



Computing Fourth Atom-Bond Connectivity Index(ABC₄) and Fifth Geometric–Arithmetic(GA₅) Index of Para-Line Graph of Two-Dimensional Molecular Lattice, Nanotubes, And Nanotorus Of TUC₄C₈

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Abstract: The features of molecular structures have been studied using a variety of topological indices. Here, a significant nanomaterial's atom bond connectivity index and geometric-arithmetic index is computed. In this paper, ABC₄ and GA₅ for the para-line graph of two-dimensional molecular lattice, nanotubes, and nanotorus of TUC₄C₈ (m, n) is discussed.

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Key words: Molecular graphs, nanostructures, fourth atom bond connectivity index, fifth geometric-arithmetic index.

1. Introduction:

The multi-walled structures of pure carbon are called carbon nanotubes, were first identified in 1991 [6]. Many theoretical and experimental studies have been done on them, and they exhibit amazing mechanical properties. They are obviously suited for advanced composites given their mechanical properties. A single-wall carbon nanotube is a cylindrical structure of a few nanometres in diameter. It is periodic along its axis and resembles a honeycomb lattice that has been rolled up. Solid-state physics researchers are interested in studying nanotubes because of the potential nanotechnology uses for them. Their symmetry has been studied and is significant in theoretical inquiries. Because of their remarkable symmetry, carbon nanotubes have made it easier to theoretically study the physical phenomena that take place in these materials.

A trivalent decoration known as a C₄C₈ net is created by alternating C₄ squares and C₈ octagons. The leapfrog method can be used to create such a covering from a square net. Some scientists have recently become interested in the topological indices of C₄C₈ nanotubes and nanotorous materials; for more information, see [8–12]. They calculated several topological distance indices for these nanotubes and nanotorous. The TUC₄C₈ nanotube is a geometric marvel made of squares and octagons (see figure 1(b)).

A simple graph termed a molecular graph, in which atoms are the vertices and atomic boundaries are the edges, can be used to depict a chemical complex. Chemical graph theory is one of the numerous subfields of graph theory. In a new breakthrough called cheminformatics, the relationship between structural traits and quantitative structural activities is looked at to predict the biological activities of the structure [1,2,3,4].

In mathematical chemistry, a molecular network without a path between every pair of vertices and the hydrogen atoms is disregarded [1, 2]. A topological index is a numerical value taken from a graph with molecular structure. With a vertex set V and an edge set E , let G be a simple, finite, connected graph. Let the number of vertices adjacent to a vertex u be its degree $d(u)$.

Harold Wiener created the best-known topological descriptor in 1947, which marked the start of the use of topological indices in chemistry [14].

The Randic index was the most popular and commonly used topological indicators for more than 40 years ago [14,15,16].

Atom-Bond connectivity index was developed by Furtula et al. and has been used to examine the stability of alkanes and the strain energy of cycloalkanes[15].

The index is defined as,

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$$

M.Ghorbani et al [16,17,18] introduced Fourth Atom-Bond Connectivity index $ABC_4(G)$

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_s(u)+d_s(v)-2}{d_s(u)d_s(v)}} \dots\dots\dots (1)$$

Geometric-Arithmetic index was developed by Vukicevic et.al[15].

$$GA(G) = \sum_{uv \in E(G)} 2 \frac{\sqrt{d(u)d(v)}}{d(u)+d(v)}$$

Grovac et al introduced Fifth Geometric-Arithmetic index $GA_5(G)$ [16].

$$GA_5(G) = \sum_{uv \in E(G)} 2 \frac{\sqrt{d_s(u)d_s(v)}}{d_s(u)+d_s(v)} \dots\dots\dots (2)$$

Where $d_s(u)$ denotes the total sum of degrees of vertices which are adjacent vertex u .

The line graph $L(G)$ of G represents the vertex set corresponds to edges of that graph such that two of its vertices are adjacent.

The graph found by introducing a vertex in every edge of G is known as the subdivision graph of G .

The Para-line graph is the line graph of sub-division graph of G i.e., $L(S(G))$

2. Results and discussion:

In this study, we computed a few well-known topological indices, including the fourth atom bond connectivity index and the geometric-arithmetic index of the 2d lattice, nanotube and nanotorus of $TUC_4C_8(4,3)$.

We considered the structures of Nanotube and Nanotorus of $TUC_4C_8(m,n)$ graph of a two-dimensional molecular lattice, where m stands for the number of squares in a column and n for the number of square in row[14-20]. See the figure 1(a), 2(a) and 3(a).

