Analysis of Sombor and Harmonic Indices of Thorn Cog-Graphs

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1. INTRODUCTION

In the past two decades, mathematical chemistry, most often in the guise of applied theoretical and computational chemistry, has endowed practical applications in many fields. Chemical graph theory is an exciting field connecting mathematics and chemistry. Graph theoretical applications with chemistry are mainly used in “Quantity Structure Activity Relationship (QSAR) and Quantity Structure-Property Relationship (QSPR) studies.” Both “QSAR and QSPR” are effective weapons in contemporary chemical and medicinal research: because of these studies, topological indices have become more feasible to predict the biochemical activities of specific compounds. ‘QSAR’ represent predictive models formed from the application of statistical tools correlating the biological activity of chemicals, it may be drugs/toxics/environmenal pollutants with descriptor representative of molecular structure and properties. The topological index describes the chemical structure mathematically in an unambiguous way. It is mainly applied in theoretical chemistry for designing molecular compounds which correlate physico-chemical, pharmaceutical and biological activities. These topological descriptors are derived from hydrogen suppressed molecular graphs in which the atoms and bonds represent the vertices and edges, respectively. Till now, more than 3000 types of topological indices have been identified. The indices are based on three types, namely distance, degree and eccentricity-based indices.

Wiener in his research work, used topological index for the first time to determine the boiling point of paraffin [1]. “Consider an n-vertex simple connected graph $G=(V, E)$, where $V(G)$ and $E(G)$ denote the vertex and the edge set, respectively. Let $M=\{a_1, a_2, ..., a_n\}$ be the n number of non-negative integers. The thorn graph $G_M$ is simply obtained from the connected graph $G$ by attaching $a_i$ number of pendant vertices to the vertex $v_i$ of $G$, where $i$ ranges from 1, 2, ..., $n$. In the vertices $V_i$ of $G$, these pendant vertices $a_i$ are fixed and it is known as the thorns of $G$. Now we denote the set of $a_i$ as the number of pendant vertices to $v_i$ of $G$ and it is denoted by $V_p$ and $p = \{1, 2, 3, ..., n\}$. $V(G_M) = V(G) \cup V_1(G) \cup V_2(G) \cup ... \cup V_n(G)$. For more graph theoretic terminology, refer [2, 3]. In 1998, Gutman laid the foundation for the thorn graph [4]. For a detailed analysis of thorn graphs, it can be found from studies [5-8]. Though there are several indices, Gutman recently introduced a new index known as the Sombor index in the year 2020 and it is examined in the study [9]. The concept of Randic energy was given by Gao in the study [10]. Fajtlowicz gave the concept of harmonic index in his research work [11]. Gutman and Trinajsic, in the year 1972, proposed the idea of dealing graph theory with orbital electrons [12]. Havare, in his research paper, gave a clear picture correlating regression analysis with Quantity Structure-Property Relationship (QSPR) studies [13]. Randic [14] introduced the Randic index and Sombor index on the directed graph given by Cruz et al. [15]. Topological indices have a significant part in chemoinformatics and it includes various subjects such as...
physics, chemistry, mathematics, information science and molecular biology [16, 17]. Chemoinformatics combined with molecular descriptors helps to develop computational models resulting in quality drug design and optimization of new drugs. Also, Rajeswari and Parvathi discussed the Zagreb indices correlating nanotubes [18] and detailed studies on nanotechnology can be found from studies [19, 20]. The application relating drug delivery and topological indices provides a key role in COVID-19 treatment [21-25]. Ortega et al. gave a brief explanation on MATLAB based particle size distribution to understand the physical properties of compounds [26].

The primary aim of the research is to analyze some standard thorn graphs, such as the thorn cog-complete graph, the thorn cog-star graph and the thorn cog-wheel graph, using the Sombor and harmonic indices.

2. PRELIMINARIES

Here in this article, fundamental formulae are discussed.

Definition 1. The Sombor index of a connected graph $G$ is given by:

$$SO(G) = \sum_{u \neq v \in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$$

where, $d_G(u)$ and $d_G(v)$ denote the degree of a vertex of $u$ and $v$ in $G$, respectively.

