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Operations of Nanostructures via SDD, ABC_4 and GA_5 indices

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Abstract

Recently, nanostructures have opened new dimensions in industry, electronics, and pharmaceutical and biological therapeutics. The topological indices are numerical tendencies that often depict quantitative structural activity/property/toxicity relationships and correlate certain physico-chemical properties such as boiling point, stability, and strain energy, of respective nanomaterial. In this article, we established closed forms of various degree-based topological indices of semi-total line graph of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[r,s]$.

Keywords: Topological indices, $2D$-lattice, nanotube, nanotorus, semi-total line operator.
AMS 2010 codes: AMS Subject Classification: 05C90, 05C35, 05C12.

1 Introduction and Preliminaries

In this article, we will consider only the simple graphs G, that are without loops and multiple edges, with vertex set $V(G)$ and edge set $E(G)$. The degree d_u of a vertex u is the number of edges that are incident to it and $S_u = \sum_{v \in N_u} d_v$ where $N_u = \{v \in V(G) | uv \in E(G)\}$. N_u is also known as the set of neighbor vertices of the vertex u or the neighborhood of u. The semi-total (line) graph $T_1(G)$ of G is the graph whose vertex set is $V(G) \bigcup E(G)$

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where two vertices of $T_1(G)$ are adjacent if and only if **(i)** they are adjacent edges of G or **(ii)** one is a vertex of G and the other is an edge of G incident to that vertex (see also [19]).

The idea of a topological index first appears in the work of H. Wiener in 1947, [27], in which he was working on boiling points of paraffins. He called this index as path number, and later it was called as Wiener index. Since then, the theory of topological indices has begun to have great importance as the topological indices are the mathematical measures which correspond to the structure of any simple finite graph. They are invariant under the graph isomorphisms. The significance of topological indices is usually associated with quantitative structures property relationship (QSPR)/quantitative structure activity relationship (QSAR) [23].

In the study of QSAR/QSPR, [3], topological indices such as Shultz index, generalized Randic index, [14], Zagreb index, general sum-connectivity index, atom-bond connectivity (ABC) index, [2,4], geometric-arithmetic (GA) index, [14], and harmonic index, [15, 18, 22], are exploited to estimate the bioactivity of chemical compounds. A topological index attaches a chemical structure with a numeric number. There are numerous applications of graph theory in this field of research called molecular or chemical graph theory, [28].

Recently [25, 26], D. Vukicevic revealed the set of 148 discrete Adriatic indices. They were analyzed on the testing sets provided by the International Academy of Mathematical Chemistry and it had been shown that they have good predictive properties in many cases. There was a vast research regarding various properties of these topological indices.

Muhammad Faisal Nadeem et. al., [17], computed generalized Randic, general Zagreb, general sum-connectivity, ABC, GA, ABC_4, and GA_5 indices of the line graphs of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$ by using the concept of subdivision.

Sunil Hosamani [12], worked on computing sanskruti index of certain nanostructures. Computed the expressions for the Sanskruti index of the line graph of subdivision graph of the 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$.

Recently, C. K. Gupta and et. al., [7, 8], worked on symmetric division deg index for bounds and operations are discussed in detail.

Symmetric division deg index is one of the discrete Adriatic indices, [25, 26]. It is a good predictor of total surface area for polychlorobiphenyls and is defined as

$$SDD(G) = \sum_{uv \in E(G)} \frac{d_u \cdot d_v}{d_u + d_v}.$$

The fourth member of the class of ABC indices was introduced by Ghorbani and Hosseinzadeh in [5]:

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

The fifth member of geometric-arithmetic (GA_5) index was introduced by Graovac et. al. in [6] as

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

The aim of this paper is to compute the SDD index, fourth member of atom-bond connectivity (ABC_4) indices and fifth member of geometric-arithmetic (GA_5) indices of semi-total (line) graph of the $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[r,s]$, where r and s denote the number of squares in a row and the number of rows of squares respectively. The construction of nanostructure is shown in Figure 1 and the $2D$-lattice, nanotube and nanotorus of the $TUC_4C_8[r,s]$ are shown in Figure 2.

