Hindawi
Journal of Mathematics
Volume 2021, Article ID 5520619, 10 pages
https://doi.org/10.1155/2021/5520619

Research Article

On Distance-Based Topological Descriptors of Chemical Interconnection Networks

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Received 8 January 2021; Revised 24 February 2021; Accepted 1 March 2021; Published 16 March 2021

Academic Editor: Ghulam Mustafa

Structure-based topological descriptors of chemical networks enable us the prediction of physico-chemical properties and the bioactivities of compounds through QSAR/QSPR methods. Topological indices are the numerical values to represent a graph which characterises the graph. One of the latest distance-based topological index is the Mostar index. In this paper, we study the Mostar index, Szeged index, PI index, ABC_{GG} index, and NGG index, for chain oxide network COX_n, chain silicate network CS_n, ortho chain S_n, and para chain Q_n, for the first time. Moreover, analytically closed formulae for these structures are determined.

1. Introduction and Preliminary Results

All the graphs G in this paper are considered to be finite, undirected, and loopless. Graph G is the set made up of vertices (also called the nodes) which are connected with the edges (also called links). It consists on two sets V and E, where V is called the vertex set and E is called the edge set. In order to understand the properties and information contained in the connectivity pattern of graphs, there are many numbers of numerical quantities, known as structure invariants, topological indices, or topological descriptors, which have been derived and studied over the past few decades. The topological indices have vast number of applications in the chemical graph theory which is the special branch of mathematical chemistry.Graph theory has a wide range of applications in engineering due to its diagrammatic nature. It is used in computer science to study the algorithms and flow of information. In engineering, it is used to model the graphics and designs of different networks by converting them in the form of graph.

The topological indices are very much used for characterizing the chemical graphs on the basis of their numerical values. They establish the relationship between the structure and properties of molecule. Topological indices are widely used in QSAR and QSPR research studies [1]. Till now, many topological indices have been derived. For any two graphs G and H which are isomorphic to each other, then $\mathrm{Top}(G) = \mathrm{Top}(H)$ [2]. Due to the success of simple topological indices, such as Wiener Index [3], Zagreb index [4], and Szeged index [5], motivated others, hundreds of topological indices are introduced. Wiener index is one of the first index which was introduced by Harold Wiener in 1947 [6], when he was working on the boiling point of paraffins. The Wiener index [7] of a graph G is defined as the sum of all the distances between pairs of vertices of G:

$$W(G) = \sum_{(u,v)\subseteq V(G)} d(u,v), \tag{1}$$

where $d(u,v)$ denotes the shortest-path distance in G.

The Szeged index is defined as

$$S_z(G) = \sum_{e=uv\in E(G)} n_u n_v, \tag{2}$$

where n_u denotes the number of vertices of G closer to u than to v and n_v is defined as the number of vertices of G closer to v than to u. This was first studied by Gutman. Later, it is known as the Szeged index [8].

The PI index [9], of a graph G, is defined as

$$PI_v(G) = \sum_{e=uv\in E(G)} n_u + n_v. \tag{3}$$

The Graovac–Ghorbani index is defined as

$$\mathrm{ABC}_{\mathrm{GG}}(G) = \sum_{e=uv\in E(G)} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}}, \tag{4}$$

and this index is introduced by Graovac and Ghorbani [10], and Furtula [11] used the name Graovac–Ghorbani index.

The normalized $\mathrm{ABC}_{\mathrm{GG}}$ index is NGG index, first studied by Dimitrov et al. [12], and is defined as

$$\mathrm{NGG}(G) = \sum_{e=uv\in E(G)} \frac{1}{\sqrt{n_u n_v}}. \tag{5}$$

A chemical graph is a simple graph in which atoms correspond to the vertices and edge denotes the bond between two atoms. A topological index, specially, the Mostar index is one of the latest topological index, derived in 2018 [13]. Previously, Arockiaraj [14] found the Mostar indices of carbon nanostructures, and Hayata and Zhou [15] calculated the large Mostar index on cacti. The Mostar index for a graph G is defined as the sum of all the absolutes values of the difference between n_u and n_v, where u and v are the adjacent vertices of an edge:

$$\mathrm{Mo}(G) = \sum_{e=uv\in E(G)} |n_u - n_v|. \tag{6}$$

2. Main Results

The main goal of this article is to compute the Mostar index of ortho chain and para chain using the edge cut method; also, we find the Mostar index, Szeged index, PI index, $\mathrm{ABC}_{\mathrm{GG}}$ index, and NGG index of oxide chains, chain silicates, ortho chain, and para chain by using the technique of edge partition. The notations used in this paper are standard and taken from the book of west [16]. For the concepts and terms not defined here, we refer the reader to concern with the book of Harary [17] and also concern with [18–25].

2.1. Results for the Chain Oxide Network COX_n. In this section, we discuss COX_n and compute the exact results for Szeged, PI, $\mathrm{ABC}_{\mathrm{GG}}$, NGG, and Mostar index. If we remove the silicon atom from the silicate network, then the resulting network is an oxide network [26], which consists of three oxygen atoms. Oxide network has the triangular structure. If an oxide network shares its oxygen with other oxide network linearly, then the oxide chain is formed, as shown in Figure 1.

