

FULL PAPER

Study of middle graph for certain classes of graph by applying degree-based topological indices

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Topological indices are extremely useful for analyzing various physical and chemical properties associated with a chemical compound. A topological index describes molecular structures by converting them into certain real numbers. Topological indices are used in the development of quantitative structure-activity relationships (QSARs) in which the biological activity of molecule correlated with their chemical structure. The chemical shape of benzene molecule is very common in nano-science, chemistry, and physics. The circumcoronene collection of benzenoid (H_s) generates from the benzene molecules. Jahangir graph ($J_{(m,t)}$) is a generalized wheel graph that consists of (m, t) circular vertices and a center vertex connected to every mt vertex on the circle. In this article, we will compute the topological indices of the middle graph of the circumcoronene series of benzenoids (H_s) and Jahangir graph ($J_{(m,t)}$). In addition, comparison of the middle graph of the circumcoronene series of benzenoid (H_s) and Jahangir graph ($J_{(3,t)}$) are presented numerically and graphically.

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KEYWORDS

Topological Indices; circumcoronene series of benzenoid; middle graph; Jahangir graph.

Introduction

Consider a molecular graph $G = (V, E)$, such a graph with vertex set $V(G)$ indicates the atoms and edge set $E(G)$ indicates chemical bonds. A degree is represented by $d_\theta \{ \theta \in V(G) \}$ which is defined as the number of edges incident with θ . (For unspecified terminologies and more details [1]).

Graph theory is branch of mathematics that has been applied in virtually every field of study. The usage of topological indices in QSPR/QSAR studies has taken important concentration in recent years. Graph theory is used to assess the linkage among several topological indices of certain graphs that generated by some graph operations that are middle graph, total graph, semi-total graph, and the strong double graph etc. Topological indices are numerical parameters of a graph

molecule that characterize its topology [2]. The first topological index to be applied in chemistry is the Wiener index. To be more precisely, Harold Wiener introduced this intriguing index in 1947 to assess the physical characteristics of the type of alkane known as paraffin [3].

The symmetric division degree index (SD) of connected graph (G) [4] is defined as follows:

$$SD(G) = \sum_{\theta\omega \in E(G)} \frac{d_\theta^2 + d_\omega^2}{d_\theta d_\omega} \quad (1)$$

Where, d_θ and d_ω are the degrees of vertex θ and ω in G .

The sum-Connectivity index [5] is defined as follows:

$$SC(G) = \sum_{\theta\omega \in E(G)} \frac{1}{\sqrt{d_\theta + d_\omega}}. \quad (2)$$

Randic connectivity index is widely used in mathematical chemistry, due to its wide applications in both mathematics and chemistry. It is defined [6] in the following equation:

$$RC(G) = \sum_{\theta\omega \in E(G)} \frac{1}{\sqrt{d_\theta d_\omega}}. \quad (3)$$

The First-Zagreb index [7] is defined as: (4)

$$M_1(G) = \sum_{\theta\omega \in E(G)} (d_\theta + d_\omega)$$

The second-Zagreb index [7] is defined as:

$$M_2(G) = \sum_{\theta\omega \in E(G)} (d_\theta d_\omega). \quad (5)$$

Zhong introduced the harmonic index in 2012 which is defined [8] as follows:

$$H(G) = \sum_{\theta\omega \in E(G)} \frac{2}{(d_\theta + d_\omega)}. \quad (6)$$

For more wide-ranging and comprehensive details, we offer the readers to follow the following articles [9-13, 17-40].

Definition 1.1. A graph that contains a cycle C_{mt} having an extra vertex which is adjacent to t vertices of C_{mt} at the distance m to each other on the C_{mt} . In Jahngir graph [14] ($J_{m,t}$), where $t \geq 2$ and $m \geq 3$. The number of vertices and edges is $mt + 1$ and $mt + m$ respectively. Jahangir graphs $J_{(3,2)}$, $J_{(3,3)}$, and $J_{(3,t)}$ are displayed in Figure 1.

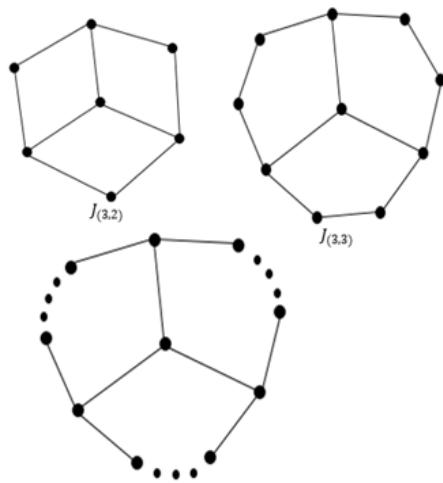


FIGURE 1 Jahangir graph

Definition 1.2. Circumcoronene series of benzenoid (H_s) where, ($s \geq 1$) is one family that is generated from benzene C_6 on circumference [15]. The number of vertices are $6s^2$ and edges are $9s^2 - 3s$, in this series of benzenoids. The Circumcoronene series of benzenoids are designated in Figure 2.