3. Two dimensional molecular lattice of $TUC_4C_8(4,3)$ & its Para-line graph $L(S(G))$.

Here Two dimensional molecular lattice of $TUC_4C_8(4,3)$ and its para-line graph is considered.

We have taken 4 squares in column and 3 squares in a row for the study which is shown in the figure 1(a) and figure 1(b) represents the line graph of subdivision graph of $TUC_4C_8(4,3)$.

For further detailed study on nanostructure you can refer [8-12,21,22].

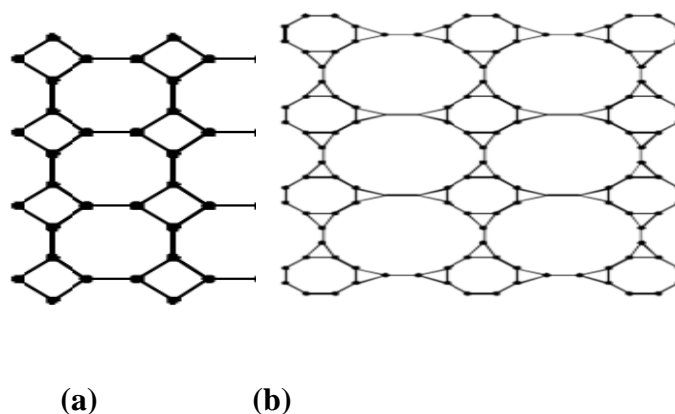


Figure 1: (a) Two dimensional molecular lattice of TUC_4C_8 (4, 3) (b) Para-line graph of TUC_4C_8 (4, 3)

Theorem 1A

Let $L(S(G))$ be para-line graph of two dimensional molecular lattice TUC_4C_8 (m, n) graph then

$$I. ABC_4(L(S(G))) = 2\left(\frac{3}{2}\right)^{\frac{1}{2}} + 4\left(\frac{7}{5}\right)^{\frac{1}{2}} + \frac{4}{5}(m+n-4)\sqrt{2} + 2(m+n-2)\left(\frac{11}{10}\right)^{\frac{1}{2}} + \frac{4}{3}(m+n-2)\left(\frac{15}{2}\right)^{\frac{1}{2}} + \frac{4}{9}(18mn - 19m - 19n + 20) \text{ if } m > 1, n > 1.$$

$$II. GA_5(L(S(G))) = \frac{32}{9}(5)^{\frac{1}{2}} + \frac{16}{13}(m+n-2)(10)^{\frac{1}{2}} + \frac{96}{17}(m+n-2)\sqrt{2} + 18(mn - m - n - 1) - 2 \text{ if } m > 1, n > 1.$$

Proof:

Let $L(S(G))$ be para-line graph of two dimensional molecular lattice TUC_4C_8 (m, n)

(figure 1(b)), has $2(mn - m - n)$ vertices and $18mn - 5m - 5n$ of edges.

In this table, the number of edges considered with respect to $d_s(u)$ & $d_s(v)$

Sl.no.	$d_s(u)$ & $d_s(v)$	No. of edges
1	4 & 4	4
2	4 & 5	8
3	5 & 5	$2(m+n-4)$
4	5 & 8	$4(m+n-2)$
5	8 & 9	$8(m+n-2)$
6	9 & 9	$18mn - 19m - 19n - 20$

I. From the definition of ABC_4 index

$$\text{Consider the formula (1), } ABC_4(L(S(G))) = \sum_{uv \in E(L(S(G)))} \sqrt{\frac{d_s(u)+d_s(v)-2}{d_s(u)d_s(v)}}$$

Consider the table values and substitute in the formula (1), we get

$$\begin{aligned}
 ABC_4(L(S(G))) &= 4\sqrt{\frac{4+4-2}{4 \times 4}} + 8\sqrt{\frac{4+5-2}{4 \times 5}} + 2(m+n-4)\sqrt{\frac{5+5-2}{5 \times 5}} + 4(m+n-2)\sqrt{\frac{5+8-2}{5 \times 8}} \\
 &\quad + 8(m+n-2)\sqrt{\frac{8+9-2}{8 \times 9}} + (18mn - 19m - 19n - 2)\sqrt{\frac{9+9-2}{9 \times 9}} \\
 ABC_4(L(S(G))) &= 2\left(\frac{3}{2}\right)^{\frac{1}{2}} + 4\left(\frac{7}{5}\right)^{\frac{1}{2}} + \frac{4}{5}(m+n-4)\sqrt{2} + 2(m+n-2)\left(\frac{11}{10}\right)^{\frac{1}{2}} \\
 &\quad + \frac{4}{3}(m+n-2)\left(\frac{15}{2}\right)^{\frac{1}{2}} + \frac{4}{9}(18mn - 19m - 19n + 20) \text{ if } m > 1, n > 1.
 \end{aligned}$$

