Computation of neighbourhood degree based topological indices for circumcoronene series of benzenoid

A. Gayathri* | D. Narasimhan* | M. Fathima* | F. Vincy*

*Department of Mathematics, Srinivasa Ramanujan Centre, SASTRA Deemed to be University, Kumbakonam, Tamil Nadu 612001, India.

Abstract Benzene is present in a group of chemical compounds known as the Circumcoronene series. Their regular hexagon-shaped benzene ring structure around the circle serves as a distinguishing feature. This article examines the several index types for this series according to the degrees of open and closed neighborhoods. Furthermore, we estimate indices to the benzenoid Circumcoronene family based on reduced reverse degrees. Using MATLAB, the distributions of these indices are also compared and analysed.

Keywords: open neighbourhood degree based topological index, closed neighbourhood degree based topological index, reduced reverse degree based topological index

1. Introduction

Chemical network theory is a branch of applied mathematics that aspires to replicate the structure-activity correlations that exist in the real world of chemicals. It has gained increasing prominence within the scientific community over the past century, owing to advancements in organic chemistry and theoretical chemistry. One of the most widely recognized topological descriptors was first introduced by chemist Harold Wiener in 1947. These indices are typically graph invariants, and they provide insights into the topology of chemical structures. The neighborhood degree of a node, denoted as \( \delta(x) \), represents the sum of degrees of all neighboring nodes connected to \( x \) (Ravi V, 2021). In this study, we compute several topological descriptors, including the Modified Randic Index and Inverse Sum Index, based on both open and closed neighborhood criteria, as well as the Reduced Reverse Index, for the Circumcoronene series within the Benzenoid family (Gao Y, 2018). The topological descriptors of the chemical graphs are very useful to study and analyze various chemical properties mathematically. In 1947, chemist Harold Wiener proposed one of the most well-known topological descriptors, giving rise to topological indices in chemistry. While Wiener was looking for structural connections among paraffin boiling points, he performed innovative studies that gave rise to the notion of topological index.

2. Equations and mathematical definitions

The formulations of certain topological indices relying on open neighborhood degree, referred to as \( SK_N^c(G) \), \( SK1_N^c(G) \), \( SK2_N^c(G) \), \( mR_N^c(G) \), \( ISI_N^c(G) \) are given below:

\[
SK_N^c(G) = \sum_{xy \in E(G)} \frac{\delta(x) + \delta(y)}{2} \tag{1}
\]

\[
SK1_N^c(G) = \sum_{xy \in E(G)} \frac{\delta(x) + \delta(y)}{2} \tag{2}
\]

\[
SK2_N^c(G) = \sum_{uv \in E(G)} \left[ \frac{\delta(x) + \delta(y)}{2} \right]^2 \tag{3}
\]

\[
mR_N^c(G) = \sum_{xy \in E(G)} \frac{1}{\max \{\delta(x), \delta(y)\}} \tag{4}
\]

\[
ISI_N^c(G) = \sum_{uv \in E(G)} \frac{\delta(u) \cdot \delta(v)}{\delta(u) + \delta(v)} \tag{5}
\]

Where \( \delta(x) = \sum_{y \in N(x)} \deg(y) \), \( N(x) \) is the neighborhood set of the vertex \( x \).

The closed neighborhood counterparts of the aforementioned topological indices are labeled as \( SK_N^c(G) \), \( SK1_N^c(G) \), \( SK2_N^c(G) \), \( mR_N^c(G) \), \( ISI_N^c(G) \) and their reciprocals are given below:
\[ SK^C_2(G) = \sum_{xy \in E(G)} \frac{\delta[x] + \delta[y]}{2} \quad (6) \]
\[ SK^C_1(G) = \sum_{xy \in E(G)} \frac{\delta[x] \cdot \delta[y]}{2} \quad (7) \]
\[ SK^C_0(G) = \sum_{uv \in E(G)} \left[ \frac{\delta[x] + \delta[y]}{2} \right]^2 \quad (8) \]
\[ mR^C_0(G) = \sum_{xy \in E(G)} \frac{1}{\max \{\delta[x], \delta[y]\}} \quad (9) \]
\[ ISI^C_0(G) = \sum_{xy \in E(G)} \frac{\delta[x] \cdot \delta[y]}{\delta[x] + \delta[y]} \quad (10) \]
\[ rSK^C_2(G) = \sum_{xy \in E(G)} \frac{2}{\delta[x] + \delta[y]} \quad (11) \]
\[ rSK^C_1(G) = \sum_{xy \in E(G)} \frac{2}{\delta[x] \cdot \delta[y]} \quad (12) \]
\[ rSK^C_0(G) = \sum_{xy \in E(G)} \left( \frac{2}{\delta[x] + \delta[y]} \right)^2 \quad (13) \]
\[ rmR^C_0(G) = \sum_{xy \in E(G)} \max \{\delta[x], \delta[y]\} \quad (14) \]
\[ rISI^C_0(G) = \sum_{uv \in E(G)} \frac{\delta[x] \cdot \delta[y]}{\delta[x] \cdot \delta[y]} \quad (15) \]

Where \( \delta[x] = \left[ \sum_{y \in (x)} \deg(y) \right] + \deg(x) \), \( N(x) \) is the neighborhood of the vertex \( x \).

