TOPOLOGICAL PROPERTIES OF BENZENOID GRAPHS

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Topological index is a quantity uniquely defined for a graph which gives a correlation with physio chemical properties of the graph. In this paper we compute certain topological indices which depend on degree of vertices in the graph like Randic index, geometric arithmetic (GA) index, atom_bond connectivity index for rhombic benzenoid system, as well as zigzag benzenoid chain using edge partition. The ABC_4 and GA_5 indices for the benzenoid systems are also discussed in this paper.[4]*

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1. Introduction

Mathematical chemistry is a branch of theoretical chemistry which deals with the chemical structure to predict the physio chemical properties of compounds using mathematical tools. Chemical graph theory is being widely used to model the chemical phenomenon mathematically. This theory plays a prominent role in the fields of chemical sciences.

A topological index is a molecular graph descriptor which contains information about the physico-chemical properties of a compound and also help in mathematical modeling of biological reactivity of chemicals. Overtime hundreds of topological indices have been introduced. Most of them depend on degree of vertices and distance between vertices of chemical graphs.

A molecular graph is a simple graph in which the vertices denote atoms and the edges represent chemical bonds between these atoms. Consider a molecular graph, say, G with vertex set $V(G)$ and edge set $E(G)$. Two vertices of a graph are called adjacent vertices if they are joined by an edge.

Number of vertices attached to a given vertex, say, v is called degree of v, denoted by d_v and:

$$s_u = \sum_{v \in N_u} d(v) \text{ where } N_u = \{v \in V(G) \mid uv \in E(G)\} .$$

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The first degree based topological index is Randic index $\chi(G)$, introduced by Milan Randic [1] in 1975, and is defined as:

$$\chi(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{dudv}} \ .$$

The general Randic index was proposed by Bollobás and Erdös [4] in 1998, defined as:

$$R_\alpha(G) = \sum_{uv\in E(G)} (d_u d_v)^\alpha .$$

Obviously Randic index is the particular case of $R_\alpha(G)$ when $\alpha = -\frac{1}{2}$.

The widely used atom-bond connectivity (ABC) index is introduced by Estrada et al. [2] and is defined:

$$\text{ABC(G)} = \sum_{uv\in E(G)} \sqrt{\frac{d_{u} + d_v - 2}{d_u d_v}}.$$

Sum connectivity index(SCI) introduced by Zhou and Trinajsti´c [3] as

$$\text{SCI(G)} = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_{u} + d_v}} .$$

Fourth Atom bond connectivity index depends upon sum of degrees of neighboring vertices, denoted by s_u for a vertex u. It is given by following relation:

$$ABC_4 = \sum_{uv\varepsilon E(G)} \sqrt{\frac{s_u + s_{v} - 2}{s_u s_v}} .$$

The fifth geometric-arithmetic index (GA_5) was introduced by Graovac et al. [6] in 2011 and is defined as:

$$GA_5\text{(G)} = \sum_{uv\varepsilon E(G)} \frac{2\sqrt{s_u s_v}}{s_u + s_v} .$$

2. Main Results and Discussion

Consider the graph of Rhombic Benzenoid system, say, R_n, where n represents number of hexagons along each boundary of the rhomb. The graph has $2n(n+2)$ vertices and $3n^2 + 4n - 1$ edges. Different computational aspects have been discussed in literature [8,9]. Degree based topological indices of R_n are computed using the edge partition below.

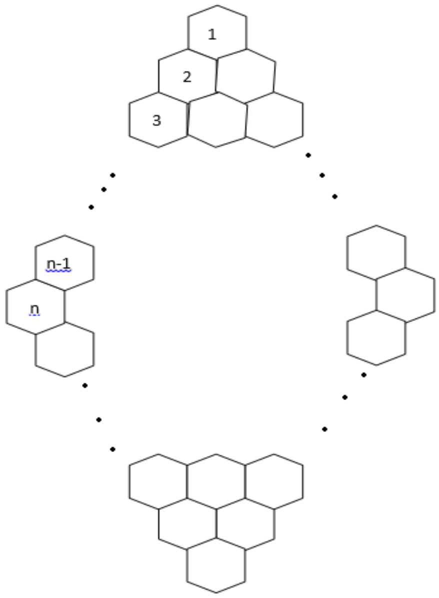

Fig.1: Graph of rhombi benzenoid R_n with n hexagons along each boundary

Table 1

Edge partition of benzenoid system R_n based on degree of end vertices of each edge

