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Analysis of Sombor and Harmonic Indices of Thorn Cog-Graphs

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ABSTRACT

In the realm of chemical graph theory, a topological index is a numerical parameter derived from a molecular graph. This index offers a streamlined approach to numerically calculate and compare various physico-chemical properties of chemical compounds, such as melting point, boiling point, viscosity, size, shape, atom count, bond strength, enthalpy, and geometric characteristics. Traditional scientific exploration of these properties, conducted in a laboratory setting, is often time-intensive, costly, and demands expertise in the respective field. Chemical graph theory provides a more cost-effective and straightforward solution, enabling the correlation of topological indices with chemistry. This approach allows for the computational analysis of any chemical species using mathematical tools, circumventing the need for laboratory-based experiments. This approach offers considerable benefits in chemical science, as it employs mathematical and theoretical methods to estimate a molecule's physico-chemical properties. The primary objective of this paper is to elucidate the correlation between thorn graphs and topological indices, utilizing the methods of vertex degrees and edge partitioning. The paper conducts a rigorous analysis of thorn graphs using mathematical calculations, deriving the relationship between the indices. These indices play a pivotal role in a diverse array of research areas, including chemoinformatics, pharmaceutical industry applications, and toxicity prediction among others.

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/toxicants/environmental 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 $M=\{a_1, a_2, \ldots, a_n\}$ 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 $p=\{1,2,3,\ldots,n\}$. $V(G_M)=V(G)\cup V_1(G)\cup V_2(G)\ldots\ldots V_n(G)$. 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 Trinajstic, 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:

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

where, $\boldsymbol{d_G\ (u)}$ and $\boldsymbol{d_G\ (v)}$ denote the degree of a vertex of $\boldsymbol{u}$ and $\boldsymbol{v}$ in *G*, respectively.

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

$$H\ (G) = \sum_{uv\in E\ (G)} \left(\frac{2}{d_G\ (u) + d_G\ (v)}\right).$$

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

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

where, α is a real number.

Definition 4. A complete graph denoted by K_x 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_M 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 $1, 2, \dots, y$, which exists at each vertex v_i for i ranges from $1, 2, \dots, x$ 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 $(K_x)_S$, where $S = \{u_1, u_2, \dots\dots, u_y\}$. 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 $q = \frac{x(x-1)}{2} + \sum_{i=1}^{y} u_i$.

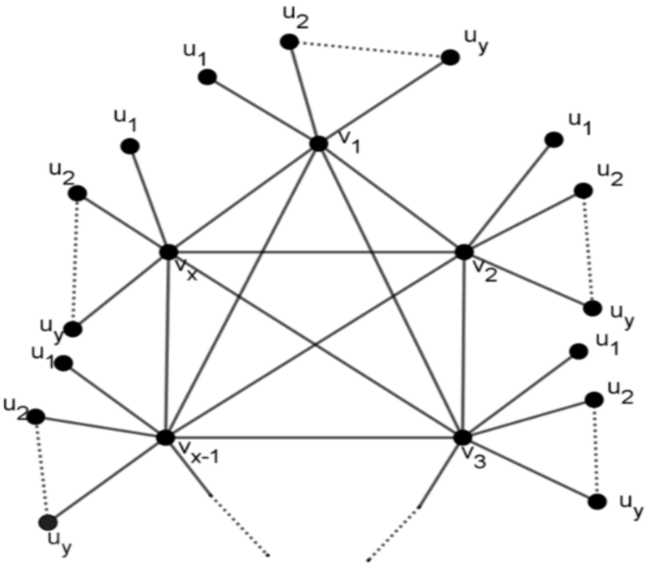

Figure 1. Thorn complete graph $K_{x,y}$

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

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

Proof

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

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

Then the Sombor index is calculated as follows:

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

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

$$x_i y_j \sqrt{y_j^2 + x^2 + 2(xy_j - x - y_j + 1)} + \sqrt{2} x_i (y_j + x - 1)$$

Theorem 3.2 Consider the thorn complete graph, the harmonic index with $(x + xy)$ number of vertices is given by:

$$H(K_{x,y}) = \left(\frac{2x_i y_j}{y_j + x}\right) + \left(\frac{x_i}{y_j + x - 1}\right)$$

