An Analysis of Thorn Graph on Topological Indices

K. Vijaya Lakshmi and N. Parvathi*

Abstract—Topological index and molecular structure are cardinal topics in graph theory that connect many real-life situations. Mathematical chemistry is a part of theoretical and computational chemistry in which the assertion is primarily based on the mathematical tool rather than focusing on quantum mechanics. The main concept behind the topological indices is that they relate to various non-identical physicochemical characteristics of chemical compounds. Topological indices are utilized to examine the molecular structure of a chemical compound. These topological indices correlate the molecular properties of graphs, such as boiling point, melting point, temperature, pressure, heat of evaporation, chemical reactivity, biological activity and so on. The integration of graph theory and chemistry plays a dominant role in many fields. Topological indices are extensively used in computational chemistry and the pharmaceutical industry for manufacturing new medications, particularly in the areas of toxicology, risk assessment and drug design. In this research paper, the computation of the Sombor index, harmonic index, inverse sum index and symmetric division deg index of a simple connected graph called the thorn graph is analyzed relating to the thorn family, namely thorn ring, thorn path and thorn star and thorn multi-star. The primary objective of this research work is to connect the thorn graph with the topological indices to facilitate numerous real-time applications.

Index Terms—Sombor index, harmonic index, inverse sum index, symmetric division deg index, degree-based index, thorn graph.

I. INTRODUCTION

 \checkmark ONSIDER an *n* vertex simple connected graph G =(V, E), where V(G) and E(G) denote the vertex set and edge set, respectively. For $a \in V(G)$, the degree of a vertex $d_G(a)$ or d_a is the number of vertices adjacent to a in G. In the same way, for $a \in V(G)$, the neighborhood denoted by $N_G(a)$ or N_a is the vertex set adjacent to a in G. A pendant vertex is a one-degree vertex and it is also termed as a thorn. An edge, incident with the pendant vertex is known as a pendant edge. Let $P = (p_1, p_2, \dots, p_n)$ be an n-tuple with non-negative integers. The thorn graph denoted by G_P is the graph obtained from G by attaching p_i pendant vertices to the vertex v_i of G, for i = 1, 2, ..., n (Shiladhar Pawar and Soner N.D)[1]. The p_i pendant vertices attached to the vertex v_i are called the thorn of v_i . The set of p_i thorns of v_i is denoted by V_i , for i = 1, 2, ..., n. Also, $V(G_P) = V(G) \cup V_1(G) \cup V_2(G) \cup \cdots \cup V_n(G).$

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K. Vijaya Lakshmi is a Research Scholar in Department of Mathematics, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur - 603203, Tamil Nadu, India. (e-mail: vk5033@srmist.edu.in).

N. Parvathi is a Professor in Department of Mathematics, Faculty of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur - 603203, Tamil Nadu, India. (corresponding author; phone: 9443004036; e-mail: parvathn@srmist.edu.in).

Gutman et al. [2] conceptualized the thorn graph in the year 1998 and in due course, its application in the field of chemistry extended to multiple disciplines, which were discussed by Bonchev, Bytautas and Vukicevic [3], [4], [5] in their research work. For a detailed analysis of graph theory and applications, refer [6]. The present paper has been motivated by earlier research work conducted by Damir Vukicevic [7] to study and analyze the thorn graph.

Topological indices measure the physicochemical characteristics of a specific compound by combining a unique number with chemical graphs. In this molecular structure, atoms and bonds represent the vertices and edges, respectively. Moreover, the topological index is a numerical parameter derived mathematically from the graphical system. There are distinct categories of topological indices, namely degreebased, distance-based and eccentricity-based indices. However, these indices have been broadly studied by researchers and documented in the mathematical and chemical literature. Harold Wiener [8] introduced the oldest topological index, which bore his name. Wiener index was mainly used in the ancient days to calculate the physical properties of paraffin. Manso et al. [9] proposed the F_i index and discussed the prediction of the normal boiling point of hydrocarbon in his research. Zagreb index [10], introduced by Gutman, was extensively used for chemical applications and is a degreebased topological index. The Estrada index was introduced by Peña et al. in 2007 [11]. The correlation between energy bounds and the spectrum of graphs in the Estrada index was discussed by Bo Zhou, cited in his study [12]. Topological indices are employed to specify the characteristics of chemical compounds, particularly in Quantitative Structure-Property Relationship(QSPR) studies reported by Havare, Shafiei and Vukicevic [13], [14], [15], [16], [17]. Detailed investigation on thorn trees relating modified Wiener index was carried out and discussed by Zhou B [18]. Wiener index on line graph and inverse problem on the Wiener index was introduced by Nathan Cohen and Stephen Wagner, respectively, in 2010 [19], [20]. Sumathi et al. [21] described the MATLAB coding of the thorn graph using Wiener index. The theory relating to the Szeged index on the polynomial chain was discussed by Gao et al. [22] in 2015. Discussions on the Kirchhoff index were presented by Liu et al. [23], while an analysis of weighted Kirchoff was given by Mitsuhashi et al. [24]. Hued colorings of cartesian products of cycles and paths were discussed by Shao et al. [25] in 2018. The Wiener index of the wheel graph was discussed by Arathi Bhat [26] in 2022. Gao et al. provided detailed application of topological indices on nanostars, refer [27]. Further, for the clear explanation of bounds and indices, refer [28], [29], presented by Fajtlowicz and Yang Yang. The new topological index, known as the Sombor index, was introduced by Ivan Gutman in the year 2021; the index throws light on a significant number of publications correlating mathematical properties and chemical applications reported by Gutman and Roberto Cruz in the literature [30], [31]. In the present research, topological indices are connected with the thorn graph and the corresponding values are computed.