II. From the definition of GA₅ index

Consider the formula (2), $GA_5(L(S(G))) = \sum_{uv \in E(L(S(G)))} 2 \frac{\sqrt{d_s(u)d_s(v)}}{d_s(u)+d_s(v)}$

Consider the table values and substitute in the formula (2), we get

$$\begin{aligned}
 GA_5(L(S(G))) &= 2 \left\{ 4 \frac{\sqrt{4 \times 4}}{4+4} + 8 \frac{\sqrt{4 \times 5}}{4+5} + 2(m+n-4) \frac{\sqrt{5 \times 5}}{5+5} + 4(m+n-2) \frac{\sqrt{5 \times 8}}{5+8} \right. \\
 &\quad \left. + 8(m+n-2) \frac{\sqrt{8 \times 9}}{8+9} + (18mn - 19m - 19n - 20) \frac{\sqrt{9 \times 9}}{9+9} \right\} \\
 GA_5(L(S(G))) &= \frac{32}{9}(5)^{\frac{1}{2}} + \frac{16}{13}(m+n-2)(10)^{\frac{1}{2}} + \frac{96}{17}(m+n-2)\sqrt{2} \\
 &\quad + 18(mn - m - n - 1) - 2 \text{ if } m > 1, n > 1.
 \end{aligned}$$

Hence proved the results.

Theorem 1B

Let $L(S(G))$ be a para-line graph of two dimensional molecular lattice $TUC_4C_8(m, n)$ as shown in fig 1, then

$$\begin{aligned}
 \text{I. } ABC_4(L(S(G))) &= \frac{3}{2}(6)^{\frac{1}{2}} + 2\left(\frac{7}{5}\right)^{\frac{1}{2}} + \frac{4}{5}(m-2)(2)^{\frac{1}{2}} + 2(m-1)\left(\frac{11}{10}\right)^{\frac{1}{2}} \\
 &\quad + \frac{1}{4}(m-1)(14)^{\frac{1}{2}} + \frac{2}{3}(m-1)(15)^{\frac{1}{2}} + \frac{4}{9}(m-1) \text{ if } m > 1, n = 1. \\
 \text{II. } GA_5(L(S(G))) &= \frac{16}{9}(5)^{\frac{1}{2}} + \frac{16}{13}(m-1)(10)^{\frac{1}{2}} + \frac{48}{17}(m-1)\sqrt{2} + (3m+2) \text{ if } m > 1, n = 1.
 \end{aligned}$$

Proof:

The Para-line graph $L(S(G))$ of two dimensional molecular lattice $TUC_4C_8(m, n)$ has $2(mn - m - n)$ vertices and $18mn - 5m - 5n$ of edges. [1, 19]

In the table, the number of edges is considered with respect to the sum of degrees of all vertices that are adjacent to vertex u and v .

Sl.no.	$d_s(u) \& d_s(v)$	No. of edges
1	4 & 4	6
2	4 & 5	4

3	5 & 5	$2(m - 2)$
4	5 & 8	$4(m - 1)$
5	8 & 8	$2(m - 1)$
6	8 & 9	$4(m - 1)$
7	9 & 9	$m - 1$

I. From the definition of ABC₄ index

$$\text{Consider the formula (1), } ABC_4(L(S(G))) = \sum_{uv \in E(L(S(G)))} \sqrt{\frac{d_s(u)+d_s(v)-2}{d_s(u)d_s(v)}}$$

Consider the table values and substitute in the formula (1), we get

$$\begin{aligned} ABC_4(L(S(G))) &= 6 \sqrt{\frac{4+4-2}{4 \times 4}} + 4 \sqrt{\frac{4+5-2}{4 \times 5}} + 2(m-2) \sqrt{\frac{5+5-2}{5 \times 5}} + 4(m-1) \sqrt{\frac{5+8-2}{5 \times 8}} \\ &\quad + 2(m-1) \sqrt{\frac{8+8-2}{8 \times 8}} + 4(m-1) \sqrt{\frac{8+9-2}{8 \times 9}} + (m-1) \sqrt{\frac{9+9-2}{9 \times 9}} \\ ABC_4(L(S(G))) &= \frac{3}{2}(6)^{\frac{1}{2}} + 2\left(\frac{7}{5}\right)^{\frac{1}{2}} + \frac{4}{5}(m-2)(2)^{\frac{1}{2}} + 2(m-1)\left(\frac{11}{10}\right)^{\frac{1}{2}} \\ &\quad + \frac{1}{4}(m-1)(14)^{\frac{1}{2}} + \frac{2}{3}(m-1)(15)^{\frac{1}{2}} + \frac{4}{9}(m-1) \text{ if } m > 1, n = 1. \end{aligned}$$

