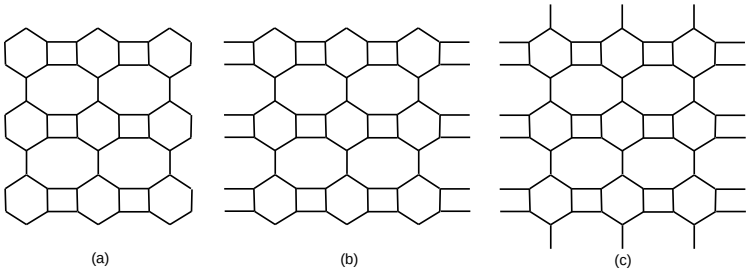

Figure 1: (a) The $2D$-lattice $TUC_4C_6C_8[3, 3]$; (b) The $TUC_4C_6C_8[3, 3]$ nanotube; (c) The $TUC_4C_6C_8[3, 3]$ nanotorus.

Table 1: The order and size of V-phenylenic nanostructures.

Graph	Order	Size
$2D$-lattice $TUC_4C_6C_8[m, n]$	$6mn$	$9mn - m - 2n$
$TUC_4C_6C_8[m, n]$ nanotube	$6mn$	$9mn - m$
$TUC_4C_6C_8[m, n]$ nanotorus	$6mn$	$9mn$

3 Main Results

In this section, we derive the topological indices for the para-line graphs of V-Phenylenic nanostructures by using their symmetric structures. The para-line graphs of these structures are presented in Figure 2 (a), (b) and (c) respectively.

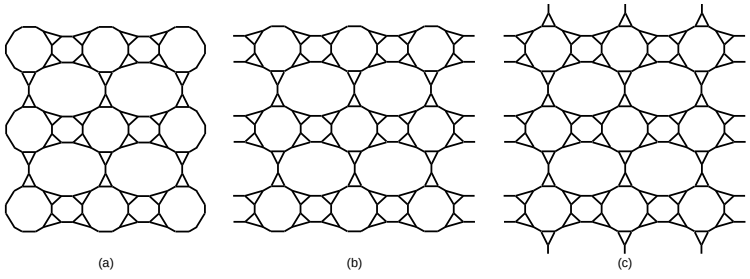

Figure 2: (a) The para-line graph G; (b) The Para-line graph H; (c) The Para-line graph K.

3.1 *TI*'s of the para-line graph of $2D$-lattice $TUC_4C_6C_8[m, n]$

Theorem 1. *Consider the graph G of* 2D*-lattice* $TUC_4C_6C_8[m, n]$. *Then*

$$R_\alpha(G) = 2.4^\alpha(m + 3n + 2) + 4.6^\alpha(m + n - 2) + 9^\alpha(27mn - 11m - 20n + 4)$$
$$M_\alpha(G) = 2^{\alpha+2}(m + 2n) + 2.3^{\alpha+1}(3mn - m - 2n)$$
$$\chi_\alpha(G) = 2.4^\alpha(m + 3n + 2) + 4.5^\alpha(m + n - 2) + 6^\alpha(27mn - 11m - 20n + 4)$$
$$ABC(G) = \sqrt{2}(3m + 5n - 2) + 18mn - \frac{22}{3}m - \frac{40}{3}n + \frac{8}{3}$$
$$GA(G) = -9m - 14n + 8 + \frac{8}{5}(m + n - 2)\sqrt{6} + 27mn$$

Proof. The para-line graph G of 2D-lattice $TUC_4C_6C_8[m, n]$ is presented in Figure 2 (a). It can easily be checked that $|V_G| = 2(9mn - m - 2n)$. Among them, there are $4(m + 2n)$ and $6(3mn - m - 2n)$ vertices of degree 2 and 3 respectively. By using the handshaking lemma, we have

$$4(m + 2n)(2) + 6(3mn - m - 2n)(3) = 2|E_G|$$
$$|E_G| = 27mn - 5m - 10n$$

So, we have the following disjoint edge partite subsets of E_G with respect to the degree of the end vertices.

$$E_{(2,2)} = \{pq \in E_G | d_p = d_q = 2\}$$
$$E_{(2,3)} = \{pq \in E_G | d_p = 2 \text{ and } d_q = 3\}$$
$$E_{(3,3)} = \{pq \in E_G | d_p = d_q = 3\}$$

We use cardinalities of partite sets given in Table 2 and by choosing the corresponding function $F(d_p, d_q)$ in

Table 2: The cardinalities of the edge partite subsets of E_G with respect to degree of end vertices.