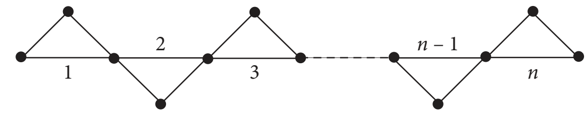

Figure 1: Oxide network.

Theorem 1. *Let G_1 be the oxide network of n order, then its Szeged index is $2n^3 + 6n^2 + n/3$.*

Proof. Let $G_1 \cong \mathrm{OX}(n)$, where $n \geq 2$; also, n is an integer.

$$\begin{aligned} Sz(G_1) &= \sum_{e\in E(G_1)} n_u n_v, \\ Sz(G_1) &= \sum_{e\in E(G_1)} n_2 n_2 + \sum_{e\in E(G_1)} n_2 n_4 + \sum_{e\in E(G_1)} n_4 n_4. \end{aligned} \tag{7}$$

By using Table 1, we have

$$\begin{aligned} Sz(G_1) &= 2 + 2n^2 + 4n - 4 + \frac{2n^3 - 11n + 6}{3}, \\ Sz(G_1) &= \frac{2n^3 + 6n^2 + n}{3}, \end{aligned} \tag{8}$$

which is required. □

Theorem 2. *Let G_1 be the oxide network of n order; then, its PI index is $4n^2 + 2n$.*

Proof. Let $G_1 \cong \mathrm{OX}(n)$, where $n \geq 2$; also, n is an integer:

$$\begin{aligned} \mathrm{PI}_v(G_1) &= \sum_{e\in E(G_1)} n_u + n_v, \\ \mathrm{PI}_v(G_1) &= \sum_{e\in E(G_1)} n_2 + n_2 + \sum_{e\in E(G_1)} n_2 + n_4 + \sum_{e\in E(G_1)} n_4 + n_4. \end{aligned} \tag{9}$$

By using Table 2, we have

$$\begin{aligned} \mathrm{PI}_v(G_1) &= 4 + 2n^2 + 6n - 4 + 2n^2 - 4n, \\ \mathrm{PI}_v(G_1) &= 4n^2 + 2n, \end{aligned} \tag{10}$$

which is required. □

Theorem 3. *Let G_1 be the oxide network of n order; then, its ABC_{GG} index is $1 + \sqrt{n^2 + 3n - 3/n^2 + 2n - 2} + \sqrt{6n^2 - 12n - 6/2n^3 - 11n + 6}$.*

Table 1: Edge partition of oxide network of n order.

Edge partition d_u, d_v	Number of edges	Szeged index
2, 2	2	2
2, 4	$2n$	$2n^2 + 4n - 4$
4, 4	$n - 2$	$2n^3 - 11n + 6/3$

Table 2: Edge partition of oxide network of n order.

Edge partition d_u, d_v	Number of edges	PI index
2, 2	2	4
2, 4	$2n$	$2n^2 + 6n - 4$
4, 4	$n - 2$	$2n^2 - 4n$

Proof. Let $G_1 \cong \mathrm{OX}(n)$, where $n \geq 2$; also, n is an integer:

$$\mathrm{ABC}_{\mathrm{GG}}(G_1) = \sum_{e\in E(G_1)} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}},$$
$$\mathrm{ABC}_{\mathrm{GG}}(G_1) = \sum_{e\in E(G_1)} \sqrt{\frac{n_2 + n_2 - 2}{n_2 n_2}} + \sum_{e\in E(G_1)} \sqrt{\frac{n_2 + n_4 - 2}{n_2 n_4}} + \sum_{e\in E(G_1)} \sqrt{\frac{n_4 + n_4 - 2}{n_4 n_4}}. \quad (11)$$

By using Table 3, we have

$$\mathrm{ABC}_{\mathrm{GG}}(G_1) = 1 + \sqrt{\frac{n^2 + 3n - 3}{n^2 + 2n - 2}} + \sqrt{\frac{6n^2 - 12n - 6}{2n^3 - 11n + 6}}, \quad (12)$$

which is required. □

Theorem 4. *Let G_1 be the oxide network of n order; then, its $NGG(G_1)$ index is $1/\sqrt{2} + 1/\sqrt{2n^2 + 4n - 4} + \sqrt{3/2n^3 - 11n + 6}$.*

Proof. Let $G_1 \cong \mathrm{OX}(n)$, where $n \geq 2$; also, n is an integer:

$$\mathrm{NGG}(G_1) = \sum_{e\in E(G_1)} \frac{1}{\sqrt{n_u n_v}},$$
$$\mathrm{NGG}(G_1) = \sum_{e\in E(G_1)} \frac{1}{\sqrt{n_2 n_2}} + \sum_{e\in E(G_1)} \frac{1}{\sqrt{n_2 n_4}} + \sum_{e\in E(G_1)} \frac{1}{\sqrt{n_4 n_4}}. \quad (13)$$

By using Table 4, we have

$$\mathrm{NGG}(G_1) = \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2n^2 + 4n - 4}} + \sqrt{\frac{3}{2n^3 - 11n + 6}}, \quad (14)$$

which is required. □

Theorem 5. *Let G_1 be the oxide network of even order; then, its Mostar index is $3n^2 - 2n$.*

Proof. Let $G_1 \cong \mathrm{OX}(n)$, where $n \geq 2$; also, n is even:

Table 3: Edge partition of oxide network of n order.