II. From the definition of GA₅ index

$$\text{Consider the formula (2), } GA_5(L(S(G))) = \sum_{uv \in E(L(S(G)))} 2 \frac{\sqrt{d_s(u)d_s(v)}}{d_s(u)+d_s(v)}$$

Consider the table values and substitute in the formula (2), we get

$$\begin{aligned} &GA_5(L(S(G))) \\ &= 2 \left\{ 6 \frac{\sqrt{4 \times 4}}{4+4} + 4 \frac{\sqrt{4 \times 5}}{4+5} + 2(m-2) \frac{\sqrt{5 \times 5}}{5+5} + 4(m-1) \frac{\sqrt{5 \times 8}}{5+8} + 2(m-1) \frac{\sqrt{8 \times 8}}{8+8} \right. \\ &\quad \left. + 4(m-1) \frac{\sqrt{8 \times 9}}{8+9} + (m-1) \frac{\sqrt{9 \times 9}}{9+9} \right\} \end{aligned}$$

$$GA_5(L(S(G))) = \frac{16}{9}(5)^{\frac{1}{2}} + \frac{16}{13}(m-1)(10)^{\frac{1}{2}} + \frac{48}{17}(m-1)\sqrt{2} + (3m+2) \text{ if } m > 1, n = 1.$$

Hence proved the results.

Here we discussed the results in two cases.

Case I: ABC₄(L(S(G))) and GA₅(L(S(G))) if $m > 1, n > 1$ in theorem 1A.

Case II: ABC₄(L(S(G))) and GA₅(L(S(G))) if $m > 1, n = 1$ in theorem 1B.

4. Nanotube of TUC₄C₈ (m, n) & its para-line graph L(S(H))

Here Nanotube of TUC₄C₈ (4, 3) and its para-line graph is considered.

We have taken 4 squares in column and 3 squares in a row for the study which is shown in the figure 2(a) and figure 2(b) represents the line graph of subdivision graph of TUC_4C_8 (4, 3). For further detailed study on nanostructure you can refer [8-12,21,22].

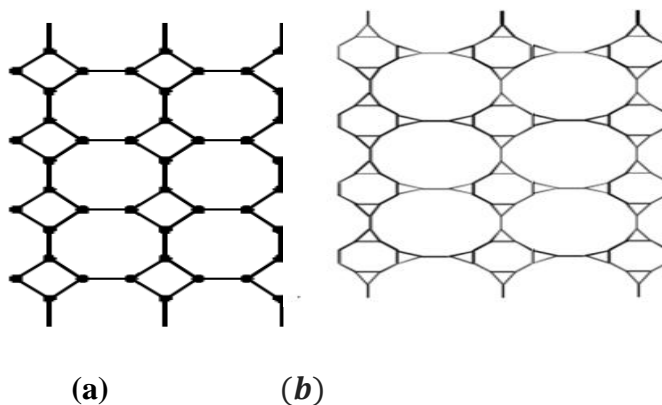


Figure 2: (a) Nanotube TUC_4C_8 (4, 3) (b) Para-line graph nanotube TUC_4C_8 (4, 3)

Theorem 2A

Let $L(S(H))$ be a Nanotube TUC_4C_8 (m, n) graph, then

- I. $ABC_4(L(S(H))) = \frac{4}{5}m\sqrt{2} + 2m\sqrt{\frac{11}{10}} + \frac{4}{3}m\sqrt{\frac{15}{2}} + \frac{4}{9}(18mn - 19m)$ if $m > 1, n > 1$.
- II. $GA_5(L(S(H))) = \frac{16}{13}m(10)^{\frac{1}{2}} + \frac{96}{17}m\sqrt{2} + (18mn - 17m)$ if $m > 1, n > 1$.