Definition 2. For a connected graph $G$, the harmonic index is given by:

$$H(G) = \sum_{u \neq v \in E(G)} \frac{2}{d_G(u) + d_G(v)}$$

Definition 3. Randic index of a simple connected graph $G$ is defined as:

$$R_\alpha(G) = \sum_{u \neq v \in E(G)} (d_G(u) d_G(v))^{\alpha}$$

where, $\alpha$ is a real number.

Definition 4. A complete graph denoted by $K_n$ is a graph where each distinct pair of vertices is connected by a single edge. Moreover, the graph contains $x$ number of vertices and edges equal to $\frac{x(x-1)}{2}$.

3. MAIN RESULTS

Here the relationship between the Sombor index, harmonic index of $G$ and $G_{x,y}$ are examined with the thorn families. The paper demonstrates an explicit formula for the topological index and the values are computed with the family of thorn graphs. Initially, we find the vertex degree for each graph, then we proceed with the edge partition to procure the required result.

3.1 Results on thorn complete graph

Here Sombor and harmonic index are computed for the thorn complete graph.

3.1.1 Thorn complete graph $K_{x,y}$

The $y$-thorn complete graph $K_{x,y}$ has a parent $K_x$ and $(y-x)$ thorns and pendant vertices $u_i$, where $i$ ranges from 1,2,..., $y$, which exists at each vertex $v_i$ for $i$ ranges from 1,2,..., $x$ of $K_x$. Also, the value of $x$ and $y$ is strictly greater than two. The $y$-thorn complete graph $K_{x,y}$ (depicted in Figure 1) is considered as the thorn graph ($K_{x,y}$), where $S = \{u_1, u_2, \ldots, u_y\}$. Here the vertices and edges of the $y$-thorn complete graph $K_{x,y}$ are given as $p = x + \sum_{i=1}^{y} u_i$ and $q = x(y-1) + \sum_{i=1}^{y} u_i$.

![Figure 1. Thorn complete graph $K_{x,y}$](image)

Theorem 3.1 Consider the thorn complete graph, the Sombor index with $(x + xy)$ number of vertices is given by:

$$SO(K_{x,y}) = x y \sqrt{y^2 + x^2 + 2(xy - x - y + 1) + 2x(y + x - 1)}$$

Proof

Here the pair of vertices of $K_x$ are examined independently between the pair of vertices of $u_i$ whereas $i$ ranges between 1,2,3,......,$y$ of the $y$-thorn complete graph $K_{x,y}$ together with the pair of vertices belonging to $K_x$ and otherwise the pendant vertex.

Let the vertices of the complete graph $K_x$ be denoted by $v_1, v_2, \ldots, v_x$ and let the vertices of the pendant degree vertex of $K_x$ be denoted by $u_1, u_2, \ldots, u_y$ where $i$ ranges from 1,2,3,......,$y$ (which is depicted in Figure 1). Let $d(v_i) = (y_j + x - 1)$ and $d(u_i) = 1$.

Then the Sombor index is calculated as follows:

$$SO(K_{x,y}) = \sum_{i,j=1}^{x,y} \sqrt{(d(v_i))^2 + (d(u_j))^2} + \sum_{i=1}^{x} \sqrt{(d(v_i))^2 + (d(v_i))^2}$$

$$= \sum_{i,j=1}^{x,y} \sqrt{(y_j + x - 1)^2 + 1} + \sum_{i=1}^{x} \sqrt{(y_j + x - 1)^2 + (y_j + x - 1)^2}$$

$$= x y \sqrt{y^2 + x^2 + 2(xy - x - y + 1) + 2x(y + x - 1)}$$
**Theorem 3.2** Consider the thorn complete graph, the harmonic index with \((x + xy)\) number of vertices is given by:

\[
H(K_{x,y}) = \left(\frac{2x y y}{y + x} \right) + \left(\frac{x}{y + x - 1}\right)
\]

**Proof**
Here the pair of vertices of \(K_x\) are examined independently between the pair of vertices of \(u_i\) whereas \(i\) ranges between 1, 2, 3, ..., \(y\) of the \(y\)-thorn complete graph \(K_{x,y}\) together with the pair of vertices belonging to \(K_x\) and otherwise the pendant vertex. Let the vertices of the complete graph \(K_x\) be denoted by \(v_1, v_2, ..., v_x\) and let the vertices of the pendant degree vertex of \(K_x\) be denoted by \(u_1, u_2, ..., u_y\) where \(i\) ranges from 1, 2, 3, ..., \(y\) (which is depicted in Figure 1). Let \(d(v_i) = y_j + x - 1\) and \(d(u_j) = 1\).