II. PRELIMINARIES

In this section, some basic definitions regarding the topological indices and their related formulae are discussed.

Definition 2.1: [32] For a molecular graph G, the Sombor index is defined as

$$SO(G) = \sum_{ab \in E(G)} \sqrt{d_a^2 + d_b^2}$$

where d_a and d_b are the degrees of the vertex of a and b in G, respectively.

Definition 2.2: [33] Randic index of a simple connected graph G is defined as

$$R_{\alpha}(G) = \sum_{ab \in E(G)} ((d_a)(d_b))^{\alpha}$$

where α is a real number.

Definition 2.3: [34] For a simple connected graph G, the harmonic index is defined as

$$H(G) = \sum_{ab \in E(G)} \left(\frac{2}{d_a + d_b}\right).$$

Definition 2.4: [35] Inverse sum index of a connected graph G is defined as follows

$$IS(G) = \sum_{ab \in E(G)} \left(\frac{d_a d_b}{d_a + d_b} \right).$$

Definition 2.5: [36] Symmetric division deg index of a connected graph G is defined as follows

$$SDD(G) = \sum_{ab \in E(G)} \left(\frac{(d_a)^2 + (d_b)^2}{(d_a)(d_b)} \right).$$

III. MAIN RESULTS

The relation between the Sombor index, harmonic index, inverse sum index and symmetric division deg index of G and G_P is examined within the thorn families. The paper presents an explicit formula for different topological indices and the values are computed.

Thorn ring

The *m*-thorn ring $C_{n,m}$ contains a cycle C_n considered as the parent. Here, every cycle vertex contains m-2 thorns, where m > 2. The thorn ring is acquired by adding pendant vertices to each cycle vertex, which is shown in Fig.1. The *m*-thorn ring $C_{n,m}$ can be observed as the thorn graph, which is denoted by $(C_n)_P$, where *P* represents the *n*-tuple, $P = (m-2, m-2, \ldots, m-2)$ (Gutman [5]).



Fig. 1. Thorn ring C_n^* .

Remark: Here, C_n denotes the vertices of the cycle and the vertices are labeled as v_1, v_2, \ldots, v_n . C_n^* denotes the pendant vertices, labeled as u_1, u_2, \ldots, u_m attached to each vertex of the cycle C_n .

Theorem 3.1: Let G_P be the thorn graph with *n*-tuple obtained from the connected graph G. Then, the Sombor index of a thorn ring with *n* ring vertices is given by $SO(C_{n,m}) = n[m\sqrt{m^2 + 4m + 5} + \sqrt{2}(m+2)].$

Proof:

Take the vertices from C_n and C_n^* .

Initially, we consider separately between pair of vertices belonging to C_n and between pair of pendant vertices of C_n^* . The next to be considered is a pair of vertices, of which one is from C_n and the other is the pendant vertex.

Let v_1, v_2, \ldots, v_n be the vertices of a cycle and let $u_1, u_2, u_3, \ldots, u_m$ belong to pendant vertices of a cycle, as denoted in Fig.1.

Here, *n* refers to the vertices of the cycle and also $n \ge 3$ (Since in cycle, 1 and 2 vertices are not applicable). Also, *m* refers to the pendant vertices of the cycle.

Let $d(v_i) = m + 2$, $d(u_j) = 1$ and $d(v_{n+1}) = v_1$. Then, the Sombor index is calculated as follows. Sombor $index(G) = \sum_{ab \in E(G)} \sqrt{d_a^2 + d_b^2}$.

$$SO(C_{n,m}) = \sum_{i=1}^{n} \sum_{i=1}^{m} \sqrt{d(v_i)^2 + d(u_j)^2} + \sum_{i=1}^{n} \sqrt{d(v_i)^2 + d(v_{i+1})^2} = \sum_{i=1}^{n} \sum_{i=1}^{m} \sqrt{(m+2)^2 + 1} + \sum_{i=1}^{n} \sqrt{(m+2)^2 + (m+2)^2} = n.m\sqrt{m^2 + 4m + 5} + n\sqrt{2(m+2)^2} = n[m\sqrt{m^2 + 4m + 5} + \sqrt{2}(m+2)].$$

Hence the proof.

Theorem 3.2: Let G_P be the thorn graph with *n*-tuple obtained from the connected graph G. Then, the harmonic index of a thorn ring with *n* ring vertices is given by $H(C_{n,m}) = nm\left(\frac{2}{m+3}\right) + \left(\frac{n}{m+2}\right)$.

Proof: Take the vertices from C_n and C_n^* .

Initially, we consider separately between pair of vertices belonging to C_n and between pair of pendant vertices of C_n^* . The next to be considered is a pair of vertices, of which one is from C_n and the other is the pendant vertex.

Let $v_1, v_2, v_3, \ldots, v_n$ be the vertices of a cycle and $u_1, u_2, u_3, \ldots, u_m$ belong to pendant vertices of a cycle as it is denoted in Fig.1.

Let $d(v_i) = m + 2$, $d(u_j) = 1$ and $d(v_{n+1}) = v_1$.

Then, the harmonic index is calculated as follows.

$$Harmonic \ index(G) = \sum_{ab \in E(G)} \left(\frac{2}{d_a + d_b}\right)$$

$$H(C_{n,m}) = \sum_{i=1}^{n} \sum_{i=1}^{m} \left(\frac{2}{d(v_i) + d(u_j)}\right) \\ + \sum_{i=1}^{n} \left(\frac{2}{d(v_i) + d(v_{i+1})}\right) \\ = \sum_{i=1}^{n} \sum_{i=1}^{m} \left(\frac{2}{m+2+1}\right) \\ + \sum_{i=1}^{n} \left(\frac{2}{m+2+m+2}\right) \\ = nm\left(\frac{2}{m+3}\right) + \left(\frac{n}{m+2}\right).$$

Hence the proof.