Proof:

Let $L(S(H))$ be a Nanotube TUC_4C_8 (m, n) graph as shown in fig 2(b)

From the observations made, the $L(S(H))$ graph of Nanotube TUC_4C_8 (m, n) has $10mn - m$ vertices and $12mn - 2m$ of edges.

In this table, the number of edges considered with respect to $d_s(u)$ & $d_s(v)$

Sl.no.	$d_s(u)$ & $d_s(v)$	No. of edges
1	5 & 5	$2m$
2	5 & 8	$4m$
3	8 & 9	$8m$
4	9 & 9	$18mn - 19m$

I. From the definition of ABC_4 index

Consider the formula (1), $ABC_4(L(S(H))) = \sum_{uv \in E(L(S(H)))} \sqrt{\frac{d_s(u)+d_s(v)-2}{d_s(u)d_s(v)}}$

Consider the table values and substitute in the formula (1), we get

$$ABC_4(L(S(H))) = 2m \sqrt{\frac{5+5-2}{5 \times 5}} + 4m \sqrt{\frac{5+8-2}{5 \times 8}} + 8m \sqrt{\frac{8+9-2}{8 \times 9}} + (18mn - 19m) \sqrt{\frac{9+9-2}{9 \times 9}}$$

$$ABC_4(L(S(H))) = \frac{4}{5}m\sqrt{2} + 2m\sqrt{\frac{11}{10}} + \frac{4}{3}m\sqrt{\frac{15}{2}} + \frac{4}{9}(18mn - 19m) \text{ if } m > 1, n > 1.$$

II. From the definition of GA₅ index

$$\text{Consider the formula (2), } GA_5(L(S(H))) = \sum_{uv \in E(L(S(H)))} 2 \frac{\sqrt{d_s(u)d_s(v)}}{d_s(u)+d_s(v)}$$

Consider the table values and substitute in the formula (2), we get

$$GA_5(L(S(H))) = 2 \left\{ 2m \frac{\sqrt{5 \times 5}}{5+5} + 4m \frac{\sqrt{5 \times 8}}{5+8} + 8m \frac{\sqrt{8 \times 9}}{8+9} + (18mn - 19m) \frac{\sqrt{9 \times 9}}{9+9} \right\}$$

$$GA_5(L(S(H))) = \frac{16}{13}m(10)^{\frac{1}{2}} + \frac{96}{17}m\sqrt{2} + (18mn - 17m) \text{ if } m > 1, n > 1.$$

Hence proved the results.

Theorem 2B

Let $L(S(H))$ be Nanotube $TUC_4C_8(m, n)$ graph, then

$$\text{I. } ABC_4(L(S(H))) = \frac{4}{5}m\sqrt{2} + 2m\sqrt{\frac{11}{10}} + \frac{1}{4}m\sqrt{14} + \frac{2m}{3}\sqrt{\frac{15}{2}} + \frac{4}{9}m \text{ if } m > 1, n = 1$$

$$\text{II. } GA_5(L(S(H))) = \frac{16}{13}m(10)^{\frac{1}{2}} + \frac{48}{17}m\sqrt{2} + 5m \text{ if } m > 1, n = 1$$

Proof:

Let $L(S(H))$ be a Nanotube $TUC_4C_8(m, n)$ graph as shown in fig 2(b)

From the observations made, the $L(S(H))$ graph of Nanotube $TUC_4C_8(m, n)$ has $10mn - m$ vertices and $12mn - 2m$ of edges.

In this table, the number of edges considered with respect to $d_s(u) \& d_s(v)$

Sl.no.	$d_s(u) \& d_s(v)$	No. of edges
1	5 & 5	$2m$
2	5 & 8	$4m$
3	8 & 8	$2m$
4	8 & 9	$4m$
5	9 & 9	m

I. From the definition of ABC₄ index

$$\text{Consider the formula (1), } ABC_4(L(S(H))) = \sum_{uv \in E(L(S(H)))} \sqrt{\frac{d_s(u)+d_s(v)-2}{d_s(u)d_s(v)}}$$

Consider the table values and substitute in the formula (1), we get

$$\begin{aligned}
 ABC_4(L(S(H))) &= 2m\sqrt{\frac{5+5-2}{5 \times 5}} + 4m\sqrt{\frac{5+8-2}{5 \times 8}} + 2m\sqrt{\frac{8+8-2}{8 \times 8}} + 4m\sqrt{\frac{8+9-2}{8 \times 9}} \\
 &\quad + m\sqrt{\frac{9+9-2}{9 \times 9}}
 \end{aligned}$$

$$ABC_4(L(S(H))) = \frac{4}{5}m\sqrt{2} + 2m\sqrt{\frac{11}{10}} + \frac{1}{4}m\sqrt{14} + \frac{2m}{3}\sqrt{\frac{15}{2}} + \frac{4}{9}m \text{ if } m > 1, n = 1.$$