Then the harmonic index is calculated as follows:

\[
H(K_{x,y}) = \sum_{i,j=1}^{x y} \left(\frac{2}{d(v_i) + d(u_j)}\right) + \sum_{i=1}^{y} \frac{2}{d(u_j) + d(v_i)} = \sum_{i,j=1}^{x y} \left(\frac{x_i}{y_j + x - 1}\right) + \sum_{i=1}^{y} \frac{x_i}{y_j + x - 1}
\]

**3.2 Results on thorn cog-complete graph**

Here Sombor and harmonic index are computed for the thorn cog-complete graph

**3.2.1 Cog-complete graph \((K_x^c)\)**

The graph \(K_x^c\) is obtained from a complete graph \(K_x(x \geq 2)\) consisting of vertices denoted by \(\{v_1, v_2, ..., v_x\}\), in addition, it contains \(y\) number of vertices namely \(u_1, u_2, ..., u_y\) and it has 2\(y\) number of edges denoted by \(\{u_i v_i, u_i v_{i+1}\} i = 1, 2, 3, ..., x; j = 1, 2, 3, ..., y\). Also, \(v_{x+1} = v_1\), which is clearly depicted in Figure 2. The number of vertices and edges are \(p(K_x^c) = 2(x + y)\) and \(q(K_x^c) = \frac{x(x + 3)}{2}\) respectively.

**Figure 2. Cog-complete graph \(K_x^c\)**

**3.2.2 Thorn cog-complete graph \((K_x^c)^*\)**

The graph \((K_x^c)^*\) is obtained from the cog-complete graph \(K_x^c\) with \(2y\) number of additional pendant vertex namely \(\{w_1^k, w_2^k, ..., w_{2y}^k\}\) for \(k = 1, 2, ..., 2y\), whereas the edges are identified by \(\{u_j w_{2k-1}, u_j w_{2k}\} i, j = 1, 2, 3, ..., y\) which is represented in Figure 3.

**Figure 3. Thorn Cog-complete graph \((K_x^c)^*\)**

**Theorem 3.3** Consider the thorn cog-complete graph, the Sombor index with \((x + 3y)\) number of vertices is given by:

\[
S(O(K_x^c_{y,x})) = x y j \sqrt{x^2 + 2x + 17} + \sqrt{2} x (x + 1) + 2 j y y k \sqrt{17}
\]

**Proof**
Here the pair of vertices of \(K_x\) are examined independently between the pair of vertices of \(u_i\) whereas \(i\) ranges between 1, 2, 3, ..., \(y\) of graph \(K_x^c\) together with the pair of vertices belonging to \(K_x\) and between pair of vertices of \(u_i\) for \(i\) ranges from 1, 2, 3, ..., \(y\) of \(K_x^c\) together with the pair of \(K_x^c_{y,x}\).

Let the vertices of the complete graph \(K_x\) be denoted by \(\{v_1, v_2, ..., v_x\}\) where \(i\) ranges from 2, 3, 4, ..., \(x\) and additional vertices of \(K_x^c\) be denoted by \(u_1, u_2, ..., u_y\) where \(j\) ranges from 1, 2, 3, ..., \(y\).