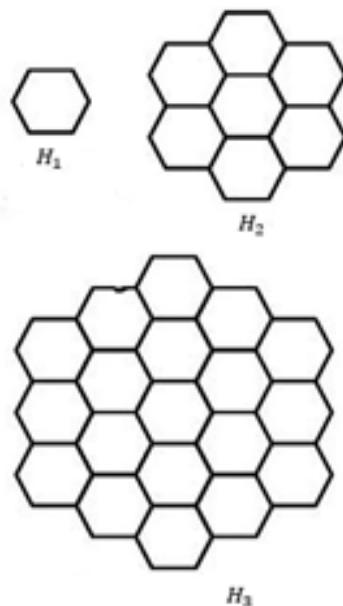


FIGURE 2 Circumcoronene series of benzenoid

Definition 1.3. The middle graph [16] of any graph G is attained by adding a new vertex to each of its edge and connecting by edges any pairs of those new vertices which lie on the adjacent edges of the graph. The middle graph of graph G is represented by $M(G)$. For example, the middle graph of the Jahangir graph ($J_{(3,3)}$) is depicted in Figure 3.

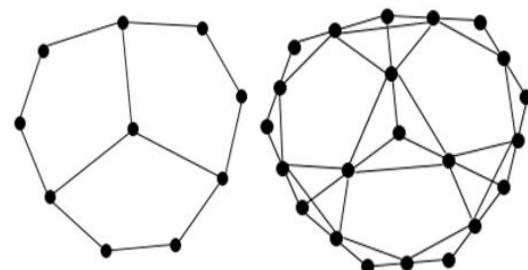


FIGURE 3 Jahangir Graph ($J_{(3,3)}$) and its middle graph [$M(J_{(3,3)})$]

Result for the Middle Graph of Jahangir graph ($J_{(3,t)}$)

In this section, we calculate degree-based indices of the middle graph of Jahangir graph ($J_{(3,t)}$), where $t \geq 3$.

Theorem 2.1. Let $[M(J_{(3,t)})]$ be the middle graph of Jahangir graph. Then,

$$\begin{aligned} 1. SD[M(J_{(3,t)})] &= \frac{3(14t+23)}{2}. \\ 2. SC[M(J_{(3,t)})] &= \sqrt{6}t + \frac{3t}{\sqrt{8}} - 2\sqrt{6} - \frac{9}{\sqrt{8}} + 4 \\ &+ \frac{6}{\sqrt{7}} + \frac{3}{\sqrt{2}} + \frac{3}{\sqrt{10}} + \frac{6}{\sqrt{11}} + \frac{\sqrt{3}}{2}. \\ 3. RC[M(J_{(3,t)})] &= \frac{((4\sqrt{3}+12)\sqrt{5}+30t-40)\sqrt{2}}{20} \\ &+ \frac{(8\sqrt{3}+12)\sqrt{5}+15t-23}{20}. \end{aligned}$$

TABLE 1 Edge division

$E[d_u, d_v]$	$E_{(2,4)}$	$E_{(2,5)}$	$E_{(3,5)}$	$E_{(3,6)}$	$E_{(4,4)}$	$E_{(4,5)}$	$E_{(5,5)}$	$E_{(5,6)}$	$E_{(6,6)}$
Number of edges	$6t - 12$	6	6	6	$3t - 9$	6	3	6	3

By using Table 1 and the Equation (1), we get the desired results, i.e.,

$$\begin{aligned} SD[M(J_{(3,t)})] &= \sum_{\theta, \omega \in E(M(J_{(3,t)}))} \frac{d_\theta^2 + d_\omega^2}{d_\theta d_\omega} \\ SD[M(J_{(3,t)})] &= E_{(2,4)} \sum_{\theta, \omega \in E(M(J_{(3,t)}))} \frac{d_\theta^2 + d_\omega^2}{d_\theta d_\omega} \\ &+ E_{(2,5)} \sum_{\theta, \omega \in E(M(J_{(3,t)}))} \frac{d_\theta^2 + d_\omega^2}{d_\theta d_\omega} \\ &+ E_{(3,5)} \sum_{\theta, \omega \in E(M(J_{(3,t)}))} \frac{d_\theta^2 + d_\omega^2}{d_\theta d_\omega} \\ &+ E_{(3,6)} \sum_{\theta, \omega \in E(M(J_{(3,t)}))} \frac{d_\theta^2 + d_\omega^2}{d_\theta d_\omega} \\ &+ E_{(4,4)} \sum_{\theta, \omega \in E(M(J_{(3,t)}))} \frac{d_\theta^2 + d_\omega^2}{d_\theta d_\omega} \\ &+ E_{(4,5)} \sum_{\theta, \omega \in E(M(J_{(3,t)}))} \frac{d_\theta^2 + d_\omega^2}{d_\theta d_\omega} \end{aligned}$$

$$\begin{aligned} 4. H[M(J_{(3,t)})] &= \frac{11t}{4} + \frac{8417}{4620}. \\ 5. M_1[M(J_{(3,t)})] &= 60t + 186. \\ 6. M_2[M(J_{(3,t)})] &= 96t + 501. \end{aligned}$$

Proof: The middle graph of Jahangir graph $M(J_{(3,t)})$ has 4 vertices of degree 3 and 6 vertices of degree 5, $3(t-2)$ vertices of degree 4, $3t-3$ vertices of degree 2 and 3 vertices of degree 6.