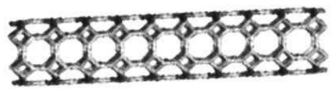
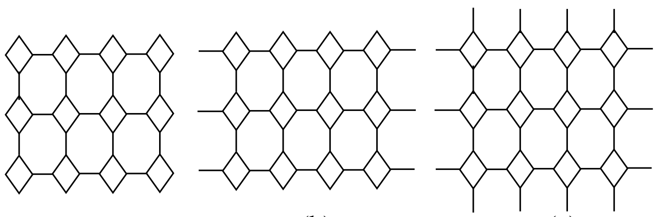


Fig. 1 Nanostructure



(a) (b) (c)

Figure 2: $2D$-Lattice, Nanotube, Nanotorus of TUC_4C_8

This paper is organised as follows. Section 1 consists of a brief introduction which is essential for the development of main results. Section 2 will consist of the *SDD* index of the $2D$-lattice, nanotube and nanotorus of the $TUC_4C_8[r,s]$ using semi-total (line) graph operator and final section concentrates on the results about the neighborhood degree based indices such as ABC_4 and GA_5 of $2D$-lattice, nanotube and nanotorus of the $TUC_4C_8[r,s]$ using the semi-total (line) graph operator.

2 Symmetric division deg index of semi-total(line) graph of $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[r,s]$

In this section, we computed the general expressions for the *SDD* index of $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[r,s]$ using semi-total (line) graph operator and the structure of the graph depicted in Figure 3.

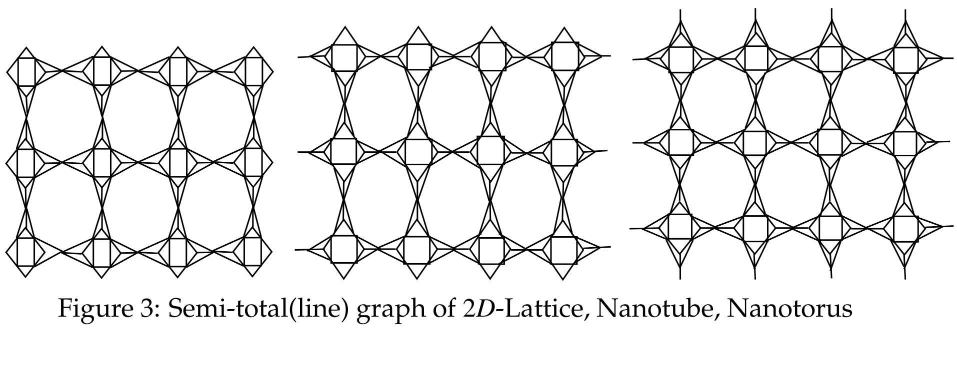


Figure 3: Semi-total(line) graph of $2D$-Lattice, Nanotube, Nanotorus

In $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[r,s]$, the number of vertices are $4rs$ and the number of edges are $6rs-r-s$, $6rs-s$ and $6rs$, respectively. The following Tables 1(a,b), 2(a,b) and 3(a,b) indicates the algebraic method, i.e., the partitioned edges will be helpful to compute the results.

Table 1: Edge partition of Semi-total(line) graph of 2D-Lattice

(a) $r > 1$and $s = 1$

Edges Partitioned	(2,4)	(2,5)	(3,5)	(3,6)	(4,4)	(4,5)	(5,5)	(5,6)
No of Edges	8	4(r-1)	4(r-1)	2(r-1)	2	4	2(2r-3)	4(r-1)

(b) $r > 1$ and $s > 1$

Edges Partitioned	(2,4)	(4,5)	(2,5)	(3,5)	(3,6)	(5,5)	(5,6)	(6,6)
No of Edges	8	8	4(r+s-2)	4(r+s-2)	2[s(r+s) +5(r+s-4)]	2(r+s-4)	8(r+s-2)	2[(s+3) (r+s)-16]

