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Molecular topological invariants of certain chemical networks

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Abstract: Topological descriptors are the graph invariants that are used to explore the molecular topology of the molecular/chemical graphs. In QSAR/QSPR research, physico-chemical characteristics and topological invariants including Randić, atom-bond connectivity, and geometric arithmetic invariants are utilized to correlate and estimate the structure relationship and bioactivity of certain chemical compounds. Graph theory and discrete mathematics have discovered an impressive utilization in the area of research. In this article, we investigate the valency-dependent invariants for certain chemical networks like generalized Aztec diamonds and tetrahedral diamond lattice. Moreover, the exact values of invariants for these categories of chemical networks are derived.

Keywords: atom-bond connectivity index, geometric-arithmetic index, generalized Aztec diamond, tetrahedral diamond lattice

1 Introduction

There are many diverse applications of mathematics in electronic and electrical engineering. It relies upon what specific region of electronic and electrical designing you are interested, for instance, there is a masses

abstract mathematics involved in communication, signal processing, network theory, etc. Networks use vertices for communicating with each other. The theory of networking includes the investigation of the most ideal method of executing a network. Graph theory has given chemists beneficial tools and techniques, such as molecular topological descriptors and molecular topological polynomials. The structure of a molecular graph is constructed with help of molecules and molecular compounds. A molecular graph represents the structural result of a chemical compound in forms of graph theory, in which vertices are denoted by atoms and edges correlate to chemical bonds between their atoms. A newly famous area is cheminformatics which is a common region of mathematics, chemistry, and information science. This new subject describes a relationship between the QSAR and QSPR that are utilized to investigate (in certain degree of accuracy) the theoretical and biological activities of several chemical compounds. In the QSAR/QSPR investigation, the topological invariants like *ABC* index is known for the prediction of bioactivity of a given chemical compounds.

A topological descriptor is a numeric number achieved from different properties of graphs. It also describes the molecular topology of that graph and is not changed under the graph automorphism. The topological indices are generally of two types: one is degree-related and the other is distance-related. In the degree-related indices, it depends upon the vertex-degree of all vertices and in the distance-related indices, it depends on the distance among the each pair of vertices. It is important to know that a theoretical chemist Wiener (1947) gave the idea of topological indices when he was investigating the characteristics of boiling point of paraffin. Firstly, he termed it as path number but after a bit, it was changed to *Wiener index* (Wiener, 1947) and the research of topological invariants started.

Here, $V(B)$ and $E(B)$ are the vertex and the edge sets of a network B . Some of the terminologies which are used in this paper are given as follows: $d(\alpha)$ presents the degree of $\alpha \in V(B)$ and $S_\alpha = \sum_{\beta \in N_B(\alpha)} d(\beta)$ where

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$N_B(\alpha) = \{\beta \in V(B) : \alpha\beta \in E(B)\}$. All the terminologies used in this manuscript are acquired from books (Diudea et al. 2001, Gutman and Polansky, 1986).

Estrada et al. (1998) gave the concept of renowned degree related topological invariant atom-bond connectivit and described as:

$$ABC(B) = \sum_{\alpha\beta \in E(B)} \sqrt{\frac{d(\alpha) + d(\beta) - 2}{d(\alpha)d(\beta)}} \quad (1)$$

The other notable degree dependend invariant is *geometric-arithmetic* index established by Vukičević et al. (2009) and interpreted as:

$$GA(B) = \sum_{\alpha\beta \in E(B)} \frac{2\sqrt{d(\alpha)d(\beta)}}{d(\alpha) + d(\beta)} \quad (2)$$

In both these indices, first we find the possible degree of all the vertices and then partitined the edges of B depending upon the degree of every end vertex adjacent to edge.

Later, Ghorbani and Hosseinzadeh (2010) presented the 4th kind of ABC invariant by generalizing the idea of ABC index. It is interpreted as:

$$ABC_4(B) = \sum_{\alpha\beta \in E(B)} \sqrt{\frac{S_\alpha + S_\beta - 2}{S_\alpha S_\beta}} \quad (3)$$

Graovac et al. (2011) generalized the geometric index by defining the fifth kind of GA index in a same way as ABC_4 index. The index is written as:

$$GA_5(B) = \sum_{\alpha\beta \in E(B)} \frac{2\sqrt{S_\alpha S_\beta}}{S_\alpha + S_\beta} \quad (4)$$

In both these indices, first we find the possible degree of all vertices and then partitined the edges of B depending upon the degree of vertices adjacent to every end vertex of each edge.