In $M(J_{(3,t)})$, we get edges of type $E_{(2,4)}$, $E_{(2,5)}$, $E_{(3,5)}$, $E_{(3,6)}$, $E_{(4,4)}$, $E_{(4,5)}$, $E_{(5,5)}$, $E_{(5,6)}$, and $E_{(6,6)}$. The number of edges of these types are given in Table 1.

$$\begin{aligned} &+ E_{(5,5)} \sum_{\theta, \omega \in E(M(J_{(3,t)}))} \frac{d_\theta^2 + d_\omega^2}{d_\theta d_\omega} \\ &+ E_{(5,6)} \sum_{\theta, \omega \in E(M(J_{(3,t)}))} \frac{d_\theta^2 + d_\omega^2}{d_\theta d_\omega} \\ &+ E_{(6,6)} \sum_{\theta, \omega \in E(M(J_{(3,t)}))} \frac{d_\theta^2 + d_\omega^2}{d_\theta d_\omega}. \\ SD[M(J_{(3,t)})] &= (6t - 12) \frac{(2)^2 + (4)^2}{8} \\ &+ (6) \frac{(2)^2 + (5)^2}{10} \\ &+ (6) \frac{(3)^2 + (5)^2}{15} \\ &+ (6) \frac{(3)^2 + (6)^2}{18} \\ &+ (3t - 9) \frac{(4)^2 + (4)^2}{16} \\ &+ (6) \frac{(4)^2 + (5)^2}{20} \\ &+ (3) \frac{(5)^2 + (5)^2}{25} \\ &+ (6) \frac{(5)^2 + (6)^2}{30} \\ &+ (3) \frac{(6)^2 + (6)^2}{36} \end{aligned}$$

$$SD[M(J_{(3,t)})] = (3t - 6)5 + \frac{216}{5} + (3t - 9)2 + 27 + \frac{123}{10}$$

$$SD[M(J_{(3,t)})] = 21t + 29.5.$$

$$SC(G) = \sum_{\theta\omega \in E(G)} \frac{1}{\sqrt{d_\theta + d_\omega}}$$

$$\begin{aligned} SC[M(J_{(3,t)})] &= E_{(2,4)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{1}{\sqrt{d_\theta + d_\omega}} \\ &+ E_{(2,5)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{1}{\sqrt{d_\theta + d_\omega}} \\ &+ E_{(3,5)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{1}{\sqrt{d_\theta + d_\omega}} \\ &+ E_{(3,6)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{1}{\sqrt{d_\theta + d_\omega}} \\ &+ E_{(4,4)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{1}{\sqrt{d_\theta + d_\omega}} \\ &+ E_{(4,5)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{1}{\sqrt{d_\theta + d_\omega}} \\ &+ E_{(5,5)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{1}{\sqrt{d_\theta + d_\omega}} \\ &+ E_{(5,6)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{1}{\sqrt{d_\theta + d_\omega}} \\ &+ E_{(6,6)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{1}{\sqrt{d_\theta + d_\omega}} \end{aligned}$$

$$\begin{aligned} SC[M(J_{(3,t)})] &= (6t - 12) \frac{1}{\sqrt{6}} + (6) \frac{1}{\sqrt{7}} \\ &+ (6) \frac{1}{\sqrt{8}} + (6) \frac{1}{\sqrt{9}} \\ &+ (3t - 9) \frac{1}{\sqrt{8}} + (6) \frac{1}{\sqrt{9}} \\ &+ (3) \frac{1}{\sqrt{10}} + (6) \frac{1}{\sqrt{11}} \\ &+ (3) \frac{1}{\sqrt{12}}. \end{aligned}$$

$$\begin{aligned} SC[M(J_{(3,t)})] &= \sqrt{6}t + \frac{3t}{\sqrt{8}} - 2\sqrt{6} - \frac{9}{\sqrt{8}} + 4 \\ &+ \frac{6}{\sqrt{7}} + \frac{3}{\sqrt{2}} + \frac{3}{\sqrt{10}} + \frac{6}{\sqrt{11}} \\ &+ \frac{\sqrt{3}}{2}. \end{aligned}$$

$$RC(G) = \sum_{\theta\omega \in E(G)} \frac{1}{\sqrt{d_\theta d_\omega}}$$

$$\begin{aligned} RC[M(J_{(3,t)})] &= E_{(2,4)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{1}{\sqrt{d_\theta d_\omega}} \\ &+ E_{(2,5)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{1}{\sqrt{d_\theta d_\omega}} \\ &+ E_{(3,5)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{1}{\sqrt{d_\theta d_\omega}} \\ &+ E_{(3,6)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{1}{\sqrt{d_\theta d_\omega}} \\ &+ E_{(4,4)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{1}{\sqrt{d_\theta d_\omega}} \\ &+ E_{(4,5)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{1}{\sqrt{d_\theta d_\omega}} \\ &+ E_{(5,5)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{1}{\sqrt{d_\theta d_\omega}} \\ &+ E_{(5,6)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{1}{\sqrt{d_\theta d_\omega}} \\ &+ E_{(6,6)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{1}{\sqrt{d_\theta d_\omega}}. \end{aligned}$$

$$\begin{aligned} RC[M(J_{(3,t)})] &= (6t - 12) \frac{1}{\sqrt{8}} + (6) \frac{1}{\sqrt{10}} \\ &+ (6) \frac{1}{\sqrt{15}} + (6) \frac{1}{\sqrt{18}} \\ &+ (3t - 9) \frac{1}{\sqrt{16}} + (6) \frac{1}{\sqrt{20}} \\ &+ (3) \frac{1}{\sqrt{25}} + (6) \frac{1}{\sqrt{30}} \\ &+ (3) \frac{1}{\sqrt{36}}. \end{aligned}$$