$(d_u, d_v)$where $uv \in E(G)$	(2,2)	(2,3)	(3,3)
Number or edge	6	8(n-1)	n(3n-4)+1

Theorem 1. *C*onsider the Rhombic benzenoid graph R_n, then its Randic index is:

$$R_{1/2}(R_n) = \begin{cases} 9n^2 + (8\sqrt{6} - 12)(n-1) & for \quad \alpha = \frac{1}{2} \\ n^2 + (\sqrt{6} - 1)\frac{4}{3}n + \left(\frac{10}{3} - \frac{8}{\sqrt{6}}\right) & for\ \alpha = -\frac{1}{2} \end{cases}$$

Proof. Using the edge partition in Table1, we compute the general Randic index of R_n as:

$$R_{1/2}(R_n) = \sum_{uv\varepsilon E(G)} \sqrt{d_u d_v}$$

$$= 6\sqrt{2 \times 2} + 8(n-1)\sqrt{2 \times 3} + n(3n-4)\sqrt{3 \times 3}$$

Simplifying, we get:

$$R_{1/2}(R_n) = 9n^2 + (8\sqrt{6} - 12)(n-1)$$

Now we find the value of general Randic index for $= -\frac{1}{2}$.

$$R_{-1/2}(R_n) = \sum_{uv\varepsilon E(G)} \frac{1}{\sqrt{d_u d_v}}$$

This implies that:

$$R_{-1/2}(R_n) = (6)\frac{1}{\sqrt{2\times 2}} + 8(n-1)\frac{1}{\sqrt{2\times 3}} + n(3n-4)\frac{1}{\sqrt{3\times 3}}$$

$$= sn^2 + (\sqrt{6}-1)\frac{4}{3}n + (\frac{10}{3} - \frac{8}{\sqrt{6}})$$

Theorem 2. The ABC index of R_n is given by

$$\text{ABC}(R_n) = 2n^2 + (\frac{1}{\sqrt{2}} - \frac{1}{3})8\text{n} + (3\sqrt{2} + \frac{2}{3})$$

Proof: We compute the Atom Bond Connectivity index ABC of R_n as:

$$\text{ABC}(R_n) = \sum_{uv\varepsilon E(G)} \sqrt{\frac{d_{u+}d_v - 2}{d_u d_v}}$$

Using edge partition in table 1, we get:

$$\text{ABC}(R_n) = 6\sqrt{\frac{2+2-2}{2\times 2}} + 8(n-1)\sqrt{\frac{2+3-2}{2\times 3}} + (3n^2 - 4n + 1)\sqrt{\frac{3+3-2}{3\times 3}}$$

After simplification, we get:

$$\text{ABC}(R_n) = 2n^2 + (\frac{1}{\sqrt{2}} - \frac{1}{3})8n + (3\sqrt{2} + \frac{2}{3})$$

Theorem 3. Consider the rhombic benzenoid graph R_n, then its sum connectivity index SCI is:

$$\text{SCI}(R_n) = \frac{3}{\sqrt{6}}n^2 + (\frac{8}{\sqrt{5}} - \frac{4}{\sqrt{6}})n + (3 + \frac{1}{\sqrt{6}} - \frac{8}{\sqrt{5}})$$

Proof: We compute the sum connectivity index (SCI) of benzenoid graph, which is given as:

$$\text{SCI}(R_n) = \sum_{uv\varepsilon E(G)} \frac{1}{\sqrt{d_u + d_v}}$$

This implies that:

$$\mathrm{SCI}(R_n) = 6\frac{1}{\sqrt{2+2}} + 8(n-1)\frac{1}{\sqrt{2+3}} + (3n^2-4n+1)\frac{1}{\sqrt{3+3}}$$

After simplification, we get:

$$\mathrm{SCI}(R_n) = \frac{3}{\sqrt{6}}n^2 + (\frac{8}{\sqrt{5}} - \frac{4}{\sqrt{6}})n + (3 + \frac{1}{\sqrt{6}} - \frac{8}{\sqrt{5}})$$

Theorem 4. Consider the rhombic benzenoid graph R_n, then its geometric-arithmetic index is:

$$\mathrm{GA}(R_n) = 3n^2 + 4(\frac{4\sqrt{6}-5}{5})n + (7 - \frac{16\sqrt{6}}{5})$$

Proof: we compute geometric-arithmetic index as follows:

$$\mathrm{GA}(R_n)\,) = \sum_{uv \varepsilon E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

This implies that:

$$\mathrm{GA}(R_n) = (6)\frac{2\sqrt{2x2}}{2+2} + 8(n-1)\frac{2\sqrt{2x3}}{2+3} + (3n^2-4n+1)\frac{2\sqrt{3x3}}{3+3}$$

After simplification, we get:

$$\mathrm{GA}(R_n) = 3n^2 + 4(\frac{4\sqrt{6}-5}{5})n + (7 - \frac{16\sqrt{6}}{5})$$

Now to compute fourth version of atom bond connectivity index and fifth Geometric Arithmetic index, we first find edge partition of the graph.

