

Reversed degree-based topological indices for Benzenoid systems

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Abstract

Topological indices are numerical values that correlate the chemical structures with physical properties. In this article, we compute some reverse topological indices namely reverse Atom-bond connectivity index and reverse Geometric-arithmetic index for four different types of Benzenoid systems.

Keywords: Topological indices, Reverse topological indices, Benzenoid systems.

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1. Introduction

Chemical graph theory is an effective branch of mathematics that provides us tools to gain information about chemical structures [1, 2]. A topological index is a numeric quantity, that best describe the topology of chemical graph.[3, 4].

Estrada [5] introduced the idea of Atom-bond connectivity index. Actually, Atom-bond connectivity index is the amended version of the first genuine degree-based topological index, that was put forward by Milan Randić in 1975, in his seminal paper [6], On characterization of molecular branching named as Branching index but after some period of time it was named as connectivity index. Now a days it in known as Randić index. Atom-bond connectivity index can be abbreviated as ABC index. It is defined as

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

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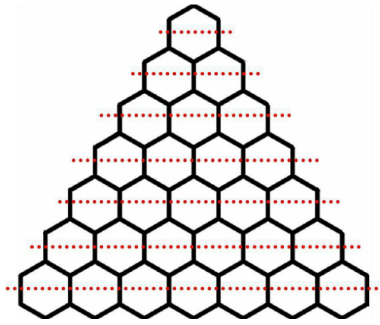


Figure 1: Triangular benzenoid system

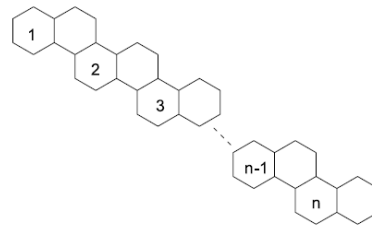


Figure 2: Zigzag benzenoid system

For explanation of further properties of ABC index, we refer [6].

Another degree based topological index that utilizes the difference between the geometric and arithmetic means [7, 8] was invented in [9] as

$$GA(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u \cdot d_v}}{\frac{1}{2}[d_u + d_v]}.$$

Motivated by the idea of reverse topological indices [10], the idea of reverse Atom-bond connectivity index and reverse Geometric-arithmetic index was put forward in [11] as

$$CABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{c_u + c_v - 2}{c_u \cdot c_v}},$$

and

$$CGA(G) = \sum_{uv \in E(G)} \frac{\sqrt{c_u \cdot c_v}}{\frac{1}{2}[c_u + c_v]},$$

where, $c_u = \Delta(G) - d_G(v) + 1$. For more about topological indices one can find [12, 13, 14].

In this paper, we aim to compute some reverse topological indices namely reverse Atom-bond connectivity index and reverse Geometric-arithmetic index for four different types of Benzenoid Systems.

2. Computational Results

In this section, we compute reversed Atom-bond connectivity index (CABC) and reverse Geometric-arithmetic index (CGA) for Triangular benzenoid system T_n (Figure 1), Zigzag benzenoid system Z_n (Figure 2), Rhombic benzenoid system R_n (Figure 3) and Hourglass benzenoid system X_p (Figure 4).

2.1. Triangular Benzenoid System T_n

Let T_n be a Triangular benzenoid system where n is the number of hexagons in graph and total quantity of hexagons in T_n is $\frac{1}{2}n(n + 1)$ The vertex and edge set of T_n are