$$RC[M(J_{(3,t)})] = \left(\frac{3}{4} + \frac{3}{\sqrt{2}}\right)t + \frac{3}{\sqrt{5}} - 2\sqrt{2} + \sqrt{\frac{6}{5}} + 2\sqrt{\frac{3}{5}} + 3\sqrt{\frac{2}{5}} - \frac{23}{20}.$$

$$\begin{aligned} H(G) &= \sum_{\theta\omega \in E(G)} \frac{2}{(d_\theta + d_\omega)}. \\ H[M(J_{(3,t)})] &= E_{(2,4)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{2}{(d_\theta + d_\omega)} \\ &+ E_{(2,5)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{2}{(d_\theta + d_\omega)} \\ &+ E_{(3,5)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{2}{(d_\theta + d_\omega)} \\ &+ E_{(3,6)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{2}{(d_\theta + d_\omega)} \\ &+ E_{(4,4)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{2}{(d_\theta + d_\omega)} \\ &+ E_{(4,5)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{2}{(d_\theta + d_\omega)} \\ &+ E_{(5,5)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{2}{(d_\theta + d_\omega)} \\ &+ E_{(5,6)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{2}{(d_\theta + d_\omega)} \\ &+ E_{(6,6)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{2}{(d_\theta + d_\omega)}. \end{aligned}$$

$$\begin{aligned} H[M(J_{(3,t)})] &= (6t - 12)\frac{2}{6} + (6)\frac{2}{7} + (6)\frac{2}{8} \\ &+ (6)\frac{2}{9} + (3t - 9)\frac{2}{8} + (6)\frac{2}{9} \\ &+ (3)\frac{2}{10} + (6)\frac{2}{11} + (3)\frac{2}{12}. \end{aligned}$$

$$\begin{aligned} H[M(J_{(3,t)})] &= (2t - 4) + \frac{12}{7} + \frac{3}{2} + \frac{4}{3} \\ &+ (3t - 9)\frac{1}{4} + \frac{4}{3} + \frac{3}{5} + \frac{12}{11} + \frac{1}{2} \\ H[M(J_{(3,t)})] &= \frac{11t}{4} + \frac{8417}{4620}. \end{aligned}$$

$$M_1(G) = \sum_{\theta\omega \in E(G)} (d_\theta + d_\omega).$$

$$\begin{aligned} M_1[M(J_{(3,t)})] &= E_{(2,4)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} (d_\theta + d_\omega) \\ &+ E_{(2,5)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} (d_\theta \\ &+ d_\omega) \\ &+ E_{(3,5)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} (d_\theta \\ &+ d_\omega) \\ &+ E_{(3,6)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} (d_\theta \\ &+ d_\omega) \\ &+ E_{(4,4)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} (d_\theta \\ &+ d_\omega) \\ &+ E_{(4,5)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} (d_\theta \\ &+ d_\omega) \\ &+ E_{(5,5)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} (d_\theta \\ &+ d_\omega) \\ &+ E_{(5,6)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} (d_\theta \\ &+ d_\omega) \\ &+ E_{(6,6)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} (d_\theta \\ &+ d_\omega). \end{aligned}$$

$$\begin{aligned} M_1[M(J_{(3,t)})] &= (6t - 12)6 + (6)7 + (6)8 \\ &+ (6)9 + (3t - 9)8 + (6)9 \\ &+ (3)10 + (6)11 + (3)12. \end{aligned}$$

$$\begin{aligned} M_1[M(J_{(3,t)})] &= 36t - 72 + 42 + 48 + 54 \\ &+ 24t - 72 + 54 + 30 + 66 \\ &+ 36. \end{aligned}$$

$$M_1[M(J_{(3,t)})] = 60t + 186.$$

$$M_2(G) = \sum_{\theta\omega \in E(G)} (d_\theta d_\omega)$$

$$\begin{aligned}
 M_2[M(J_{(3,t)})] &= E_{(2,4)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} (d_\theta d_\omega) \\
 &\quad + E_{(2,5)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} (d_\theta d_\omega) \\
 &\quad + E_{(3,5)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} (d_\theta d_\omega) \\
 &\quad + E_{(3,6)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} (d_\theta d_\omega) \\
 &\quad + E_{(4,4)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} (d_\theta d_\omega) \\
 &\quad + E_{(4,5)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} (d_\theta d_\omega) \\
 &\quad + E_{(5,5)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} (d_\theta d_\omega) \\
 &\quad + E_{(5,6)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} (d_\theta d_\omega) \\
 &\quad + E_{(6,6)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} (d_\theta d_\omega).
 \end{aligned}$$

$$\begin{aligned}
 M_2[M(J_{(3,t)})] &= (6t - 12)8 + (6)10 + (6)15 \\
 &\quad + (6)18 + (3t - 9)16 + (6)20 \\
 &\quad + (3)25 + (6)30 + (3)36. \\
 M_2[M(J_{(3,t)})] &= 48t - 96 + 60 + 90 + 108 \\
 &\quad + 48n - 144 + 120 + 75 \\
 &\quad + 180 + 108. \\
 M_2[M(J_{(3,t)})] &= 96t + 501.
 \end{aligned}$$

Comparison

In this section, we give comparison of the above-computed topological indices numerically and the graphically. The numerical comparison of the middle graph of Jahangir graph $J_{(3,t)}$ is demonstrated in Table 2, where $t = 2, 3, \dots, 10$ and graphically comparison is depicted in the Figure 4.