Theorem 3.3: Let G_P be the thorn graph with *n*-tuple obtained from the connected graph G. Then, the inverse sum index of a thorn ring with *n* ring vertices is given by $IS(C_{n,m}) = nm\left(\frac{m+2}{m+3}\right) + n\left(\frac{m+2}{2}\right)$.

Proof: Take the vertices from C_n and C_n^* .

Initially, we consider separately between pair of vertices belonging to C_n and between pair of pendant vertices of C_n^* . The next to be considered are a pair of vertices, of which one is from C_n and the other is the pendant vertex.

Let $v_1, v_2, v_3, \ldots, v_n$ be the vertices of a cycle and $u_1, u_2, u_3, \ldots, u_m$ belong to pendant vertices of a cycle, as it is denoted in Fig.1.

Let $d(v_i) = m + 2$, $d(u_j) = 1$ and $d(v_{n+1}) = v_1$. Then, the inverse sum index is calculated as follows.

$$Inverse \ sum \ index(G) = \sum_{ab \in E(G)} \left(\frac{d_a d_b}{d_a + d_b} \right)$$

$$IS(C_{n,m}) = \sum_{i=1}^{n} \sum_{i=1}^{m} \left(\frac{d(v_i)d(u_j)}{d(v_i) + d(u_j)} \right) \\ + \sum_{i=1}^{n} \left(\frac{d(v_i)d(v_{i+1})}{d(v_i) + d(v_{i+1})} \right) \\ = \sum_{i=1}^{n} \sum_{i=1}^{m} \left(\frac{(m+2)(1)}{m+2+1} \right) \\ + \sum_{i=1}^{n} \left(\frac{(m+2)(m+2)}{m+2+m+2} \right) \\ = nm \left(\frac{m+2}{m+3} \right) + n \left(\frac{m+2}{2} \right)$$

Hence the proof is completed.

Theorem 3.4: Let G_P be the thorn graph with *n*-tuple obtained from the connected graph G. Then, the symmetric division deg index of a thorn ring with *n* ring vertices is given by $SDD(C_{n,m}) = nm\left(\frac{m^2+4m+5}{m+2}\right) + 2n(m+2)$.

Proof: Take the vertices from C_n and C_n^* .

Initially, we consider separately between pair of vertices belonging to C_n and between pair of pendant vertices of C_n^* . The next to be considered are a pair of vertices, of which one is from C_n and the other is the pendant vertex.

Let $v_1, v_2, v_3, \ldots, v_n$ be the vertices of a cycle and $u_1, u_2, u_3, \ldots, u_m$ belong to pendant vertices of a cycle, as it is denoted in Fig.1.

Let $d(v_i) = m + 2$, $d(u_j) = 1$ and $d(v_{n+1}) = v_1$.

Then, the symmetric division deg index is calculated as follows.

Symmetric division deg index(G) =
$$\sum_{ab \in E(G)} \left(\frac{(d_a)^2 + (d_b)^2}{(d_a)(d_b)} \right)$$

$$SDD(C_{n,m}) = \sum_{i=1}^{n} \sum_{i=1}^{m} \left(\frac{(d(v_i))^2 + (d(u_j))^2}{d(v_i)d(u_j)} \right) + \sum_{i=1}^{n} \left(\frac{(d(v_i))^2 + (d(v_{i+1}))^2}{d(v_i)d(v_{i+1})} \right)$$

$$=\sum_{i=1}^{n}\sum_{i=1}^{m}\left(\frac{(m+2)^{2}+1}{m+2}\right)$$
$$+\sum_{i=1}^{n}\left(\frac{(m+2)^{2}+(m+2)^{2}}{(m+2)}\right)$$

$$=nm\left(\frac{m^2+4m+5}{m+2}\right)+2n(m+2).$$

Hence the proof is completed.

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Fig. 2. Example of thorn cycle with 5-thorn ring $C_{3,5}$.

Example: Consider the 5-thorn ring (with m - 2 = 3 thorns) $C_{3,5}$, given in Fig.2.

Then the Sombor index of a thorn cycle, $SO(C_{3,5})$ is calculated as $15\sqrt{50} + 21\sqrt{2}$.

The harmonic index of a thorn cycle, $H(C_{3,5})$ is calculated as $\frac{15}{4} + \frac{3}{7}$.

The inverse sum index of a thorn cycle, $IS(C_{3,5})$ is calculated as $\frac{105}{8} + \frac{21}{2}$.

The symmetric division deg index of a thorn cycle, $SDD(C_{3,5})$ is calculated as $\frac{750}{7} + 21$.

Thorn path

The thorn path, represented by $P_{n,r,s}$ is initially extracted from the parent P_n by adding q pendant vertices to the intermediate vertices and u pendant vertices to the end vertices, which can be seen in Fig.3. The labeling of the vertices in the route P_n is done in such a way that the nonterminal vertices have labels ranging from $2, 3, \ldots, n - 1$ and the end part is labeled as 1 and n. The path $P_{n,r,s}$ indicated by $(P_n)_P$, is then referred to as 'the thorn graph.' Here, P is observed as the n-tuple [3], $P = (s, r, \ldots, r, s)$.



Fig. 3. Thorn path $P_{n,r,s}$.

Theorem 3.5: Let G_P be the thorn graph with *n*-tuple obtained from the connected graph G. Then, the Sombor index of a thorn path $P_{n,r,s}$, with $n \ge 3$ vertices is given by $SO(P_{n,r,s}) = 2u\sqrt{(u+1)^2 + 1} + 2\sqrt{(u+1)^2 + (q+2)^2} + (n-3)\sqrt{2}(q+2) + (n-2)q\sqrt{(q+2)^2 + 1}$.