Table 2: Semi-total line graph of nanotube

(a) $r > 1$ and $s = 1$

Edges Partitioned	(2,5)	(3,3)	(3,5)	(3,6)	(5,5)	(5,6)
No of Edges	4r	2	4(r+1)	2(r-1)	4r	4(r-1)

(b) $r > 1$ and $s > 1$

Edges Partitioned	(2,5)	(3,3)	(3,5)	(3,6)	(5,5)	(5,6)	(6,6)
No of Edges	4r	2s	4(r+1)	14(r-2)+26(s-2) +2r(s-2)(r+s-4)+28	2r	4(2r-1)	10(r-2)+20(s-2) +2r(s-2)(r+s-4)+16

Table 3: Edge Partition for Semi-total(line) graph of Nanotorus

(a) $r > 1$ and $s = 1$

Edges Partitioned	(3,3)	(3,6)	(6,6)
No of Edges	$2(r+1)$	$2(7r+1)$	$4(2r-1)$

(b) $r > 1$ and $s > 1$

Edges Partitioned	(3,3)	(3,6)	(6,6)
No of Edges	$2(r+s)$	$[2r(s-2)+26](r+s-4)+56$	$[2r(s-2)+20](r+s-4)+32$

Theorem 1. *Let G=$TUC_4C_8[r,s]$ be the semi-total (line) graph of 2D-lattice graph of $TUC_4C_8[r,s]$, then*

$$SDD(G) = \begin{cases} 5.933r + 60.93s + rs(9s+42) - 41s^2 - 103.467 & \textit{when } r > 1 \textit{ and } s > 1 \\ 41.8r - 13.6 & \textit{when } r > 1 \textit{ and } s = 1 \end{cases}$$

Proof. **Case (i):** Let $r > 1$ and $s > 1$.

Let G be the semi-total (line) graph of the 2D-lattice graph of $TUC_4C_8[r,s]$. The number of vertices and edges of the 2D-Lattice graph G is equal to $|V| = 2(s-2)(r+s-3)+3r-s+8rs$ and $|E| = 2(2s+17)(r+s)$.

Hence the edge partition on the degree sum of vertices of each vertex is obtained, as shown in Table 1(b). We apply the topological indices to the edge partitions to get the required results.

Case (ii): Let $r > 1$ and $s = 1$.

It can be observed that in G, $|V| = (9r-1)$ and $|E| = 6(3r-s)$. Hence utilizing Table 1(a) and *SDD* index, we can obtain the expressions of *SDD* index of G.

Theorem 2. *Let H be the semi-total (line) graph of the $TUC_4C_8[r,s]$ nanotube, then*

$$SDD(H) = \begin{cases} 40.93r + 4s + 55(r-2) + 105(s-2) + 9r(s-2)(r+s-4) + 102.93 \\ \text{when } r > 1 \text{ and } s > 1 \\ \\ 27.733r + 4.933 \quad \text{when } r > 1 \text{ and } s = 1 \end{cases}$$

Proof. Let H be the semi-total (line) graph of nanotube of $TUC_4C_8[r,s]$ nanotube. Vertices and edges of H graph are equal to $|V|$=$(9r+1)$ and $|E|$=$18r$ for $r > 1$, $s = 1$ and $|V|$=$9rs + r + s + (s-2)(r+s-3)$ and $|E|$=$4r(r(s-2)+s(s-6)) + 74r + 48s - 56$ for the case and $r > 1$, $s > 1$. Hence computing the results using the Table 2(a)and 2(b)and *SDD* index, we get the required result.

Theorem 3. *Let K be the semi-total (line) graph of the $TUC_4C_8[r,s]$ nanotorus. Then*

$$SDD(K) = \begin{cases} 4(r+s) + (r+s-4)[9r(s-2)+105] + 204 \quad \text{when } r > 1 \text{ and } s > 1 \\ \\ 55r + 1 \quad \text{when } r > 1 \text{ and } s = 1 \end{cases}$$

Proof. Let K be semi-total (line) graph of the nanotorus of $TUC_4C_8[r,s]$. The number of vertices and edges of the graph K are equal to $|V| = (11r+1)$, $|E| = 32r$; and $|V| = 10rs + r + s$ and $|E| = 4r(s-2) + 134$ respectively, in the cases of $r > 1$, $s = 1$; and $r > 1$, $s > 1$. Hence computing the results using the Table 3(a) and 3(b) and *SDD* definition, we get the required result.