Edge partition d_u, d_v	Number of edges	$\mathrm{ABC}_{\mathrm{GG}}$ index
2,2	2	1
2,4	$2n$	$\sqrt{n^2 + 3n - 3/n^2 + 2n - 2}$
4,4	$n - 2$	$\sqrt{6n^2 - 12n - 6/2n^3 - 11n + 6}$

Table 4: Edge partition of oxide network of n order.

Edge partition d_u, d_v	Number of edges	NGG index
2, 2	2	$1/\sqrt{2}$
2, 4	$2n$	$1/\sqrt{2n^2 + 4n - 4}$
4, 4	$n - 2$	$\sqrt{3/2n^3 - 11n + 6}$

$$\mathrm{Mo}(G_1) = \sum_{uv\in E(G_1)} |n_u - n_v|,$$
$$\mathrm{Mo}(G_1) = \sum_{uv\in E(G_1)} |n_2 - n_2| + \sum_{uv\in E(G_1)} |n_2 - n_4| + \sum_{uv\in E(G_1)} |n_4 - n_4|. \quad (15)$$

By using Table 5, we have

$$\mathrm{Mo}(G_1) = 0 + 2n^2 + 2n - 4 + n^2 - 4n + 4,$$
$$\mathrm{Mo}(G_1) = 3n^2 - 2n, \quad (16)$$

which is required. □

Theorem 6. *Let G_1 be the oxide network of odd order; then, its Mostar index is $3n^2 - 2n - 1$.*

Proof. Let $G_1 \cong \mathrm{OX}(n)$, where $n \geq 1$; also, n is odd:

$$\mathrm{Mo}(G_1) = \sum_{uv\in E(G_1)} n_u - n_v,$$
$$\mathrm{Mo}(G_1) = \sum_{uv\in E(G_1)} |n_2 - n_2| + \sum_{uv\in E(G_1)} |n_2 - n_4| + \sum_{uv\in E(G_1)} |n_4 - n_4|. \quad (17)$$

By using Table 6, we have

$$\mathrm{Mo}(G_1) = 0 + 2n^2 + 2n - 4 + n^2 - 4n + 3,$$
$$\mathrm{Mo}(G_1) = 3n^2 - 2n - 1, \quad (18)$$

which is required. □

2.2. Results for the Chain Silicate Network CS_n. In this section, we discuss CS_n and compute the exact results for Szeged, PI, $\mathrm{ABC}_{\mathrm{GG}}$, NGG, and Mostar index. Silicates are the

Table 5: Edge partition of oxide network of even order.

Edge partition d_u, d_v	Number of edges	Mostar index
2, 2	2	0
2, 4	$2n$	$2n^2 + 2n - 4$
4, 4	$n - 2$	$n^2 - 4n + 4$

Table 6: Edge partition of oxide network of odd order.

Edge partition d_u, d_v	Number of edges	Mostar index
2, 2	2	0
2, 4	$2n$	$2n^2 + 2n - 4$
4, 4	$n - 2$	$n^2 - 4n + 3$

compounds which consist of silicon and oxygen, having the tetrahedron structure with bond angle of 109.5°. SiO_4 is found in almost all of the silicates. A single tetrahedron has a shape like a pyramid with triangular base. It has four oxygen atoms at its corners, and silicon atom is bounded equally with oxygen atoms with bond length of 162 pm. A single tetrahedron is shown in Figure 2(a). If a single tetrahedron shares its oxygen with other tetrahedrons; then, a linear silicate chain [27] is formed, as shown in Figure 2(b).

Theorem 7. *Let G_2 be the chain silicate network of n order; then, its Szeged index is $3n^3 + 9n^2/2$.*

Proof. Let $G_2 \cong CS_n$, where $n \geq 2$; also, n is an integer:

$$\mathrm{Sz}(G_2) = \sum_{e \in E(G_2)} n_u n_v,$$
$$\mathrm{Sz}(G_2) = \sum_{e \in E(G_2)} n_3 n_3 + \sum_{e \in E(G_2)} n_3 n_6 + \sum_{e \in E(G_2)} n_6 n_6. \quad (19)$$

By using Table 7, we have

$$\mathrm{Sz}(G_2) = n + 4 + 6n^2 + 4n - 8 + \frac{3n^3 - 3n^2 - 10n + 8}{2},$$
$$\mathrm{Sz}(G_2) = \frac{3n^3 + 9n^2}{2}, \quad (20)$$

which is required. □

Theorem 8. *Let G_2 be the chain silicate network of n order; then, its PI index is $9n^2 + 3n$.*

Proof. Let $G_2 \cong CS_n$, where $n \geq 2$; also, n is an integer:

$$\mathrm{PI_v}(G_2) = \sum_{e \in E(G_2)} n_u + n_v,$$
$$\mathrm{PI_v}(G_2) = \sum_{e \in E(G_2)} n_3 + n_3 + \sum_{e \in E(G_2)} n_3 + n_6 + \sum_{e \in E(G_2)} n_6 + n_6. \quad (21)$$