Proof: Let $P_{n,r,s}$, $n \geq 3$ denote the thorn path acquired from the parent P_n that is, for each non-terminal vertex, r_q neighbors are added, while for each terminal vertex, s_u neighbors are added.

Path vertices are denoted by $v_1, v_2, v_3, \ldots, v_n$ and $s_1, s_2, s_3, \ldots, s_u$ are the pendant end vertices of the path. Furthermore, $r_1, r_2, r_3, \ldots, r_q$ belong to the pendant intermediate vertices. This is highlighted in Fig.3. Let $d(v_1) = d(v_n) = u + 1$, $d(v_i) = q + 2$, for all i = 2, 3..., n - 1. $d(s_j) = d(r_k) = 1$, where j = 2, 3..., u and k = 1, 2..., q.

$$SO(P_{n,r,s}) = \sum_{i=1,n} \sum_{j=1}^{u} \sqrt{(d(s_j))^2 + (d(v_i))^2} + \sum_{i=1,n-1} \sqrt{(d(v_i))^2 + (d(v_{i+1}))^2} + \sum_{i=2}^{n-2} \sqrt{(d(v_i))^2 + (d(v_{i+1}))^2} + \sum_{i=2}^{n-1} \sum_{k=1}^{q} \sqrt{(d(v_i))^2 + (d(r_k))^2}$$

$$= \sum_{i=1,n} \sum_{j=1}^{u} \sqrt{1 + (u+1)^2} \\ + \sum_{i=1,n-1} \sqrt{(u+1)^2 + (q+2)^2} \\ + \sum_{i=2}^{n-2} \sqrt{(q+2)^2 + (q+2)^2} \\ + \sum_{i=2}^{n-1} \sum_{k=1}^{q} \sqrt{(q+2)^2 + 1}$$

$$\begin{split} =& 2u\sqrt{(u+1)^2+1} \\ &+ 2\sqrt{(u+1)^2+(q+2)^2} \\ &+ (n-3)\sqrt{2}(q+2) \\ &+ (n-2)q\sqrt{(q+2)^2+1}. \end{split}$$

Hence the proof.

Theorem 3.6: Let G_P be the thorn graph with *n*-tuple obtained from the connected graph G. Then, the harmonic index of a thorn path, $P_{n,r,s}$, having $n \ge 3$ vertices is given by

$$H(P_{n,r,s}) = \left(\frac{4u}{u+2}\right) + \left(\frac{4}{u+q+3}\right) + \left(\frac{n-3}{q+2}\right) + \left(\frac{2q(n-2)}{q+3}\right).$$
Proof:

Let $P_{n,r,s}$, $n \ge 3$ denote the thorn path acquired from the parent P_n , that is, for each non-terminal vertex, r_q neighbors are added while for each terminal vertex, s_u neighbors are added.

Path vertices are denoted by $v_1, v_2, v_3, \ldots, v_n$ and $s_1, s_2, s_3, \ldots, s_u$ are the pendant end vertices of the path.

Furthermore, $r_1, r_2, r_3, \ldots, r_q$ belong to the pendant intermediate vertices. This is highlighted in Fig.3.

Let $d(v_1) = d(v_n) = u + 1$, $d(v_i) = q + 2$, for all i = 2, 3..., n - 1. $d(s_j) = d(r_k) = 1$, where j = 2, 3..., u and k = 1, 2..., q.

$$H(P_{n,r,s}) = \sum_{i=1,n} \sum_{j=1}^{u} \left(\frac{2}{d(s_j) + d(v_i)}\right) \\ + \sum_{i=1,n-1} \left(\frac{2}{d(v_i) + d(v_{i+1})}\right) \\ + \sum_{i=2}^{n-2} \left(\frac{2}{d(v_i) + d(v_{i+1})}\right) \\ + \sum_{i=2}^{n-1} \sum_{k=1}^{q} \left(\frac{2}{d(v_i) + d(r_k)}\right) \\ = \sum_{i=1,n} \sum_{j=1}^{u} \left(\frac{2}{1 + u + 1}\right) \\ + \sum_{i=1,n-1} \left(\frac{2}{u + 1 + q + 2}\right) \\ + \sum_{i=2}^{n-2} \left(\frac{2}{q + 2 + q + 2}\right) \\ + \sum_{i=2}^{n-1} \sum_{k=1}^{q} \left(\frac{2}{q + 2 + 1}\right) \\ = \left(\frac{4u}{u + 2}\right) + \left(\frac{4}{u + q + 3}\right) \\ + \left(\frac{n - 3}{q + 2}\right) \\ + \left(\frac{2q(n - 2)}{q + 3}\right).$$

Hence the proof.

Theorem 3.7: Let G_P be the thorn graph with *n*-tuple obtained from the connected graph G. Then, the inverse sum index of a thorn path, $P_{n,r,s}$, having $n \ge 3$ vertices is given by $\left(\frac{2u(u+1)}{u+2}\right) + \left(\frac{2(u+1)(q+2)}{u+q+3}\right) + \left(\frac{(n-3)(q+2)}{2}\right) + \left(\frac{(n-2)q(q+2)}{q+3}\right)$. *Proof:*

Let $P_{n,r,s}$, $n \ge 3$ denote the thorn path acquired from the parent P_n , that is, for each non-terminal vertex, r_q neighbors are added, while for each terminal vertex, s_u neighbors are added.

Path vertices are denoted by $v_1, v_2, v_3, \ldots, v_n$ and $s_1, s_2, s_3, \ldots, s_u$ are the pendant end vertices of the path.

Furthermore, $r_1, r_2, r_3, \ldots, r_q$ belong to the pendant intermediate vertices. This is highlighted in Fig.3.