The Zagreb Indices based on Reduced Reverse Vertex Degrees, designated as \( RRM_1(G), RRM_2(G), RRMH_1(G), RRMH_2(G), RRF(G) \), are given below:

\[ RRM_1(G) = \sum_{xy \in E(G)} \left[ R_R x + R_R y \right] \quad (16) \]
\[ RRM_2(G) = \sum_{xy \in E(G)} \left[ R_R x \ast R_R y \right] \quad (17) \]
\[ RRMH_1(G) = \sum_{xy \in E(G)} \left[ R_R x + R_R y \right]^2 \quad (18) \]
\[ RRMH_2(G) = \sum_{xy \in E(G)} \left[ R_R x \ast R_R y \right]^2 \quad (19) \]
\[ RRF(G) = \sum_{xy \in E(G)} \left[ R_R x^2 + R_R y^2 \right] \quad (20) \]
\[ RRABC(G) = \sum_{xy \in E(G)} \left[ \frac{R_R x + R_R y - 2}{R_R x \ast R_R y} \right] \quad (21) \]

2.1. Reduced Reverse degree

Let \( G \) be a Graph and \( v \) be a vertex of \( G \). The reduced reverse degree is defined as

\[ RR_v = \Delta(G) - d_v + 2. \]

3. Results and discussions

3.1. Results on Open Neighborhood degree:

The way they classify a wide range of topological indices is based on the structural characteristics of the graphs that they compute. Graph topological indices can be generically classified into three types: distance-based, degree-based, and counting-related indices. Because of their consistent predictive potential, degree-based topological indices have been used to construct multi-linear regression models for statistical characteristic correlation.

The tabulated data in Table 1 shows how a set of edge degree pairs usually are arranged inside layers H \( (H > 2) \).

1. The \( SK^C_N(G) \) index of the Circumcoronene series of benzenoid with H layer is given by

\[ SK^C_N(G) = \begin{cases} 
24 & \text{if } H = 1 \\
81H^2 - 63H + 6 & \text{if } H \geq 2 
\end{cases} \]
Proof:

Let $SK_N^{\xi}(G) = \sum_{x,y \in E(G)} \frac{\delta(x)+\delta(y)}{2}$

For $H = 1$, $SK_N^{\xi}(G) = 6 \left( \frac{4+4}{2} \right) = 24$.

For $H \geq 2$, consider the edge partition in Table 1.

<table>
<thead>
<tr>
<th>$(\delta(x), \delta(y))$</th>
<th>General Pattern</th>
</tr>
</thead>
<tbody>
<tr>
<td>(5,5)</td>
<td>6</td>
</tr>
<tr>
<td>(5,7)</td>
<td>12</td>
</tr>
<tr>
<td>(6,7)</td>
<td>$12(H-1)$</td>
</tr>
<tr>
<td>(7,9)</td>
<td>$6(H-1)$</td>
</tr>
<tr>
<td>(9,9)</td>
<td>$9H^2 - 21H + 12$</td>
</tr>
</tbody>
</table>

$SK_N^{\xi}(G) = 6 \left( \frac{5+5}{2} \right) + 12 \left( \frac{5+7}{2} \right) + 12(H-2) \left( \frac{6+7}{2} \right) + 6(H-1) \left( \frac{7+9}{2} \right) + (9H^2 - 21H + 12) \left( \frac{9+9}{2} \right)$

$= 30 + 72 + 78(H-2) + 48(H-1) + 9(9H^2 - 21H + 12)$

$= 81H^2 - 63H + 6$.

Hence for both the cases, the value of the defined index for the Circumcoronene series of benzenoid is obtained.

2. The $SK1_N^{\xi}(G)$ index of the Circumcoronene series of benzenoid with H layer is given by

$$SK1_N^{\xi}(G) = \begin{cases} 24 & \text{if } H = 1 \\ \frac{1}{2}(729H^2 - 819H + 156) & \text{if } H \geq 2 \end{cases}$$

Proof:

Let $SK1_N^{\xi}(G) = \sum_{x,y \in E(G)} \frac{\delta(x)+\delta(y)}{2}$

For $H = 1$, $SK1_N^{\xi}(G) = 6 \left( \frac{4+4}{2} \right) = 24$.

For $H \geq 2$, consider the edge partition in Table 1.

$SK1_N^{\xi}(G) = 6 \left( \frac{5+5}{2} \right) + 12 \left( \frac{5+7}{2} \right) + 12(H-2) \left( \frac{6+7}{2} \right) + 6(H-1) \left( \frac{7+9}{2} \right) + (9H^2 - 21H + 12) \left( \frac{9+9}{2} \right)$

$= \frac{1}{2}(729H^2 - 819H + 156)$.

For this reason, the value of the chosen index of the benzenoid Circumcoronene series has been estimated for each instance.

3. The $SK2_N^{\xi}(G)$ index of the Circumcoronene series of benzenoid with H layer is given by

$$SK2_N^{\xi}(G) = \begin{cases} 96 & \text{if } H = 1 \\ 729H^2 - 810H + 156 & \text{if } H \geq 2 \end{cases}$$

Proof:

Let $SK2_N^{\xi}(G) = \sum_{x,y \in E(G)} \left[ \frac{\delta(x)+\delta(y)}{2} \right]^2$

For $H = 1$, $SK2_N^{\xi}(G) = 6 \left( \frac{4+4}{2} \right)^2 = 96$.