The *first Zagreb index* M_1 and the *second Zagreb index* M_2 (Reti et al., 2019) for a graph G can be defined as:

$$M_1(G) = \sum_{v \in V(G)} (d(v))^2 = \sum_{uv \in E(G)} (d(u) + d(v)),$$

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

The neighborhood first and second Zagreb indices (first defined by Reti et al. (2019)) are as follows:

$$NM_1(G) = \sum_{v \in V(G)} (S_v)^2,$$

$$NM_2(G) = \sum_{uv \in E(G)} S_u S_v$$

For more discussion about invariants, see: Ahmad et al. (2017), Alikhani et al. (2014), Akhter and Imran (2016a, 2016b), Akhter et al. (2018, 2019), Bača et al. (2015), Baig et al. (2015a, 2015b), Guirao et al. (2020), Hameed et al. (2019), Hayat and Imran (2014, 2015a, 2015b, 2015c), Imran et al. (2020), Iranmanesh and Zeraatkar (2010), Lin et al. (2014), Manzoor (2015), and Yang et al. (2019).

In this article, we derive the certain degree related molecular topological invariants for chemical networks like generalized Aztec diamonds, tetrahedral diamond lattice, and certain infinite classes of nanostar dendrimers. We compute the analytical formulas for above families of chemically applicable networks.

2 ABC , GA , ABC_4 , GA_5 , NM_1 , and NM_2 indices of generalized Aztec diamonds

In this part of the article, we discuss the degree-based topological descriptors for the generalized Aztec diamonds.

For any two graphs W and F , the tensor product of the graphs W and F is interpreted by $W \otimes F$. The vertex set of $W \otimes F$ is $V(W) \times V(F)$ and $E(W \otimes F) = \{(w, f)(s, e) | ws \in E(W) \text{ and } fe \in E(F)\}$.

The tensor product of two paths L_p and L_q is described by $L_p \otimes L_q$. It is a graph on $p \times q$ vertices with vertex set is defined as:

$$\{(x_1, y_1) : 1 \leq x_1 \leq q, 1 \leq y_1 \leq p\}$$

and an edge between the (x_1, y_1) and (x_2, y_2) exists if and only if:

$$|x_1 - x_2| + |y_1 - y_2| = 1.$$

The graph $L_p \otimes L_q$ is known as a generalized Aztec diamond with vertex cardinality pq . $L_9 \otimes L_{10}$ is depicted in Figure 1. In the next theorem, the ABC index for generalized Aztec diamond graphs has been computed.

Theorem 2.1

The ABC index of generalized Aztec diamond graph $G = L_p \otimes L_q$ for $p, q \geq 2$, is:

$$ABC(L_p \otimes L_q) = \frac{\sqrt{6}}{2}pq + \left(1 - \frac{3\sqrt{3}}{4}\right)2\sqrt{2}p + \left(1 - \frac{3\sqrt{3}}{4}\right)2\sqrt{2}q + 2\left(\sqrt{3} + \sqrt{2} - 6\sqrt{2} + \frac{9\sqrt{6}}{4}\right).$$

Proof: Firstly, we identify that the graph G has vertices having degree one, two, and four. Thus, the graph G has only edges with end vertices have degree one, two, or four. So possible edges are of type (1,4), (2,2), (2,4), and (4,4), where by edge of type $(d(m), d(n))$, we mean end vertices of the edge with degrees m and n . In Table 1, all the edges of type (1,4), (2,2), (2,4), and (4,4) are counted. Now, by appying the information shown in Table 1, the ABC index of $L_p \otimes L_q$ is derived as:

$$\begin{aligned} ABC(G) &= \sum_{\alpha\beta \in E(G)} \sqrt{\frac{d(\alpha)+d(\beta)-2}{d(\alpha)d(\beta)}}. \\ ABC(L_p \otimes L_q) &= 4\sqrt{\frac{1+4-2}{1 \times 4}} + 4\sqrt{\frac{2+2-2}{2 \times 2}} \\ &\quad + 4(p+q-6)\sqrt{\frac{2+4-2}{2 \times 4}} \\ &\quad + 2(p-3)(q-3)\sqrt{\frac{4+4-2}{4 \times 4}}. \end{aligned}$$

Figure 1: The partition of the edges of $L_9 \otimes L_{10}$ that depend on the degree of every end vertex of each edge.

Table 1: The cardinality of edges of type $(d(m), d(n))$ of $L_p \otimes L_q$, where m and n are degrees of adjacent vertices of every edge

$(d(m), d(n))$ with $mn \in E(G)$	Quantity of edges
(1,4)	4
(2,2)	4
(2,4)	$4(p+q-6)$
(4,4)	$2(p-3)(q-3)$

After simplification of above calculations, we acquire the following result of ABC index:

$$ABC(L_p \otimes L_q) = \frac{\sqrt{6}}{2}pq + \left(1 - \frac{3\sqrt{3}}{4}\right)2\sqrt{2}p + \left(1 - \frac{3\sqrt{3}}{4}\right)2\sqrt{2}q + 2\left(\sqrt{3} + \sqrt{2} - 6\sqrt{2} + \frac{9\sqrt{6}}{4}\right).$$

In Theorem 2.2, we have computed the GA invariant of generalized Aztec diamond.