TABLE 2 Numerical result of middle graph of Jahangir graph $J_{(3,t)}$

t	$SD[M(J_{(3,t)})]$	$SC[M(J_{(3,t)})]$	$RC[M(J_{(3,t)})]$	$H[M(J_{(3,t)})]$	$M_1[M(J_{(3,t)})]$	$M_2[M(J_{(3,t)})]$
2	76.5	10.0476	7.6478	7.3218	306	693
3	97.5	13.5578	10.5191	10.0718	366	789
4	118.5	17.0679	13.3905	12.8218	426	885
5	139.5	20.5781	16.2618	15.5718	486	981
6	160.5	24.0882	19.1331	18.3218	546	1077
7	181.5	27.5984	22.0044	21.0718	606	1173
8	202.5	31.1085	24.8757	23.8218	666	1269
9	223.5	34.6187	27.7471	26.5718	726	1365
10	244.5	38.1288	30.6184	29.3218	786	1461

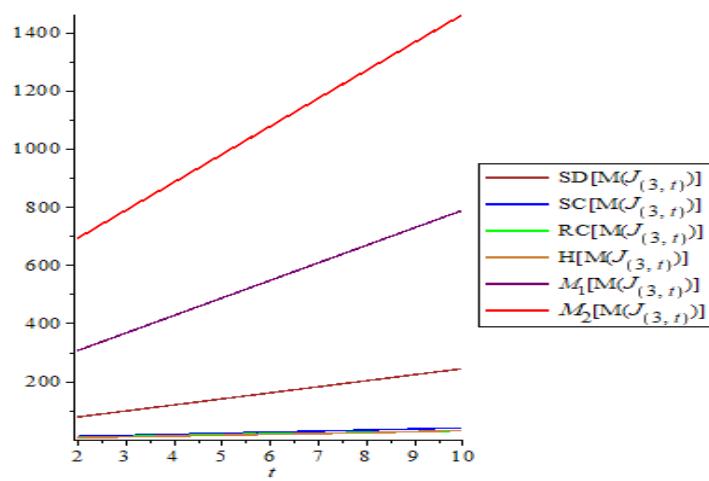


FIGURE 4 Graphical representation of middle graph of Jahangir graph $J_{(3,t)}$

Result for the Middle Graph of Circumcoronene Series of Benzenoid Graph (H_s)

In this section, we calculate the degree-based indices of the middle graph of (H_s), where $s \geq 2$.

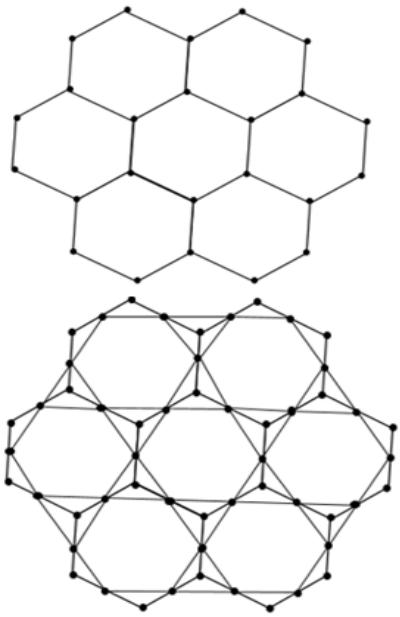


FIGURE 5 Circumcoronene series of benzenoid (H_2) and its middle graph $M(H_2)$

Theorem 4.1. Let $[M(H_s)]$ be the middle graph of circumcoronene series of benzenoid. Then,

$$SD[M(H_s)] = \frac{273}{5} + (s-1) \left(\frac{174}{5} + \frac{136}{5} + \frac{122}{5} \right) + (18s^2 - 30s + 12) \frac{5}{2} - 48s + 36s^2.$$

$$SC[M(H_s)] = \frac{12}{\sqrt{6}} + (s-1) \left(\frac{12}{\sqrt{7}} + \frac{6}{\sqrt{2}} + \frac{12}{\sqrt{11}} \right) + 6s^2 - 10s + 8 + \frac{6(2s-3)}{\sqrt{10}} + \frac{9(s^2-2s+1)}{\sqrt{3}}.$$

$$RC[M(H_s)] = \frac{6}{\sqrt{2}} + (s-1) \left(\frac{12}{\sqrt{10}} + \frac{12}{\sqrt{15}} + \frac{12}{\sqrt{30}} \right) + (6s^2 - 10s + 4) \frac{1}{\sqrt{2}} + \frac{6}{\sqrt{5}} + (2s-3) \frac{6}{5} + 3s^2 - 6s + 3.$$

$$H[M(H_s)] = \frac{1913}{1155}s + \frac{142}{1155} + 7s^2.$$

$$M_1[M(H_s)] = 378s^2 - 270s + 12.$$

$$M_2[M(H_s)] = 972s^2 - 876s + 90.$$

Proof: The middle graph of circumcoronene series of benzenoid $M(H_s)$ where, $s \geq 2$ has $6s$ vertices of degree 2, $6s(s-1)$ vertices of degree 3, 6 vertices of degree 4, $6s$ vertices of degree 5 and $9s^2 - 9s - 6$ vertices of degree 6.

In $M(H_s)$, we get edge of type $E_{(2,4)}, E_{(2,5)}, E_{(3,5)}, E_{(3,6)}, E_{(4,5)}, E_{(5,5)}, E_{(5,6)}$, and $E_{(6,6)}$. Table 3 lists the number of edges.