Let $d(v_1) = d(v_n) = u + 1$, $d(v_i) = q + 2$, for all i = 2, 3..., n - 1.

$$d(s_j) = d(r_k) = 1$$
, where $j = 2, 3..., u$ and $k = 1, 2..., q$.

$$IS(P_{n,r,s}) = \sum_{i=1,n} \sum_{j=1}^{u} \left(\frac{d(s_j)d(v_i)}{d(s_j) + d(v_i)} \right) \\ + \sum_{i=1,n-1} \left(\frac{d(v_i)d(v_{i+1})}{d(v_i) + d(v_{i+1})} \right) \\ + \sum_{i=2}^{n-2} \left(\frac{d(v_i)d(v_{i+1})}{d(v_i) + d(v_{i+1})} \right) \\ + \sum_{i=2}^{n-1} \sum_{k=1}^{q} \left(\frac{d(v_i)d(r_k)}{d(v_i) + d(r_k)} \right)$$

$$= \sum_{i=1,n} \sum_{j=1}^{u} \left(\frac{(1)(u+1)}{1+u+1} \right) \\ + \sum_{i=1,n-1} \left(\frac{(u+1)(q+2)}{u+1+q+2} \right) \\ + \sum_{i=2}^{n-2} \left(\frac{(q+2)(q+2)}{q+2+q+2} \right) \\ + \sum_{i=2}^{n-1} \sum_{k=1}^{q} \left(\frac{(1)(q+2)}{1+q+2} \right) \\ = \left(\frac{2u(u+1)}{u+2} \right) + \left(\frac{2(u+1)(q+2)}{u+q+3} \right) \\ + \left(\frac{(n-3)(q+2)}{2} \right) + \left(\frac{(n-2)q(q+2)}{q+3} \right)$$

Hence the proof.

Theorem 3.8: Let G_P be the thorn graph with *n*-tuple obtained from the connected graph G. Then, the symmetric division deg index of a thorn path, $P_{n,r,s}$, having $n \ge 3$ vertices is given by $2u\left(\frac{1+(u+1)^2}{u+1}\right) + 2\left(\frac{(u+1)^2+(q+2)^2}{(u+1)(q+2)}\right) + 2(n-3) + (n-2)q\left(\frac{(q+2)^2+1}{q+2}\right)$. *Proof:* Let $P_{n,r,s}$, $n \ge 3$ denote the thorn path acquired from the parent P that is formula.

Proof: Let $P_{n,r,s}$, $n \ge 3$ denote the thorn path acquired from the parent P_n , that is, for each non-terminal vertex, r_q neighbors are added, while for each terminal vertex, s_u neighbors are added.

Path vertices are denoted by $v_1, v_2, v_3, \ldots, v_n$ and $s_1, s_2, s_3, \ldots, s_u$ are the pendant end vertices of the path. Furthermore, $r_1, r_2, r_3, \ldots, r_q$ belong to the pendant intermediate vertices. This is highlighted in Fig.3.

Let $d(v_1) = d(v_n) = u + 1$, $d(v_i) = q + 2$, for all i = 2, 3..., n - 1. $d(s_i) = d(r_k) = 1$, where i = 2, 3..., u and k = 1, 2..., q.

$$d(s_j) = d(r_k) = 1$$
, where $j = 2, 3..., u$ and $k = 1, 2..., q$.

$$SDD(P_{n,r,s}) = \sum_{i=1,n} \sum_{j=1}^{a} \left(\frac{(d(s_j))^2 + (d(v_i))^2}{d(s_j)d(v_i)} \right) \\ + \sum_{i=1,n-1} \left(\frac{(d(v_i))^2 + (d(v_{i+1}))^2}{d(v_i)d(v_{i+1})} \right) \\ + \sum_{i=2}^{n-2} \left(\frac{(d(v_i))^2 + (d(v_{i+1}))^2}{d(v_i)d(v_{i+1})} \right) \\ + \sum_{i=2}^{n-1} \sum_{k=1}^{q} \left(\frac{(d(v_i))^2 + (d(r_k))^2}{d(v_i)d(r_k)} \right) \\ = \sum_{i=2}^{n} \sum_{k=1}^{u} \left(\frac{1 + (u+1)^2}{u(u+1)} \right)$$

$$= \sum_{i=1,n} \sum_{j=1}^{n} \left(\frac{\frac{1+(u+2)}{u+1}}{u+1} \right) \\ + \sum_{i=1,n-1}^{n-2} \left(\frac{(u+1)^2 + (q+2)^2}{(u+1)(q+2)} \right) \\ + \sum_{i=2}^{n-2} \left(\frac{(q+2)^2 + (q+2)^2}{(q+2)(q+2)} \right) \\ + \sum_{i=2}^{n-1} \sum_{k=1}^{q} \left(\frac{(q+2)^2 + 1}{q+2} \right)$$

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$$=2u\left(\frac{1+(u+1)^2}{u+1}\right) + 2\left(\frac{(u+1)^2+(q+2)^2}{(u+1)(q+2)}\right) + 2(n-3) + (n-2)q\left(\frac{(q+2)^2+1}{q+2}\right).$$

Hence the theorem.



Fig. 4. Example of thorn path $P_{4,3,5}$.

Example: Consider the example of thorn path $P_{4,3,5}$, given in Fig.4.

Then the Sombor index of a thorn path, $P_{4,3,5}$ is calculated as $2\sqrt{61} + 10\sqrt{37} + 6\sqrt{26} + \sqrt{50}$.

The harmonic index of a thorn path, $P_{4,3,5}$ is calculated as $\frac{20}{7} + \frac{4}{11} + 2 + \frac{1}{5}$.

The inverse sum index of a thorn path, $P_{4,3,5}$ is calculated as $\frac{60}{7} + \frac{60}{11} + \frac{5}{2} + 5$.