By using Table 8, we have

$$\mathrm{PI_v}(G_2) = 2n + 8 + 6n^2 + 8n - 10 + 3n^2 - 7n + 2,$$
$$\mathrm{PI_v}(G_2) = 9n^2 + 3n, \quad (22)$$

which is required. □

Theorem 9. *Let G_2 be the chain silicate network of n order then its ABC_{GG} index is $\sqrt{2n+6/n+4} + \sqrt{3n^2+4n-6/3n^2+2n-4} + \sqrt{6n^2-14n/3n^3-3n^2-10n+8}$.*

Proof. Let $G_2 \cong CS_n$, where $n \geq 2$; also, n is an integer:

$$\mathrm{ABC_{GG}}(G_2) = \sum_{e \in E(G_2)} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}},$$
$$\mathrm{ABC_{GG}}(G_2) = \sum_{e \in E(G_2)} \sqrt{\frac{n_3 + n_3 - 2}{n_3 n_3}} + \sum_{e \in E(G_2)} \sqrt{\frac{n_3 + n_6 - 2}{n_3 n_6}} + \sum_{e \in E(G_2)} \sqrt{\frac{n_6 + n_6 - 2}{n_6 n_6}}. \quad (23)$$

By using Table 9, we have

$$\mathrm{ABC_{GG}}(G_2) = \sqrt{\frac{2n+6}{n+4}} + \sqrt{\frac{3n^2 + 4n - 6}{3n^2 + 2n - 4}} + \sqrt{\frac{6n^2 - 14n}{3n^3 - 3n^2 - 10n + 8}}, \quad (24)$$

which is required. □

Theorem 10. *Let G_2 be the chain silicate network of n order; then, its NGG index is $1/\sqrt{n+4} + 1\ /\sqrt{6n^2+4n-8} + \sqrt{2/3n^3-3n^2-10n+8}$.*

Proof. Let $G_2 \cong CS_n$, where $n \geq 2$; also, n is an integer:

$$\mathrm{NGG}(G_2) = \sum_{e \in E(G_2)} \frac{1}{\sqrt{n_u n_v}},$$
$$\mathrm{NGG}(G_2) = \sum_{e \in E(G_2)} \frac{1}{\sqrt{n_3 n_3}} + \sum_{e \in E(G_2)} \frac{1}{\sqrt{n_3 n_6}} + \sum_{e \in E(G_2)} \frac{1}{\sqrt{n_6 n_6}}. \quad (25)$$

By using Table 10, we have

$$\mathrm{NGG}(G_2) = \frac{1}{\sqrt{n+4}} + \frac{1}{\sqrt{6n^2 + 4n - 8}} + \sqrt{\frac{2}{3n^3 - 3n^2 - 10n + 8}}, \quad (26)$$

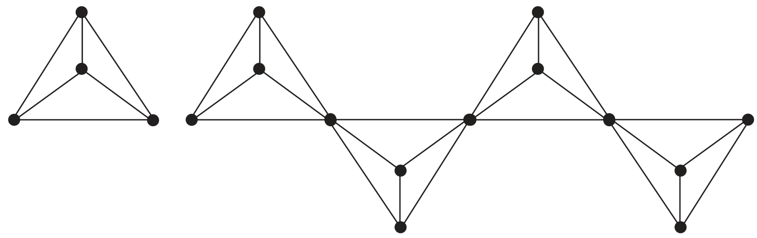
(a) (b)

Figure 2: (a) Single silicate and (b) chain silicate.

Table 7: Edge partition of chain silicate network of n order.

Edge partition d_u, d_v	Number of edges	Szeged index
3, 3	$n+4$	$n+4$
3, 6	$2(2n-1)$	$6n^2+4n-8$
6, 6	$n-2$	$3n^3-3n^2-10n+8/2$

Table 8: Edge partition of chain silicate network of n order.

Edge partition d_u, d_v	Number of edges	PI index
3, 3	$n+4$	2n+8
3, 6	$2(2n-1)$	$6n^2+8n-10$
6, 6	$n-2$	$3n^2-7n+2$

Table 9: Edge partition of chain silicate network of n order.

Edge partition d_u, d_v	Number of edges	ABC_{GG} index
3, 3	$n+4$	$\sqrt{2n+6/n+4}$
3, 6	$2(2n-1)$	$\sqrt{3n^2+4n-6/3n^2+2n-4}$
6, 6	$n-2$	$\sqrt{6n^2-14n/3n^3-3n^2-10n+8}$

Table 10: Edge partition of chain silicate network of n order.

Edge partition d_u, d_v	Number of edges	ABC_{GG} index
3, 3	$n+4$	$1/\sqrt{n+4}$
3, 6	$2(2n-1)$	$1/\sqrt{6n^2+4n-8}$
6, 6	$n-2$	$\sqrt{2/3n^3-3n^2-10n+8}$

which is required. □

Theorem 11. *Let G_2 be the chain silicate network of even order; then, its Mostar index is $15n^2-12n/2$.*

Proof. Let $G_2 \cong CS_n$, where $n \geq 2$; also, n is even.

$$\mathrm{Mo}(G_2) = \sum_{uv\in E(G_2)} |n_u - n_v|,$$
$$\mathrm{Mo}(G_2) = \sum_{uv\in E(G_2)} |n_3 - n_3| + \sum_{uv\in E(G_2)} |n_3 - n_6| + \sum_{uv\in E(G_2)} |n_6 - n_6|. \quad (27)$$

By using Table 11, we have

$$\mathrm{Mo}(G_2) = 0 + 6n^2 - 6 + \frac{3n^2-12n+12}{2},$$
$$\mathrm{Mo}(G_2) = \frac{15n^2-12n}{2}, \quad (28)$$

Table 11: Edge partition of chain silicate network of even order.