3 ABC_4 and GA_5 indices of semi-total (line) graph of $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[r,s]$

In this section, ABC_4 and GA_5 by using semi-total (line) graph of the $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[r,s]$ are determined by means of the neighborhood vertex degree indices.

Table 4: Edge Partition of Semi-total(line) graph of 2D-Lattice for Neighborhood vertices

(a) $r > 1$ and $s = 1$

Edges Partitioned	No of Edges
(8,13) (9,13) (13,20) (9,20) (16,20) (20,26)	4
(13,13) (20,20)	2
(16,26)	2(r-1)
(16,21) (10,21) (21,21) (21,26)	4(r-2)

(b) $r > 1$ and $s > 1$

Edges Partitioned	No of Edges
(9,14) (9,21) (14,21) (17,21) (28,28)	8
(21,28)	16
(17,28)	$4(r+s)$
(17,22) (22,29) (10,22) (22,28) (17,29) (28,29)	$4(r+s-4)$
(22,22)	$2(r+s-4)$
(29,29) (18,30)	$2(r+s-4)[1+r/3(s-2)]$
(18,29) (29,30)	$4(r+s-4)[1+r/3(s-2)]$

Theorem 4. *Let G_1 be the semi-total (line) graph of the 2D-lattice, then*

$$ABC_4(G_1) = \begin{cases} 8.99(r+s)+3.316(r+s-4)[1+r/3(s-2)]-11.754 \\ \qquad \text{when } r>1 \text{ and } s>1 \\ \\ 5.751r-2.119 \quad \text{when } r>1 \text{ and } s=1 \end{cases}$$

$$GA_5(G_1) = \begin{cases} 29.347(r+s)+11.822(r+s-4)[1+r/3(s-2)]-43.101 \\ \qquad \text{when } r>1 \text{ and } s>1 \\ \\ 17.622r-5.873 \quad \text{when } r>1 \text{ and } s=1 \end{cases}$$

Proof. To compute the $ABC_4(G_1)$ and $GA_5(G_1)$ indices of the 2D-lattice of $TUC_4C_8[r,s]$, we need an edge partition of the 2D-lattice of $TUC_4C_8[r,s]$, based on the degree sum of neighbors of the two end vertices of each edge. We presented these partitions with their cardinalities in Tables 4(a) and 4(b). Hence using the definitions of the ABC_4 and GA_5, and Table 4(a) and 4(b), we obtained required results.

Table 5: Semi-total(line) graph of Nanotube for Neighborhood vetices

(a) $r>1$ and $s=1$

Edges Partitioned	No of Edges
(13,13) (18,18)	2
(10,18) (18,21)	4
(13,18)	8
(10,21) (16,21) (21,26)	$4(r-1)$
(16,26)	$2(r-1)$
(21,21)	$2(2r-3)$

(b) $r>1$ and $s>1$

Edges Partitioned	No of Edges
(14,13)	$2s$
(19,26) (26,29) (26,18) (26,30) (19,10) (13,26) (14,19) (14,26) (13,19) (19,22)	4
(10,22) (22,17) (17,29) (18.29) (22,29) (17,28) (29,30) (22,28) (28,29)	$4(r-1)$
(22,22) (29,29)	$2(r-2)$
(13,27) (14,27) (18,27)	$4(s-2)$
(27,27)	$2(s-2)$
(18,30)	$2(r+s-2)+12(s-2)(r+s-4)$
(30,30)	$[12(s-2)(r+s-4)]-2$

