Research Article

On Computation Degree-Based Topological Descriptors for Planar Octahedron Networks

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A molecular graph is used to represent a chemical molecule in chemical graph theory, which is a branch of graph theory. A graph is considered to be linked if there is at least one link between its vertices. A topological index is a number that describes a graph’s topology. Cheminformatics is a relatively young discipline that brings together the field of sciences. Cheminformatics helps in establishing QSAR and QSPR models to find the characteristics of the chemical compound. We compute the first and second modified K-Banhatti indices, harmonic K-Banhatti index, symmetric division index, augmented Zagreb index, and inverse sum index and also provide the numerical results.

1. Introduction

Graph theory provides topological indices, which are a useful tool. Cheminformatics is a contemporary academic discipline that brings together chemistry, mathematics, and information science. It investigates the connections between quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR), which are used to predict biological activities and chemical compound characteristics.

The silicate structures [1] formed from the POH network, TP network, and hex POH network [2] are discussed in this article.

The following is the procedure for making POH networks.

Step 1: consider a m-dimensional silicate network.
Step 2: connect new vertices in the centre of each triangular face to existing vertices in the adjacent triangular face.
Step 3: all of the new centre vertices in the same silicate cell must be connected.
Step 4: for the m dimension, the resultant graph is known as the planar octahedron network as shown in Figure 1. Remove all silicon vertices from the graph. The triangle prism network as shown in Figure 2 and the hex POH network as shown in Figure 3 are also possible.

Let ψ represent a graph. Then, modified first and second K-Banhatti indices [3] can be defined as

\[ MK_1B(\psi) = \sum_{ab \in E(\psi)} \left( \frac{1}{d_a + d_b} \right), \]  \hspace{1cm} (1)

\[ MK_2B(\psi) = \sum_{ab \in E(\psi)} \left( \frac{1}{d_a \times d_b} \right). \]  \hspace{1cm} (2)

Harmonic K-Banhatti index [4] of a graph ψ is defined as
Symmetric division index of a graph \[5\] is defined as

\[
\text{SD}(\psi) = \sum_{ab \in E(\psi)} \left( \frac{d_a + d_b}{d_a d_b} \right) .
\]  

(4)

Augmented Zagreb index of a graph \[4\] is defined as

\[
\text{AG}(\psi) = \sum_{ab \in E(\psi)} \left( \frac{d_a \times d_b}{d_a + d_b - 2} \right)^3 .
\]  

(5)

Inverse sum index of a graph \[\psi\] is defined as

\[
I(\psi) = \sum_{ab \in E(\psi)} \left( \frac{d_a \times d_b}{d_a + d_b} \right) .
\]  

(6)

2. Main Results

We research different indices on different kinds of planar octahedron networks. Nowadays, extensive research studies are being conducted in the field of chemical graph theory for further studying topological indices of various graphs [6–13]. For the basic notations and definitions, see [14, 15].

2.1. Results for Planar Octahedron Network POH (m).

The planar octahedron network is the resulting graph for the \(m\) dimension. All silicon vertices should be removed from the scene. There are also the triangular prism network and the hex POH network. Now, we calculate several key indices for the POH network in the following theorems.

**Theorem 1.** Consider the planar octahedral network POH \((m)\); then, its first and second modified K-Banhatti indices are equal to

\[
\text{MK}_1(\psi_1) = \frac{51}{8} m^2 + \frac{3}{4} m,
\]  

(7)

\[
\text{MK}_2(\psi_1) = \frac{81}{32} m^2 + \frac{9}{16} m.
\]  

Proof. Let \(\psi_1 \equiv \text{POH}(m)\). From equation (1), we have
Theorem 2. The harmonic K-Banhatti and symmetric division indices are equal in the POH \((m)\) network.

\[
\text{MK}_1 B(\psi) = \sum_{\text{ab} \in E(\psi)} \left( \frac{1}{(d_a + d_b)} \right). \tag{8}
\]