Edge partition d_u, d_v	Number of edges	Mostar index
3, 3	$n+4$	0
3, 6	$2(2n-1)$	$6n^2-6$
6, 6	$n-2$	$3n^2-12n+12/2$

which is required. □

Theorem 12. *Let G_2 be the chain silicate network of odd order; then, its Mostar index is $15n^2-12n-3/2$.*

Proof. Let $G_2 \cong CS_n$, where $n \geq 1$; also, n is odd:

$$\mathrm{Mo}(G_2) = \sum_{uv\in E(G_2)} |n_u - n_v|,$$
$$\mathrm{Mo}(G_2) = \sum_{uv\in E(G_2)} |n_3 - n_3| + \sum_{uv\in E(G_2)} |n_3 - n_6| + \sum_{uv\in E(G_2)} |n_6 - n_6|. \quad (29)$$

By using Table 12, we have

$$\mathrm{Mo}(G_2) = 0 + 6n^2 - 6 + \frac{3n^2-12n+9}{2},$$
$$\mathrm{Mo}(G_2) = \frac{15n^2-12n-3}{2}, \quad (30)$$

Table 12: Edge partition of chain silicate network of odd order.

Edge partition d_u, d_v	Number of edges	Mostar index
3, 3	$n+4$	0
3, 6	$2(2n-1)$	$6n^2-6$
6, 6	$n-2$	$3n^2-12n+9/2$

which is required. □

2.3. Results for the Ortho Chain S_n. In this section, we discuss S_n and compute the exact results for Szeged, PI, ABC_{GG}, NGG, and Mostar index. The single molecule of para and ortho chain has the same structure. Basically, it is a cycle graph having 4 sides denoted as C_4 and represented as a four-sided regular polygon. The ortho chain has a zig-zag structure where each corner of C_4 is attached linearly, as shown in Figure 3. The para chain has a structure in which each C_4 is attached at corner to corner with other C_4 but not linearly, as shown in Figure 4 [28].

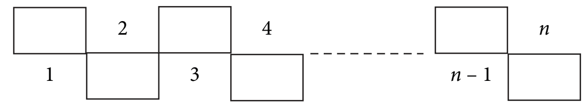

Figure 3: Ortho chain of n vertices.

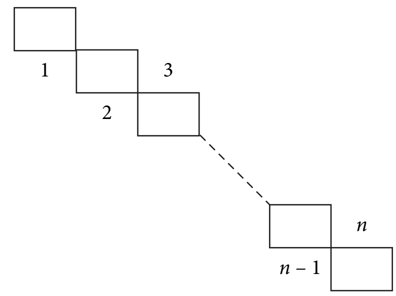

Figure 4: Para chain of n order.

Theorem 13. *Let G_3 be the ortho chain of n order; then, its Szeged index is $3n^3+15n^2-2n$.*

Proof. Let $G_3 \cong S_n$, where $n \geq 2$; also, n is an integer.

$$\mathrm{Sz}(G_3) = \sum_{e\in E(G_3)} n_u n_v,$$
$$\mathrm{Sz}(G_3) = \sum_{e\in E(G_3)} n_2 n_2 + \sum_{e\in E(G_3)} n_2 n_4 + \sum_{e\in E(G_3)} n_4 n_4. \quad (31)$$

By using Table 13, we have

$$\mathrm{Sz}(G_3) = \frac{3n^3+3n^2+26n-8}{2} + 12n^2 - 4n + \frac{3n^3+3n^2-22n+8}{2},$$
$$\mathrm{Sz}(G_3) = 3n^3+15n^2-2n, \quad (32)$$

which is required. □

Theorem 14. *Let G_3 be the ortho chain of n order; then, its PI index is $12n^2+4n$.*

Proof. Let $G_3 \cong S_n$, where $n \geq 2$; also, n is an integer:

$$\mathrm{PI}_v(G_3) = \sum_{e\in E(G_3)} n_u + n_v,$$
$$\mathrm{PI}_v(G_3) = \sum_{e\in E(G_3)} n_2 + n_2 + \sum_{e\in E(G_3)} n_2 + n_4 + \sum_{e\in E(G_3)} n_4 + n_4. \quad (33)$$

By using Table 14, we have

$$\mathrm{PI}_v(G_3) = 3n^2+7n+2+6n^2+2n+3n^2-5n-2,$$
$$\mathrm{PI}_v(G_3) = 12n^2+4n, \quad (34)$$

Table 13: Edge partition of ortho chain of n order.

Edge partition d_u, d_v	Number of edges	Szeged index
2, 2	$n+2$	$3n^3+3n^2+26n-8/2$
2, 4	$2n$	$12n^2-4n$
4, 4	$n-2$	$3n^3+3n^2-22n+8/2$

Table 14: Edge partition of ortho chain of n order.