Table 2

Edge partition of rhombic benzenoid system based on degree sum of neighbors of end vertices of each edge

(s_u, s_v) where $uv \in E(G)$	Number of edges
(4,5)	4
(5,5)	2
(5,7)	8
(6,7)	$8(n-2)$
(7,9)	$4(n-1)$
(9,9)	$3n^2-8n+5$

Theorem 5. For the rhombic benzenoid graph R_n, its ABC_4 index is equal to:

$$ABC_4(R_n) = \frac{4}{3}n^2 + (8\sqrt{\frac{11}{42}} + \frac{4}{3}\sqrt{2} - \frac{32}{9})n + (2\sqrt{\frac{7}{5}} + \frac{4}{5}\sqrt{2} + 8\sqrt{\frac{2}{7}} - 16\sqrt{\frac{11}{42}} - \frac{4}{3}\sqrt{2} + \frac{20}{9})$$

Proof: we compute ABC_4 index using edge partition given in table 2:

$$ABC_4(R_n) = \sum_{uv\varepsilon E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}$$

This implies that:

$$ABC_4(R_n) = (4)\sqrt{\frac{4+5-2}{4\times 5}} + (2)\sqrt{\frac{5+5-2}{5\times 5}} + (8)\sqrt{\frac{5+7-2}{5\times 7}} + 8(n-2)\sqrt{\frac{6+7-2}{6\times 7}} + 4(n-1)\sqrt{\frac{7+9-2}{7\times 9}} + (3n^2-8n+5)\sqrt{\frac{9+9-2}{9\times 9}}$$

After simplification, we get:

$$ABC_4(R_n) = \frac{4}{3}n^2 + (8\sqrt{\frac{11}{42}} + \frac{4}{3}\sqrt{2} - \frac{32}{9})n + (2\sqrt{\frac{7}{5}} + \frac{4}{5}\sqrt{2} + 8\sqrt{\frac{2}{7}} - 16\sqrt{\frac{11}{42}} - \frac{4}{3}\sqrt{2} + \frac{20}{9}) .$$

Theorem 6: The GA_5 index of the rhombic benzenoid graph R_n is

$$GA_5(R_n) = 3n^2 + (\frac{16}{13}\sqrt{42} + \frac{\sqrt{63}}{2} - 8)n + (\frac{16}{9}\sqrt{5} + \frac{4}{3}\sqrt{35} - \frac{\sqrt{63}}{2} - \frac{32}{13}\sqrt{42} + 7)$$

Proof: We compute $GA_5(R_n)$ index defined as:

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

This implies that:

$$GA_5(R_n) = (4)\frac{2\sqrt{4\times 5}}{4+5} + (2)\frac{2\sqrt{5\times 5}}{5+5} + (8)\frac{2\sqrt{5\times 7}}{5+7} + (8n-16)\frac{2\sqrt{6\times 7}}{6+7} + 4(n-1)\frac{2\sqrt{7\times 9}}{7+9} + (3n^2-8n+5)\frac{2\sqrt{9\times 9}}{9+9}$$

After simplification, we get:

$$GA_5(R_n) = 3n^2 + (\tfrac{16}{13}\sqrt{42} + \tfrac{\sqrt{63}}{2} - 8)n + (\tfrac{16}{9}\sqrt{5} + \tfrac{4}{3}\sqrt{35} - \tfrac{\sqrt{63}}{2} - \tfrac{32}{13}\sqrt{42} + 7)$$

Consider the graph of zigzag benzenoid chain, say, Z_n. Here n denote number of rows in Z_n and there are two hexagons in each row of the system. Z_n has $8n+2$ vertices and $10n+1$ edges. Such hexagonal chains have been investigated for many topological indices [10,11].