For $H \geq 2$, consider the edge partition in Table 1.

$SK2_N^{\xi}(G) = 6 \left( \frac{5+5}{2} \right)^2 + 12 \left( \frac{5+7}{2} \right)^2 + 12(H-2) \left( \frac{6+7}{2} \right)^2 + 6(H-1) \left( \frac{7+9}{2} \right)^2 + (9H^2 - 21H + 12) \left( \frac{9+9}{2} \right)^2$

$= \frac{1}{16}(10^2) + 12(12^2) + 12(H-2)(13^2) + 6(H-1)(16^2) + 18(9H^2 - 21H + 12)$

$= 729H^2 - 810H + 156$

Therefore, the specified numerical values of the index have been derived for all feasible values of H.

4. The $mR_N^{\xi}(G)$ index of the Circumcoronene series of benzenoid with H layer is given by
\[ mR^G_N(H) = \begin{cases} 
\frac{1.5}{H} + \frac{16}{105} & \text{if } H = 1 \\
\frac{H^2}{21} + \frac{16}{105} & \text{if } H \geq 2 
\end{cases} \]

Proof:
Let \( mR^G_N(G) = \sum_{x,y \in E(G)} \frac{1}{\max(\delta(x),\delta(y))} \)
For \( H = 1 \), \( mR^G_N(G) = 6 \left( \frac{1}{\max(4,4)} \right) = 1.5. \)
For \( H \geq 2 \), consider the edge partition in Table 1.
\[
mR^G_N(G) = \frac{6}{\max(5,5)} + \frac{12}{\max(5,7)} + \frac{12(H - 2)}{\max(6,7)} + \frac{6(H - 1)}{\max(7,9)} + \frac{9H^2 - 21H + 12}{\max(9,9)} = \frac{H^2}{21} + \frac{16}{105} \]

As a result, the given calculation is used to determine the index value for the Circumcoronene series of benzenoids.

5. The \( ISI^G_N(G) \) index of the Circumcoronene series of benzenoid with H layer is given by
\[
ISI^G_N(G) = \begin{cases} 
\frac{12}{H^2} - \frac{3339}{104} - \frac{295}{104} & \text{if } H = 1 \\
\text{if } H \geq 2 
\end{cases} \]

Proof:
Let \( ISI^G_N(G) = \sum_{u \in \delta(N_G)} \frac{\sum_{v \in \delta(N_G)} - \sum_{e \in \delta(N_G)}}{\delta(u) + \delta(v)} \)
For \( H = 1 \), \( ISI^G_N(G) = 6 \left( \frac{24x}{(x+4)} \right) = 12 \)
For \( H \geq 2 \), consider the edge partition in Table 1.
\[
ISI^G_N(G) = 6 \left( \frac{5 + 5}{5 + 5} \right) + 12 \left( \frac{5 + 7}{5 + 7} \right) + 12(H - 2) \left( \frac{6 + 7}{6 + 7} \right) + 6(H - 1) \left( \frac{7 + 9}{7 + 9} \right) + (9H^2 - 21H + 12) \left( \frac{9 + 9}{9 + 9} \right) = \frac{15 + 35 + 504}{13(\frac{81}{\frac{2}{H^2} - \frac{295}{104}})} = \frac{1008}{189} + \frac{189}{81} - \frac{8}{2H^2} - \frac{8}{2H + 54} = \frac{5}{2H^2} - \frac{295}{104} 
\]

Accordingly, the Circumcoronene series of benzenoid yields the indicated index value. Figure 1 displays the visual and numerical representations. As one looks at Table 2 and the picture, it becomes clear that every index has an increasing H value and is arranged in an ascending manner.

<table>
<thead>
<tr>
<th>( H )</th>
<th>( SK^G_N(G) )</th>
<th>( SK^G_N(G) )</th>
<th>( SK^G_N(G) )</th>
<th>( mR^G_N(G) )</th>
<th>( ISI^G_N(G) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>204</td>
<td>717</td>
<td>1452</td>
<td>4.2476</td>
<td>100.625</td>
</tr>
<tr>
<td>3</td>
<td>546</td>
<td>2130</td>
<td>4287</td>
<td>9.2952</td>
<td>271.019</td>
</tr>
<tr>
<td>4</td>
<td>1050</td>
<td>4272</td>
<td>8580</td>
<td>16.3429</td>
<td>522.413</td>
</tr>
<tr>
<td>5</td>
<td>1716</td>
<td>7143</td>
<td>14331</td>
<td>25.3904</td>
<td>854.808</td>
</tr>
<tr>
<td>6</td>
<td>2544</td>
<td>10743</td>
<td>21540</td>
<td>36.4381</td>
<td>1268.202</td>
</tr>
<tr>
<td>7</td>
<td>3534</td>
<td>15072</td>
<td>30207</td>
<td>49.4857</td>
<td>1762.596</td>
</tr>
<tr>
<td>8</td>
<td>4686</td>
<td>20130</td>
<td>40332</td>
<td>64.5333</td>
<td>2337.990</td>
</tr>
<tr>
<td>9</td>
<td>6000</td>
<td>25917</td>
<td>51915</td>
<td>81.5810</td>
<td>2994.385</td>
</tr>
<tr>
<td>10</td>
<td>7476</td>
<td>32433</td>
<td>64956</td>
<td>100.6286</td>
<td>3731.779</td>
</tr>
<tr>
<td>11</td>
<td>9114</td>
<td>39678</td>
<td>79455</td>
<td>121.6762</td>
<td>4550.173</td>
</tr>
</tbody>
</table>

Figure 1 depicts the graphical representations of open neighborhood degree-based indices obtained from results 2.1 to 5. It shows that SK1 and SK2 indices have more deviation from the other three, such as SK, MR, and ISI.