Edge partition d_u, d_v	Number of edges	PI index
2, 2	$n+2$	$3n^2+7n+2$
2, 4	$2n$	$6n^2+2n$
4, 4	$n-2$	$3n^2-5n-2$

which is required. □

Theorem 15. *Let G_3 be the ortho chain of n order; then, its ABC_{GG} index is $\sqrt{6n^2+14n/3n^3+3n^2+26n-8}$ $+\sqrt{3n^2+n-1/6n^2-2n}+\sqrt{6n^2-10n-8/3n^3+3n^2-22n}$ $+8$.*

Proof. Let $G_3 \cong S_n$, where $n \geq 2$; also, n is an integer:

$$\mathrm{ABC}_{GG}(G_3) = \sum_{e\in E(G_3)} \sqrt{\frac{n_u+n_v-2}{n_u n_v}},$$
$$\mathrm{ABC}_{GG}(G_3) = \sum_{e\in E(G_3)} \sqrt{\frac{n_2+n_2-2}{n_2 n_2}} + \sum_{e\in E(G_3)} \sqrt{\frac{n_2+n_4-2}{n_2 n_4}} + \sum_{e\in E(G_3)} \sqrt{\frac{n_4+n_4-2}{n_4 n_4}}. \quad (35)$$

By using Table 15, we have

Table 15: Edge partition of ortho chain of n order.

Edge partition d_u, d_v	Number of edges	ABC_{GG} index
2, 2	$n+2$	$\sqrt{6n^2+14n/3n^3+3n^2+26n-8}$
2, 4	$2n$	$\sqrt{3n^2+n-1/6n^2-2n}$
4, 4	$n-2$	$\sqrt{6n^2-10n-8/3n^3+3n^2-22n+8}$

$$\mathrm{ABC}_{GG}(G_3) = \sqrt{\frac{6n^2+14n}{3n^3+3n^2+26n-8}} + \sqrt{\frac{3n^2+n-1}{6n^2-2n}} + \sqrt{\frac{6n^2-10n-8}{3n^3+3n^2-22n+8}}, \tag{36}$$

which is required. □

Theorem 16. *Let G_3 be the ortho chain of n order; then, its $NGG(G_3)$ index is $\sqrt{2/3n^3+3n^2+26n-8}+1/2\sqrt{3n^2-n}+\sqrt{2/3n^3+3n^2-22n+8}$.*

Proof. Let $G_3 \cong S_n$, where $n \geq 2$; also, n is an integer:

$$\mathrm{NGG}(G_3) = \sum_{e\in E(G_3)} \frac{1}{\sqrt{n_u n_v}},$$

$$\mathrm{NGG}(G_3) = \sum_{e\in E(G_3)} \frac{1}{\sqrt{n_2 n_2}} + \sum_{e\in E(G_3)} \frac{1}{\sqrt{n_2 n_4}} + \sum_{e\in E(G_3)} \frac{1}{\sqrt{n_4 n_4}}. \tag{37}$$

By using Table 16, we have

$$\mathrm{NGG}(G_3) = \sqrt{\frac{2}{3n^3+3n^2+26n-8}} + \frac{1}{2\sqrt{3n^2-n}} + \sqrt{\frac{2}{3n^3+3n^2-22n+8}}, \tag{38}$$

which is required. □

Theorem 17. *Let G_3 be the ortho chain of even order; then, its Mostar index is $9n^2-6n$.*

Proof. Let $G_3 \cong S_n$, where $n \geq 2$; also, n is even:

$$\mathrm{Mo}(G_3) = \sum_{uv\in E(G_3)} |n_u - n_v|,$$
$$\mathrm{Mo}(G_3) = \sum_{uv\in E(G_3)} |n_2 - n_2| + \sum_{uv\in E(G_3)} |n_2 - n_4| + \sum_{uv\in E(G_3)} |n_4 - n_4|. \tag{39}$$

By using Table 17, we have

Table 16: Edge partition of oxide network of n order.

Edge partition d_u, d_v	Number of edges	NGG index
2, 2	$n+2$	$\sqrt{2/3n^3+3n^2+26n-8}$
2, 4	$2n$	$1/2\sqrt{3n^2-n}$
4, 4	$n-2$	$\sqrt{2/3n^3+3n^2-22n+8}$

Table 17: Edge partition of ortho chain of even order.

Edge partition d_u, d_v	Number of edges	Mostar index
2, 2	$n+2$	$3n^2+12n-12/2$
2, 4	$2n$	$6n^2-6n$
4, 4	$n-2$	$3n^2-12n+12/2$

$$\mathrm{Mo}(G_3) = \frac{3n^2+12n-12}{2} + 6n^2 - 6n + \frac{3n^2-12n+12}{2},$$
$$\mathrm{Mo}(G_3) = 9n^2 - 6n, \tag{40}$$

which is required. □

Theorem 18. *Let G_3 be the ortho chain of odd order; then, its Mostar index is $9n^2-6n-3$.*

Proof. Let $G_3 \cong S_n$, where $n \geq 1$; also, n is odd:

$$\mathrm{Mo}(G_3) = \sum_{uv\in E(G_3)} |n_u - n_v|,$$
$$\mathrm{Mo}(G_3) = \sum_{uv\in E(G_3)} |n_2 - n_2| + \sum_{uv\in E(G_3)} |n_2 - n_4| + \sum_{uv\in E(G_3)} |n_4 - n_4|. \tag{41}$$

By using Table 18, we have

$$\mathrm{Mo}(G_3) = \frac{3n^2+12n-15}{2} + 6n^2 - 6n + \frac{3n^2-12n+9}{2},$$
$$\mathrm{Mo}(G_3) = 9n^2 - 6n - 3, \tag{42}$$

which is required. □

2.4. Results for the Para Chain Q_n. In this section, we discuss Q_n and compute the exact results for Szeged, PI, ABC_{GG}, NGG, and Mostar index.