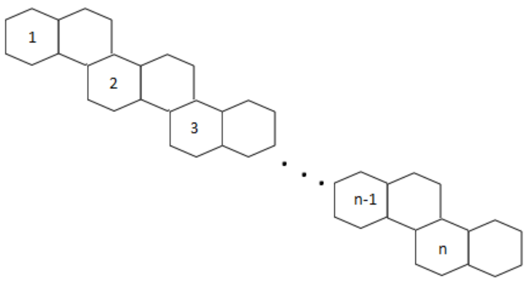

Fig. 2: Graph of zigzag benzenoid chain Z_n.

Table 3

Edge partition of benzenoid graph Z_n based on degree of end vertices of each edge

(d_u, d_v) where $uv \in E(G)$	(2,2)	(2,3)	(3,3)
Number of edge	$2(n+2)$	$4n$	$4n-3$

Theorem 7. The general Randic index of zigzag benzenoid graph Z_n is given by:

$$R_\alpha(R_n) = \begin{cases} n(16+4\sqrt{6})-1 & for \quad \alpha = \frac{1}{2} \\ n(\frac{42+12\sqrt{6}}{18}) + 1 & for\ \alpha = -\frac{1}{2} \end{cases}$$

Proof. Let Z_n be the graph of zigzag benzenoid chain. Now by using the edge partition based on the degree of end vertices of each edge of benzenoid graph given in table 3, we compute the Randic index as:

$$R_{1/2}(R_n) = \sum_{uv\varepsilon E(G)} \sqrt{d_u d_v}$$

$$= 2(n+2)\sqrt{2\times 2} + 4n\sqrt{2\times 3} + (4n-3)\sqrt{3\times 3}$$

Simplifying this, we get:

$$R_{1/2}(Z_n) = n(16+4\sqrt{6})-1$$

Now we compute general Randic index, which is equal to Randic index for:

$$\alpha = -\frac{1}{2}\ .$$

$$R_{-\frac{1}{2}}(Z_n) = \sum_{uv\varepsilon E(G)} \frac{1}{\sqrt{d_u d_v}}$$

This implies that:

$$R_{-\frac{1}{2}}(Z_n) = 2(n+2)\frac{1}{\sqrt{2\times 2}} + (4n)\frac{1}{\sqrt{2\times 3}} + (4n-3)\frac{1}{\sqrt{3\times 3}}$$

After an easy simplification, we get:

$$R_{-\frac{1}{2}}(Z_n) = n(\frac{42+12\sqrt{6}}{18}) + 1$$

Theorem 8: Consider the zigzag benzenoid chain Z_n, then its atom bond connectivity index is:

$$ABC(Z_n) = n\left(\frac{18\sqrt{2}+16}{6}\right) + \left(\frac{4\sqrt{2}-4}{2}\right).$$

Proof: Atom Bond Connectivity index of benzenoid graph is given as:

$$ABC(Z_n) = \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

This implies that:

$$ABC(Z_n) = (2n+4)\sqrt{\frac{2+2-2}{2\times 2}}\ (4n)\sqrt{\frac{2+3-2}{2\times 3}} + (4n-3)\sqrt{\frac{3+3-2}{3\times 3}}$$

After an easy simplification, we get:

$$ABC(Z_n) = n(\frac{18\sqrt{2}+16}{6}) + (\frac{4\sqrt{2}-4}{2})$$

Theorem 9. The sum connectivity index of Z_n is given by:

$$SCI(Z_n) = n\left(\frac{\sqrt{30}+4\sqrt{6}+4\sqrt{5}}{\sqrt{30}}\right) + (\frac{2\sqrt{6}-3}{\sqrt{6}})$$

Proof: We compute the sum connectivity index SCI of Z_n as:

$$SCI(Z_n) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_{u+}\, d_v}}$$

Using table 2, we get:

$$SCI(Z_n) = (2n+4)\frac{1}{\sqrt{2+2}} + (4n)\frac{1}{\sqrt{2+3}} + (4n-3)\frac{1}{\sqrt{3+3}}$$

After simplification, we have:

$$SCI(Z_n) = n\left(\frac{\sqrt{30}+4\sqrt{6}+4\sqrt{5}}{\sqrt{30}}\right) + (\frac{2\sqrt{6}-3}{\sqrt{6}})$$