Theorem 2.2

For

$$\begin{aligned} p, q \geq 2, GA(L_p \otimes L_q) &= 2pq + 2\left(\frac{4\sqrt{2}}{3} - 3\right)p + 2\left(\frac{4\sqrt{2}}{3} - 3\right)q \\ &\quad + 2\left(\frac{63}{5} - \frac{6\sqrt{2}}{3}\right). \end{aligned}$$

Proof: Again, by using the information given in Table 1, the GA invariant of generalized Aztec diamond is derived follows; since:

$$\begin{aligned} GA(G) &= \sum_{\alpha\beta \in E(G)} 2\frac{\sqrt{d(\alpha)d(\beta)}}{(d(\alpha)+d(\beta))} \\ GA(L_p \otimes L_q) &= 4 \times \frac{2\sqrt{1 \times 4}}{1+4} + 4 \times \frac{2\sqrt{2 \times 2}}{2+2} \\ &\quad + 4(p+q-6)\frac{2\sqrt{2 \times 4}}{2+4} \\ &\quad + 2(p-3)(q-3)\frac{2\sqrt{4 \times 4}}{4+4}. \end{aligned}$$

From an easy simplification, we acquired:

$$GA(L_p \otimes L_q) = 2pq + 2 \left(\frac{4\sqrt{2}}{3} - 3 \right) p + 2 \left(\frac{4\sqrt{2}}{3} - 3 \right) q + 2 \left(\frac{63}{5} - \frac{6\sqrt{2}}{3} \right).$$

Similarly, the ABC_4 index of the generalized Aztec diamond can be computed by using Table 1.

Theorem 2.3

For $p, q \geq 2$, the ABC_4 index of $L_p \otimes L_q$ is calculated as:

$$ABC_4(L_p \otimes L_q) = \frac{\sqrt{30}}{8} pq + \left(\sqrt{3} + \sqrt{14} - \frac{5\sqrt{30}}{8} \right) p + \left(\sqrt{3} + \sqrt{14} - \frac{3\sqrt{30}}{4} \right) q + \left(\frac{2\sqrt{11}}{3} + \frac{2\sqrt{10}}{3} + \frac{2\sqrt{30}}{3} + \frac{\sqrt{22}}{3} + \frac{68\sqrt{30}}{16} + 8\sqrt{2} - 10\sqrt{3} - 10\sqrt{14} \right).$$

Proof: In the ABC_4 index, we first find possible degrees of all the vertices connected to end vertices of each edge. An edge with sum of the degrees of end vertices is m and n , and is interpreted as (S_m, S_n) – type edges. Thus, the possible edges are of type type (4,9), (6,6), (9,8), (8,12), (12,16), (16,16), (6,12), (9,16), and (12,12). In Table 2, all the edges of type (4,9), (6,6), (9,8), (8,12), (12,16), (16,16), (6,12), (9,16), and (12,12) are counted. Now, by applying the

Table 2: The cardinality of edges of type (S_m, S_n) of $L_p \otimes L_q$, where m and n are sum of degrees of all neighboring vertices of end vertices of each edge

(S_m, S_n) with $mn \in E(G)$	Number of edges
(4, 9)	4
(6, 6)	4
(6, 12)	8
(8, 12)	$4(p + q - 10)$
(9, 8)	8
(9, 16)	4
(12, 12)	4
(12, 16)	$4(p + q - 10)$
(16, 16)	$2(p - 6)(q - 5) + 8$

information interpreted in Table 2, the ABC_4 invariant of $L_p \otimes L_q$ is computed as follows; since:

$$ABC_4(G) = \sum_{\alpha\beta \in E(G)} \sqrt{\frac{S_\alpha + S_\beta - 2}{S_\alpha S_\beta}}$$

By an easy calculation, the above equation can be written as:

$$ABC_4(L_p \otimes L_q) = \frac{\sqrt{30}}{8} pq + \left(\sqrt{3} + \sqrt{14} - \frac{5\sqrt{30}}{8} \right) p + \left(\sqrt{3} + \sqrt{14} - \frac{3\sqrt{30}}{4} \right) q + \left(\frac{2\sqrt{11}}{3} + \frac{2\sqrt{10}}{3} + \frac{2\sqrt{30}}{3} + \frac{\sqrt{22}}{3} + \frac{68\sqrt{30}}{16} + 8\sqrt{2} - 10\sqrt{3} - 10\sqrt{14} \right).$$

The following theorem gives the GA_5 index of generalized Aztec diamond $L_p \otimes L_q$.