II. From the definition of GA₅ index

$$\text{Consider the formula (2), } GA_5(L(S(H))) = \sum_{uv \in E(L(S(H)))} 2 \frac{\sqrt{d_s(u)d_s(v)}}{d_s(u)+d_s(v)}$$

Consider the table values and substitute in the formula (2), we get

$$\begin{aligned}
 GA_5(L(S(H))) &= 2 \left\{ 2m \frac{\sqrt{5 \times 5}}{5+5} + 4m \frac{\sqrt{5 \times 8}}{5+8} + 2m \frac{\sqrt{8 \times 8}}{8+8} + 4m \frac{\sqrt{8 \times 9}}{8+9} + m \frac{\sqrt{9 \times 9}}{9+9} \right\} \\
 GA_5(L(S(H))) &= \frac{16}{13}m(10)^{\frac{1}{2}} + \frac{48}{17}m\sqrt{2} + 5m \text{ if } m > 1, n = 1
 \end{aligned}$$

Hence proved the results.

Here we discussed the results in two cases.

Case I: $ABC_4(L(S(H)))$ and $GA_5(L(S(H)))$ if $m > 1, n > 1$ in theorem 2A.

Case II: $ABC_4(L(S(H)))$ and $GA_5(L(S(H)))$ if $m > 1, n = 1$ in theorem 2B.

5. Nanotorus of TUC₄C₈ (m, n) & its para-line graph L(S(R))

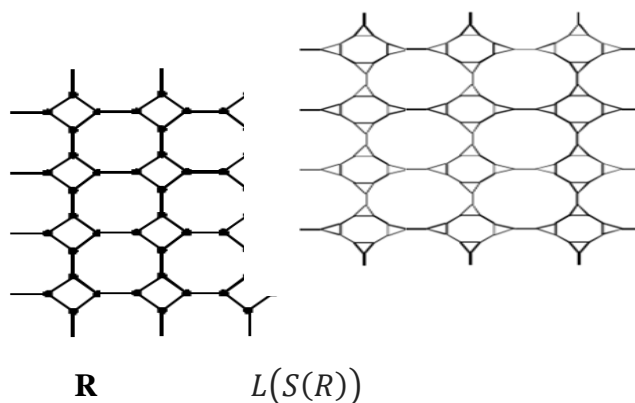


Fig.3

Theorem 3

Consider $L(S(R))$ of Nanotorus TUC₄C₈ (m, n) graph as shown in fig 3, then

I. $ABC_4(L(S(R))) = 8mn.$

$$\text{II. } GA_5(L(S(R))) = 18mn$$

Proof:

From the analysis, the $L(S(R))$ of Nanotorus $TUC_4C_8(m, n)$ graph has $12mn$ vertices and $18mn$ edges.

Edges of graph are taken here with respect to their sum of degrees of all vertices that are adjacent to vertex u and v . Here $d_s(u) = d_s(v) = 9$, number of edges: $18mn$ with respect to the edge division .

I. From the definition of ABC₄ index

$$ABC_4(L(S(R))) = \sum_{uv \in E(L(S(R)))} \sqrt{\frac{d_s(u) + d_s(v) - 2}{d_s(u)d_s(v)}} = (18mn) \sqrt{\frac{9 + 9 - 2}{9 \times 9}}$$

$$ABC_4(L(S(R))) = 8mn.$$

II. From the definition of GA₅ index

$$GA_5(L(S(H))) = \sum_{uv \in E(L(S(H)))} 2 \frac{\sqrt{d_s(u)d_s(v)}}{d_s(u) + d_s(v)}$$

$$GA_5(L(S(H))) = 2 \left\{ 18mn \frac{\sqrt{9 \times 9}}{9 + 9} \right\}$$

$$GA_5(L(S(R))) = 18mn$$

Hence proved the results.

6. Conclusion

This paper discusses the results of the fourth atom-bond connectivity index (ABC₄) and fifth geometric-arithmetic index (GA₅) for para-line graph of the two-dimensional molecular lattice, nanotubes, and nanotorus of $TUC_4C_8(m, n)$. In subsequent studies, the computation of the second, fourth ABC & GA indices of various notable nanostructures with wide-ranging chemical applications will be done.

7. Acknowledgment

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