Furthermore, let \(w_1, w_2, ..., w_{2y}\) for \(k = 1, 2, 3, ..., 2y\) of \(K_x^c_{y,x}\) be another \(2y\) number of pendant vertices of \(K_x^c_{y,x}\) which is depicted in Figure 3. Let \(d(v_i) = (x + 1)\) and \(d(u_j) = 4\) and \(d(w_k) = 1\).

\[
S(O(K_x^c_{y,x})) = \sum_{i,j=1}^{x y} \sqrt{(d(v_i))^2 + (d(u_j))^2} + \sum_{i=1}^{y} \sqrt{(d(u_j))^2 + (d(v_i))^2} + \sum_{j,k=1}^{y} j k \sqrt{(d(u_j))^2 + (d(w_k))^2}
\]

\[
= x y j \sqrt{x^2 + 2x + 17} + \sqrt{2} x (x + 1) + 2 j y y k \sqrt{17} j y y k
\]

**Theorem 3.4** Consider the thorn cog-complete graph, the harmonic index with \((x + 3y)\) number of vertices is given by:

\[
H(K_x^c_{y,x}) = \left(\frac{2x y y}{x + 5}\right) + \left(\frac{x}{x + 1}\right) + \left(\frac{4 j y y k}{5}\right)
\]
Proof
Here the pair of vertices of \( K_s \) are examined independently between the pair of vertices of \( u_i \) whereas \( i \) ranges between \( 1,2,3,\ldots, y \) of \( K_x^* \) together with the pair of vertices belonging to \( K_y \) and between pair of vertices of \( u_j \) for \( j \) ranges from \( 1,2,3,\ldots, y \) of \( K_x^* \) together with the pair of pendant degree vertices of \( K_y^* \). Let the vertices of the complete graph \( K_x^* \) be denoted by \( \{v_1, v_2, \ldots, v_x\} \) where \( i \) ranges from \( 2,3,4,\ldots, x \) and the additional vertices of \( K_x^* \) be denoted by \( u_1, u_2, \ldots, u_y \) where \( j \) ranges from \( 1,2,3,\ldots, y \).

Furthermore, let \( w, w_2, \ldots, w_{2y} \) for \( k = 1,2,3,\ldots, 2y \) of \( K_y^* \) be another \( 2y \) number of pendant vertices of \( K_y^* \) which is depicted in Figure 3. Let \( d(v_i) = (x + 1) \) and \( d(u_j) = 4 \) and \( d(w_k) = 1 \).

\[
H(K_x^* y_x^*) = \sum_{i,j=1}^{x,y_i} \left( \frac{2}{d(v_i)+d(u_j)} \right) + \sum_{i=1}^{x} \left( \frac{2}{d(v_i)+d(u_j)} \right) + \\
\sum_{i,j=1}^{x,y_i} \left( \frac{2}{d(u_j)+d(v_i)} \right) + \sum_{i=1}^{x} \left( \frac{2}{d(u_j)+d(v_i)} \right) + \\
\sum_{i,j=1}^{x,y_i} \left( \frac{2}{d(v_i)+d(w_k)} \right) + \sum_{j=1}^{y} \left( \frac{2}{d(w_k)+d(v_i)} \right)
\]

3.3 Results on thorn cog star graph

Here Sombor and harmonic index are computed for the thorn cog-star graph.

3.3.1 Cog-stargraph \( S^C_x \)
The graph \( S^C_x \) is obtained from the star graph \( S_x \) \((x\geq 2)\), consisting of the vertex set \( \{v_1, v_2, \ldots, v_x, v_x\} \) and also \((y - 1)\) set of vertices namely \( u_1, u_2, \ldots, u_y \) and \( 2y \) edges mentioned as \( \{u_jw_{i+1}, u_jw_{i+2} : i = 1, 2, 3, \ldots, x, j = 1, 2, 3, \ldots, y - 1\} \). Also, \( v_x+1 = v_2 \) and it is clearly depicted in Figure 4. The number of vertices and edges are given by \( p(S^C_x) = (x + y - 1) \) and \( q(S^C_x) = (x + 2y - 3) \).

![Figure 4. Cog-star graph \( S^C_x \)](image)

3.3.2 Thorn cog-star graph \( \{S^C_x^* \} \)
The graph \( S^C_x^* \) is acquired from the star graph \( S^C_x \) \((x\geq 2)\), consisting of \( \{v_1, v_2, \ldots, v_x, v_x, u_1u_x, \ldots, u_yv_x\} \) where \( i \) ranges from \( 1,2,3,\ldots,x \) and \( j \) from \( 1,2,3,\ldots,(y - 1) \) in addition with \( 2(y - 1) \) number of vertices such that \( \{w_1, w_2, \ldots, w_{2y-3}, w_{2y-2}\} \) and the number of edges are denoted by \( \{u_jw_{j-1}, w_jw_{j+1} : j = 1, 2, 3, \ldots, (y - 1)\} \) as depicted in the Figure 5.