Theorem 2.4

For $p, q \geq 2$, the GA_5 index of generalized Aztec diamond $G = L_p \otimes L_q$ is:

$$GA_5(G) = 2pq + 2 \left(\frac{2\sqrt{6}}{5} + \frac{2\sqrt{3}}{7} - 3 \right) p + 4 \left(\frac{2\sqrt{6}}{5} + \frac{2\sqrt{3}}{7} - 3 \right) q + 4 \left(\frac{24\sqrt{2}}{17} - 4\sqrt{6} + \frac{2\sqrt{2}}{3} - \frac{20\sqrt{3}}{7} + \frac{6631}{325} \right).$$

Proof: By applying the information given in Table 2 on Eq. 2, we get:

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

$$GA_5(L_p \otimes L_q) = \frac{2\sqrt{4 \times 9}}{4+9} \times 4 + \frac{2\sqrt{6 \times 6}}{6+6} \times 4 + \frac{2\sqrt{9 \times 8}}{9+8} \times 8 + \frac{2\sqrt{8 \times 12}}{8+12} \times 4(p+q-10) + \frac{2\sqrt{6 \times 12}}{6+12} \times 4 + \frac{2\sqrt{16 \times 16}}{16+16} \left[2(p-6)(q-5) + 8 \right] + \frac{2\sqrt{12 \times 16}}{12+16} \times 4(p+q-10) + \frac{2\sqrt{9 \times 16}}{9+16} \times 4 + \frac{2\sqrt{12 \times 12}}{12+12} \times 4$$

After simplification, we get:

$$GA_5(L_p \otimes L_q) = 2pq + 2\left(\frac{2\sqrt{6}}{5} + \frac{2\sqrt{3}}{7} - 3\right) \\ p + 4\left(\frac{2\sqrt{6}}{5} + \frac{2\sqrt{3}}{7} - 3\right) \\ q + 4\left(\frac{24\sqrt{2}}{17} - 4\sqrt{6} + \frac{2\sqrt{2}}{3} - \frac{20\sqrt{3}}{7} + \frac{6631}{325}\right).$$

Theorem 2.5

For $p, q \geq 2$, the NM_1 index of $L_p \otimes L_q$ is calculated as:

$$NM_1(L_p \otimes L_q) = 256pq - 608p - 608q + 6748.$$

Proof: In the NM_1 index, we first find possible degrees sum of all the vertices. The possible degree sum of a vertex is either, 4 or 6 or 8 or 9 or 12. There are 4 vertices (red color in Figure 1) of degree sum is equal to 4. There are 8 vertices (green color in Figure 1) of degree sum is equal to 6. There are $2(p+q-8)$ vertices (blue color in Figure 1) of degree sum is equal to 8 and 12. There are 4 vertices (blue color in Figure 1) of degree sum is equal to 9. There are $(p-4)(q-4)$ vertices (black color in Figure 1) of degree sum is equal to 16. Now, by applying this information, the NM_1 index of $L_p \otimes L_q$ is computed as follows; since:

$$NM_1(G) = \sum_{v \in V(G)} (S_v)^2.$$

By an easy calculation, the above equation can be written as:

$$NM_1(L_p \otimes L_q) = 4(4^2) + 8(6^2) + 2(p+q-8)(8^2) \\ + 4(9^2) + 2(p+q-8)(12^2) + (p-4)(q-4)(16^2) \\ = 256(p-4)(q-4) + 416(p+q-8) + 676 \\ = 256pq - 608p - 608q + 6748$$

The following theorem gives the NM_1 index of generalized Aztec diamond $L_p \otimes L_q$.

Theorem 2.6

For $p, q \geq 2$, the NM_2 index of $L_p \otimes L_q$ is:

$$NM_2(L_p \otimes L_q) = 512pp - 1408p \\ - 1408q + 8144.$$

Proof: Since:

$$NM_2(G) = \sum_{uv \in E(G)} S_u S_v.$$

Therefore, by applying this information given in Table 2, the NM_2 index of $L_p \otimes L_q$ is computed as follows:

$$NM_2(G) = \sum_{uv \in E(G)} S_u S_v \\ NM_2(L_p \otimes L_q) = (4 \times 6) \times 4 + (6 \times 6) \\ \times 4 + (9 \times 8) \times 8 + (8 \times 12) \times 4(p+q-10) \\ + (6 \times 12) \times 4 + (16 \times 16) \left[2(p-6)(q-5) + 8 \right] \\ + (12 \times 16) \times 4(q+p-10) + (9 \times 16) \times 4 \\ + (12 \times 12) \times 4. \\ = 512pp - 1408p - 1408q + 8144.$$