Proof

Here the pair of vertices of K_x are examined independently between the pair of vertices of u_i whereas i ranges between $1, 2, 3, \dots\dots, y$ of the *y*-thorn complete graph $K_{x,y}$ together with the pair of vertices belonging to K_y and otherwise the pendant vertex. Let the vertices of the complete graph K_x be denoted by $v_{1,}\ v_2, \dots\dots,\ v_x$ and let the vertices of the pendant degree vertex of K_x be denoted by $u_{1,}\ u_2, \dots\dots,\ u_y$ where i ranges from $1, 2, 3, \dots\dots, y$ (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:

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

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 $\{v_{1,}\ v_2, \dots\dots,\ v_x\}$, in addition, it contains y number of vertices namely $u_{1,}\ u_2, \dots\dots,\ u_y$ and it has $2y$ number of edges denoted by $\{u_j v_i,\ u_j v_{i+1};\ i = 1, 2, 3, \dots\dots, x;\ j = 1, 2, 3, \dots\dots, y\}$. 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.

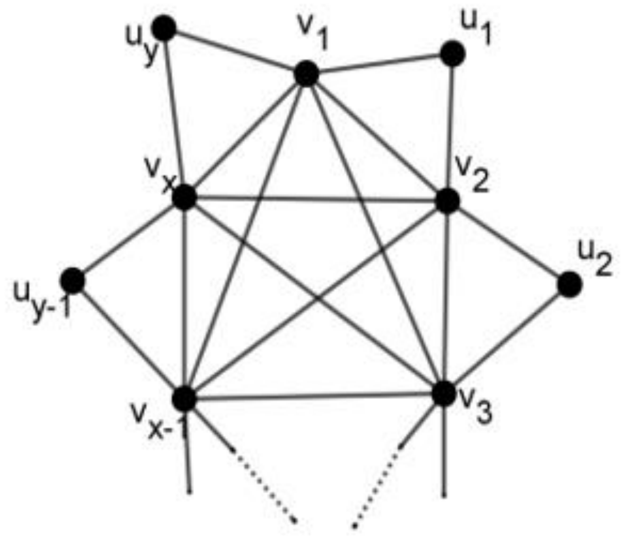

Figure 2. Cog-complete graph $K^c{}_x$

3.2.2 Thorn cog-complete graph $\left(K^{C^*}{}_x\right)$

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

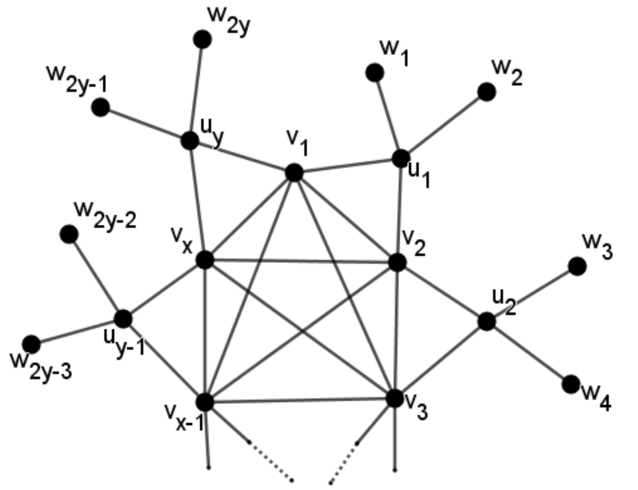

Figure 3. Thorn Cog-complete graph $\left(K^{C^*}{}_x\right)$

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

$$SO\left(K^{C^*}{}_{y,x}\right) = x_i y_j \sqrt{x^2 + 2x + 17} + \sqrt{2}x_i(x + 1) + 2(y_j y_k)\sqrt{17}.$$

Proof

Here the pair of vertices of K_x are examined independently between the pair of vertices of u_i whereas i ranges between $1, 2, 3, \dots, y$ 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 $1, 2, 3, \dots, y$ of $K^c{}_x$ together with the pair of $K_{y,x}^C$.

Let the vertices of the complete graph K_x be denoted by $\{v_{1,}\ v_2, \dots\dots, v_x\}$ where i ranges from $2, 3, 4, \dots, x$ and additional vertices of $K^c{}_x$ be denoted by $u_{1,}\ u_2, \dots\dots,\ u_y$ where j ranges from 1, 2, 3, ..., y.