Now by using Table 3 and the Equation (1), we obtain the desired results, i.e.,

TABLE 3 Edge division

$E[d_u, d_v]$	Number of edges
$E_{(2,4)}$	12
$E_{(2,5)}$	$12(s-1)$
$E_{(3,5)}$	$12(s-1)$
$E_{(3,6)}$	$18s^2 - 30s + 12$
$E_{(4,5)}$	12
$E_{(5,5)}$	$6(2s-3)$
$E_{(5,6)}$	$12(s-1)$
$E_{(6,6)}$	$18(s^2 - 2s + 1)$

$$SD[M(J_{(3,t)})] = \sum_{\theta \omega \in E(G)} \frac{d_\theta^2 + d_\omega^2}{d_\theta d_\omega},$$

$$\begin{aligned}
SD[M(H_s)] &= E_{(2,4)} \sum_{\theta\omega \in E(M(H_s))} \frac{d_\theta^2 + d_\omega^2}{d_\theta d_\omega} \\
&+ E_{(2,5)} \sum_{\theta\omega \in E(M(H_s))} \frac{d_\theta^2 + d_\omega^2}{d_\theta d_\omega} \\
&+ E_{(3,5)} \sum_{\theta\omega \in E(M(H_s))} \frac{d_\theta^2 + d_\omega^2}{d_\theta d_\omega} \\
&+ E_{(3,6)} \sum_{\theta\omega \in E(M(H_s))} \frac{d_\theta^2 + d_\omega^2}{d_\theta d_\omega} \\
&+ E_{(4,5)} \sum_{\theta\omega \in E(M(H_s))} \frac{d_\theta^2 + d_\omega^2}{d_\theta d_\omega} \\
&+ E_{(5,5)} \sum_{\theta\omega \in E(M(H_s))} \frac{d_\theta^2 + d_\omega^2}{d_\theta d_\omega} \\
&+ E_{(5,6)} \sum_{\theta\omega \in E(M(H_s))} \frac{d_\theta^2 + d_\omega^2}{d_\theta d_\omega} \\
&+ E_{(6,6)} \sum_{\theta\omega \in E(M(H_s))} \frac{d_\theta^2 + d_\omega^2}{d_\theta d_\omega}.
\end{aligned}$$

$$\begin{aligned}
SD[M(H_s)] &= (12) \frac{(2)^2 + (4)^2}{8} + 12(s-1) \frac{(2)^2 + (5)^2}{10} + 12(s-1) \frac{(3)^2 + (5)^2}{15} + (18s^2 - 30s + 12) \frac{(3)^2 + (6)^2}{18} \\
&+ (12) \frac{(4)^2 + (5)^2}{20} + 6(2s-3) \frac{(5)^2 + (5)^2}{25} + 12(s-1) \frac{(5)^2 + (6)^2}{30} + 18(s^2 - 2s + 1) \frac{(6)^2 + (6)^2}{36}.
\end{aligned}$$

$$SD[M(H_s)] = 81s^2 - \frac{183s}{5} - \frac{9}{5}.$$

$$SC(G) = \sum_{\theta\omega \in E(G)} \frac{1}{\sqrt{d_\theta d_\omega}}.$$

$$\begin{aligned}
SC[M(H_s)] &= E_{(2,4)} \sum_{\theta\omega \in E(M(H_s))} \frac{1}{\sqrt{d_\theta + d_\omega}} \\
&+ E_{(2,5)} \sum_{\theta\omega \in E(M(H_s))} \frac{1}{\sqrt{d_\theta + d_\omega}} \\
&+ E_{(3,5)} \sum_{\theta\omega \in E(M(H_s))} \frac{1}{\sqrt{d_\theta + d_\omega}} \\
&+ E_{(3,6)} \sum_{\theta\omega \in E(M(H_s))} \frac{1}{\sqrt{d_\theta + d_\omega}} \\
&+ E_{(4,5)} \sum_{\theta\omega \in E(M(H_s))} \frac{1}{\sqrt{d_\theta + d_\omega}} \\
&+ E_{(5,5)} \sum_{\theta\omega \in E(M(H_s))} \frac{1}{\sqrt{d_\theta + d_\omega}} \\
&+ E_{(5,6)} \sum_{\theta\omega \in E(M(H_s))} \frac{1}{\sqrt{d_\theta + d_\omega}} \\
&+ E_{(6,6)} \sum_{\theta\omega \in E(M(H_s))} \frac{1}{\sqrt{d_\theta + d_\omega}}
\end{aligned}$$

$$\begin{aligned}
SC[M(H_s)] &= (12) \frac{1}{\sqrt{6}} + 12(s-1) \frac{1}{\sqrt{7}} + 12(s-1) \frac{1}{\sqrt{8}} + (18s^2 - 30s + 12) \frac{1}{\sqrt{9}} + 6(2s-3) \frac{1}{\sqrt{10}} + 12(s-1) \frac{1}{\sqrt{11}} + 18(s^2 - 2s + 1) \frac{1}{\sqrt{12}}.
\end{aligned}$$

$$\begin{aligned}
SC[M(H_s)] &= \frac{12}{\sqrt{6}} + (s-1) \left(\frac{12}{\sqrt{7}} + \frac{6}{\sqrt{2}} + \frac{12}{\sqrt{11}} \right) + 6s^2 - 10s + 8 + \frac{6(2s-3)}{\sqrt{10}} + \frac{9(s^2 - 2s + 1)}{\sqrt{3}}.
\end{aligned}$$