3 ABC , GA , ABC_4 , GA_5 , NM_1 , and NM_2 indices of tetrahedral diamond lattice

The structure of tetrahedral diamond lattice (Manuel et al., 2015) of t dimension is constructed by t layers, every one interpreted as L_t . The starting layer has just a single vertex and the next one have 4 vertices, which is isomorphic to S_4 . For $t \geq 3$, every layer l has $\sum_{k=1}^{l-2} k$ hexagons with 3 pendent vertices. According to depth first labeling, we can construct every next layer for vertices. More precisely, we can use that layer l presented the labels form $\sum_{k=1}^{l-1} k^2 + 1$ to $\sum_{k=1}^l k^2$.

The vertex set of tetrahedral diamond of dimension t has $\sum_{k=1}^t k^2$ vertices and the edge set has $\frac{2}{3}(t^2 - t)$ edges. There is no any odd cycle in Tetrahedral diamond, so it is a bipartite graph.

The tetrahedral diamond lattice of dimension t is constructed with the help of t -layers in the following ways. The vertex in the first (starting) layer with label 1 is connected with a vertex in layer 2 with label 3. The layers l and $l+1$, $l \geq 2$, are connected as:

- (i) The vertex having label $\sum_{k=1}^{l-1} k^2 + (\sum_{m=1}^i 2(l-m)) + (2f-1) + 1$ in layer l is connected to the vertex which has label $\sum_{k=1}^l k^2 + 2f$ in layer $l+1$ for all $1 \leq f \leq l$.
- (ii) The vertex with label $\sum_{k=1}^{l-1} k^2 + (\sum_{m=1}^i 2(l-m)) + (2f-1) + 1$ in layer l is connected to the vertex which has label $\sum_{k=1}^l k^2 + (\sum_{m=1}^i 2(l-m)) + 3 + (2f)$ in layer $l+1$ where $1 \leq i \leq l-1$ and $1 \leq f \leq l-i$.

Figure 2 depicts a 5-dimension tetrahedral diamond.

In Theorem 3.1, the value of ABC_4 invariant of tetrahedral diamond lattice is derived.

Theorem 3.1

For $t \geq 1$, the ABC index of tetrahedral diamond lattice G with dimension t is:

$$ABC(G) = \sqrt{15}t^2 + (6\sqrt{2} - 5\sqrt{15})t + 2(\sqrt{3} - 6\sqrt{2} + 3\sqrt{15}) + \sum_{k=5}^t (k-4)(k-3)\sqrt{6}.$$

Figure 2: The graph of 5-dimension tetrahedral diamond lattice.

Proof: The graph G contains only vertices of degree one, two, three and four. The edges of the graph G of dimension t are of the form $(1,4)$, $(2,4)$, $(3,4)$, and $(4,4)$. The construction of graph indicates that the number of edges of tupe $(1,4)$ are four for every layer. There are $6t-12$ vertices of 2 degree, and two edges are induced by an each vertex. So, number of $(2,4)$ -type edges is $12(t-2)$. Also by induction argument, the number of $(3, 4)$ -type edges is:

$$\frac{9(t-2)(t-3)}{2} + 3 \frac{(t-2)(t-3)}{2} = 6(t-2)(t-3).$$

Note that the quantity of $(4,4)$ -type edges can be obtained by removing all edges of type $(1,4)$, $(2,4)$, $(3,4)$ from G . Thus, the quantity of $(4, 4)$ - type edges is:

$$\begin{aligned} |E(G)| - ((1,4) + (2,4) + (3,4)) \\ &= \frac{2}{3}(t^3 - t) - (4 + 12t - 24 + 6t^2 - 30t + 36) \\ &= \frac{2}{3}(t^3 - 9t^2 + 26t - 24). \end{aligned}$$

From Table 3, the formula for ABC index can be deduced to:

$$\begin{aligned} ABC(G) &= 4\sqrt{\frac{1+4-2}{1 \times 4}} + 12(t-2)\sqrt{\frac{2+4-2}{2 \times 4}} \\ &\quad + 6(t-2)(t-3)\sqrt{\frac{3+4-2}{3 \times 4}} \\ &\quad + \frac{2}{3}(t^3 - 9t^2 + 26t - 24)\sqrt{\frac{4+4-2}{4 \times 4}}. \end{aligned}$$

Table 3: The quantity of (m, n) -type edges of tetrahedral diamond G , where m and n are degrees of the adjacent vertices of each edge

$(d(m), d(n))$ with $mn \in E(G)$	Number of edges
$(1,4)$	4
$(2,4)$	$12(t-2)$
$(3,4)$	$6(t-2)(t-3)$
$(4,4)$	$\frac{2}{3}(t^3 - 9t^2 + 26t - 24)$