Using Table 1, we have

\[
\text{MK}_1 B(\psi) = \frac{1}{4 + 4} |E_1(\text{POH}(m))| + \frac{1}{4 + 8} |E_2(\text{POH}(m))| + \frac{1}{8 + 8} |E_3(\text{POH}(m))|,
\]

\[
= \frac{1}{8} |E_1(\text{POH}(m))| + \frac{1}{12} |E_2(\text{POH}(m))| + \frac{1}{16} |E_3(\text{POH}(m))| \tag{9}
\]

We get the following value after calculations:

\[
\Rightarrow \text{MK}_1 B(\psi) = \frac{51}{8} m^2 + \frac{3}{4} m. \tag{10}
\]

Let \(\psi \equiv \text{POH}(m)\). From equation (2), we have

\[
\text{MK}_2 B(\psi) = \sum_{\text{ab} \in E(\psi)} \left( \frac{1}{(d_a + d_b)} \right). \tag{11}
\]

Using Table 1, we have

\[
\text{MK}_2 B(\psi) = \frac{1}{4 \times 4} |E_1(\text{POH}(m))| + \frac{1}{4 \times 8} |E_2(\text{POH}(m))| + \frac{1}{8 \times 8} |E_3(\text{POH}(m))|,
\]

\[
= \frac{1}{16} |E_1(\text{POH}(m))| + \frac{1}{32} |E_2(\text{POH}(m))| + \frac{1}{64} |E_3(\text{POH}(m))| \tag{12}
\]

We get the following value after calculations:

\[
\Rightarrow \text{MK}_2 B(\psi) = \frac{81}{32} m^2 + \frac{9}{16} m. \tag{13}
\]

Table 1: Edge partition.

| \(E_i\) | Number of edges |
|-------|----------------|
| \((4, 4)\) | \(18m^2 + 12m\) |
| \((4, 8)\) | \(36m^2 - 48m + 12\) |
| \((8, 8)\) | \(18m^2 - 36m + 18\) |

\[\text{HKB}(\psi) = \sum_{\text{ab} \in E(\psi)} \frac{2}{(d_a + d_b)}. \tag{15}\]

Using Table 1, we have

\[\text{HKB}(\psi) = \frac{51}{4} m^2 + \frac{3}{2} m, \tag{14}\]

\[\text{SD}(\psi) = 162m^2.\]

Proof. Let \(\psi \equiv \text{POH}(m)\) network; from equation (3),

\[
\text{HKB}(\psi) = \sum_{\text{ab} \in E(\psi)} \left( \frac{2}{(d_a + d_b)} \right). \tag{15}
\]

Using Table 1, we have

\[
\text{HKB}(\psi) = \frac{2}{4 + 4} |E_1(\text{POH}(m))| + \frac{2}{4 + 8} |E_2(\text{POH}(m))| + \frac{2}{8 + 8} |E_3(\text{POH}(m))|,
\]

\[
= \frac{2}{8} |E_1(\text{POH}(m))| + \frac{2}{12} |E_2(\text{POH}(m))| + \frac{2}{16} |E_3(\text{POH}(m))| \tag{16}
\]

We get the following value after calculations:

\[
\Rightarrow \text{HKB}(\psi) = \frac{51}{4} m^2 + \frac{3}{2} m. \tag{17}
\]
For the symmetric division index of a graph using equation (3),

\[ \text{SD}(\psi) = \sum_{a \in E(\psi)} \left( \frac{d_a}{d_b} + \frac{d_b}{d_a} \right). \]  

(18)

Using Table 1, we have

\[ \text{SD}(\psi_1) = \left( \frac{4}{4} + \frac{4}{4} \right) |E_1(\text{POH}(m))| + \left( \frac{4}{8} + \frac{8}{4} \right) |E_2(\text{POH}(m))| + \left( \frac{8}{8} + \frac{8}{8} \right) |E_3(\text{POH}(m))| \]

\[ = 2|E_1(\text{POH}(m))| + \left( \frac{1}{2} + \frac{2}{1} \right) |E_2(\text{POH}(m))| + 2|E_3(\text{POH}(m))| \]

\[ = 2 \left( 18m^2 + 12m \right) + \frac{5}{2} \left( 36m^2 - 48m + 12 \right) + 2 \left( 18m^2 - 36m + 18 \right). \]  