$$V(T_n) = n^2 + 4n + 1,$$

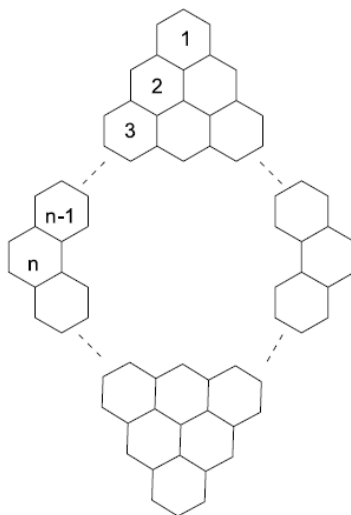


Figure 3: Rhombic benzenoid system

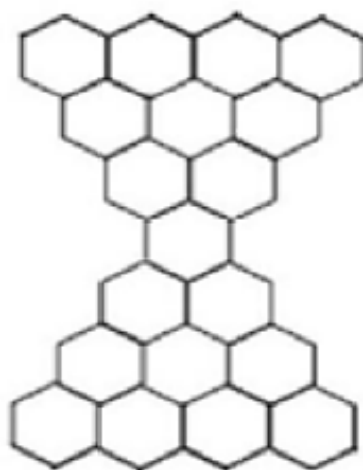


Figure 4: Hourglass benzenoid System

and

$$E(T_n) = \frac{3}{2}n(n + 3)$$

respectively.

For the Triangular benzenoid system T_n there are following three types of edges in edge set of T_n ;

$$\begin{aligned} E_1(T_n) &= \{uv \in E(T_n); d_u = 2, d_v = 2\} \ ; \ |E_1(T_n)| = 6, \\ E_2(T_n) &= \{uv \in E(T_n); d_u = 2, d_v = 3\} \ ; \ |E_2(T_n)| = 6(n - 1), \\ E_3(T_n) &= \{uv \in E(T_n); d_u = 3, d_v = 3\} \ ; \ |E_3(T_n)| = \frac{3}{2}n(n - 1). \end{aligned}$$

The reverse edge set of T_n is given as,

$$\begin{aligned} CE_1(T_n) &= \{uv \in E(T_n); d_u = 2, d_v = 2\} \ ; \ |CE_1(T_n)| = 6, \\ CE_2(T_n) &= \{uv \in E(T_n); d_u = 2, d_v = 1\} \ ; \ |CE_2(T_n)| = 6(n - 1), \\ CE_3(T_n) &= \{uv \in E(T_n); d_u = 1, d_v = 1\} \ ; \ |CE_3(T_n)| = \frac{3}{2}n(n - 1). \end{aligned}$$

Theorem 2.1. *Let T_n be the Triangular benzenoid System, then we have*

1. $CABC(T_n) = \frac{6}{\sqrt{2}}n$,
2. $CGA(T_n) = \frac{3}{2}n^2 + \frac{1}{2}(8\sqrt{2} - 3)n + 2(3 - 2\sqrt{2})$.

Proof. Using the reverse edge partition of T_n we have following computations for our results;

1.

$$\begin{aligned} CABC(T_n) &= \sum_{uv \in E(T_n)} \sqrt{\frac{c_u(T_n) + c_v(T_n) - 2}{c_u(T_n) \cdot c_v(T_n)}} \\ &= \sum_{uv \in E_1(T_n)} \sqrt{\frac{c_u(T_n) + c_v(T_n) - 2}{c_u(T_n) \cdot c_v(T_n)}} + \sum_{uv \in E_2(T_n)} \sqrt{\frac{c_u(T_n) + c_v(T_n) - 2}{c_u(T_n) \cdot c_v(T_n)}} \\ &\quad + \sum_{uv \in E_3(T_n)} \sqrt{\frac{c_u(T_n) + c_v(T_n) - 2}{c_u(T_n) \cdot c_v(T_n)}} \\ &= (6)\sqrt{\frac{2+2-2}{2.2}} + [6(n-1)]\sqrt{\frac{2+1-2}{2.1}} + \left[\frac{3}{2}n(n-1)\right]\sqrt{\frac{1+1-2}{1.1}} \\ &= \frac{6}{\sqrt{2}}n. \end{aligned}$$

2.