$$RC(G) = \sum_{\theta\omega \in E(G)} \frac{1}{\sqrt{d_\theta d_\omega}}$$

$$\begin{aligned}
RC[M(H_s)] &= E_{(2,4)} \sum_{\theta\omega \in E(M(H_s))} \frac{1}{\sqrt{d_\theta d_\omega}} \\
&\quad + E_{(2,5)} \sum_{\theta\omega \in E(M(H_s))} \frac{1}{\sqrt{d_\theta d_\omega}} \\
&\quad + E_{(3,5)} \sum_{\theta\omega \in E(M(J_{(3,t)}))} \frac{1}{\sqrt{d_\theta d_\omega}} \\
&\quad + E_{(3,6)} \sum_{\theta\omega \in E(M(H_s))} \frac{1}{\sqrt{d_\theta d_\omega}} \\
&\quad + E_{(4,5)} \sum_{\theta\omega \in E(M(H_s))} \frac{1}{\sqrt{d_\theta d_\omega}} \\
&\quad + E_{(5,5)} \sum_{\theta\omega \in E(M(H_s))} \frac{1}{\sqrt{d_\theta d_\omega}} \\
&\quad + E_{(5,6)} \sum_{\theta\omega \in E(M(H_s))} \frac{1}{\sqrt{d_\theta d_\omega}} \\
&\quad + E_{(6,6)} \sum_{\theta\omega \in E(M(H_s))} \frac{1}{\sqrt{d_\theta d_\omega}}. \\
RC[M(H_s)] &= \frac{12}{\sqrt{8}} + 12(s-1) \frac{1}{\sqrt{10}} + 12(s-1) \frac{1}{\sqrt{15}} + (18s^2 - 30s + 12) \frac{1}{\sqrt{18}} + \frac{12}{\sqrt{20}} + 6(2s-3) \frac{1}{\sqrt{25}} + 12(s-1) \frac{1}{\sqrt{30}} + 18(s^2 - 2s + 1) \frac{1}{\sqrt{36}}. \\
RC[M(H_s)] &= \frac{6}{\sqrt{2}} + (s-1) \left(\frac{12}{\sqrt{10}} + \frac{12}{\sqrt{15}} + \frac{12}{\sqrt{30}} \right) + (6s^2 - 10s + 4) \frac{1}{\sqrt{2}} + \frac{6}{\sqrt{5}} + (2s-3) \frac{6}{5} + 3s^2 - 6s + 3. \\
H(G) &= \sum_{\theta\omega \in E(G)} \frac{2}{(d_\theta + d_\omega)}.
\end{aligned}$$

$$\begin{aligned}
H[M(H_s)] &= E_{(2,4)} \sum_{\theta\omega \in E(M(H_s))} \frac{2}{(d_\theta + d_\omega)} \\
&\quad + E_{(2,5)} \sum_{\theta\omega \in E(M(H_s))} \frac{2}{(d_\theta + d_\omega)} \\
&\quad + |E_{(3,5)}| \sum_{\theta\omega \in E(M(H_s))} \frac{2}{(d_\theta + d_\omega)} \\
&\quad + E_{(3,6)} \sum_{\theta\omega \in E(M(H_s))} \frac{2}{(d_\theta + d_\omega)} \\
&\quad + E_{(4,5)} \sum_{\theta\omega \in E(M(H_s))} \frac{2}{(d_\theta + d_\omega)} \\
&\quad + E_{(5,5)} \sum_{\theta\omega \in E(M(H_s))} \frac{2}{(d_\theta + d_\omega)} \\
&\quad + E_{(5,6)} \sum_{\theta\omega \in E(M(H_s))} \frac{2}{(d_\theta + d_\omega)} \\
&\quad + E_{(6,6)} \sum_{\theta\omega \in E(M(H_s))} \frac{2}{(d_\theta + d_\omega)}. \\
H[M(H_s)] &= \frac{24}{6} + 12(s-1) \frac{2}{7} + 12(s-1) \frac{2}{8} + (18s^2 - 30s + 12) \frac{2}{9} + (12) \frac{2}{9} + 6(2s-3) \frac{2}{10} + 12(s-1) \frac{2}{11} + 18(s^2 - 2s + 1) \frac{2}{12}. \\
H[M(H_s)] &= (s-1) \frac{24}{7} + 3(s-1) + (6s^2 - 10s + 4) \frac{2}{3} + (2s-3) \frac{6}{5} + (s-1) \frac{24}{11} + 3(s^2 - 2s + 1) \frac{20}{3}. \\
H[M(H_s)] &= \frac{1913}{1155}s + \frac{142}{1155} + 7s^2. \\
M_1(G) &= \sum_{\theta\omega \in E(G)} (d_\theta + d_\omega).
\end{aligned}$$