(19)

After calculations,

\[ \Rightarrow \text{SD}(\psi_1) = 162m^2. \]  

(20)

**Theorem 3.** Then, augmented Zagreb and inverse sum indices are equal to the POH network.

\[ \text{AG}(\psi_1) = \frac{416820244}{128625} m^2 - \frac{2836480}{3087}m, \]  

(21)

\[ I(\psi_1) = 204m^2 - 24m. \]

After some calculations, we get

\[ \Rightarrow \text{AG}(\psi_1) = \frac{416820244}{128625} m^2 - \frac{2836480}{3087}m. \]  

(24)

For the inverse sum index and by using equation (6), we have

\[ I(\psi_1) = \left( \frac{16}{8} \right) |E_1(\text{POH}(m))| + \left( \frac{32}{12} \right) |E_2(\text{POH}(m))| + \left( \frac{64}{16} \right) |E_3(\text{POH}(m))| \]

\[ = 2 \left( 18m^2 + 12m \right) + \left( \frac{32}{12} \right) \left( 36m^2 - 48m + 12 \right) + 4 \left( 18m^2 - 36m + 18 \right). \]  

(26)

After calculations,

\[ \Rightarrow I(\psi_1) = 204m^2 - 24m. \]  

(27)
2.2. Results for Triangular Prism Network TP\((m)\). In this part, we propose the theorem for the TP network.

**Theorem 4.** The first and second modified K-Banhatti indices are equal to the TP network:

\[
\begin{align*}
\text{MK}_1B(\psi_2) &= \frac{13}{2}m^2 + \frac{2}{3}m, \\
\text{MK}_2B(\psi_2) &= \frac{7}{2}m^2 + \frac{2}{3}m. 
\end{align*}
\]

Proof. Let \(\psi_2 \equiv \text{TP}(m)\). From equation (1), we have

\[
\text{MK}_1B(\psi_2) = \frac{1}{3+3} \left| E_1 (\text{TP}(m)) \right| + \frac{1}{3+6} \left| E_2 (\text{TP}(m)) \right| + \frac{1}{6+6} \left| E_3 (\text{TP}(m)) \right| \\
= \frac{1}{6} \left| E_1 (\text{TP}(m)) \right| + \frac{1}{9} \left| E_2 (\text{TP}(m)) \right| + \frac{1}{12} \left| E_3 (\text{TP}(m)) \right| \\
= \frac{1}{6} (18m^2 + 6m) + \frac{1}{9} (18m^2 + 6m) + \frac{1}{12} (18m^2 - 36m + 18).
\]

After some calculations, we get

\[
\Rightarrow \text{MK}_1B(\psi_2) = \frac{13}{2}m^2 + \frac{2}{3}m. 
\]

Let \(\psi_2 \equiv \text{TP}(m)\). From equation (2), we have

\[
\text{MK}_2B(\psi_2) = \frac{1}{3 \times 3} \left| E_1 (\text{TP}(m)) \right| + \frac{1}{3 \times 6} \left| E_2 (\text{TP}(m)) \right| + \frac{1}{6 \times 6} \left| E_3 (\text{TP}(m)) \right| \\
= \frac{1}{9} \left| E_1 (\text{TP}(m)) \right| + \frac{1}{18} \left| E_2 (\text{TP}(m)) \right| + \frac{1}{36} \left| E_3 (\text{TP}(m)) \right| \\
= \frac{1}{9} (18m^2 + 6m) + \frac{1}{18} (18m^2 + 6m) + \frac{1}{36} (18m^2 - 36m + 18).
\]

After calculations,

\[
\Rightarrow \text{MK}_2B(\psi_2) = \frac{7}{2}m^2 + \frac{2}{3}m. 
\]

**Theorem 5.** In the POH \((m)\) network, the harmonic K-Banhatti and symmetric division indices are equal to

\[
\begin{align*}
\text{HKB}(\psi_2) &= 13m^2 + \frac{4}{3}m, \\
\text{SD}(\psi_2) &= 117m^2 + 3m.
\end{align*}
\]