3.2. Results On Closed Neighborhood degree

Indices reveal chemical structural topology, generally graph invariants. Its neighborhood degree is the total number of surrounding nodes connected to a node 'n'. The chemical structures' qualities and properties will be better identified by indices defined using neighborhood degree-based methodology.

https://www.malque.pub/ojs/index.php/msj
The general arrangement of a set of edge degree pairs within the closed neighborhood of the circumcoronene series of benzenoids for layer \(H\) \((h > 2)\) is stated in Table 3.

### Table 3 Edge pattern based on closed neighborhood.

<table>
<thead>
<tr>
<th>((δ[x], δ[y]))</th>
<th>General Pattern</th>
</tr>
</thead>
<tbody>
<tr>
<td>(7,7)</td>
<td>6</td>
</tr>
<tr>
<td>(7,10)</td>
<td>12</td>
</tr>
<tr>
<td>(8,10)</td>
<td>(12(H - 1))</td>
</tr>
<tr>
<td>(10,12)</td>
<td>(6(H - 1))</td>
</tr>
<tr>
<td>(12,12)</td>
<td>(9H^2 - 21H + 12)</td>
</tr>
</tbody>
</table>

6. The \(SK^C_N(G)\) index of the Circumcoronene series of benzenoid with H layer is given by

\[
SK^C_N(G) = \begin{cases} 
36 & \text{if } H = 1 \\
648H^2 - 672H + 111 & \text{if } H \geq 2 
\end{cases}
\]

**Proof:**

Let \(SK^C_N(G) = \sum_{xy \in E(G)} \frac{δ[x] + δ[y]}{2}\)

For \(H = 1, SK^C_N(G) = 6 \left(\frac{6 + 6}{2}\right) = 36.\)

For \(H \geq 2,\) consider the edge partition in Table 3.

\[
SK^C_N(G) = 6 \left(\frac{7 + 7}{2}\right) + 12 \left(\frac{7 + 10}{2}\right) + 12(H - 2) \left(\frac{8 + 10}{2}\right) + 6(H - 1) \left(\frac{10 + 12}{2}\right) + (9H^2 - 21H + 12) \left(\frac{12 + 12}{2}\right)
\]

\[
= 6(7) + 12 \left(\frac{17}{2}\right) + 12(H - 2)(9) + 6(H - 1)(11) + 12(9H^2 - 21H + 12)
\]

\[
= 648H^2 - 672H + 111.
\]

As a result, the statement’s numerical value for the index of the benzenoid Circumcoronene series is obtained for every case.

7. The \(SK^C_1(G)\) index of the Circumcoronene series of benzenoid with H layer is given by

\[
SK^C_1(G) = \begin{cases} 
108 & \text{if } H = 1 \\
648H^2 - 672H + 111 & \text{if } H \geq 2 
\end{cases}
\]

**Proof:**

Let \(SK^C_1(G) = \sum_{xy \in E(G)} \frac{δ[x] + δ[y]}{2}\)

For \(H = 1, SK^C_1(G) = 6 \left(\frac{6 + 6}{2}\right) = 108.\)

For \(H \geq 2,\) consider the edge partition in Table 3.
Let \( SK1_S^C(G) = 6 \left( \frac{7 \* 7}{2} \right) + 12 \left( \frac{7 \* 10}{2} \right) + 12(H - 2) \left( \frac{8 \* 10}{2} \right) + 6(H - 1) \left( \frac{10 \* 12}{2} \right) + (9H^2 - 21H + 12) \left( \frac{12 \* 12}{2} \right) \)

\[ = 147 + 420 + 480(H - 2) + 3360(H - 1) + 72(9H^2 - 21H + 12) \]

\[ = 648H^2 - 672H + 111. \]

Thus, the value of the index of the Circumcoronene series of benzenoid is calculated as stated.