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

$$SO\left(K^{C^*}{}_{y,x}\right) = \sum_{i,j=1}^{x_i,y_j}\sqrt{\left(d(v_i)\right)^2 + \left(d(u_j)\right)^2} + \sum_{i=1}^{x_i}\sqrt{\left(d(v_i)\right)^2 + \left(d(v_i)\right)^2} + \sum_{j,k=1}^{y_j,2y_k}\sqrt{\left(d(u_j)\right)^2 + \left(d(w_k)\right)^2} = \sum_{i,j=1}^{x_i,y_j}\sqrt{(x+1)^2 + 4^2} + \sum_{i=1}^{x_i}\sqrt{(x+1)^2 + (x+1)^2} + \sum_{j,k=1}^{y_j,2y_k}\sqrt{1 + 4^2} = x_i y_j\sqrt{x^2 + 2x + 17} + \sqrt{2}x_i(x+1) + 2\sqrt{17}(y_j y_k).$$

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

$$H\left(K^{C^*}{}_{y,x}\right) = \left(\frac{2x_i y_j}{x + 5}\right) + \left(\frac{x_i}{x + 1}\right) + \left(\frac{4y_j y_k}{5}\right).$$

Proof

Here the pair of vertices of K_x are examined independently between the pair of vertices of u_i whereas i ranges between $1, 2, 3, \dots, y$ of $K^c{}_x$ together with the pair of vertices belonging to K_x and between pair of vertices of u_i for i ranges from $1, 2, 3, \dots, y$ of K_x^C together with the pair of pendant degree vertices of $K^{C^*}{}_{y,x}$. Let the vertices of the complete graph K_x be denoted by $\{v_{1,} v_2, \dots\dots, v_x\}$ where i ranges from $2, 3, 4, \dots, x$ and the additional vertices of K_x^C be denoted by $u_{1,} u_2, \dots\dots, u_y$ where j ranges from $1, 2, 3, \dots\dots, y$.

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

$$H\left(K^{C^*}{}_{y,x}\right) = \sum_{i,j=1}^{x_i, y_j} \left(\frac{2}{d(v_i)+d(u_j)}\right) + \sum_{i=1}^{x_{i,}} \left(\frac{2}{d(v_i)+d(v_i)}\right) + \sum_{i,j=1}^{y_j, 2y_k} \left(\frac{2}{d(u_j)+d(w_k)}\right) = \sum_{i,j=1}^{x_i, y_j} \left(\frac{2}{x+1+4}\right) + \sum_{j=1}^{x_i} \left(\frac{2}{x+1+x+1}\right) + \sum_{\mathrm{i,j=1}}^{\mathrm{y_j}, 2y_k} \left(\frac{2}{4+1}\right) = \left(\frac{2x_i y_j}{x+5}\right) + \left(\frac{x_i}{x+1}\right) + \left(\frac{4y_j y_k}{5}\right).$$

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≥2)*, consisting of the vertex set $\{v_{1,} v_2, \dots\dots, v_{x-1,} v_x\}$ and also $(y-1)$ set of vertices namely $u_{1,} u_2, \dots\dots, u_{y-1}$ and $2y$ edges mentioned as $\{u_j w_{i+1}, u_j v_{i+2} : i = 1, 2, 3, \dots, x,\ j = 1, 2, 3, \dots\dots, (y-1)\}$. Also, $v_{x+1} = v_2$ and it is clearly depicted in Figure 4. The number of vertices and edges are given by $p(S_x^C) = (x + y - 1)$ and $q(S_x^C) = (x + 2y - 3)$.