The symmetric division deg index of a thorn path, $P_{4,3,5}$ is calculated as $\frac{185}{3} + \frac{61}{15} + 2 + \frac{156}{5}$.

Thorn star $S_{n,q,u}$

The thorn star is generated from the star S_n by joining u pendant vertices to the central vertex v_0 and by joining q pendant vertices to its end vertices, as depicted in Fig. 5. On considering the star S_n , labeling for vertices is done in such a way that, the end vertices take the labels as $1, 2, \ldots, n-1$ and similarly, mid-vertex of the star, v_0 is numbered as n, which is also depicted in Fig. 5. Then, the star $S_{n,q,u}$ is named as the thorn graph and is denoted by $(S_n)_P$, where P indicates the n-tuple [3], $P = (q, q, \ldots, q, u)$.



Fig. 5. THORN STAR GRAPH $S_{n,q,u}$.

Theorem 3.9: Let G_P be the thorn graph with *n*-tuple obtained from the connected graph G. Then, the Sombor

index of a thorn star $S_{n,q,u}$ is given by $u\sqrt{1+(u+n)^2}+n\sqrt{(u+n)^2+(q+1)^2}+nq\sqrt{(q+1)^2+1}.$

Proof: From the star S_n , the thorn star denoted by $S_{n,q,u}$, is obtained.

Consider the central vertex of S_n as v_0 .

Let $v_1, v_2, v_3, \ldots, v_n$ be the end vertices numbered as $1, 2, \ldots, n-1, n$ and the pendant vertices be denoted by $r_1, r_2, r_3, \ldots, r_q$, similarly, v_0 contains pendant vertices, namely $s_1, s_2, s_3, \ldots, s_q$.

Here P = (q, q, q, ..., q, u), where P denotes the n-tuple and it is depicted in Fig.5. Let $d(v_0) = (u+n)$, $d(v_i) = q+1$, where i ranges from 1, 2, 3, ..., n, $d(s_j) = d(r_k) = 1$.

$$O(S_{n,q,u}) = \sum_{j=1}^{u} \sqrt{d(s_j)^2 + d(v_0)^2} + \sum_{i=1}^{n} \sqrt{d(v_0)^2 + d(v_i)^2} + \sum_{i=1}^{n} \sum_{k=1}^{q} \sqrt{d(v_i)^2 + d(r_k)^2} = \sum_{j=1}^{u} \sqrt{1 + (u+n)^2} + \sum_{i=1}^{n} \sqrt{(u+n)^2 + (q+1)^2} + \sum_{i=1}^{n} \sum_{k=1}^{q} \sqrt{(q+1)^2 + 1} = u\sqrt{1 + (u+n)^2} + n\sqrt{(u+n)^2 + (q+1)^2} + nq\sqrt{(q+1)^2 + 1}.$$

This completes the proof.

S

Theorem 3.10: Let G_P be the thorn graph with *n*-tuple obtained from the connected graph G. Then the harmonic index of a thorn star $S_{n,q,u}$ is given by $u\left(\frac{2}{u+n+1}\right) + n\left(\frac{2}{u+n+q+1}\right) + nq\left(\frac{2}{q+2}\right)$.

Proof:

From the star S_n , the thorn star denoted by $S_{n,q,u}$, is obtained.

Consider the central vertex of S_n as v_0 .

Let $v_1, v_2, v_3, \ldots, v_n$ be the end vertices and it is numbered as $1, 2, \ldots, n - 1, n$ and let the pendant vertices be denoted by $1, 2, 3, \ldots, q$. Here $P = (r, r, r, \ldots, r, q)$, where P denotes the *n*-tuple. This is depicted in Fig.5.

Let $d(v_0) = (u+n)$, $d(v_i) = q+1$, where *i* ranges from 1, 2, 3, ..., n, $d(s_j) = d(r_k) = 1$.

Then, it proceeds as follows,

$$H(S_{n,q,u}) = \sum_{j=1}^{u} \left(\frac{2}{d(s_j) + d(v_0)}\right) + \sum_{i=1}^{n} \left(\frac{2}{d(v_0) + d(v_i)}\right)$$
$$+ \sum_{i=1}^{n} \sum_{k=1}^{q} \left(\frac{2}{d(v_i) + d(r_k)}\right)$$
$$= \sum_{j=1}^{u} \left(\frac{2}{1 + u + n}\right) + \sum_{i=1}^{n} \left(\frac{2}{u + n + q + 1}\right)$$
$$+ \sum_{i=1}^{n} \sum_{k=1}^{q} \left(\frac{2}{q + 1 + 1}\right)$$
$$= u \left(\frac{2}{u + n + 1}\right) + n \left(\frac{2}{u + n + q + 1}\right)$$
$$+ nq \left(\frac{2}{q + 2}\right).$$

This completes the theorem.

Theorem 3.11: Let G_P be the thorn graph with *n*-tuple obtained from the connected graph G. Then the inverse sum index of a thorn star $S_{n,q,u}$ is given by $u\left(\frac{u+n}{u+n+1}\right) +$

 $n\left(\frac{(u+n)(q+1)}{u+n+q+1}\right) + nq\left(\frac{q+1}{q+2}\right).$ Proof: From the star S_n , the thorn star denoted by $S_{n,q,u}$, is obtained.

Consider the central vertex of S_n as v_0 .

Let $v_1, v_2, v_3, \ldots, v_n$ be the end vertices numbered as $1, 2, \ldots, n-1, n$ and the pendant vertices be denoted by $1, 2, 3, \ldots, q$. Here, $P = (r, r, r, \ldots, r, q)$, where P denotes the *n*-tuple and it is depicted in Fig.5.