Proof. Let \(\psi_2 \equiv \text{TP}(m)\) network, and by using equation (3), we have
Using Table 2, we have

\[
HKB(\psi) = \sum_{ab \in E(\psi)} \frac{2}{d_a + d_b}. \tag{36}
\]

Using Table 2, we have

\[
HKB(\psi) = \frac{2}{3 + 3} |E_1(\text{TP}(m))| + \frac{2}{3 + 6} |E_2(\text{TP}(m))| + \frac{2}{6 + 6} |E_3(\text{TP}(m))|
= \frac{2}{6} |E_1(\text{TP}(m))| + \frac{2}{9} |E_2(\text{TP}(m))| + \frac{2}{12} |E_3(\text{TP}(m))|
= \frac{1}{3} \left(18m^2 + 6m\right) + \frac{2}{9} \left(18m^2 + 6m\right) + \frac{1}{6} \left(18m^2 - 36m + 18\right). \tag{37}
\]

After calculations,

\[
\Rightarrow HKB(\psi) = 13m^2 + \frac{4}{3}m. \tag{38}
\]

For the symmetric division index of a graph using equation (3), we have

\[
SD(\psi) = \sum_{ab \in E(\psi)} \frac{d_a + d_b}{d_a \cdot d_b}. \tag{39}
\]

Using Table 2, we have

\[
SD(\psi) = \left(\frac{3}{3} + \frac{3}{3}\right) |E_1(\text{TP}(m))| + \left(\frac{3}{6} + \frac{6}{3}\right) |E_2(\text{TP}(m))| + \left(\frac{6}{6} + \frac{6}{6}\right) |E_3(\text{TP}(m))|
= 2|E_1(\text{TP}(m))| + \left(\frac{1}{2} + 2\right) |E_2(\text{TP}(m))| + 2|E_3(\text{TP}(m))|
= 2\left(18m^2 + 6m\right) + \frac{5}{2} \left(18m^2 + 6m\right) + 2 \left(18m^2 - 36m + 18\right). \tag{40}
\]

After some calculations, we get

\[
\Rightarrow SD(\psi) = 117m^2 + 3m. \tag{41}
\]

\[\Box\]

**Theorem 6.** The augmented Zagreb and inverse sum indices are equal to the TP network.

\[
AG(\psi) = \frac{1853423451}{1372000}m^2 - \frac{534408759}{1372000}m, \tag{42}
\]

\[
I(\psi) = 204m^2 - 24m.
\]

\[
AG(\psi) = \left(\frac{9}{4}\right)^3 |E_1(\text{TP}(m))| + \left(\frac{18}{7}\right)^3 |E_2(\text{TP}(m))| + \left(\frac{36}{10}\right)^3 |E_3(\text{TP}(m))|
= \left(\frac{9}{4}\right)^3 \left(18m^2 + 6m\right) + \left(\frac{18}{7}\right)^3 \left(18m^2 + 6m\right) + \left(\frac{36}{10}\right)^3 \left(18m^2 - 36m + 18\right). \tag{44}
\]

We get the following value after calculations:

\[
\Rightarrow AG(\psi) = \frac{1853423451}{1372000}m^2 - \frac{534408759}{1372000}m. \tag{45}
\]
For the inverse sum index and by using equation (6), we have

\[ I(\psi) = \sum_{ab \in E(\psi)} \left( \frac{d_a \times d_b}{d_a + d_b} \right). \]  

(46)

Using Table 2, we have

\[ I(\psi) = \left(\frac{9}{6}\right) \left| E_1(TP(m)) \right| + 2\left| E_2(TP(m)) \right| + 3\left| E_3(TP(m)) \right| \]

\[ = \left(\frac{9}{6}\right) (18m^2 + 6m) + 2(18m^2 + 6m) + 3(18m^2 - 36m + 18). \]  

(47)

After calculations,

\[ \Rightarrow I(\psi) = 117m^2 - 15m. \]  

(48)

\[ \square \]