$$\begin{aligned} CGA(T_n) &= \sum_{uv \in E(T_n)} \frac{\sqrt{c_u(T_n) \cdot c_v(T_n)}}{\frac{1}{2}[c_u(T_n) + c_v(T_n)]} \\ &= \sum_{uv \in E_1(T_n)} \frac{\sqrt{c_u(T_n) \cdot c_v(T_n)}}{\frac{1}{2}[c_u(T_n) + c_v(T_n)]} + \sum_{uv \in E_2(T_n)} \frac{\sqrt{c_u(T_n) \cdot c_v(T_n)}}{\frac{1}{2}[c_u(T_n) + c_v(T_n)]} \\ &\quad + \sum_{uv \in E_3(T_n)} \frac{\sqrt{c_u(T_n) \cdot c_v(T_n)}}{\frac{1}{2}[c_u(T_n) + c_v(T_n)]} \\ &= (6)\frac{\sqrt{2.2}}{\frac{1}{2}[2+2]} + [6(n-1)]\frac{\sqrt{2.1}}{\frac{1}{2}[2+1]} + \left[\frac{3}{2}n(n-1)\right]\frac{\sqrt{1.1}}{\frac{1}{2}[1+1]} \\ &= \frac{3}{2}n^2 + \frac{1}{2}(8\sqrt{2} - 3)n + 2(3 - 2\sqrt{2}). \end{aligned}$$

□

2.2. Zigzag benzenoid system Z_p

Zigzag benzenoid system is denoted by Z_p , where p is the number of rows in graph of Z_p and each row consists of two hexagons as shown in Figure 2. For the Zigzag Benzenoid System Z_p there are following three types of edges;

$$\begin{aligned} E_1(Z_p) &= \{uv \in E(Z_p); d_u = 2, d_v = 2\} \quad ; \quad |E_1(Z_p)| = 2p + 4, \\ E_2(Z_p) &= \{uv \in E(Z_p); d_u = 2, d_v = 3\} \quad ; \quad |E_2(Z_p)| = 4p, \\ E_3(Z_p) &= \{uv \in E(Z_p); d_u = 3, d_v = 3\} \quad ; \quad |E_3(Z_p)| = 4p - 3. \end{aligned}$$

The maximum edge degree in edge set of T_n is 3 so the reverse edge set of Z_p is given as,

$$\begin{aligned} CE_1(Z_p) &= \{uv \in E(Z_p); d_u = 2, d_v = 2\} \quad ; \quad |CE_1(Z_p)| = 2p + 4, \\ CE_2(Z_p) &= \{uv \in E(Z_p); d_u = 2, d_v = 1\} \quad ; \quad |CE_2(Z_p)| = 4p, \\ CE_3(Z_p) &= \{uv \in E(Z_p); d_u = 1, d_v = 1\} \quad ; \quad |CE_3(Z_p)| = 4p - 3. \end{aligned}$$

Theorem 2.2. Let Z_p be the graph of Zigzag benzenoid system, then we have

1. $CABC(Z_p) = 3\sqrt{2}p + 2\sqrt{2}$,
2. $CGA(Z_p) = \frac{2}{3}(9 + 4\sqrt{2})p + 1$.

Proof. Using the reverse edge partition of Z_p we have following computations for our results;

1.

$$\begin{aligned} CABC(Z_p) &= \sum_{uv \in E(Z_p)} \sqrt{\frac{c_u(Z_p) + c_v(Z_p) - 2}{c_u(Z_p) \cdot c_v(Z_p)}} \\ &= \sum_{uv \in E_1(Z_p)} \sqrt{\frac{c_u(Z_p) + c_v(Z_p) - 2}{c_u(Z_p) \cdot c_v(Z_p)}} + \sum_{uv \in E_2(Z_p)} \sqrt{\frac{c_u(Z_p) + c_v(Z_p) - 2}{c_u(Z_p) \cdot c_v(Z_p)}} \\ &\quad + \sum_{uv \in E_3(Z_p)} \sqrt{\frac{c_u(Z_p) + c_v(Z_p) - 2}{c_u(Z_p) \cdot c_v(Z_p)}} \\ &= (2p + 4)\sqrt{\frac{2 + 2 - 2}{2 \cdot 2}} + (4p)\sqrt{\frac{2 + 1 - 2}{2 \cdot 1}} + (4p - 3)\sqrt{\frac{1 + 1 - 2}{1 \cdot 1}} \\ &= 3\sqrt{2}p + 2\sqrt{2}. \end{aligned}$$