Theorem 10. The Geometric -Arithmetic index of benzenoid graph Z_n:

$$GA(Z_n) = n\,(6+\frac{8\sqrt{6}}{5}) + 1$$

Proof: We compute geometric-arithmetic index of Z_n as:

$$GA(Z_n) = \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

This implies that:

$$GA(Z_n) = (2n+4)\frac{2\sqrt{2\times 2}}{2+2} + (4n)\frac{2\sqrt{2\times 3}}{2+3} + (4n-3)\ \frac{2\sqrt{3\times 3}}{3+3}\ ,$$

which yields:

$$GA(Z_n) = n\,(6+\frac{8\sqrt{6}}{5}) + 1$$

Table 4

Edge partition of zigzag benzenoid system based on degree sum of neighbors of end vertices of each edge

(s_u, s_v) where uv ∈ E(G)	Number of edges
(4,4)	2
(4,5)	4
(5,5)	2(n-1)
(5,7)	4
(5,8)	4(n-1)
(7,8)	2
(8,8)	4n-5

Theorem 11 Consider the zigzag benzenoid system Z_n, then its ABC_4 index is given by:

$$ABC_4(Z_n) = n(\frac{2\sqrt{8}}{5} + 4\sqrt{\frac{11}{40}} + 4\frac{\sqrt{14}}{8}) + (\frac{\sqrt{6}}{2} + 4\sqrt{\frac{7}{20}} - \frac{2}{5}\sqrt{8} + 4\sqrt{\frac{2}{7}} - 4\sqrt{\frac{11}{40}} + 2\sqrt{\frac{13}{56}} - \frac{5\sqrt{14}}{8})$$

Proof: We compute ABC_4 index of Z_n using Table 4, as follows:

$$ABC_4(Z_n) = \sum_{uv\varepsilon E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}$$

This implies that:

$$ABC_4(Z_n) = (2)\sqrt{\frac{4+4-2}{4\times 4}} + (4)\sqrt{\frac{4+5-2}{4\times 5}} + 2(n-1)\sqrt{\frac{5+5-2}{5\times 5}} + (4)\sqrt{\frac{5+7-2}{5\times 7}} + 4(n-1)\sqrt{\frac{5+8-2}{5\times 8}} + (2)\sqrt{\frac{7+8-2}{7\times 8}} + (4n-5)\sqrt{\frac{8+8-2}{8\times 8}}$$

It can be simplified to:

$$ABC_4(Z_n) = n(\frac{2\sqrt{8}}{5} + 4\sqrt{\frac{11}{40}} + 4\frac{\sqrt{14}}{8}) + (\frac{\sqrt{6}}{2} + 4\sqrt{\frac{7}{20}} - \frac{2}{5}\sqrt{8} + 4\sqrt{\frac{2}{7}} - 4\sqrt{\frac{11}{40}} + 2\sqrt{\frac{13}{56}} - \frac{5\sqrt{14}}{8})$$

Theorem 12: Fifth Geometric Arithmetic index GA_5 of benzenoid graph Z_n is given by:

$$GA_5(Z_n) = n(\frac{8}{13}(\sqrt{40} + 6) + (\frac{4}{\sqrt{5}} + \frac{2\sqrt{35}}{3} - \frac{16\sqrt{10}}{13} + \frac{8\sqrt{14}}{15} - 5).$$

Proof: We compute GA_5 index of Z_n using Table 4 as:

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

This implies that:

$$GA_5(Z_n) = (2)\frac{2\sqrt{4\times 4}}{4+4} + (4)\frac{2\sqrt{4\times 5}}{4+5} + (2n-2)\frac{2\sqrt{5\times 5}}{5+5} + (4)\frac{2\sqrt{5\times 7}}{5+7} + (4n-4)\frac{2\sqrt{5\times 8}}{5+8} + (2)\frac{2\sqrt{7\times 8}}{7+8}$$

After an easy simplification, we get:

$$GA_5(Z_n) = n(\frac{8}{13}(\sqrt{40} + 6) + (\frac{4}{\sqrt{5}} + \frac{2\sqrt{35}}{3} - \frac{16\sqrt{10}}{13} + \frac{8\sqrt{14}}{15} - 5).$$

3. Concluding Remarks

In this paper we computed topological descriptors of two important benzenoid graph that are rhombic benzenoid system and zigzag benzenoid chain. We gave exact expressions for Randic index, ABC index, sum connectivity index, GA index for these two important classes of graphs. We also computed fourth version of ABC index and fifth version of GA index for the graphs. This will be quite helpful in understanding the chemical properties of the graphs and their underlying topologies. In future we are interested to find other topological invariants of these structures.

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