Theorem 19. *Let G_4 be the para chain of n order; then, its Szeged index is $6n^3+6n^2+4n$.*

Proof. Let $G_4 \cong Q_n$, where $n \geq 2$; also, n is an integer.

Table 18: Edge partition of ortho chain of odd order.

Edge partition d_u, d_v	Number of edges	Mostar index
2, 2	$n+2$	$3n^2 + 12n - 15/2$
2, 4	$2n$	$6n^2 - 6n$
4, 4	$n-2$	$3n^2 - 12n + 9/2$

$$\mathrm{Sz}(G_4) = \sum_{e\in E(G_4)} n_u n_v,$$
$$\mathrm{Sz}(G_4) = \sum_{e\in E(G_4)} n_2 n_2 + \sum_{e\in E(G_4)} n_2 n_4. \tag{43}$$

By using Table 19, we have

$$\mathrm{Sz}(G_4) = 24n - 8 + 6n^3 + 6n^2 - 20n + 8,$$
$$\mathrm{Sz}(G_4) = 6n^3 + 6n^2 + 4n, \tag{44}$$

which is required. □

Theorem 20. *Let G_4 be the para chain of n order; then, its PI index is $12n^2 + 4n$.*

Proof. Let $G_4 \cong Q_n$, where $n \geq 2$; also, n is an integer:

$$\mathrm{PI}_v(G_4) = \sum_{e\in E(G_4)} n_u + n_v,$$
$$\mathrm{PI}_v(G_4) = \sum_{e\in E(G_4)} n_2 + n_2 + \sum_{e\in E(G_4)} n_2 + n_4. \tag{45}$$

By using Table 20, we have

$$\mathrm{PI}_v(G_4) = 12n + 4 + 12n^2 - 8n - 4,$$
$$\mathrm{PI}_v(G_4) = 12n^2 + 4n, \tag{46}$$

which is required. □

Theorem 21. *Let G_4 be the para chain of n order; then, its ABC_{GG} index is $\sqrt{6n+1/12n-4} + \sqrt{6n^2-4n-3/3n^3+3n^2-10n+4}$.*

Proof. Let $G_4 \cong \mathrm{OX}(n)$, where $n \geq 2$; also, n is an integer:

$$\mathrm{ABC_{GG}}(G_4) = \sum_{e\in E(G_4)} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}},$$
$$\mathrm{ABC_{GG}}(G_4) = \sum_{e\in E(G_4)} \sqrt{\frac{n_2 + n_2 - 2}{n_2 n_2}} + \sum_{e\in E(G_4)} \sqrt{\frac{n_2 + n_4 - 2}{n_2 n_4}}. \tag{47}$$

By using Table 21, we have

$$\mathrm{ABC_{GG}}(G_4) = \sqrt{\frac{6n+1}{12n-4}} + \sqrt{\frac{6n^2 - 4n - 3}{3n^3 + 3n^2 - 10n + 4}}, \tag{48}$$

which is required. □

Table 19: Edge partition of para chain of n order.

Edge partition d_u, d_v	Number of edges	Szeged index
2, 2	4	$24n - 8$
2, 4	$4n - 4$	$6n^3 + 6n^2 - 20n + 8$

Table 20: Edge partition of para chain of n order.

Edge partition d_u, d_v	Number of edges	PI index
2, 2	4	$12n + 4$
2, 4	$4n - 4$	$12n^2 - 8n - 4$

Table 21: Edge partition of para chain of n order.

Edge partition d_u, d_v	Number of edges	$\mathrm{ABC_{GG}}$ index
2, 2	4	$\sqrt{6n+1/12n-4}$
2, 4	$4n - 4$	$\sqrt{6n^2-4n-3/3n^3+3n^2-10n+4}$

Theorem 22. *Let G_4 be the para chain of n order; then, its $NGG(G_4)$ index is $1/2\sqrt{6n-2} + 1/\sqrt{6n^3+6n^2-20n+8}$.*

Proof. Let $G_4 \cong Q_n$, where $n \geq 2$ also n is an integer:

$$\mathrm{NGG}(G_4) = \sum_{e\in E(G_4)} \frac{1}{\sqrt{n_u n_v}},$$
$$\mathrm{NGG}(G_4) = \sum_{e\in E(G_4)} \frac{1}{\sqrt{n_2 n_2}} + \sum_{e\in E(G_4)} \frac{1}{\sqrt{n_2 n_4}}. \tag{49}$$

By using Table 22, we have

$$\mathrm{NGG}(G_4) = \frac{1}{2\sqrt{6n-2}} + \frac{1}{\sqrt{6n^3 + 6n^2 - 20n + 8}}, \tag{50}$$

which is required. □

Theorem 23. *Let G_4 be the para chain of even order; then, its Mostar index is $6n^2$.*