8. The \( SK2_S^C(G) \) index of the Circumcoronene series of benzenoid with H layer is given by

\[ SK2_S^C(G) = \begin{cases} 216 & \text{if } H = 1 \\ 1296H^2 - 1326H + 219 & \text{if } H \geq 2 \end{cases} \]

Proof:
Let \( SK2_S^C(G) = \sum_{uv \in E(G)} \left[ \delta(x) + \delta(y) \right]^2 \)

For \( H = 1 \), \( SK2_S^C(G) = 6 \left( \frac{6+6}{2} \right)^2 = 216. \)

For \( H \geq 2 \), consider the edge partition in Table 3.

\[ SK2_S^C(G) = 6 \left( \frac{7 + 7}{2} \right)^2 + 12 \left( \frac{7 + 10}{2} \right)^2 + 12(H - 2) \left( \frac{8 + 10}{2} \right)^2 + 6(H - 1) \left( \frac{10 + 12}{2} \right)^2 + (9H^2 - 21H + 12) \left( \frac{12 + 12}{2} \right)^2 \]

\[ = \frac{1}{4} [1176 + 3468 + 3888(H - 2) + 2904(H - 1) + 1728(3H^2 - 7H + 4)] \]

\[ = \frac{1}{4} [5184H^2 - 5304H + 876] \]

\[ = 1296H^2 - 1326H + 219 \]

As a result, the value of the index for the benzenoid Circumcoronene series defined in the statement is obtained.

9. The \( mR_S^C(G) \) index of the Circumcoronene series of benzenoid with H layer is given by

\[ mR_S^C(G) = \begin{cases} 3 \left( \frac{4}{H^2} - \frac{1}{20}H + \frac{11}{70} \right) & \text{if } H = 1 \\ \frac{3}{4}H^2 - \frac{1}{20}H + \frac{11}{70} & \text{if } H \geq 2 \end{cases} \]

Proof:
Let \( mR_S^C(G) = \sum_{xy \in E(G)} \frac{1}{\max \{ \delta(x), \delta(y) \}} \)

For \( H = 1 \), \( mR_S^C(G) = 6 \left( \frac{1}{\max(6,6)} \right) = 1. \)

For \( H \geq 2 \), consider the edge partition in Table 3.

\[ mR_S^C(G) = 6 \left( \frac{\max(7,7)}{\max(7,10)} \right) + 12 \left( \frac{\max(7,10)}{\max(8,10)} \right) + \frac{12(H - 2)}{\max(10,12)} + \frac{6(H - 1)}{\max(10,12)} + (9H^2 - 21H + 12) \left( \frac{9}{\max(12,12)} \right) \]

\[ = \frac{6}{7} + \frac{12}{10} + \frac{12}{10}H - \frac{24}{10} + \frac{6}{12}H - \frac{6}{12} + \frac{9}{12}H^2 - \frac{21}{12}H + 1 \]

\[ = \frac{3}{4}H^2 - \frac{1}{20}H + \frac{11}{70} \]

Hence from the edge partition values defined in table.3 the value of index of the Circumcoronene series of benzenoid are estimated.

10. The \( ISI_S^C(G) \) index of the Circumcoronene series of benzenoid with H layer is given by

\[ ISI_S^C(G) = \begin{cases} 24 \left( \frac{54H^2}{33} - \frac{1318}{561}H + \frac{1693}{561} \right) & \text{if } H = 1 \\ \frac{24}{54H^2} - \frac{1318}{33}H + \frac{1693}{561} & \text{if } H \geq 2 \end{cases} \]

Proof:
Let \( ISI_S^C(G) = \sum_{xy \in E(G)} \frac{\delta(x) \* \delta(y)}{\max \{ \delta(x), \delta(y) \}} \)

For \( H = 1 \), \( ISI_S^C(G) = 6 = 24. \)

For \( H \geq 2 \), consider the edge partition in Table 3.
\[ I_{SI}^{\mathcal{F}}(G) = 6 \left( \frac{7 \times 7}{7 + 7} \right) + 12 \left( \frac{7 \times 10}{7 + 10} \right) + 12(H - 2) \left( \frac{8 \times 10}{8 + 10} \right) + 6(H - 1) \left( \frac{10 \times 12}{10 + 12} \right) + (9H^2 - 21H + 12) \left( \frac{12 \times 12}{12 + 12} \right) \]
\[ = 54H^2 - \frac{1318}{33}H + \frac{1693}{561}. \]

Hence from the edge partition values defined index of the Circumcoronene series of benzenoid with \( H \) layer are estimated.

### 3.3. Results on Reciprocal of Closed Neighborhood degree

As the indices so far discussed depends on closed and open neighborhoods, we may consider that the values obtained will be more suitable than those defined using a degree-based methodology.

11. The \( r_{SK}^{\mathcal{C}}(G) \) index of the Circumcoronene series of benzenoid with \( H \) layer is given by

\[ r_{SK}^{\mathcal{C}}(G) = \begin{cases} 
1 & \text{if } H = 1 \\
648H^2 - 672H + 111 & \text{if } H \geq 2 
\end{cases} \]

Proof:

Let \( r\text{SK}^{\mathcal{C}}(G) = \sum_{xy \in E(G)} \frac{2}{\delta(x) + \delta(y)} \)

For \( H = 1 \), \( r\text{SK}^{\mathcal{C}}(G) = 6 \left( \frac{2}{3} \right) = 2 \).

For \( H \geq 2 \), consider the edge partition in Table 3.

\[ r_{SK}^{\mathcal{C}}(G) = 6 \left( \frac{2}{7 + 7} \right) + 12 \left( \frac{2}{7 + 10} \right) + 12(H - 2) \left( \frac{2}{18} \right) + 6(H - 1) \left( \frac{2}{22} \right) + (9H^2 - 21H + 12) \left( \frac{2}{24} \right) \]
\[ = \frac{6}{7} + \frac{24}{17} + \frac{4}{3}H - \frac{8}{11} + \frac{6}{11}H - \frac{9}{12}H^2 - \frac{21}{24}H + \frac{12}{12} \]
\[ = \frac{3}{4}H^2 + \frac{13}{132}H + \frac{3565}{1309}. \]

Hence from the edge partition values defined in Table 3 the value of index for the Circumcoronene series of benzenoid are estimated for all layers.