2.3. Results for Hexagonal Planar Octahedron (HPOH) Network. In this part, we propose the theorem for the HPOH network.

**Theorem 7.** The first and second modified K-Banhatti indices are equal to the hex POH network:

\[ MK_1B(\psi) = \frac{51}{8}m^2 - 4m - \frac{13}{8}, \]

\[ MK_2B(\psi) = \frac{81}{32}m^2 - \frac{15}{16}m - \frac{39}{32}. \]  

(49)

**Proof.** Let \( \psi \equiv HPOH(m) \). From equation (1), we have

\[ MK_1B(\psi) = \sum_{ab \in E(\psi)} \left( \frac{1}{(d_a + d_b)} \right). \]  

(50)

Using Table 3, we have

\[ MK_1B(\psi) = \frac{51}{8}m^2 - 4m - \frac{13}{8}. \]  

(51)

\[ MK_2B(\psi) = \frac{81}{32}m^2 - \frac{15}{16}m - \frac{39}{32}. \]  

(52)

We get the following value after calculations:

\[ \Rightarrow MK_1B(\psi) = \frac{51}{8}m^2 - 4m - \frac{13}{8}. \]  

(53)

Let \( \psi \equiv HPOH(m) \). From equation (2), we have

\[ MK_2B(\psi) = \frac{1}{4 \times 4} \left| E_1(HPOH(m)) \right| + \frac{1}{4 \times 4} \left| E_2(HPOH(m)) \right| + \frac{1}{8 \times 8} \left| E_3(HPOH(m)) \right| \]

\[ = \frac{1}{16} \left| E_1(HPOH(m)) \right| + \frac{1}{32} \left| E_2(HPOH(m)) \right| + \frac{1}{64} \left| E_3(HPOH(m)) \right| \]  

(54)

Using Table 3, we have

\[ MK_2B(\psi) = \frac{1}{16} (18m^2 + 18m - 30) + \frac{1}{32} (36m^2 - 48m + 12) + \frac{1}{64} (18m^2 - 36m + 18). \]
We get the following value after calculations:
\[ \Rightarrow MK_2B(\psi_3) = \frac{81}{32} m^2 - \frac{15}{16} m - \frac{39}{32} \] (55)

**Theorem 8.** Then, harmonic K-Banhatti and symmetric division indices are equal to the hex POH network:

\[ HKB(\psi_3) = \frac{51}{4} m^2 - 8m - \frac{13}{4}, \] (56)
\[ SD(\psi_3) = 162m^2 - 156m + 6. \] (57)

**Proof.** Let \( \varphi_1 \equiv HPOH(m) \) network, and from equation (3),
\[ \text{HKB}(\psi) = \sum_{abc \in E(\psi)} \frac{2}{d_a + d_b}, \] (57)

Using Table 3, we have
\[ \Rightarrow \text{HKB}(\psi_3) = \frac{51}{4} m^2 - 8m - \frac{13}{4} \] (59)

For the symmetric division index of a graph using equation (3), we have
\[ \text{SD}(\psi) = \sum_{abc \in E(\psi)} \frac{d_a + d_b}{d_a d_b}, \] (60)

Using Table 3, we have
\[ \Rightarrow \text{SD}(\psi_3) = 162m^2 - 156m + 6. \] (62)

**Theorem 9.** The augmented Zagreb and inverse sum indices are equal to the hex POH network:

\[ HKB(\psi_3) = \frac{51}{4} m^2 - 8m - \frac{13}{4}, \] (56)
\[ SD(\psi_3) = 162m^2 - 156m + 6. \] (57)

Using Table 3, we have
\[ \Rightarrow \text{HKB}(\psi_3) = \frac{51}{4} m^2 - 8m - \frac{13}{4} \] (59)

For the symmetric division index of a graph using equation (3), we have
\[ \text{SD}(\psi) = \sum_{abc \in E(\psi)} \frac{d_a + d_b}{d_a d_b}, \] (60)

