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

Keywords: General Randić index, Molecular Graphs, Edges, Atom-bond connectivity (ABC) index, Geometric-arithmetic (GA) index, Sum Connectivity(SCI) index

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:

$$s_u = \sum_{u \in N(v)} d(v)$$ 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:

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

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:

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

Sum connectivity index (SCI) introduced by Zhou and Trinajst´ic [3] as

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

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:

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

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

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

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.** Consider the Rhombic benzenoid graph $R_n$, then its Randic index is:

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

**Proof.** Using the edge partition in Table 1, we compute the general Randic index of $R_n$ as:

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

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

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

$$R_{-1/2}(R_n) = \sum_{u,v \in E(G)} \frac{1}{d_u d_v}$$

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

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

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

$$ABC(R_n) = \sum_{u,v \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

Using edge partition in table 1, we get:

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

$$+ 1) \sqrt{\frac{3 + 3 - 2}{3 \times 3}}$$

After simplification, we get:

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

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

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

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

$$SCI(R_n) = \sum_{u,v \in E(G)} \frac{1}{d_u + d_v}$$
This implies that:

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

After simplification, we get:

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

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

\[
\text{GA}(R_n) = 3n^2 + 4 \left( \frac{4\sqrt{6} - 5}{5} \right) n + (7 - \frac{16\sqrt{6}}{5})
\]

**Proof:** we compute geometric-arithmetic index as follows:

\[
\text{GA}(R_n) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}
\]

This implies that:

\[
\text{GA}(R_n) = (6) \frac{2\sqrt{2x^2}}{2 + 2} + 8(n - 1) \frac{2\sqrt{2x^3}}{2 + 3} + (3n^2 - 4n + 1) \frac{2\sqrt{3x^3}}{3 + 3}
\]

After simplification, we get:

\[
\text{GA}(R_n) = 3n^2 + 4 \left( \frac{4\sqrt{6} - 5}{5} \right) n + (7 - \frac{16\sqrt{6}}{5})
\]

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

**Table 2**

<table>
<thead>
<tr>
<th>((s_u, s_v)) where (uv \in E(G))</th>
<th>Number of edges</th>
</tr>
</thead>
<tbody>
<tr>
<td>(4,5)</td>
<td>4</td>
</tr>
<tr>
<td>(5,5)</td>
<td>2</td>
</tr>
<tr>
<td>(5,7)</td>
<td>8</td>
</tr>
<tr>
<td>(6,7)</td>
<td>8(n - 2)</td>
</tr>
<tr>
<td>(7,9)</td>
<td>4(n - 1)</td>
</tr>
<tr>
<td>(9,9)</td>
<td>3n^2 - 8n + 5</td>
</tr>
</tbody>
</table>

**Theorem 5.** For the rhombic benzenoid graph \( R_n \), its \( ABC_4 \) index is equal to:
Proof: we compute $ABC_4$ index using edge partition given in table 2:

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

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

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

Proof: We compute $GA_5(R_n)$ index defined as:
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\[ GA_5(R_n) = \sum_{e=uv \in E(G)} \frac{2\sqrt{S_uS_v}}{S_u + S_v} \]

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:

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

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].

![Graph of zigzag benzenoid chain \( Z_n \).](image)

**Table 3**

| Edge partition of benzenoid graph \( Z_n \) based on degree of end vertices of each edge |
|---------------------------------------------|----------------|----------------|
| \((d_u, d_v)\) where \( uv \in E(G) \)     | \((2,2)\)     | \((2,3)\)     |
| Number of edge                             | \(2(n + 2)\)  | \(4n\)        | \(4n - 3\)    |

**Theorem 7.** The general Randic index of zigzag benzenoid graph \( Z_n \) is given by:
\[ R_{\alpha}(R_n) = \begin{cases} 
\frac{n(16 + 4\sqrt{6})}{18} + 1 & \text{for } \alpha = -\frac{1}{2} \\
\frac{n(16 + 4\sqrt{6})}{4} - 1 & \text{for } \alpha = \frac{1}{2} 
\end{cases} \]

**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:

\[ R_{1/2}(R_n) = \sum_{uv \in E(G)} \sqrt{d_u d_v} \]

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

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 \( \alpha = -\frac{1}{2} \):

\[ R_{-1/2}(Z_n) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} \]

This implies that:

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

After an easy simplification, we get:

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

**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:
\[ ABC(Z_n) = (2n + 4) \left( \frac{2 + 2 - 2}{2 \times 2} (4n) \sqrt{\frac{2 + 3 - 2}{2 \times 3}} + (4n - 3) \sqrt{\frac{3 + 3 - 2}{3 \times 3}} \right) \]

After an easy simplification, we get:

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

**Theorem 9.** The sum connectivity index of \( Z_n \) is given by:

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

**Proof:** We compute the sum connectivity index SCI of \( Z_n \) as:

\[ SCI(Z_n) = \sum_{u \neq v \in \mathcal{G}} \frac{1}{\sqrt{d_u + d_v}} \]

Using table 2, we get:

\[ SCI(Z_n) = (2n + 4) \left( \frac{1}{\sqrt{2} + 2} \right) + (4n) \left( \frac{1}{\sqrt{2} + 3} \right) + (4n - 3) \left( \frac{1}{\sqrt{3} + 3} \right) \]

After simplification, we have:

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

**Theorem 10.** The geometric-arithmetic index of benzenoid graph \( Z_n \):

\[ GA(Z_n) = n \left( 6 + \frac{8\sqrt{6}}{5} \right) + 1 \]

**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:

\[ GA(Z_n) = n \left( 6 + \frac{8\sqrt{6}}{5} \right) + 1 \]
Table 4

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<td>2</td>
</tr>
<tr>
<td>(8,8)</td>
<td>4n-5</td>
</tr>
</tbody>
</table>

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

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

**Proof:** We compute \( ABC_4 \) index of \( Z_n \) using Table 4, as follows:

\[
ABC_4(Z_n) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}
\]

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:
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\[ \text{ABC}_4(Z_n) = n \left( \frac{2\sqrt{8}}{5} + 4 \left( \frac{11}{40} + \frac{\sqrt{14}}{8} \right) + \left( \frac{\sqrt{6}}{2} \right) + 4 \left( \frac{7}{20} - \frac{2}{5} \sqrt{8} + \frac{2}{7} \right) \right. \]
\[ \left. - 4 \left( \frac{11}{40} + 2 \left( \frac{13}{56} - \frac{5\sqrt{14}}{8} \right) \right) \right] \]

**Theorem 12:** Fifth Geometric Arithmetic index \( GA_5 \) of benzenoid graph \( Z_n \) is given by:

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

**Proof:** We compute \( GA_5 \) index of \( Z_n \) using Table 4 as:

\[ GA_5(Z_n) = \sum_{e=uv \in E(G)} \frac{2\sqrt{S_uS_v}}{S_u + S_v} \]

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:

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

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.
REFERENCES