$E_{(p,q)}$	$E_{(2,2)}$	$E_{(2,3)}$	$E_{(3,3)}$
$\lvert E_{(p,q)}\rvert$	$2p + 6q + 4$	$4p + 4q - 8$	$27pq - 11p - 20q + 4$

equation (1) to obtain the required results. □

Theorem 2. *Consider the graph G of 2D-lattice $TUC_4C_6C_8[m, n]$. Then for $m > 1$ and $n \geq 1$*

$$ABC_4(G) = \frac{\sqrt{6}}{2}(n + 4) + \frac{2\sqrt{35}}{5}n + \frac{4\sqrt{2}}{5}(m - 2) + \frac{\sqrt{110}}{5}(m + n - 2)$$
$$+\frac{2\sqrt{30}}{3}(m + n - 2) + 12mn - \frac{76}{9}m - \frac{112}{9}n + \frac{80}{9}$$
$$GA_5(G) = -17m - 26n + \frac{16\sqrt{5}}{9}n + \frac{16\sqrt{10}}{13}(m + n - 2) + \frac{96\sqrt{2}}{17}(m + n - 2) + 27mn + 24$$

Proof. For $m > 1$ and $n \geq 1$, it can easily be checked from Figure 2 (a) that in G $|V_4| = 4(n + 2)$, $|V_5| = 4(m + n - 2)$, $|V_8| = 4(m + n - 2)$ and $|V_9| = 2(9mn - 5m - 8n + 4)$. So, we have the following disjoint edge partite subsets of E_G which consist of edges having end vertices labeled by the degree sum of adjacent vertices and their cardinalities are given in Table 3.

$$\delta_{(4,4)} = \{pq \in E_G | S_p = S_q = 4\}$$
$$\delta_{(4,5)} = \{pq \in E_G | S_p = 4 \text{ and } S_q = 5\}$$
$$\delta_{(5,5)} = \{pq \in E_G | S_p = 5 \text{ and } S_q = 5\}$$
$$\delta_{(5,8)} = \{pq \in E_G | S_p = 5 \text{ and } S_q = 8\}$$
$$\delta_{(8,9)} = \{pq \in E_G | S_p = 8 \text{ and } S_q = 9\}$$
$$\delta_{(9,9)} = \{pq \in E_G | S_p = S_q = 9\}$$

By using Table 3 and choosing the corresponding function $F(S_p, S_q)$ in equation (2), we get the required results. □

3.2 *TI*'s of the para-line graph of $TUC_4C_6C_8[m, n]$ nanotube

Theorem 3. *Consider the para-line graph H of $TUC_4C_6C_8[m, n]$ nanotube. Then for $m \geq 1$ and $n \geq 1$*

$$R_\alpha(H) = 2.4^\alpha m + 4.6^\alpha m + 9^\alpha(27mn - 11m)$$

Table 3: The cardinalities of the edge partite subsets of E_G with respect to degree sum of adjacent vertices.

$\delta_{(p,q)}$	$\delta_{(4,4)}$	$\delta_{(4,5)}$	$\delta_{(5,5)}$	$\delta_{(5,8)}$	$\delta_{(8,9)}$	$\delta_{(9,9)}$
$\lvert\delta_{(p,q)}\rvert$	$2(n+4)$	$4n$	$2(m-2)$	$4(m+n-2)$	$8(m+n-2)$	$27mn-19m-28n+20$

Table 4: The cardinalities of the edge partite subsets of E_H with respect to degree of end vertices.