Using Table 3, we have
\[ \Rightarrow \text{SD}(\psi_3) = 162m^2 - 156m + 6. \] (62)
Proof. Let $\varphi_1 \equiv \text{HPOH} (m)$ network. Using equation (5) for the augmented Zagreb index,

$$\text{AG} (\psi_3) = \frac{416820224}{128625} m^2 - \frac{600773632}{128625} m + \frac{595764224}{385875}. \quad (63)$$

Using Table 3, we have

$$\begin{align*}
\text{AG} (\psi_3) &= \left(16 \right)^3 |E_1 (\text{HPOH} (m))| + \left(\frac{32}{10} \right)^3 |E_2 (\text{HPOH} (m))| + \left(\frac{64}{14} \right)^3 |E_3 (\text{HPOH} (m))| \\
&= \left(16 \right)^3 \left(18m^2 + 18m - 30\right) + \left(\frac{32}{10} \right)^3 \left(36m^2 - 48m + 12\right) + \left(\frac{64}{14} \right)^3 \left(18m^2 - 36m + 18\right). \quad (65)
\end{align*}$$

We get the following value after calculations:

$$\Rightarrow \text{AG} (\psi_3) = \frac{416820224}{128625} m^2 - \frac{600773632}{128625} m + \frac{595764224}{385875}. \quad (66)$$

For the inverse sum index and by using equation (6), we have

$$I (\psi_3) = \sum_{a \neq b \in \psi_1} \left(\frac{d_a \times d_b}{d_a + d_b - 2}\right)^3. \quad (64)$$

Using Table 3, we have

$$\begin{align*}
\text{AG} (\psi_3) &= \left(16 \right)^3 |E_1 (\text{HPOH} (m))| + \left(\frac{32}{10} \right)^3 |E_2 (\text{HPOH} (m))| + \left(\frac{64}{14} \right)^3 |E_3 (\text{HPOH} (m))| \\
&= \left(16 \right)^3 \left(18m^2 + 18m - 30\right) + \left(\frac{32}{10} \right)^3 \left(36m^2 - 48m + 12\right) + \left(\frac{64}{14} \right)^3 \left(18m^2 - 36m + 18\right). \quad (65)
\end{align*}$$

We get the following value after calculations:

$$\Rightarrow \text{AG} (\psi_3) = \frac{416820224}{128625} m^2 - \frac{600773632}{128625} m + \frac{595764224}{385875}. \quad (66)$$

For the inverse sum index and by using equation (6), we have

$$I (\psi_3) = \sum_{a \neq b \in \psi_1} \left(\frac{d_a \times d_b}{d_a + d_b - 2}\right)^3. \quad (64)$$
Figure 6: For TP 1.

Figure 7: For TP 2.

Figure 8: For hex POH 1.
Using Table 3, we have

\[ I(\psi_3) = \left( \frac{16}{8} \right) |E_1(\text{HPOH}(m))| + \left( \frac{32}{12} \right) |E_2(\text{HPOH}(m))| + \left( \frac{64}{16} \right) |E_3(\text{HPOH}(m))| \]

\[ = 2(18m^2 + 18m - 30) + \left( \frac{32}{12} \right) (36m^2 - 48m + 12) + 4(18m^2 - 36m + 18). \]

After calculations,

\[ \Rightarrow I(\psi_3) = 204m^2 - 236m + 44. \]  

(69)

3. Comparison of Indices through Graphs

The comparison of the first and second K-Banhatti, harmonic K-Banhatti, symmetric division, augmented Zagreb, and inverse sum indices for the POH network, TP network, and HPOH network is conducted for different values. The comparison graphs are shown in Figures 4–9.

4. Conclusion

In this paper, first and the second K-Banhatti, harmonic K-Banhatti, symmetric division, augmented Zagreb, and inverse sum indices have been computed for the planar octahedron networks. From a chemical standpoint, these findings might be useful for computer scientists and chemists, who come across these networks. Additional multiplicative degree-based indices should be computed soon.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Authors’ Contributions

Wang Zhen was responsible for software Parvez Ali contributed in collection of data. Haidar Ali contributed to original draft preparation. Ghulam Dustigeer was responsible for methodology. Jia-Bao Liu reviewed and edited the manuscript.

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