Let $d(v_0) = (u+n)$, $d(v_i) = q+1$, where i ranges from $1, 2, 3, \ldots, n, d(s_i) = d(r_k) = 1.$

$$IS(S_{n,q,u}) = \sum_{j=1}^{u} \left(\frac{d(s_j)d(v_0)}{d(s_j) + d(v_0)} \right) + \sum_{i=1}^{n} \left(\frac{d(v_0)d(v_i)}{d(v_0) + d(v_i)} \right)$$
$$+ \sum_{i=1}^{n} \sum_{k=1}^{q} \left(\frac{d(v_i)d(r_k)}{d(v_i) + d(r_k)} \right)$$
$$= \sum_{i=1}^{q} \left(\frac{(1)(u+n)}{u+n+1} \right) + \sum_{i=1}^{n} \left(\frac{(u+n)(q+1)}{u+n+q+1} \right)$$
$$+ \sum_{i=1}^{n} \sum_{k=1}^{q} \left(\frac{(q+1)(1)}{q+1+1} \right)$$
$$= u \left(\frac{u+n}{u+n+1} \right) + n \left(\frac{(u+n)(q+1)}{u+n+q+1} \right)$$
$$+ nq \left(\frac{q+1}{q+2} \right).$$

Hence the proof.

Theorem 3.12: Let G_P be the thorn graph with *n*-tuple obtained from the connected graph G. Then, the symmetric division deg index of a thorn star $S_{n,q,u}$ is given by $\frac{\left(\frac{(u+n)^2+1}{u+n}\right)}{Proof: \text{ From the star } S_n, \text{ thorn star denoted by } S_{n,q,u}, }$ u

is obtained.

Consider the central vertex of S_n as v_0 .

Let $v_1, v_2, v_3, \ldots, v_n$ be the end vertices numbered as $1, 2, \ldots, n - 1, n$ and the pendant vertices be denoted by $r_1, r_2, r_3, \ldots, r_q$, similarly, v_0 contains pendant vertices namely, $s_1, s_2, s_3, \ldots, s_q$.

Here $P = (q, q, q, \dots, q, u)$, where P denotes the n-tuple and it is depicted in Fig.5.

Let $d(v_0) = u + n$, $d(v_i) = q + 1$, where i ranges from $1, 2, 3, \ldots, n, d(s_i) = d(r_k) = 1.$

$$SDD(S_{n,q,u}) = \sum_{j=1}^{u} \left(\frac{(d(s_j))^2 + (d(v_0))^2}{d(s_j)d(v_0)} \right) \\ + \sum_{i=1}^{n} \left(\frac{(d(v_0))^2 + (d(v_i))^2}{d(v_0)d(v_i)} \right) \\ + \sum_{i=1}^{n} \sum_{k=1}^{q} \left(\frac{(d(v_i))^2 + (d(r_k))^2}{d(v_i)d(r_k)} \right) \\ = \sum_{j=1}^{u} \left(\frac{1 + (u+n)^2}{u+n} \right) \\ + \sum_{i=1}^{n} \left(\frac{(u+n)^2 + (q+1)^2}{(u+n)(q+1)} \right) \\ + \sum_{i=1}^{n} \sum_{k=1}^{q} \left(\frac{(q+1)^2 + 1}{(q+1)} \right) \\ = u \left(\frac{(u+n)^2 + (q+1)^2}{(u+n)(q+1)} \right) \\ + nq \left(\frac{(q+1)^2 + 1}{q+1} \right).$$

Hence the proof.



Fig. 6. Example of thorn star $S_{4,3,5}$.

Example: Consider the example of thorn star $S_{4,3,5}$, given in Fig. 6.

Then the Sombor index of a thorn star, $S_{4,3,5}$, is calculated as $4\sqrt{97} + 5\sqrt{26} + 12\sqrt{17}$.

The harmonic index of a thorn star, $S_{4,3,5}$, is calculated as $1 + \frac{8}{13} + \frac{24}{5}$.

The inverse sum index of a thorn star, $S_{4,3,5}$, is calculated as $\frac{9}{2} + \frac{144}{13} + \frac{48}{5}$.

The symmetric division deg index of a thorn star, $S_{4,3,5}$, is calculated as $\frac{410}{9} + \frac{97}{9} + 51$.

Thorn multi-star $(S_n(r_1, r_2, ..., r_{q-1}, r_q))$

From the star S_n , the thorn star is acquired by connecting q_i extreme vertices to the vertex *i* of S_n , where *i* ranges from $1, 2, 3, \ldots, n - 1, n$. Here, v_o denotes the vertex in the middle of the star and the remaining vertices, namely $v_1, v_2, \ldots, v_{n-1}, v_n$ are formed by connecting the central vertex v_0 and each vertex has q_n pendant vertices, which is shown in Fig.7.



Fig. 7. Thorn multi-star $(S_n(r_1, r_2, ..., r_{q-1}, r_q))$.

Theorem 3.13: Let G_P be the thorn graph with *n*-tuple obtained from the connected graph G. Then, the Sombor index of a thorn multi-star $SO(S_n(r_1, r_2, \ldots, r_{q-1}, r_q))$ is given by $n\sqrt{n^2 + (q+1)^2} + qn\sqrt{(q+1)^2 + 1}$.

Proof: From the star S_n , the thorn multi-star denoted by $S_n(r_1, r_2, \ldots, r_{q-1}, r_q)$, is obtained.

This thorn multi-star is obtained by connecting q_i extreme vertices to the vertex i of S_n , where i ranges from $1, 2, 3, \ldots, n-1, n$, which is depicted in Fig 7.