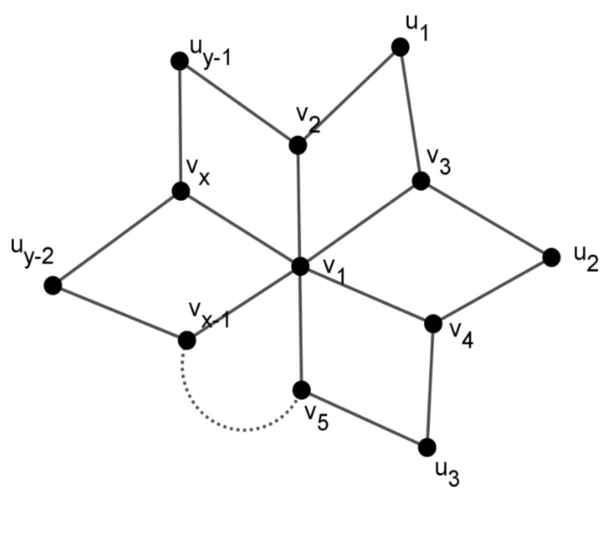

Figure 4. Cog-star graph $S^c{}_x$

3.3.2 Thorn cog-star graph $\left(S^{C^*}{}_x\right)$

The graph $S^{C^*}{}_x$, is acquired from the star graph $S^C{}_x$ (*x*≥2), consisting of $\{v_{1,} v_2, \dots\dots, v_{x-1,} v_x, u_1, u_2, \dots\dots, u_{y-1}\}$ where i ranges from $1, 2, 3, \dots, x$ and j from $1, 2, 3, \dots\dots, (y-1)$ in addition with $2(y-1)$ number of vertices such that $\{w_{1,} w_2, \dots\dots, w_{2y-3,} w_{2y-2}\}$ and the number of edges are denoted by $\{u_{j,} w_{2j-1}, u_j w_{2j} : j = 1, 2, 3, \dots, (y-1)\}$ as depicted in the Figure 5.

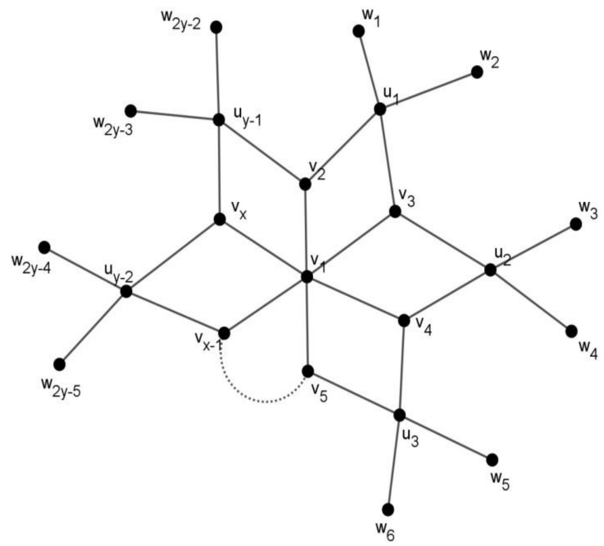

Figure 5. Thorn cog-star graph $S^{C^*}{}_x$

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

$$SO\left(S^{C^*}{}_x\right) = 5x_i(y_j - 1) + x_i\sqrt{x^2 - 2x + 10} + 2\sqrt{17}(y_j - 1)(y_k - 1).$$

Proof

Here the pair of vertices of S_x are examined independently between the pair of vertices of u_j where j ranges from $1, 2, 3, \dots (y-1)$ of S_x^C together with the pair of vertices belonging to S_x and between pair of vertices of u_j for j ranges from $1, 2, 3, \dots, \mathrm{y}$ of S_x^C together with the pair of pendant vertices of $S^{C^*}{}_x$. Let the vertices of the star graph S_x be denoted by $v_{1,} v_2, \dots\dots, v_{x-1,} v_x$, where i ranges from $1, 2, 3, \dots\dots, x$ and the additional vertices of S_x^C be denoted by $u_{1,} u_2, \dots\dots, u_{y-1,}$ where j ranges from $1, 2, 3, \dots\dots, (y-1)$.

Furthermore, let w_1, $w_2, \dots\dots, w_{2y-2}$ for $\mathrm{k} = 1, 2, 3, \dots\dots, (2y-2)$ of $S^{C^*}{}_x$ be an another $(2y-2)$ number of pendant vertices of S_x^C which is depicted in Figure 5. Let $d(v_i) = 3$, $i \epsilon \{2, 3, \dots\dots, x\}$ $d(v_1) = (x-1)$, $d(u_j) = 4$ and $d(\mathrm{w_k}) = 1$.