12. The \( r\text{SK}^{1\mathcal{C}}(G) \) index of the Circumcoronene series of benzenoid with \( H \) layer is given by

\[ r\text{SK}^{1\mathcal{C}}(G) = \begin{cases} 
1 & \text{if } H = 1 \\
\frac{H^2}{8} + \frac{13}{120}H + \frac{8}{147} & \text{if } H \geq 2 
\end{cases} \]

Proof:

Let \( r\text{SK}^{1\mathcal{C}}(G) = \sum_{xy \in E(G)} \frac{2}{\delta(x) + \delta(y)} \)

For \( H = 1 \), \( r\text{SK}^{1\mathcal{C}}(G) = 6 \left( \frac{2}{6 + 6} \right) = \frac{1}{3} \).

For \( H \geq 2 \), consider the edge partition in Table 3.

\[ r\text{SK}^{1\mathcal{C}}(G) = 6 \left( \frac{2}{7 + 7} \right) + 12 \left( \frac{2}{7 + 10} \right) + 12(H - 2) \left( \frac{2}{8 + 10} \right) + 6(H - 1) \left( \frac{2}{10 + 12} \right) + (9H^2 - 21H + 12) \left( \frac{2}{12 + 12} \right) \]
\[ = \frac{H^2}{8} + \frac{13}{120}H + \frac{8}{147} \]

Thus the closed neighbourhood topological value of index for the Circumcoronene series of benzenoid is obtained for every layer.

13. The \( r\text{SK}^{2\mathcal{C}}(G) \) index of the Circumcoronene series of benzenoid with \( H \) layer is given by

\[ r\text{SK}^{2\mathcal{C}}(G) = \begin{cases} 
1 & \text{if } H = 1 \\
\frac{H^2}{16} + \frac{2713}{52272}H + \frac{14428321}{55516784} & \text{if } H \geq 2 
\end{cases} \]
Proof: Let $rSK^2_{NH}(G) = \sum_{xy \in E(G)} \left( \frac{2}{\delta(x) + \delta(y)} \right)^2$.

For $H = 1$, $rSK^2_{NH}(G) = 6 \left( \frac{2}{6+6} \right)^2 = \frac{1}{6}$.

For $H \geq 2$, consider the edge partition in Table 3.

$$rSK^2_{NH}(G) = 4 \left( \frac{6}{7+7} \right)^2 + \frac{12}{(7+10)^2} + \frac{12(H-2)}{(8+10)^2} + \frac{6(H-1)}{(10+12)^2} + \frac{(9H^2 - 21H + 4)}{(12+12)^2}$$

$$= \frac{6}{16} + \frac{2713}{52272}H + \frac{14428321}{555167844}$$

Thus, the closed neighbourhood topological value of index of the Circumcoronene series of benzenoid is obtained for every layer.

14. The $rmR^2_{NH}(G)$ index of the Circumcoronene series of benzenoid with $H$ layer is given by

$$rmR^2_{NH}(G) = \begin{cases} 36 & \text{if } H = 1 \\ 108H^2 - 60H - 6 & \text{if } H \geq 2 \end{cases}$$

Proof: Let $rmR^2_{NH}(G) = \sum_{xy \in E(G)} \max(\delta[u], \delta[v])$.

For $H = 1$, $rmR^2_{NH}(G) = 6(\max(6,6)) = 36$.

For $H \geq 2$, consider the edge partition in Table 3.

$$rmR^2_{NH}(G) = 6(\max(7,7)) + 12(\max(7,10)) + 12(H-2)(\max(8,10)) + 6(H-1)(\max(10,12)) + (9H^2 - 21H + 12)(\max(12,12))$$

$$= 108H^2 - 60H - 6.$$

Thus, the closed neighbourhood topological value of index of the Circumcoronene series of benzenoid is obtained for every layer.

15. The $rSI^2_{NH}(G)$ index of the Circumcoronene series of benzenoid with $H$ layer is given by

$$rSI^2_{NH}(G) = \begin{cases} \frac{3}{2} & \text{if } H = 1 \\ \frac{3}{2}H^2 + \frac{3}{10}H + \frac{43}{35} & \text{if } H \geq 2 \end{cases}$$

Proof: Let $rSI^2_{NH}(G) = \sum_{uv \in E(G)} \frac{\delta[u]+\delta[v]}{\delta[u]+\delta[v]}$.

For $H = 1$, $rSI^2_{NH}(G) = 6 \left( \frac{6+6}{6+6} \right) = 2$.

For $H \geq 2$, consider the edge partition in Table 5.

$$SI^2_{NH}(G) = 6 \left( \frac{7+7}{7+7} \right) + 12 \left( \frac{7+10}{7+10} \right) + 12(H-2) \left( \frac{8+10}{8+10} \right) + 6(H-1) \left( \frac{10+12}{10+12} \right) + (9H^2 - 21H + 12) \left( \frac{12+12}{12+12} \right)$$

$$= \frac{4}{2}H^2 + \frac{3}{10}H + \frac{43}{35}$$

Therefore, the value of index of the Circumcoronene series of benzenoid is derived for all layers with reference to the partition table as provided in Table 5.