![Figure 5. Thorn cog-star graph \( S^C_x^* \)](image)

**Theorem 3.5** Consider the thorn cog-star graph, the Sombor index with \((x + 3(y - 1))\) number of vertices given by:

\[
SO(S^C_x^*) = 5x(y - 1) + x_1\sqrt{x^2 - 2x + 10} + 2\sqrt{17(y - 1)}(y - 1).
\]

**Proof**
Here the pair of vertices of \( S_x \) are examined independently between the pair of vertices of \( u_j \) where \( j \) ranges from \( 1,2,3,\ldots,(y - 1) \) of \( S^C_x \) together with the pair of vertices belonging to \( S_y \) and between pair of vertices of \( u_j \) for \( j \) ranges from \( 1,2,3,\ldots,y \) of \( S^C_x \) together with the pair of pendant vertices of \( S^C_x \). Let the vertices of the star graph \( S_x \) be denoted by \( v_1, v_2, \ldots, v_x \) where \( i \) ranges from \( 1,2,3,\ldots,x \) and the additional vertices of \( S^C_x \) be denoted by \( u_1, u_2, \ldots, u_x \) where \( j \) ranges from \( 1,2,3,\ldots,y \). Furthermore, let \( w_1, w_2, \ldots, w_{2y-2} \) for \( k = 1,2,3,\ldots, (2y - 2) \) of \( S^C_x \) be another \( (2y - 2) \) number of pendant vertices of \( S^C_x \) which is depicted in Figure 5. Let \( d(v_i) = 3 \), \( i \in \{2, 3, \ldots, x\} \) \( d(u_j) = (x - 1) \), \( d(w_k) = 4 \) and \( d(w_k) = 1 \).

**Theorem 3.6** Consider the thorn cog-star graph, the harmonic index with \((x + 3(y - 1))\) number of vertices given by:

\[
H(S^C_x^*) = \left( \frac{\sum_{i=1}^{x} d(v_i)}{x} \right)^2 + \left( \frac{\sum_{j=1}^{y} d(u_j)}{x} \right)^2 + \left( \frac{\sum_{k=1}^{2} d(w_k)}{x} \right)^2 + \left( \frac{\sum_{i=1}^{x} d(v_i)}{2x} \right)^2 + \left( \frac{\sum_{j=1}^{y} d(u_j)}{2x} \right)^2 + \left( \frac{\sum_{k=1}^{2} d(w_k)}{2x} \right)^2 + \left( \frac{\sum_{i=1}^{x} \sqrt{x+1}^2 + 4 + \sqrt{4 + 4^2} + \sqrt{4 + 4^2} + \sqrt{4 + 4^2}}{5} \right).
\]
Proof  
Here the pair of vertices of $S_x$ are examined independently between the pair of vertices of $u_i$ where $j$ ranges from $1, 2, 3, ..., y - 1$ of $S_x^C$ together with the pair of vertices belonging to $S_x$ and between pair of vertices of $u_i$ for $j$ ranges from $1, 2, 3, ..., y$ of $S_x$ together with the pair of pendant degree vertices of $S_x^C$. Let the vertices of the star graph $S_x$ be denoted by $v_1, v_2, ..., v_{x-1}, v_x$, where $i$ ranges from $1, 2, 3, ..., x$ and the additional vertices of $S_x^C$ be denoted by $u_1, u_2, ..., u_{y-1}$ where $j$ ranges from $1, 2, 3, ..., (y - 1)$.