2.

$$\begin{aligned} CGA(Z_p) &= \sum_{uv \in E(Z_p)} \frac{\sqrt{c_u(Z_p) \cdot c_v(Z_p)}}{\frac{1}{2}[c_u(Z_p) + c_v(Z_p)]} \\ &= \sum_{uv \in E_1(Z_p)} \frac{\sqrt{c_u(Z_p) \cdot c_v(Z_p)}}{\frac{1}{2}[c_u(Z_p) + c_v(Z_p)]} + \sum_{uv \in E_2(Z_p)} \frac{\sqrt{c_u(Z_p) \cdot c_v(Z_p)}}{\frac{1}{2}[c_u(Z_p) + c_v(Z_p)]} \\ &\quad + \sum_{uv \in E_3(Z_p)} \frac{\sqrt{c_u(Z_p) \cdot c_v(Z_p)}}{\frac{1}{2}[c_u(Z_p) + c_v(Z_p)]} \\ &= (2p + 4)\frac{\sqrt{2 \cdot 2}}{\frac{1}{2}[2 + 2]} + (4p)\frac{\sqrt{2 \cdot 1}}{\frac{1}{2}[2 + 1]} + (4p - 3)\frac{\sqrt{1 \cdot 1}}{\frac{1}{2}[1 + 1]} \\ &= \frac{2}{3}(9 + 4\sqrt{2})p + 1. \end{aligned}$$

□

2.3. Rhombic benzenoid system R_n

Take another benzenoid system in which hexagons are arranged to form a rhombic shape R_n , in which there are n rows of n hexagons as given in Figure 3. The vertex and edge set of Rhombic Benzenoid System R_n is given as,

$$V(R_n) = 2n(n + 2)$$

and edge set is

$$E(R_n) = 3n^2 + 4n - 1$$

respectively.

There are following type of edges in Rhombic benzenoid system R_n ;

$$\begin{aligned} E_1(R_n) &= \{uv \in E(R_n); d_u = 2, d_v = 2\} \ ; \ |E_1(R_n)| = 6, \\ E_2(R_n) &= \{uv \in E(R_n); d_u = 2, d_v = 3\} \ ; \ |E_2(R_n)| = 8(n - 1), \\ E_3(R_n) &= \{uv \in E(R_n); d_u = 3, d_v = 3\} \ ; \ |E_3(R_n)| = 3n^2 - 4n + 1. \end{aligned}$$

The maximum edge degree in edge set of R_n is 3, then the reverse edge set of R_n is given as,

$$\begin{aligned} CE_1(R_n) &= \{uv \in E(R_n); d_u = 2, d_v = 2\} \ ; \ |CE_1(R_n)| = 6, \\ CE_2(R_n) &= \{uv \in E(R_n); d_u = 2, d_v = 1\} \ ; \ |CE_2(R_n)| = 8(n - 1), \\ CE_3(R_n) &= \{uv \in E(R_n); d_u = 1, d_v = 1\} \ ; \ |CE_3(R_n)| = 3n^2 - 4n + 1. \end{aligned}$$

Theorem 2.3. Let R_n be the graph of Rhombic benzenoid system R_n , then we have

1. $CABC(R_n) = \frac{8}{\sqrt{2}}n - \sqrt{2}$,
2. $CGA(R_n) = 3n^2 + \frac{4}{3}(4\sqrt{2} - 3) + \frac{1}{3}(21 - 16\sqrt{2})$.