Figures 2 and 3 depict the numerical and graphical representations. By examining these figures along with Table 4, it becomes evident that all the indices follow an ascending order with the increase in $H$. 

https://www.malque.pub/ojs/index.php/msj
3.4. Results on Reduced Reverse degreee

The structure of the Circumcoronene series of benzene follows a honeycomb structure. The Modified Randic Index, the Inverse Sum Index, and the Reduced Reverse Randic Index are three topological descriptors we compute for the Circumcoronene series of the Benzenoid family based on open and closed neighborhood criteria.
General pattern for reduced reverse degree pairs of the edges of circumcoronene series of benzenoids for $H(H \geq 2)$ terms is shown in Table 5.

<table>
<thead>
<tr>
<th>$(d_x, d_y)$</th>
<th>$(\mathcal{RR}_x, \mathcal{RR}_y)$</th>
<th>General Pattern</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2,2)</td>
<td>(2,3)</td>
<td>6</td>
</tr>
<tr>
<td>(2,3)</td>
<td>(3,3)</td>
<td>12(H - 1)</td>
</tr>
<tr>
<td>(3,3)</td>
<td>(2,2)</td>
<td>$9H^2 - 15H + 6$</td>
</tr>
</tbody>
</table>

16. The $\mathcal{RR}_M(G)$ index of the Circumcoronene series of benzenoids with a layer of $H$ is expressed as

$$\mathcal{RR}_M(G) = \begin{cases} 24 & \text{if } H = 1 \\ 36H^2 & \text{if } H \geq 2 \end{cases}$$

Proof:
Let $\mathcal{RR}_M(G) = \sum_{xy \in E(G)}[\mathcal{RR}_x + \mathcal{RR}_y]$.
For $H = 1$, $\mathcal{RR}_M(G) = 6(2 + 2) = 24$.
For $H \geq 2$, consider the edge partition in Table 5.

$$\mathcal{RR}_M(G) = 6(3 + 3) + 12(H - 1)(3 + 2) + (9H^2 - 15H + 6)(2 + 2)$$
$$= 36 + 60H - 60 + 36H^2 - 60H + 24$$
$$= 36H^2$$

Thus the value of Zagreb Indices based on Reduced Reverse Vertex Degrees index of the Circumcoronene series of benzenoid for all layers obtained.

17. The $\mathcal{RR}_M(G)$ index of the Circumcoronene series of benzenoids with a layer of $H$ is expressed as

$$\mathcal{RR}_M(G) = \begin{cases} 24 & \text{if } H = 1 \\ 36H^2 + 32H + 6 & \text{if } H \geq 2 \end{cases}$$

Proof:
Let $\mathcal{RR}_M(G) = \sum_{xy \in E(G)}[\mathcal{RR}_x + \mathcal{RR}_y]$.
For $H = 1$, $\mathcal{RR}_M(G) = 6(2 * 2) = 24$.
For $H \geq 2$, consider the edge partition in Table 5.

$$\mathcal{RR}_M(G) = 6(3 * 3) + 12(H - 1)(3 * 2) + (9H^2 - 15H + 6)(2 * 2)$$
$$= 36H^2 + 32H + 6$$

Hence the value of Zagreb Indices based on Reduced Reverse Vertex Degrees index of the Circumcoronene series of benzenoid is calculated.

2.18 The $\mathcal{RR}_M(G)$ index of the Circumcoronene series of benzenoids with a layer of $H$ is expressed as

$$\mathcal{RR}_M(G) = \begin{cases} 96 & \text{if } H = 1 \\ 144H^2 + 60H + 12 & \text{if } H \geq 2 \end{cases}$$

Proof:
Let $\mathcal{RR}_M(G) = \sum_{xy \in E(G)}[\mathcal{RR}_x + \mathcal{RR}_y]^2$.
For $H = 1$, $\mathcal{RR}_M(G) = 6(2 + 2)^2 = 96$.
For $H \geq 2$, consider the edge partition in Table 5.

$$\mathcal{RR}_M(G) = 6(3 + 3)^2 + 12(H - 1)(3 + 2)^2 + (9H^2 - 15H + 6)(2 + 2)^2$$
$$= 144H^2 + 60H + 12$$

Therefore, the value of Zagreb Indices based on Reduced Reverse Vertex Degrees index of the circumcoronene series of benzenoid is obtained based on the edge partition defined in table 5.

19. The $\mathcal{RR}_M(G)$ index of the Circumcoronene series of benzenoids with a layer of $H$ is expressed as

$$\mathcal{RR}_M(G) = \begin{cases} 96 & \text{if } H = 1 \\ 144H^2 + 192H + 150 & \text{if } H \geq 2 \end{cases}$$

Proof:
Let $\mathcal{K}H_{M}(G) = \sum_{x \in E(G)}[\mathcal{K}R_{x} \ast \mathcal{K}R_{y}]^2$

For $H = 1$, $\mathcal{K}H_{M}(G) = 6(2 + 2)^2 = 96$.