$E_{(p,q)}$	$E_{(2,2)}$	$E_{(2,3)}$	$E_{(3,3)}$
$\lvert E_{(p,q)}\rvert$	$2m$	$4m$	$27mn-11m$

$$M_\alpha(H) = 2^{\alpha+2}m + 2.3^{\alpha+1}(3mn-m)$$
$$\chi_\alpha(H) = 2.4^\alpha m + 4.5^\alpha m + 6^\alpha(27mn-11m)$$
$$ABC(H) = 3\sqrt{2}m + \frac{\sqrt{7}}{3}(27mn-11m)$$
$$GA(H) = -9m + \frac{8\sqrt{6}}{5}m + 27mn$$

Proof. The para-line graph H of $TUC_4C_6C_8[m,n]$ nanotube and is presented in Figure 2 (b). One can easily verify that $|V_H| = 2(9pq-p)$. Among them, there are $4m$ and $6m(3n-1)$ vertices of degree 2 and 3 respectively. By using the handshaking lemma, we have

$$4m(2) + 6m(3n-1)(3) = 2|E_H|$$
$$|E_H| = 27mn - 5m$$

Therefore, we get the following disjoint edge partite subsets of E_H and present its cardinalities in Table 4.

$$E_{(2,2)} = \{pq \in E_H | d_p = d_q = 2\}$$
$$E_{(2,3)} = \{pq \in E_H | d_p = 2 \text{ and } d_q = 3\}$$
$$E_{(3,3)} = \{pq \in E_H | d_p = d_q = 3\}$$

We apply equation (1) to the information in Table 4 by choosing the corresponding functions $F(d_p, d_q)$ and get the desired results. □

Theorem 4. *Consider the para-line graph H of $TUC_4C_6C_8[m,n]$ nanotube. Then for $m \geq 1$ and $n \geq 1$*

$$ABC_4(H) = 12mn + \frac{4\sqrt{2}}{5}m + \frac{\sqrt{110}}{5}m + \frac{2\sqrt{30}}{3}m - \frac{76}{9}m$$
$$GA_5(H) = 27mn - 17m + \frac{16\sqrt{10}}{13}m + \frac{96\sqrt{2}}{17}m$$

Proof. For $m \geq 1$ and $n \geq 1$, it can easily be checked from Figure 2 (b) that in H, $|V_5| = 4m$, $|V_8| = 4m$ and $|V_9| = 2(9mn-5m)$. So, we have the following edge partite subsets of E_H which consist of edges having end vertices labeled by the degree sum of adjacent vertices and their cardinalities are given in Table 5.

$$\delta_{(5,5)} = \{pq \in E_G | S_p = 5 \text{ and } S_q = 5\}$$
$$\delta_{(5,8)} = \{pq \in E_G | S_p = 5 \text{ and } S_q = 8\}$$
$$\delta_{(8,9)} = \{pq \in E_G | S_p = 8 \text{ and } S_q = 9\}$$
$$\delta_{(9,9)} = \{pq \in E_G | S_p = S_q = 9\}$$

We apply equation (2) to Table 5 by taking the corresponding function $F(S_p, S_q)$ and get the desired indices. □

Table 5: The cardinalities of the edge partite subsets of E_H with respect to degree sum of adjacent vertices.

$\delta_{(p,q)}$	$\delta_{(5,5)}$	$\delta_{(5,8)}$	$\delta_{(8,9)}$	$\delta_{(9,9)}$
$\lvert\delta_{(p,q)}\rvert$	$2m$	$4m$	$8m$	$27mn - 19n$

3.3 *TI*'s of the para-line graph of $TUC_4C_6C_8[m, n]$ nanotorus

Theorem 5. *Consider the para-line graph K of $TUC_4C_6C_8[p, q]$ nanotorus. Then*

$$R_\alpha(G) = 27.9^\alpha mn$$
$$M_\alpha(G) = 18.3^\alpha mn$$
$$\chi_\alpha(G) = 27.6^\alpha mn$$
$$ABC(K) = 18pq$$
$$GA(K) = 27pq$$

Proof. The para-line graph of $TUC_4C_6C_8[m, n]$ nanotorus and its para-line graph K is presented in Figure 2 (c). One can easily check that in K, $|V_K| = 18mn$ and all these vertices are of degree 3. By using the handshaking lemma, we have $|E_K| = 27mn$. So, we have exactly one edge partition of E_K which is given by

$$E_{(3,3)} = \{pq \in E_K | d_p = d_q = 3\}$$

and clearly $|E_{(3,3)}| = |E_K| = 27mn$.
With this cardinality, we apply equation (1) by setting the corresponding function $F(d_p, d_q)$ and get the desired indices. □