$$SO\left(\mathrm{S^{C^*}}{}_\mathrm{x}\right) = \sum_{i=2,j=1}^{x_i, y_j - 1} \sqrt{\left(d(v_i)\right)^2 + \left(d(u_j)\right)^2} + \sum_{i=2}^{x_i} \sqrt{\left(d(v_1)\right)^2 + \left(d(v_i)\right)^2} + \sum_{i=2,j=1}^{y_j - 1, 2y_k - 2} \sqrt{\left(d(u_j)\right)^2 + \left(d(w_k)\right)^2} = \sum_{i=1}^{x_i, y_j - 1} \sqrt{3^2 + 4^2} + \sum_{i=1}^{x_i} \sqrt{(x-1)^2 + (3)^2} + \sum_{i=2,j=1}^{y_j - 1, 2y_k - 2} \sqrt{1 + (4)^2} = 5\mathrm{x_i}(\mathrm{y_j} - 1) + x_i\sqrt{\mathrm{x}^2 - 2\mathrm{x} + 10} + 2\sqrt{17}(\mathrm{y_j} - 1)(\mathrm{y_k} - 1).$$

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

$$H\left(S^{C^*}{}_x\right) = \left(\frac{2x_i(y_j - 1)}{7}\right) + \left(\frac{2x_i}{x+2}\right) + \left(\frac{4(y_j - 1)(y_k - 1)}{5}\right).$$

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_x^C together with the pair of vertices belonging to S_x and between pair of vertices of u_j for j ranges from $1, 2, 3, \ldots, y$ of S_x^C together with the pair of pendant degree vertices of ${S^{C^*}}_x$. Let the vertices of the star graph S_x be denoted by $v_{1,} v_2, \ldots, v_{x-1,} v_x$, where i ranges from $1, 2, 3, \ldots, x$ and the additional vertices of S_x^C be denoted by $u_{1,} u_2, \ldots \ldots, u_{y-1}$ where j ranges from $1, 2, 3, \ldots \ldots, (y-1)$.

Furthermore, let $w_1, w_2, \ldots \ldots, w_{2y-2}$ for $k = 1, 2, 3, \ldots \ldots, 2y-2$ of ${S^{C^*}}_x$ be $2y-2$ number of pendant vertices of S_x^C which is depicted in Figure 5. Let $d(v_i) = 3$, and $d(v_1) = x-1$, $d(u_j) = 4$ and $d(\mathrm{w_k}) = 1$.

$$H({S^{C^*}}_x) = \sum_{i=2,j=1}^{x_i,(y_j-1)} \left(\frac{2}{d(v_i)+d(u_j)}\right) + \sum_{i=2}^{x_i} \left(\frac{2}{d(v_1)+d(v_i)}\right) + \sum_{i=2,j=1}^{(y_j-1),(2y_k-2)} \left(\frac{2}{d(u_j)+d(w_k)}\right) = \sum_{i=2,j=1}^{x_i,(y_j-1)} \left(\frac{2}{3+4}\right) + \sum_{i=2}^{x_i} \left(\frac{2}{x-1+3}\right) + \sum_{i=2,j=1}^{(y_j-1),(2y_k-2)} \left(\frac{2}{1+4}\right) = \left(\frac{2x_i(y_j-1)}{7}\right) + \left(\frac{2x_i}{x+2}\right) + \left(\frac{4(y_j-1)(y_k-1)}{5}\right).$$

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 $(\mathrm{W_x})$

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

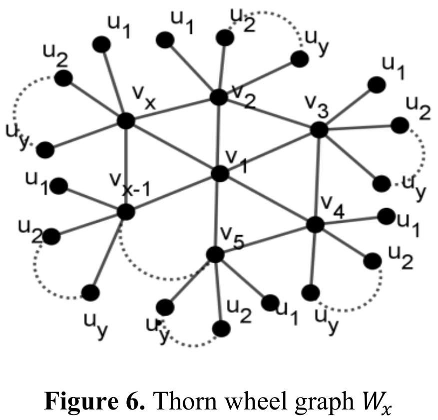

Figure 6. Thorn wheel graph W_x

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

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

Proof

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

$$SO(W_{x,y}) = \sum_{i=2,j=1}^{x_i,y_j} \sqrt{\left(d(v_i)\right)^2 + \left(d(u_j)\right)^2} + \sum_{i=2}^{x_i} \sqrt{\left(d(v_i)\right)^2 + \left(d(v_i)\right)^2} + \sum_{i=2}^{x_i} \sqrt{\left(d(v_1)\right)^2 + \left(d(v_i)\right)^2} = \sum_{i=2,j=1}^{x_i,y_j} \sqrt{(y+3)^2 + 1} + \sum_{i=2}^{x_i} \sqrt{(y+3)^2 + (y+3)^2} + \sum_{i=2}^{x_i} \sqrt{(x-1)^2 + (y+3)^2} = x_i y_j \sqrt{y^2 + 6y + 10} + \sqrt{2}\, x_i(y+3) + x_i\sqrt{x^2 + y^2 - 2x + 6y + 10}.$$