Proof. Using the reverse edge partition of R_n we have following computations for our results;

1.

$$\begin{aligned} CABC(R_n) &= \sum_{uv \in E(R_n)} \sqrt{\frac{c_u(R_n) + c_v(R_n) - 2}{c_u(R_n) \cdot c_v(R_n)}} \\ &= \sum_{uv \in E_1(R_n)} \sqrt{\frac{c_u(R_n) + c_v(R_n) - 2}{c_u(R_n) \cdot c_v(R_n)}} + \sum_{uv \in E_2(R_n)} \sqrt{\frac{c_u(R_n) + c_v(R_n) - 2}{c_u(R_n) \cdot c_v(R_n)}} \\ &\quad + \sum_{uv \in E_3(R_n)} \sqrt{\frac{c_u(R_n) + c_v(R_n) - 2}{c_u(R_n) \cdot c_v(R_n)}} \\ &= (6)\sqrt{\frac{2 + 2 - 2}{2 \cdot 2}} + 8(n - 1)\sqrt{\frac{2 + 1 - 2}{2 \cdot 1}} + (3n^2 - 4n + 1)\sqrt{\frac{1 + 1 - 2}{1 \cdot 1}} \\ &= \frac{8}{\sqrt{2}}n - \sqrt{2}. \end{aligned}$$

2.

$$\begin{aligned} CGA(R_n) &= \sum_{uv \in E(R_n)} \frac{\sqrt{c_u(R_n) \cdot c_v(R_n)}}{\frac{1}{2}[c_u(R_n) + c_v(R_n)]} \\ &= \sum_{uv \in E_1(R_n)} \frac{\sqrt{c_u(R_n) \cdot c_v(R_n)}}{\frac{1}{2}[c_u(R_n) + c_v(R_n)]} + \sum_{uv \in E_2(R_n)} \frac{\sqrt{c_u(R_n) \cdot c_v(R_n)}}{\frac{1}{2}[c_u(R_n) + c_v(R_n)]} \end{aligned}$$

$$\begin{aligned}
 & + \sum_{uv \in E_3(R_n)} \frac{\sqrt{c_u(R_n) \cdot c_v(R_n)}}{\frac{1}{2}[c_u(R_n) + c_v(R_n)]} \\
 & = (6) \frac{\sqrt{2 \cdot 2}}{\frac{1}{2}[2 + 2]} + 8(n - 1) \frac{\sqrt{2 \cdot 1}}{\frac{1}{2}[2 + 1]} + (3n^2 - 4n + 1) \frac{\sqrt{1 \cdot 1}}{\frac{1}{2}[1 + 1]} \\
 & = 3n^2 + \frac{4}{3}(4\sqrt{2} - 3) + \frac{1}{3}(21 - 16\sqrt{2}).
 \end{aligned}$$

□

2.4. Hourglass benzenoid system X_n

Let X_n be a Hourglass benzenoid system which is obtained from two copies of a triangular benzenoid T_n by overlapping their external hexagons. The vertex and edge sets of X_n are

$$V(X_n) = 2(n^2 + 4n - 2)$$

and

$$E(X_n) = 3n^2 + 9n - 4$$

respectively.

For the Triangular benzenoid system X_n there are following three types of edges in edge set of X_n ;

$$\begin{aligned}
 E_1(X_n) &= \{uv \in E(X_n); d_u = 2, d_v = 2\} \ ; \ |E_1(X_n)| = 8, \\
 E_2(X_n) &= \{uv \in E(X_n); d_u = 2, d_v = 3\} \ ; \ |E_2(X_n)| = 4(3n - 4), \\
 E_3(X_n) &= \{uv \in E(X_n); d_u = 3, d_v = 3\} \ ; \ |E_3(X_n)| = 3n^2 - 3n + 4.
 \end{aligned}$$