Furthermore, let $w_1, w_2, ..., w_{2y-2}$ for $k = 1, 2, 3, ..., 2y - 2$ of $S_x^C$ be $2y - 2$ number of pendant vertices of $S_x^C$ which is depicted in Figure 5. Let $d(v_i) = 3$, and $d(v_i) = x - 1, d(u_j) = 4$ and $d(w_k) = 1$.

$$H(S_x^C) = \sum_{i=1}^{x} \left( \frac{2}{d(v_i) + d(u_j)} + \frac{2}{d(v_i) + d(w_k)} \right) + \sum_{i=1}^{y} \left( \frac{2}{d(u_j) + d(w_k)} \right)$$

$$= \sum_{i=1}^{x} \left( \frac{2}{d(v_i) + d(u_j)} + \frac{2}{d(v_i) + d(w_k)} \right) + \sum_{i=1}^{y} \left( \frac{2}{d(u_j) + d(w_k)} \right)$$

$$= \sum_{i=1}^{x} \left(\frac{2}{x+1} + \frac{2}{y-1} \right) + \sum_{i=1}^{y} \left(\frac{2}{y-1} \right)$$

$$= \sum_{i=1}^{x} \left(\frac{2}{x+1} \right) + \sum_{i=1}^{y} \left(\frac{2}{y-1} \right)$$

3.4 Results on thorn wheel graph

Here Sombor and harmonic index are computed for the thorn wheel graph.

3.4.1 Thorn wheel graph ($W_x$)

The $y$-thorn wheel graph $W_{xy}$ has a parent graph $W_x$ and $(y - 3)$ thorns that is it has $u_i$ pendant vertices where $i$ ranges from $1, 2, 3, ..., y$ at each vertex $v_i$ for $i = 1, 2, 3, ..., x$ of $W_x$ and also $x, y > 3$. The $y$-thorn wheel graph $W_{xy}$ is considered as the thorn graph ($W_x^S$) where $S = u_1, u_2, ..., u_y$. Then $p = x + \sum_{i=1}^{y} u_i$ and $q = 2(x - 1) + \sum_{i=1}^{y} u_i$ denote the number of vertices and edges of $W_{xy}$. Also, then $W_x$ is depicted in Figure 6.

**Figure 6. Thorn wheel graph $W_x$**

Theorem 3.7 Consider the thorn wheel graph, the Sombor index with $(x + (x - 1)y)$ number of vertices is given by:

$$SO(W_{xy}) = x_1 y \sqrt{y^2 + 6y + 10} + \sqrt{2} x_i (y + 3) + x_i \sqrt{x^2 + y^2 - 2x + 6y + 10}.$$

Proof

Here the pair of vertices of $W_x$ are examined independently between the pair of vertices of $u_i$ where $i$ ranges from $1, 2, 3, ..., y$ of the $y$-thorn wheel graph $W_{xy}$ together with the pair of vertices belonging to $W_x$ and otherwise the pendant degree vertex. Let the vertices of the wheel graph $W_x$ be denoted by $v_1, v_2, ..., v_x$ and let the vertices of the pendant degree vertex of $W_{xy}$ be denoted by $u_1, u_2, ..., u_y$ where $i$ ranges from $1, 2, 3, ..., y$, as depicted in Figure 6. Let $d(v_i) = (y + 3)$, for $i = 2, 3, ..., x$, $d(v_1) = (x - 1)$ and $d(u_i) = 1$.

$$SO(W_{xy}) = \sum_{i=1}^{x} \left( \frac{2}{d(v_i)} + \frac{2}{d(u_i)} \right) + \sum_{i=1}^{x} \left( \frac{2}{d(v_i)} + \frac{2}{d(u_i)} \right)$$

$$= \sum_{i=1}^{x} \sqrt{\frac{2}{d(v_i)} + \frac{2}{d(u_i)}}$$

$$= \sum_{i=1}^{x} \sqrt{\frac{2}{d(v_i)} + \frac{2}{d(u_i)}}$$

$$= \sum_{i=1}^{x} \sqrt{\frac{2}{d(v_i)} + \frac{2}{d(u_i)}}$$

Theorem 3.8 Consider the thorn wheel graph, the harmonic index with $(x + (x - 1)y)$ number of vertices is given by:

$$H(W_{xy}) = \left( \frac{2x_1 y}{y+4} + \frac{x_1}{y+3} + \frac{2x_i}{x+y+2} \right).$$