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

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

Proof

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

$$H({K^{C^*}}_{y,x}) = \sum_{i=2,j=1}^{x_i,y_j} \left(\frac{2}{d(v_i)+d(u_j)}\right) + \sum_{i=2}^{x_i} \left(\frac{2}{d(v_i)+d(v_i)}\right) + \sum_{i=2}^{x_i} \left(\frac{2}{d(v_1)+d(v_i)}\right) = \sum_{i=2,j=1}^{x_i,y_j} \left(\frac{2}{y+3+1}\right) + \sum_{i=2}^{x_i} \left(\frac{2}{y+3+y+3}\right) + \sum_{i=2}^{x_i} \left(\frac{2}{x-1+y+3}\right) = \left(\frac{2x_i y_j}{y+4}\right) + \left(\frac{x_i}{y+3}\right) + \left(\frac{2x_i}{x+y+2}\right).$$

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 $({W^C}_x)$

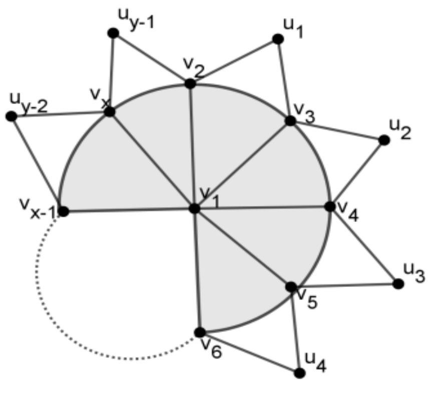

Figure 7. Cog wheel graph ${W^C}_x$

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

3.5.2 Thorn cog-wheel graph $\left({W^{C^*}}_x\right)$

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

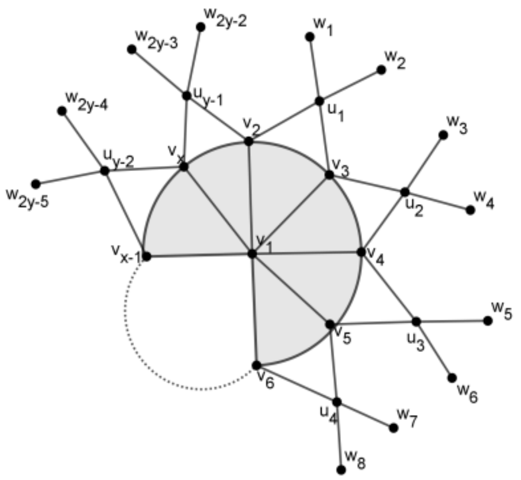

Figure 8. Thorn Cog wheel graph ${W^{C^*}}_x$

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

$$SO\left({W^{C^*}}_x\right) = \sqrt{41}x_i(y_j - 1) + x_i\sqrt{x^2 - 2x + 26} + 5\sqrt{2}x_i + 2\sqrt{17}\,(y_j - 1)(y_k - 1).$$

Proof

Here the pair of vertices of W_x are examined independently between the pair of vertices of u_j where j ranges from $1,2,3,\dots,(y-1)$ of ${W^C}_x$ together the pair of vertices belonging to W_x and between pair of vertices of of u_j where j ranges from $1,2,3,\dots,y$ 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 $v_1, v_2, \dots\dots, v_x$ where $i = 1,2,3,\dots,x$ and the number of additional vertices of ${W^C}_x$ be denoted by $u_1, u_2, \dots\dots, u_{x-1}$ where $j = 1,2,3,\dots,(y-1)$.