The maximum edge degree in edge set of X_n is 4, so the reverse edge set of X_n is given as,

$$\begin{aligned}
 CE_1(X_n) &= \{uv \in E(X_n); d_u = 2, d_v = 2\} \ ; \ |CE_1(X_n)| = 8, \\
 CE_2(X_n) &= \{uv \in E(X_n); d_u = 2, d_v = 1\} \ ; \ |CE_2(X_n)| = 4(3n - 4), \\
 CE_3(X_n) &= \{uv \in E(X_n); d_u = 1, d_v = 1\} \ ; \ |CE_3(X_n)| = 3n^2 - 3n + 4.
 \end{aligned}$$

Theorem 2.4. Let X_n be the graph of Hourglass Benzenoid System X_n , then we have

1. $CABC(X_n) = 6\sqrt{2}n - 4\sqrt{2}$,
2. $CGA(X_n) = 3n^2 + (8\sqrt{2} - 3)n + \frac{4}{3}(8\sqrt{2} + 9)$.

Proof. Using the reverse edge partition of X_n we have following computations for our results;

1.

$$\begin{aligned}
 CABC(X_n) &= \sum_{uv \in E(X_n)} \sqrt{\frac{c_u(X_n) + c_v(X_n) - 2}{c_u(X_n) \cdot c_v(X_n)}} \\
 &= \sum_{uv \in E_1(X_n)} \sqrt{\frac{c_u(X_n) + c_v(X_n) - 2}{c_u(X_n) \cdot c_v(X_n)}} + \sum_{uv \in E_2(X_n)} \sqrt{\frac{c_u(X_n) + c_v(X_n) - 2}{c_u(X_n) \cdot c_v(X_n)}} \\
 &\quad + \sum_{uv \in E_3(X_n)} \sqrt{\frac{c_u(X_n) + c_v(X_n) - 2}{c_u(X_n) \cdot c_v(X_n)}} \\
 &= (8) \sqrt{\frac{2 + 2 - 2}{2 \cdot 2}} + [4(3n - 4)] \sqrt{\frac{2 + 1 - 2}{2 \cdot 1}} + [3n^2 - 3n + 4] \sqrt{\frac{1 + 1 - 2}{1 \cdot 1}} \\
 &= 6\sqrt{2}n - 4\sqrt{2}.
 \end{aligned}$$

2.

$$\begin{aligned}
CGA(X_n) &= \sum_{uv \in E(X_n)} \frac{\sqrt{c_u(X_n) \cdot c_v(X_n)}}{\frac{1}{2}[c_u(X_n) + c_v(X_n)]} \\
&= \sum_{uv \in E_1(X_n)} \frac{\sqrt{c_u(X_n) \cdot c_v(X_n)}}{\frac{1}{2}[c_u(X_n) + c_v(X_n)]} + \sum_{uv \in E_2(X_n)} \frac{\sqrt{c_u(X_n) \cdot c_v(X_n)}}{\frac{1}{2}[c_u(X_n) + c_v(X_n)]} \\
&\quad + \sum_{uv \in E_3(X_n)} \frac{\sqrt{c_u(X_n) \cdot c_v(X_n)}}{\frac{1}{2}[c_u(X_n) + c_v(X_n)]} \\
&= (8) \frac{\sqrt{2.2}}{\frac{1}{2}[2+2]} + [4(3n-4)] \frac{\sqrt{2.1}}{\frac{1}{2}[2+1]} + [3n^2 - 3n + 4] \frac{\sqrt{1.1}}{\frac{1}{2}[1+1]} \\
&= 3n^2 + (8\sqrt{2} - 3)n + \frac{4}{3}(8\sqrt{2} + 9).
\end{aligned}$$

□

3. Conclusion

With the help of topological index, we can assign a single number to a chemical structure. In quantitative structure activity/ property relationship, knowledge of topological indices plays an important role. In this article, we compute some reverse topological indices for four benzenoid systems, namely Triangular benzenoid system T_n , Zigzag benzenoid system Z_p , Rhombic benzenoid system R_n and Hourglass benzenoid system X_n .

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