Theorem 5. *Let H_1 be the semi-total (line) graph of the $TUC_4C_8[r,s]$ nanotube, then*

$$ABC_4(H_1) = \begin{cases} 11.7r+7.151s+3.048(s-2)(r+s-4)+2(r+s-2) \\ \qquad +3.502(s-2)(r+s-4)-14.84 \text{ when } r>1 \text{ and } s>1 \\ \\ 5.749r+0.638 \quad \text{when } r>1 \text{ and } s=1 \end{cases}$$

$$GA_5(H_1) = \begin{cases} 39.21r+23.447s+12(s-2)(r+s-4)+2(r+s-2)+ \\ \qquad 11.616(s-2)(r+s-4)-66.539 \text{ when } r>1 \text{ and } s>1 \\ \\ 17.614r+0.095 \quad \text{when } r>1 \text{ and } s=1 \end{cases}$$

Proof. To compute the $ABC_4(H_1)$ and $GA_5(H_1)$ indices of the nanotube of the $TUC_4C_8[r,s]$, we need an edge partition of the nanotube of the $TUC_4C_8[r,s]$, based on the degree sum of the neighbors of the two end vertices of each edge. We presented these partitions together with their cardinalities in Tables 5(a) and 5(b). Hence using the ABC_4 and GA_5 formulae together with Table 5(a)and 5(b), we obtain the required results.

Table 6: Semi-total(line) graph of Nanotorous for Neighborhood vertices

(a) $r > 1$ and $s = 1$

Edges Partitioned	No of Edges
(15,24)	16
(24,27)	4
(24,24)	2
(15,15)	$2(r+1)$
(15,27)	$8(r-1)$
(27,27)	$2(2r-3)$
(18,30)	$2(r-1)$
(27,30) (18,27)	$4(r-1)$

(b) $r > 1$ and $s > 1$

Edges Partitioned	No of Edges
(15,24)	16
(24,27)	8
(15,15)	$2(r+s)$
(15,27) (27,30)	$8(r+s-2)$
(18,30)	$14(r+s)+8(s-2)(r+s-4)-40$
(18,27)	$4(r+s-8)$
(27,27)	$2(r+s-4)$
(30,30)	$10(r+s)+2(s-2)(r+s-4)[2(r+s-4)-2]-32$

Theorem 6. *Let K_1 be the semi-total (line) graph of the $TUC_4C_8[r,s]$ nanotorus, then*

$$ABC_4(K_1) = \begin{cases} 21.109(r+s)+2(r-s)(r+s-4)[0.508(r+s)-1.371]-26.17 \\ \qquad\qquad \text{when } r>1 \text{ and } s>1 \\ 7.103r+0.568 \quad \text{when } r>1 \text{ and } s=1 \end{cases}$$

$$GA_5(K_1) = \begin{cases} 47.123(r+s)+2(s-2)(r+s-4)[2(r+s)-4.128]-94.314 \\ \qquad\qquad \text{when } r>1 \text{ and } s>1. \\ 17.6r+5.961 \quad \text{when } r>1 \text{ and } s=1 \end{cases}$$

Proof. To compute the $ABC_4(K_1)$ and $GA_5(K_1)$ indices of the nanotorus of the $TUC_4C_8[r,s]$, we need an edge partition of the nanotorus of $TUC_4C_8[r,s]$, based on the degree sum of the neighbors of the two end vertices of each edge. We presented these partitions with their cardinalities in Tables 6(a) and 6(b). Hence using the ABC_4 and GA_5 formula together with Tables 6(a) and 6(b), we obtain required results.

4 Conclusions

In the field of chemical graph theory, the studies under the framework of semi-total (line) graph operator is a new direction in the field of structural chemistry. In this article, we computed the closed form of the $2D$-lattice, nanotubes and nanotorus of some degree-based topological indices for these structures. These indices can help us to understand the physical features, chemical and biological activities of these structures such as the boiling point, the heat of formation, the fracture toughness, the strength, the conductivity, and the hardness. From this point of view, a topological index can be regarded as a score function that maps each molecular structure to a real number and is used as a descriptor of the molecule under testing. These results can also play a vital part in the study of the nanostructures in electronics and industry which can be used in the preparation of armor due to their strength.

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