Furthermore, let $w_1, w_2, \dots\dots, w_{2y-2}$ for $k = 1,2,3,\dots\dots,(2y-2)$ of ${W^{C^*}}_x$ be another $(2y-2)$ number of pendant degree vertices of W_x^C, which is depicted in Figure 8. Let $d(v_1) = (x-1)$, $d(u_j) = 4$ $(for\; j = 1,2,3,\dots,(y-1))$, $d(v_i) = 5$ for $i = 2,3,\dots,x$ and $d(w_k) = 1$ for $k = 1,2,3,\dots,2(y-1)$.

$$SO({W^{C^*}}_x) = \sum_{i=2,j=1}^{x_i,y_j-1}\sqrt{\left(d(v_i)\right)^2 + \left(d(u_j)\right)^2} + \sum_{i=2}^{x_i}\sqrt{\left(d(v_1)\right)^2 + \left(d(v_i)\right)^2} + \sum_{i=2}^{x_i}\sqrt{\left(d(v_i)\right)^2 + \left(d(v_i)\right)^2} + \sum_{j,k=1}^{y_{j-1},2y_k-2}\sqrt{\left(d(u_j)\right)^2 + \left(d(w_k)\right)^2}$$
$$= \sum_{i=2,j=1}^{x_i,y_j-1}\sqrt{5^2+4^2} + \sum_{i=2}^{x_i}\sqrt{5^2+(x-1)^2} + \sum_{i=2}^{x_i}\sqrt{5^2+5^2} + \sum_{j,k=1}^{y_{j-1},2y_k-2}\sqrt{4^2+1} = \sqrt{41}x_i(y_j-1) + x_i\sqrt{x^2-2x+26} + 5\sqrt{2}\,x_i + 2\sqrt{17}\,(y_j-1)(y_k-1).$$

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

$$H\left({W^{C^*}}_x\right) = \left(\frac{2x_i(y_j-1)}{9}\right) + \left(\frac{2x_i}{x+4}\right) + \left(\frac{x_i}{5}\right) + \left(\frac{4(y_j-1)(y_k-1)}{5}\right).$$

Proof

Here the pair of vertices of W_x are examined independently between the pair of vertices of u_j where j ranges from $1,2,3,\dots,(y-1)$ 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 $1,2,3,\dots,y$ 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 $v_1, v_2, \dots\dots, v_x$ where $i = 1,2,3,\dots,x$ and the additional vertices of ${W^C}_x$ be denoted by $u_1, u_2, \dots\dots, u_{x-1}$ where $j = 1,2,3,\dots,(y-1)$.

Furthermore, let $w_1, w_2, \dots\dots, w_{2y-2}$ for k = $1,2,3,\dots\dots,(2y-2)$ of ${W^{C^*}}_x$ be another $(2y-2)$ number of pendant degree vertices of W_x^C which is depicted in Figure 8. Let $d(v_1) = (x-1), d(u_j) = 4$ $(\text{for } j = 1,2,3,\dots,(y-1))$, $d(v_i) = 5$ for $i = 2,3,\dots,x$ and $d(w_k) = 1$ for $k = 1,2,3,\dots,2(y-1)$.

$$\begin{aligned} H({W^{C^*}}_x) &= \sum_{i=2,j=1}^{x_i,(y_j-1)}\left(\frac{2}{d(v_i)+d(u_j)}\right) \\ &+ \sum_{i=2}^{x_i}\left(\frac{2}{d(v_1)+d(v_i)}\right) \\ &+ \sum_{i=2}^{x_i}\left(\frac{2}{d(v_i)+d(v_i)}\right) \\ &+ \sum_{j,k=1}^{y_j-1,2y_k-2}\left(\frac{2}{d(u_j)+d(w_k)}\right) \\ &= \sum_{i=2,j=1}^{x_i,(y_j-1)}\left(\frac{2}{5+4}\right) + \sum_{i=2}^{x_i}\left(\frac{2}{5+x-1}\right) \\ &+ \sum_{i=2}^{x_i}\left(\frac{2}{5+5}\right) + \sum_{j,k=1}^{y_j-1,2y_k-2}\left(\frac{2}{4+1}\right) \\ &= \left(\frac{2x_i(y_j-1)}{9}\right) + \left(\frac{2x_i}{x+4}\right) + \left(\frac{x_i}{5}\right) \\ &+ \left(\frac{4(y_j-1)(y_k-1)}{5}\right). \end{aligned}$$

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.

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NOMENCLATURE

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