$$\begin{aligned}
 M_1[M(H_s)] &= E_{(2,4)} \sum_{\theta\omega \in E(M(H_s))} (d_\theta + d_\omega) \\
 &+ E_{(2,5)} \sum_{\theta\omega \in E(M(H_s))} (d_\theta + d_\omega) \\
 &+ E_{(3,5)} \sum_{\theta\omega \in E(M(H_s))} (d_\theta + d_\omega) \\
 &+ E_{(3,6)} \sum_{\theta\omega \in E(M(H_s))} (d_\theta + d_\omega) \\
 &+ E_{(4,5)} \sum_{\theta\omega \in E(M(H_s))} (d_\theta + d_\omega) \\
 &+ E_{(5,5)} \sum_{\theta\omega \in E(M(H_s))} (d_\theta + d_\omega) \\
 &+ E_{(5,6)} \sum_{\theta\omega \in E(M(H_s))} (d_\theta + d_\omega) \\
 &+ E_{(6,6)} \sum_{\theta\omega \in E(M(H_s))} (d_\theta + d_\omega) \\
 M_1[M(H_s)] &= 72 + 12(s-1)7 + 12(s-1)8 \\
 &+ (18s^2 - 30s + 12)9 + 108 \\
 &+ 6(2s-3)10 + 12(s-1)11 \\
 &+ 18(s^2 - 2s + 1)12 \\
 M_1[M(H_s)] &= 432s + 27(6s^2 - 10s + 4) \\
 &+ 216(s^2 - 2s + 1) - 312. \\
 M_1[M(H_s)] &= 378s^2 - 270s + 12. \\
 M_2(G) &= \sum_{\theta\omega \in E(G)} (d_\theta d_\omega).
 \end{aligned}$$

$$\begin{aligned}
 M_2[M(H_s)] &= E_{(2,4)} \sum_{\theta\omega \in E(M(H_s))} (d_\theta d_\omega) \\
 &+ E_{(2,5)} \sum_{\theta\omega \in E(M(H_s))} (d_\theta d_\omega) \\
 &+ E_{(3,5)} \sum_{\theta\omega \in E(M(H_s))} (d_\theta d_\omega) \\
 &+ E_{(3,6)} \sum_{\theta\omega \in E(M(H_s))} (d_\theta d_\omega) \\
 &+ E_{(4,5)} \sum_{\theta\omega \in E(M(H_s))} (d_\theta d_\omega) \\
 &+ E_{(5,5)} \sum_{\theta\omega \in E(M(H_s))} (d_\theta d_\omega) \\
 &+ E_{(5,6)} \sum_{\theta\omega \in E(M(H_s))} (d_\theta d_\omega) \\
 &+ E_{(6,6)} \sum_{\theta\omega \in E(M(H_s))} (d_\theta d_\omega). \\
 M_2[M(H_s)] &= (12)8 + 12(s-1)10 + 12(s-1)15 + (18s^2 - 30s + 12)18 + (12)20 + 6(2s-3)25 + 12(s-1)30 \\
 &+ 18(s^2 - 2s + 1)36. \\
 M_2[M(H_s)] &= 960s + 54(6s^2 - 10s + 4) \\
 &+ 648(s^2 - 2s + 1) - 774. \\
 M_2[M(H_s)] &= 972s^2 - 876s + 90.
 \end{aligned}$$

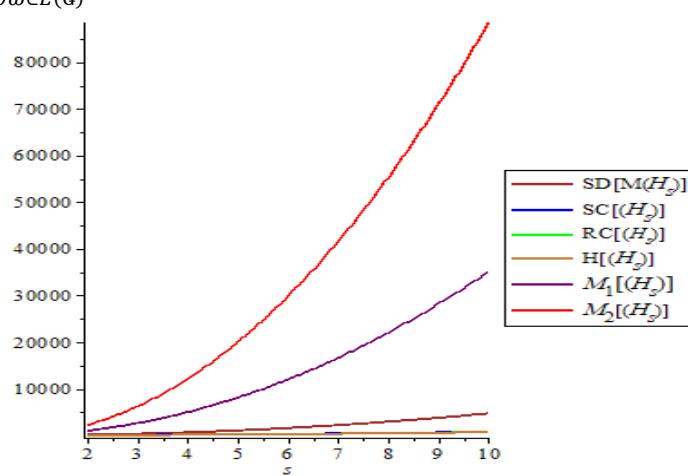


FIGURE 6 Graphical representation of middle graph of (H_s)

Comparison

In this section, we provide the comparison of the above-computed topological indices numerically and the graphically. The

numerical comparison of $M(H_s)$ where, $s = 2, 3, \dots, 10$, as presented in Table 4, and the graphical comparison is displayed in the Figure 6.

TABLE 4 Numerical results of middle graph of (H_s)

s	SD[$M(H_s)$]	SC[$M(H_s)$]	RC[$M(H_s)$]	H[$M(H_s)$]	$M_1[M(H_s)]$	$M_2[M(H_s)]$
2	129.6	32.192	24.475	24.810	984	2226
3	324.6	71.383	57.510	58.154	2604	6210
4	627.6	124.57	105.03	105.50	4980	12138
5	1038.6	191.76	167.03	166.84	8112	20010
6	1557.6	272.96	243.52	242.19	12000	29825
7	2184.6	368.15	334.50	331.53	16644	41586
8	2919.6	477.35	439.96	434.87	22044	55290
9	3762.6	600.52	559.91	552.22	28200	70938
10	4713.6	737.72	694.34	683.56	35112	88530

Conclusion

Topological indices help to understand the information about biological activity, chemical reactivity, and physical characteristics of chemical compounds. We derived the general formulas of some of the topological indices based on the degree of vertex i.e. sum connectivity index (SC), Randic connectivity index (RC), Symmetric division degree index (SD), Harmonic index (H), the first Zagreb index (M_1), and the second Zagreb index (M_2) of the middle graph of Jahangir graph $J_{(3,t)}$. These outcomes can be employed to further understand the topological characteristics of graphs. The comparison of attained analytical expressions is expressed graphically and numerically.

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Conflict of Interest

The authors declare that there is no conflict of interests regarding the publication of this manuscript.

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