Proof. Let $G_4 \cong Q_n$, where $n \geq 2$; also, n is even:

$$\mathrm{Mo}(G_4) = \sum_{uv\in E(G_4)} |n_u - n_v|,$$
$$\mathrm{Mo}(G_4) = \sum_{uv\in E(G_4)} |n_2 - n_2| + \sum_{uv\in E(G_4)} |n_2 - n_4|. \tag{51}$$

By using Table 23, we have

$$\mathrm{Mo}(G_4) = 12n - 12 + 6n^2 - 12n + 12,$$
$$\mathrm{Mo}(G_4) = 6n^2, \tag{52}$$

which is required. □

Theorem 24. *Let G_4 be the para chain of odd order; then, its Mostar index is $6n^2 - 6$.*

Table 22: Edge partition of para chain of n order.

Edge partition d_u, d_v	Number of edges	NGG index
2, 2	4	$1/2\sqrt{6n-2}$
2, 4	$4n-4$	$1/\sqrt{6n^3+6n^2-20n+8}$

Table 23: Edge partition of para chain of even order.

Edge partition d_u, d_v	Number of edges	Mostar index
2, 2	4	$12n-12$
2, 4	$4n-4$	$6n^2-12n+12$

Table 24: Edge partition of para chain of odd order.

Edge partition d_u, d_v	Number of edges	Mostar index
2, 2	4	$12n-12$
2, 4	$4n-4$	$6n^2+12n+6$

Table 25: Comparison table for chain oxide network.

OX(n)	Sz(G)	PI	ABC	NGG
1	3	6	—	—
2	14	20	—	—
3	37	42	—	—
4	76	72	2.75	1.04
5	135	110	2.71	0.95
6	218	156	2.66	0.90
7	329	210	2.62	0.86
8	472	272	2.59	0.84
9	651	342	2.56	0.83
10	870	420	2.53	0.81

Table 26: Comparison table for chain silicate.

CS_n	Sz(G)	PI	ABC	NGG
1	6	12	—	—
2	30	42	—	—
3	81	90	—	—
4	168	156	2.91	0.58
5	300	240	2.89	0.49
6	486	342	2.88	0.45
7	735	462	2.86	0.41
8	1056	600	2.83	0.38
9	1458	756	2.81	0.35
10	1950	930	2.80	0.33

Proof. Let $G_4 \cong Q_n$, where $n \geq 1$; also, n is odd:

$$\text{Mo}(G_4) \sum_{uv\in E(G_4)} |n_u - n_v|,$$
$$\text{Mo}(G_4) = \sum_{uv\in E(G_4)} |n_2 - n_2| + \sum_{uv\in E(G_4)} |n_2 - n_4|. \quad (53)$$

By using Table 24, we have

$$\text{Mo}(G_4) = 12n - 12 + 6n^2 + 12n + 6,$$
$$\text{Mo}(G_4) = 6n^2 - 6, \quad (54)$$

which is required.

Table 27: Comparison table for ortho chain.

S_n	Sz(G)	PI	ABC	NGG
1	16	16	—	—
2	80	56	—	—
3	210	120	—	—
4	424	208	1.98	0.26
5	740	320	1.88	0.19
6	1176	456	1.80	0.15
7	1750	616	1.74	0.12
8	2480	800	1.68	0.10
9	3384	1006	1.63	0.09
10	4480	1240	1.58	0.08

Table 28: Comparison table for para chain.

Q_n	Sz(G)	PI	ABC	NGG
1	16	16	—	—
2	80	56	1.61	0.32
3	228	120	1.46	0.20
4	496	208	1.37	0.16
5	920	320	1.30	0.13
6	1536	456	1.26	0.11
7	2380	616	1.22	0.10
8	3488	800	1.19	0.09
9	4896	1008	1.16	0.08
10	6640	1240	1.14	0.07

For the comparison of Szeged, PI, ABC_{GG}, and NGG index of COX_n, we computed the indices for different values of n. By increasing the values of n, we can clearly check from Table 25 that the order of Szeged and PI index is increasing while that of ABC_{GG} and *NGG* is decreasing.

For the comparison of Szeged, PI, ABC_{GG}, and NGG index of CS_n, we computed the indices for different values of n. By increasing the values of n, we can clearly check from Table 26 that the order of Szeged and PI index is increasing while that of ABC_{GG} and NGG is decreasing.

For the comparison of Szeged, PI, ABC_{GG}, and NGG index of S_n, we computed the indices for different values of n. By increasing the values of n, we can clearly check from Table 27 that the order of Szeged and PI index is increasing while that of ABC_{GG} and NGG is decreasing.

For the comparison of Szeged, PI, ABC_{GG}, and NGG index of Q_n, we computed the indices for different values of n. By increasing the values of n, we can clearly check from Table 28 that the order of Szeged and PI index is increasing while that of ABC_{GG} and NGG is decreasing. □

3. Conclusion

In this article, we have figured out several bond-additive TIs such as Szeged, PI, ABC, NGG, and Mostar index. We calculated the closed formulae for abovementioned TIs of chain silicate, oxide network, para, and ortho chain. The above outcomes contribute in the field of natural sciences and pharmaceutical science. Our exploration kept on determining new consequences of these graphs.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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