After computation, we get:

$$ABC(G) = \sqrt{15}t^2 + \left(6\sqrt{2} - 5\sqrt{15}\right)t + 2\left(\sqrt{3} - 6\sqrt{2} + 3\sqrt{15}\right) + \sum_{k=5}^t (k-4)(k-3)\sqrt{6}.$$

Theorem 3.2

The GA index of G (tetrahedral diamond lattice) of dimension t where $t \geq 1$ is given by:

$$GA(G) = 24t^2 + 4\left(2\sqrt{2} - 30\frac{\sqrt{3}}{7}\right)t + 16\left(\frac{1}{5} + 9\frac{\sqrt{3}}{7} - \sqrt{2}\right) + 2\sum_{k=5}^t (k-4)(k-3).$$

Proof: The GA index formula of tetrahedral diamond lattice G is deduced by using the information from Table 3 as:

$$GA(G) = 2\sqrt{\frac{1 \times 4}{1+4}} \times 4 + 2\sqrt{\frac{2 \times 4}{2+4}} \times 12(t-2) + 2\sqrt{\frac{3 \times 4}{3+4}} \times 6(t-2)(t-3) + 2\sqrt{\frac{4 \times 4}{4+4}} \times 2\sum_{k=5}^t (k-4)(k-3)$$

After an easy computation, we acquire:

$$GA(G) = 24t^2 + 4\left(2\sqrt{2} - 30\frac{\sqrt{3}}{7}\right)t + 16\left(\frac{1}{5} + 9\frac{\sqrt{3}}{7} - \sqrt{2}\right) + 2\sum_{k=5}^t (k-4)(k-3).$$

Now we shall calculate the ABC_4 and GA_5 index for tetrahedral diamond lattice G in upcoming theorems.

Theorem 3.3

The result for ABC_4 index of tetrahedral diamond lattice G is:

$$ABC_4(G) = \left(\frac{24}{\sqrt{10}} - \frac{20}{\sqrt{6}} - 5\sqrt{\frac{23}{29}}\right)t + \left(\frac{4}{\sqrt{6}} + \sqrt{\frac{23}{29}}\right)t^2 + 3\left(\frac{8}{\sqrt{6}} + \frac{1}{\sqrt{7}} + 2\sqrt{\frac{13}{14}} + 2\sqrt{\frac{23}{29}}\right) + \sum_{k=5}^t (k-4)(k-3)\frac{9}{2\sqrt{39}}.$$

Proof: Let S_m denote the sum of degrees of all the vertices joined with vertex m . The (S_m, S_n) -type edges are the edges with sum of degrees of neighboring vertices of the end vertices of every edge is S_m and S_n . The formula for ABC_4 index of tetrahedral diamond lattice G can be deduced by applying the edge partition of Table 4 and written as:

$$ABC_4(G) = 4\sqrt{\frac{4+7-2}{4 \times 7}} + 12\sqrt{\frac{7+8-2}{7 \times 8}} + 12(t-3)\sqrt{\frac{8+10-2}{8 \times 10}} + 4(t-2)(t-3)\sqrt{\frac{12+10-2}{12 \times 10}} + 2(t-2)(t-3)\sqrt{\frac{12+13-2}{12 \times 13}} + 2\sum_{k=5}^t (k-4)(k-3)\sqrt{\frac{16+13-2}{16 \times 13}}.$$

After simplification, we acquire:

$$ABC_4(G) = \left(\frac{24}{\sqrt{10}} - \frac{20}{\sqrt{6}} - 5\sqrt{\frac{23}{29}}\right)t + \left(\frac{4}{\sqrt{6}} + \sqrt{\frac{23}{29}}\right)t^2 + 3\left(\frac{8}{\sqrt{6}} + \frac{1}{\sqrt{7}} + 2\sqrt{\frac{13}{14}} + 2\sqrt{\frac{23}{29}}\right) + \sum_{k=5}^t (k-4)(k-3)\frac{9}{2\sqrt{39}}.$$

Table 4: The quantity of (S_m, S_n) -type edges, where m and n are sum of degrees of all neighboring vertices of the end vertices of each edge

(S_m, S_n) with $mn \in E(G)$	Number of edges
(4,7)	4
(7,8)	12
(8,10)	$12(t-3)$
(12,10)	$4(t-2)(t-3)$
(12,13)	$2(t-2)(t-3)$
(16,13)	$2\sum_{k=5}^t (k-4)(k-3)$

In upcoming theorem, we compute the ABC_4 index for tetrahedral diamond lattice.