Proof

Here the pair of vertices of $W_x$ are examined independently between the pair of vertices of $u_i$ where $i$ ranges from $1, 2, 3, ..., y$ of the $y$-thorn wheel graph $W_{xy}$ together with the pair of vertices belonging to $W_x$ and otherwise the pendant degree vertex. Let the vertices of the wheel graph $W_x$ be denoted by $v_1, v_2, ..., v_x$ and let the vertices of the pendant degree vertex of $W_{xy}$ be denoted by $u_1, u_2, ..., u_y$ where $i$ ranges from $1, 2, 3, ..., y$, as depicted in Figure 6. Let $d(v_i) = (y + 3)$, for $i = 2, 3, ..., x$, $d(v_1) = (x - 1)$ and $d(u_i) = 1$.

$$H(K_{xy}^S) = \sum_{i=1}^{x} \left( \frac{2}{d(v_i) + d(u_i)} + \frac{2}{d(v_i) + d(u_i)} \right) + \sum_{i=1}^{x} \left( \frac{2}{d(v_i) + d(u_i)} + \frac{2}{d(v_i) + d(u_i)} \right)$$

$$= \sum_{i=1}^{x} \left( \frac{2}{d(v_i) + d(u_i)} + \frac{2}{d(v_i) + d(u_i)} \right)$$

3.5 Results on thorn cog-wheel graph

Here the Sombor and harmonic index are computed for the thorn cog-wheel graph.

3.5.1 Cog-wheel graph ($W_x^C$)

**Figure 7. Cog wheel graph $W_x^C$**
Here the graph $W^C_x$, obtained from the wheel graph $W_x$ ($x \geq 4$) consisting of vertices denoted by $v_1, v_2, ..., v_{x-1}, v_x$, in addition, it contains $(y - 1)$ number of vertices, namely $u_1, u_2, ..., u_{y-1}$ and number of edges denoted by $\{u_iu_{i+1}, u_iu_{i+2} : i = 1, 2, 3, ..., (y - 1)\}$. Also, $(v_{x+1} = v_x)$ which is clearly depicted in Figure 7. The number of vertices and edges are given by $p(W^C_x) = x + y - 1$ and $q(W^C_x) = 2(x + y - 2)$.

3.5.2 Thorn cog-wheel graph ($W^C_{x}$)

Here the graph $W^C_{x}$, is obtained from the graph $W^C_x$ consisting of the vertex set $\{v_1, v_2, ..., v_{x-1}, v_x, u_1, u_2, ..., u_{y-1}\}$ where $i = 1, 2, 3, ..., x$ and $j = 1, 2, 3, ..., (y - 1)$ . In addition it contained 2 $(y - 1)$ number of vertices given by $\{w_1, w_2, ..., w_{2y-3}, w_{2y-2}\}$ and the edges are denoted by $\{u_jw_{2j-1}, u_jw_{2j} : j = 1, 2, 3, ..., (y - 1)\}$ (Figure 8).

![Figure 8. Thorn Cog wheel graph $W^C_{x}$](image)

**Theorem 3.9** Consider the thorn cog-wheel graph, the Sombor index with $(x + 3(y - 1))$ number of vertices given by:

$$SO(W^C_{x}) = \sum_{i=2, j=1}^{x,y-1} \left( \sqrt{(d(v_i))^2 + (d(u_j))^2} + \sum_{i=2}^{v_i} \sum_{j=1}^{u_j} \left( \sqrt{(d(v_i))^2 + (d(u_j))^2} \right) \right)$$

**Proof**

Here the pair of vertices of $W_x$ are examined independently between the pair of vertices of $u_j$ where $j$ ranges from 1, 2, 3, ..., $(y - 1)$ of $W^C_x$ together with the pair of vertices belonging to $W_x$ and between pair of vertices of of $u_j$ where $j$ ranges from 1, 2, 3, ..., $y$ of $W^C_x$ together with the pair of pendant degree vertices of $W^C_{x}$.

Let the vertices of the wheel graph $W_x$ be denoted by $v_1, v_2, ..., v_x$ where $i = 1, 2, 3, ..., x$ and the additional vertices of $W^C_x$ be denoted by $u_1, u_2, ..., u_{y-1}$ where $j = 1, 2, 3, ..., (y - 1)$.