Theorem 6. *Consider the para-line graph K of $TUC_4C_6C_8[p, q]$ nanotorus. Then*

$$ABC_4(K) = 12mn$$
$$GA_5(K) = 27mn$$

Proof. It is easy to see from Figure 2 (c) that $|V_9| = 18mn$. So, we have exactly one edge partition with respect to end vertices labeled by degree sum of adjacent vertices, given by

$$\delta_{(9,9)} = \{pq \in E_K | S_p = S_q = 9\}$$

and clearly $|\delta_{(9,9)}| = |E_K| = 27mn$.
With this cardinality, we apply equation (2) by choosing the corresponding function $F(S_p, S_q)$ and obtain the required results. □

4 Conclusion

In this article, well-known degree-based topological indices such as first general Zagreb, general Randić connectivity, general sum-connectivity, ABC, ABC_4, GA and GA_5 indices are studied. These indices correlate many chemical properties such as stability, heat of formation, boiling point and strain energy of chemical compounds. By using the symmetric structure property of V-phenylenic nanostructures, we present these indices for their para-line graphs which will help the people to interpret and analyze the underlying topologies of these nanostructures.

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References

[1] Rücker G., Rücker C., On topological indices, boiling points, and cycloalkanes, J. Chem. Inf. Comput. Sci., 1999, 39, 788–802.
[2] Deng H., Yang J., Xia F., A general modeling of some vertex-degree based topological indices in benzenoid systems and phenylenes, Comput. Math. Appl., 2011, 61, 3017–3023.
[3] Klein D.J., Yi E., A comparison on metric dimension of graphs, line graphs, and line graphs of the subdivision graphs, Eur. J. Pure Appl. Math., 2012, 5, 302-316.
[4] Furtula B., Gutman I., Dehmer M., On structure-sensitivity of degree-based topological indices, Appl. Math. Comput., 2013, 219, 8973–8978.
[5] Gutman I., Degree-based topological indices, Croat. Chem. Acta, 2013, 86, 351–361.
[6] Randić M., On characterization of molecular branching, J. Am. Chem. Soc., 1975, 97, 6609–6615.
[7] Li X., Zhao H., Trees with the first three smallest and largest generalized topological indices, MATCH Commun. Math. Comput. Chem., 2004, 50, 57–62.
[8] Zhou B., Trinajstić N., On a novel connectivity index, J. Math. Chem., 2009, 46, 1252–1270.
[9] Zhou B., Trinajstić N., On general sum-connectivity index, J. Math. Chem., 2010, 47, 210–218.
[10] Lučić B., Trinajstić N., Zhou, B., Comparison between the sum-connectivity index and product-connectivity index for benzenoid hydrocarbons, Chem. Phys. Lett., 2009, 475, 146–148.
[11] Estrada E., Torres L., Rodriguez L., Gutman I., An atom-bond connectivity index: modelling the enthalpy of formation of alkanes, Indian J.Chem., 1998, 37A, 849–855.
[12] Vukicevic D., Furtula B., Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, J. Math. Chem., 2009, 46, 1369–1376.
[13] Ghorbani M., Hosseinzadeh M.A., Computing ABC_4 index of nanostar dendrimers, Optoelectron. Adv. Mater. -Rapid Commun., 2010, 4(9), 1419–1422.
[14] Graovac A., Ghorbani M., Hosseinzadeh, M.A., Computing fifth geometric-arithmetic index for nanostar dendrimers, J. Math. Nanosci., 2011, 1, 33–42.
[15] Ranjini P.S., Lokesha V., Cangl I.N., On the Zagreb indices of the line graphs of the subdivision graphs, Appl. Math. Comput., 2011, 218, 699–702.
[16] Su G., Xu L., Topological indices of the line graph of subdivision graphs and their Schur-bounds, Appl. Math. Comput., 2015, 253, 395–401.
[17] Nadeem M.F., Zafar S., Zahid, Z., On certain topological indices of the line graph of subdivision graphs, Appl. Math. Comput., 2015, 271, 790-794.
[18] Nadeem M.F., Zafar S., Zahid Z., On topological properties of the line graphs of subdivision graphs of certain nanostructures, Appl. Math. Comput., 2016, 273, 125-130.
[19] Akhter S., Imran M., On molecular topological properties of benzenoid structures, Can. J. of Chem., 2016, 94(8), 687–698.
[20] Mufti Z.S., Zafar S., Zahid Z., Nadeem, F., Study of the para-line graphs of certain benzenoid structures using topological indices, MAGNT Research Report, 2017, 4(3), 110–116.