Theorem 3.4

The GA_5 index for the tetrahedral diamond lattice G is given by:

$$GA_5(G) = 4 \left(\frac{\sqrt{20}}{3} - \frac{10\sqrt{30}}{11} \right) t + 8 \left(\frac{\sqrt{30}}{11} + \frac{\sqrt{39}}{25} \right) t^2 + 4 \left(\frac{4\sqrt{7}}{11} + \frac{12\sqrt{14}}{15} - \sqrt{20} + \frac{12\sqrt{30}}{11} + \frac{12\sqrt{39}}{25} \right) + \frac{16\sqrt{13}}{29} \sum_{k=5}^t (k-4)(k-3) \quad (5)$$

Proof: By applying the information from Table 4 in Eq. 5, we derive the GA_5 index as:

$$GA_5(G) = \frac{2\sqrt{4 \times 7}}{4+7} \times 4 + \frac{2\sqrt{8 \times 7}}{8+7} \times 12 + \frac{2\sqrt{8 \times 10}}{10+8} 12(t-3) + \frac{2\sqrt{12 \times 10}}{12+10} \times 4(t-2)(t-3) + \frac{2\sqrt{12 \times 13}}{12+13} \times 2(t-2)(t-3) + \frac{2\sqrt{16 \times 13}}{16+13} \times 2 \sum_{k=5}^t (k-4)(k-3),$$

which can be deduced to:

$$GA_5(G) = 4 \left(\frac{\sqrt{20}}{3} - \frac{10\sqrt{30}}{11} \right) t + 8 \left(\frac{\sqrt{30}}{11} + \frac{\sqrt{39}}{25} \right) t^2 + 4 \left(\frac{4\sqrt{7}}{11} + \frac{12\sqrt{14}}{15} - \sqrt{20} + \frac{12\sqrt{30}}{11} + \frac{12\sqrt{39}}{25} \right) + \frac{16\sqrt{13}}{29} \sum_{k=5}^t (k-4)(k-3).$$

Theorem 3.5

The result for NM_1 index of tetrahedral diamond lattice G is:

$$NM_1(G) \approx 85t^3 - 552t^2 + 2410t - 2047.$$

Proof: Let S_m denote the sum of degrees of all the vertices joined with vertex m . The degree sum of the

vertex in the graph is either 4 or 7 or 8 or 10 or 12 or 16. The computation gives that:

$$S_4 = 4, S_7 = 4, S_8 = 6t - 12, S_{10} = 6t - 18, S_{12} = \frac{(t-2)(3t-5)}{2}, S_{16} = \frac{(t-2)(t-3)(t-4)}{3}.$$

Using this information NM_1 index of tetrahedral diamond lattice G can be calculated as follows:

$$NM_1(G) = \sum_{v \in V(G)} (S_v)^2 = 4(4^2) + 4(7^2) + (6t-12)(8^2) + (6t-18)(10^2) + \frac{(t-2)(3t-5)}{2}(12^2) + \frac{(t-2)(t-3)(t-4)}{3}(16^2) \approx 85t^3 - 552t^2 + 2410t - 2047.$$

In upcoming theorem, we compute the GA_5 index for tetrahedral diamond lattice.

Theorem 3.6

The NM_2 index for the tetrahedral diamond lattice G is given by:

$$NM_2(G) = 792t^2 - 3000t + 2656 + 416 \sum_{k=5}^t (k-4)(k-3).$$

Proof: By applying the information from Table 4 in Eq. 5, we derive the GA_5 index as:

$$NM_2(G) = \sum_{uv \in E(G)} S_u S_v = (4 \times 7) \times 4 + (8 \times 7) \times 12 + (8 \times 10) 12(t-3) + (12 \times 10) \times 4(t-2)(t-3) + (12 \times 13) \times 2(t-2)(t-3) + (16 \times 13) \times 2 \sum_{k=5}^t (k-4)(k-3) = 792t^2 - 3000t + 2656 + 416 \sum_{k=5}^t (k-4)(k-3)$$

4 Conclusion

In this article, some degree depended invariants namely ABC , GA , ABC_4 , GA_5 , NM_1 , and NM_2 indices are computed for the networks constructed from generalized Aztec diamonds and tetrahedral diamond lattices. We have found the exact values of these parameters for the said

classes of graphs. This, we believe will work in the favour of researcher working in network science to investigate the underlying topologies of given networks.

In future, it is interesting to design certain new networks and then investigate their topological properties and compute their exact values which can be fruitful in understanding of the underlying topologies.