For $H \geq 2$, consider the edge partition in Table 5.

$$\mathcal{K}H_{M}(G) = 6(3 \ast 3)^2 + 12(H - 1)(3 \ast 2)^2 + (9H^2 - 15H + 6)(2 \ast 2)^2$$

$$= 406 + 432(H - 1) + 16(9H^2 - 15H + 6) = 144H^2 + 192H + 150$$

Therefore, the value of Zagreb Indices based on Reduced Reverse Vertex Degrees of index of the Circumcoronene series of benzenoid is derived.

20. The $\mathcal{K}RF(G)$ index of the Circumcoronene series of benzenoids with a layer of $H$ is expressed as

$$\mathcal{K}RF(G) = \begin{cases} 48 & \text{if } H = 1 \\ 72H^2 + 36H & \text{if } H \geq 2 \end{cases}$$

Proof:

Let $\mathcal{K}RF(G) = \sum_{x \in E(G)}[\mathcal{K}R_{x}^2 + \mathcal{K}R_{y}^2]$

For $H = 1$, $\mathcal{K}RF(G) = 6(2^2 + 2^2) = 48$

For $H \geq 2$, consider the edge partition in Table 5.

$$\mathcal{K}RF(G) = 6(3^2 + 3^2) + 12(H - 1)(3^2 + 2^2) + (9H^2 - 15H + 6)(2^2 + 2^2)$$

$$= 108 + 156(H - 1) + 8(9H^2 - 15H + 6) = 72H^2 + 36H$$

Therefore, the value of Zagreb Indices based on Reduced Reverse Vertex Degrees index of the Circumcoronene series of benzenoid is calculated for all layers.

21. The $\mathcal{K}RABC(G)$ index of the Circumcoronene series of benzenoids with a layer of $H$ is expressed as

$$\mathcal{K}RABC(G) = \begin{cases} \frac{9}{\sqrt{2}}H^2 - \frac{3}{\sqrt{2}}H + 4 - 3\sqrt{2} & \text{if } H = 1 \\ \frac{2 + 2 - 2}{2 + 2} & \text{if } H \geq 2 \end{cases}$$

Proof:

Let $\mathcal{K}RABC(G) = \sum_{x \in E(G)}\sqrt{\mathcal{K}R_{x}^{2} + \mathcal{K}R_{y}^{2}}$

For $H = 1$, $\mathcal{K}RABC(G) = 6\sqrt{\frac{2 + 2 - 2}{2 + 2}} = 3\sqrt{2}$.

For $H \geq 2$, consider the edge partition in Table 5.

$$\mathcal{K}RF(G) = 6\left(\frac{3 + 3 - 2}{3 + 3}\right) + 12(H - 1)\left(\frac{3 + 2 - 2}{3 + 2}\right) + (9H^2 - 15H + 6)\left(\frac{2 + 2 - 2}{2 + 2}\right)$$

$$= 4 + 12H - \frac{1}{\sqrt{2}}H^2 - \frac{1}{\sqrt{2}}H^2 + 9H^2 - 15H + 6H + 6\sqrt{2}$$

$$= \frac{9}{\sqrt{2}}H^2 - \frac{3}{\sqrt{2}}H + 4 - 3\sqrt{2}$$

Hence the value of the value of Zagreb Indices based on Reduced Reverse Vertex Degrees index of the Circumcoronene series of benzenoid is obtained.

<table>
<thead>
<tr>
<th>Table 6 Indices based on reduced reverse degree.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H$</td>
</tr>
<tr>
<td>-------</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>3</td>
</tr>
<tr>
<td>4</td>
</tr>
<tr>
<td>5</td>
</tr>
<tr>
<td>6</td>
</tr>
<tr>
<td>7</td>
</tr>
<tr>
<td>8</td>
</tr>
<tr>
<td>9</td>
</tr>
<tr>
<td>10</td>
</tr>
</tbody>
</table>

Figure 4 illustrates both numerical and graphical representations.
4. Discussion

Comparison of topological indices based on Open and Closed, Closed and its Reciprocal neighborhood degrees: For the circumcoronene series of benzenoids, Figures 5-14 present a graphical and numerical comparison of topological indices, such as SK, SK1, SK2, mR, and ISI, based on open and closed neighborhood degrees, as well as closed and its reciprocal.
Figure 7 SK2 Index for Open and Closed.

Figure 8 Modified Randic Index for Open and Closed.

Figure 9 ISI Index for Open and Closed.
Figure 10 SK Index for Closed and its reciprocal.

Figure 11 SK1 Index for Closed and its reciprocal.

Figure 12 SK2 Index for Closed and its reciprocal.
5. Conclusion

Several topological indices for the benzenoids of the Circumcoronene family are computed in this work. The indicators of the study will be useful to the researchers when they investigate the molecular properties and composition of benzenoids in the Circumcoronene family. Moreover, the graphs and numerical comparisons of the discussed indices will facilitate research in the family that is comparable to the structure taken. We also use MATLAB to compare and assess these indices' distributions.

Ethical considerations

Not applicable.

Conflict of Interest

The authors declare no conflicts of interest.

Funding

This research did not receive any financial support.

References


https://www.malque.pub/ojs/index.php/msj