Furthermore, let $w_1, w_2, ..., w_{2y-2}$ for $k = 1, 2, 3, ..., (2y - 2)$ of $W^C_x$ be another $(2y - 2)$ number of pendant degree vertices of $W^C_x$ which is depicted in Figure 8. Let $d(v_i) = (x - 1)$, $d(u_j) = 4$ (for $j = 1, 2, 3, ..., (y - 1)$), $d(v_i) = 5$ for $i = 2, 3, ..., x$ and $d(w_k) = 1$ for $k = 1, 2, 3, ..., 2(y - 1)$.

**Theorem 3.10** Consider the thorn cog-wheel graph, the harmonic index with $(x + 3(y - 1))$ number of vertices given by:

$$H(W^C_{x}) = \sum_{i=2, j=1}^{x,y-1} \left( \frac{2}{(d(v_i))^2 + (d(u_j))^2} + \sum_{i=2}^{v_i} \sum_{j=1}^{u_j} \left( \frac{2}{(d(v_i))^2 + (d(u_j))^2} \right) \right)$$

**Proof**

Here the pair of vertices of $W_x$ are examined independently between the pair of vertices of $u_j$ where $j$ ranges from 1, 2, 3, ..., $(y - 1)$ of $W^C_x$ together with the pair of vertices belonging to $W_x$ and between pair of vertices of of $u_j$ where $j$ ranges from 1, 2, 3, ..., $y$ of $W^C_x$ together with the pair of pendant degree vertices of $W^C_{x}$.

Let the vertices of the wheel graph $W_x$ be denoted by $v_1, v_2, ..., v_x$ where $i = 1, 2, 3, ..., x$ and the additional vertices of $W^C_x$ be denoted by $u_1, u_2, ..., u_{y-1}$ where $j = 1, 2, 3, ..., (y - 1)$.

Furthermore, let $w_1, w_2, ..., w_{2y-2}$ for $k = 1, 2, 3, ..., (2y - 2)$ of $W^C_x$ be another $(2y - 2)$ number of pendant degree vertices of $W^C_x$ which is depicted in Figure 8. Let $d(v_i) = (x - 1)$, $d(u_j) = 4$ (for $j = 1, 2, 3, ..., (y - 1)$), $d(v_i) = 5$ for $i = 2, 3, ..., x$ and $d(w_k) = 1$ for $k = 1, 2, 3, ..., 2(y - 1)$.

4. RESULTS AND DISCUSSION

Thorn graph provides a computational approach to deal with indices namely Sombor and harmonic indices. Here, using the family of thorn graphs such as the thorn-cog complete graph, star and wheel graph, values are computed using the edge
partition method. This computational methodology creates a base for the analysis of the properties of molecular compounds in chemistry. Moreover, the methodology aids in comparing other topological indices with different graphical structure resulting in the prediction of physicochemical properties of chemical compounds without the involvement of laboratory experiments and it is a cost-effective approach.

5. CONCLUSION

This research paper has conducted an in-depth analysis of two noteworthy indices – the Sombor and harmonic index – in relation to thorn graphs. Mathematical relationships between these indices and thorn graphs have been established. Initially, the Sombor and harmonic index were examined in the context of the thorn cog complete graph. Subsequently, the focus shifted to the thorn cog-star and cog-wheel graph.

This theoretical methodology significantly contributes to the understanding of physico-chemical properties of molecules in chemistry. Future research could extend these computational and analytical techniques to other thorn families, dealing with additional topological indices. This would facilitate easier prediction and comparison of molecules.

The theoretical tools developed in this study hold the potential to foster advancements in various disciplines. These include drug design, toxicity prediction, examination of the biological properties of chemical compounds, material sciences, risk assessment, regulatory decision-making, the pharmaceutical industry, and nanotechnology.

REFERENCES


**NOMENCLATURE**

- QSPR  Quantity Structure Property Relationship
- QSAR  Quantity Structure Activity Relationship
- SO    Sombor Index
- H     Harmonic Index