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References

- Ahmad U., Sarfraz A., Yousaf R., Computation of Zagreb and Atom bond connectivity Indices of Certain Families of Dendrimers by using Automorphism. *J. Serbian Chemical Soc.*, 2017, 82, 151-162.
- Alikhani S., Hasni R., Arif N.E., On the atom-bond connectivity index of some families of dendrimers. *J. Comput. Theor. Nanosci.*, 2014, 11, 1802-1805.
- Akhter S., Imran M., On degree-based topological descriptors of strong product graphs. *Can. J. Chem.*, 2016a, 94(6), 559-565.
- Akhter S., Imran M., On molecular topological properties of benzenoid structures. *Can. J. Chem.*, 2016b, 94(8), 687-698.
- Akhter S., Imran M., Gao W., Frahani M.R., On topological indices of honeycomb networks and Graphene networks. *Hac. J. Math. Stat.*, 2018, 47(1), 1-17.
- Akhter S., Imran M., Farahani M.R., Javaid I., On topological properties of hexagonal and silicate networks. *Hac. J. Math. Stat.*, 2019, 48(3), 711-723.
- Bača M., Horváthová J., Mokrišová M., Suhányiová A., On topological indices of Fullerenes. *Appl. Math. Comput.*, 2015, 251, 154-161.
- Baig A.Q., Imran M., Ali H., Computing Omega, Sadhana and PI polynomials of benzenoid carbon nanotubes. *Optoelectron. Adv. Mater. Rapid Commun.*, 2015a, 9, 248-255.
- Baig A.Q., Imran M., Ali H., On topological indices of poly oxide, poly silicate, DOX and DSL networks. *Canad. J. Chem.*, 2015b, 93, 730-739.
- Diudea M.V., Gutman I., Lorentz J., *Molecular Topology*. Nova, Huntington, 2001.
- Estrada E., Torres L., Rodríguez L., Gutman I., An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes. *Indian J. Chem.* 1998, 37A, 849-855.
- Ghorbani M., Hosseinzadeh M.A., Computing ABC_5 index of nanostar dendrimers. *Optoelectron. Adv. Mater. Rapid Commun.*, 2010, 4, 1419-1422.
- Graovac A., Ghorbani M., Hosseinzadeh M.A., Computing fifth geometric-arithmetic index for nanostar dendrimers. *J. Math. Nanosci.*, 2011, 1, 33-42.
- Gutman I., Polansky O.E., *Mathematical concepts in organic chemistry*. Springer-Verlag, New York, 1986.
- Guirao J.L.G., Imran M., Siddiqui M.K., Akhter S., On valency-based molecular topological descriptors of subdivision vertex-edge join of three graphs. *Symmetry*, 2020, 12, 1026.
- Hameed S., Ahmad U., Extremal values in a class of basic peri-condensed benzenoids with respect to VDB topological indices. *Ars Combinatoria*, 2019, 145, 367-376.
- Hayat S., Imran M., Computation of topological indices of certain networks. *Appl. Math. Comput.*, 2014, 240, 213-228.
- Hayat S., Imran M., Computation of certain topological indices of nanotubes. *J. Comput. Theor. Nanosci.*, 2015a, 12, 70-76.
- Hayat S., Imran M., Computation of certain topological indices of nanotubes covered by C_5 and C_7 . *J. Comput. Theor. Nanosci.*, 2015b, 12, 533-541.
- Hayat S., Imran M., On some degree based topological indices of certain nanotubes. *J. Comput. Theor. Nanosci.*, 2015c, 12, 1599-1605.
- Imran M., Akhter S., Iqbal Z., Edge Mostar index of chemical structures and nanostructures using graph operations. *Int. J. Quantum. Chem.*, 2020, 120, e26259.
- Iranmanesh A., Zeraatkar M., Computing GA index for some nanotubes. *Optoelectron. Adv. Mater. Rapid Commun.*, 2010, 4, 1852-1855.
- Lin W., Chen J., Chen Q., Gao T., Lin X., Cai B., Fast computer search for trees with minimal ABC index based on tree degree sequences. *MATCH Commun. Math. Comput. Chem.*, 2014, 72, 699-708.
- Manzoor S., On Topological Indices of Certain Networks. M. Phill Dissertation, submitted to Higher Education Commission, Pakistan, 2015.
- Manuel P.D., Rajan B., Grigorious C., Stephen S., On the strong metric dimension of tetrahedral diamond lattice. *Math. Comput. Sci.*, 2015, 9, 201-208.
- Reti T., Ali A., Varga P., Bitay E., Some properties of the neighborhood first Zagreb index. *Discrete Math. Lett.*, 2019, 2, 10-17.
- Vukičević 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.
- Wiener H., Structural determination of paraffin boiling points. *J. Amer. Chem. Soc.*, 1947, 69, 17-20.
- Yang H., Imran M., Akhter S., Iqbal Z., Siddiqui M.K., On distance-based topological descriptors of subdivision vertex-edge join of three graphs. *IEEE Access*, 2019, 7, 143381-143391.