In the thorn multi-star $S_n(r_1, r_2, \ldots, r_{q-1}, r_q)$, labeling of vertices is done in such a way that, the number v_0 is the central vertex, additionally, $1, 2, 3, \ldots, n-1, n$ represents the numbering of the terminal vertices and it is denoted as $v_1, v_2, \ldots, v_{n-1}, v_n$. Let $d(v_0) = n$, $d(v_i) = q + 1$ and $d(r_k) = 1$.

$$SO(S_n(r_1, r_2, \dots, r_{q-1}, r_q)) = \sum_{i=1}^n \sqrt{d(v_0)^2 + d(v_i)^2} + \sum_{i=1}^n \sum_{k=1}^q \sqrt{d(v_i)^2 + d(r_k)^2} = n\sqrt{n^2 + (q+1)^2} + qn\sqrt{(q+1)^2 + 1}.$$

This completes the proof of the theorem.

Theorem 3.14: Let G_P be the thorn graph with *n*-tuple obtained from the connected graph G. Then, the harmonic index of a thorn multi-star $S_n(r_1, r_2, \ldots, r_{q-1}, r_q)$ is given by $n\left(\frac{2}{n+q+1}\right) + qn\left(\frac{2}{q+2}\right)$. *Proof:* From the star S_n , the thorn multi-star denoted by

Proof: From the star S_n , the thorn multi-star denoted by $S_n(r_1, r_2, \ldots, r_{q-1}, r_q)$, is obtained. This thorn multi-star is obtained by connecting q_i extreme vertices to the vertex i of S_n , for i ranges from $1, 2, 3, \ldots, n-1, n$. This is depicted in Fig. 7.

In the thorn multi-star $S_n(r_1, r_2, \ldots, r_{q-1}, r_q)$, labeling of vertices is done in such a way that, the number v_0 is the central vertex, additionally, $1, 2, 3, \ldots, n-1, n$ denotes the numbering of the terminal vertices and it is represented as $v_1, v_2, \ldots, v_{n-1}, v_n$.

Let
$$d(v_0) = n$$
, $d(v_i) = q + 1$ and $d(r_k) = 1$.

$$H(S_n(r_1, r_2, \dots, r_{q-1}, r_q)) = \sum_{i=1}^n \left(\frac{2}{d(v_0) + d(v_i)}\right) + \sum_{i=1}^n \sum_{k=1}^q \left(\frac{2}{d(v_i) + d(r_k)}\right) = n\left(\frac{2}{n+q+1}\right) + qn\left(\frac{2}{q+2}\right).$$

Theorem 3.15: Let G_P be the thorn graph with *n*-tuple obtained from the connected graph G. Then, the inverse sum index of a thorn multi-star $S_n(r_1, r_2, \ldots, r_{q-1}, r_q)$ is given by $n\left(\frac{n(q+1)}{n+q+1}\right) + nq\left(\frac{q+1}{q+2}\right)$.

Proof: From the star S_n , the thorn multi-star denoted by $S_n(r_1, r_2, \ldots, r_{q-1}, r_q)$, is obtained.

This thorn multi-star is obtained by connecting q_i extreme vertices to *i* of S_n , where *i* ranges from $1, 2, 3, \ldots, n-1, n$ and it is depicted in Fig.7.

In the thorn star $S_n(r_1, r_2, \ldots, r_{q-1}, r_q)$, labeling of vertices is done in such a way that, the number v_0 is the central vertex, additionally, $1, 2, 3, \ldots, n-1, n$ represents the numbering of the terminal vertices and it is denoted as $v_1, v_2, \ldots, v_{n-1}, v_n$. Let $d(v_0) = n$, $d(v_i) = q + 1$ and $d(r_k) = 1$.

$$IS(S_n(r_1, r_2, \dots, r_{q-1}, r_q)) = \sum_{i=1}^n \left(\frac{d(v_0)d(v_i)}{d(v_0) + d(v_i)} \right) \\ + \sum_{i=1}^n \sum_{j=1}^q \left(\frac{d(v_i)d(r_k)}{d(v_i) + d(r_k)} \right) \\ = n \left(\frac{n(q+1)}{n+q+1} \right) \\ + nq \left(\frac{q+1}{q+2} \right).$$

This completes the proof of the theorem.

Theorem 3.16: Let G_P be the thorn graph with *n*tuple obtained from the connected graph G. Then, the symmetric division deg index of a thorn multistar $S_n(r_1, r_2, \ldots, r_{q-1}, r_q)$, is given by $n\left(\frac{n^2+(q+1)^2}{n(q+1)}\right) + nq\left(\frac{(q+1)^2+1}{q+1}\right)$.

Proof: From the star S_n , the thorn multi-star denoted by $S_n(r_1, r_2, \ldots, r_{q-1}, r_q)$, is obtained.

Consider the central vertex of S_n as v_0 .

Let $v_1, v_2, v_3, \ldots, v_n$ be the end vertices numbered as $1, 2, \ldots, n - 1, n$ and the pendant vertices be denoted by $r_1, r_2, r_3, \ldots, r_q$, similarly, v_0 contains pendant vertices namely $s_1, s_2, s_3, \ldots, s_q$.

Here $P = (q, q, q, \dots, q, u)$, where P denotes the n-tuple and it is depicted in Fig. 7.

Let $d(v_0) = n$, $d(v_i) = q + 1$, where *i* ranges from 1, 2, 3, ..., n, $d(s_j) = d(r_k) = 1$. $SDD(S_n(r_1, r_2, ..., r_{q-1}, r_q))$

$$\begin{split} &= \sum_{i=1}^n \left(\frac{(d(v_0))^2 + (d(v_i))^2}{d(v_0)d(v_i)} \right) \\ &+ \sum_{i=1}^n \sum_{k=1}^q \left(\frac{(d(v_i))^2 + (d(r_k))^2}{d(v_i)d(r_k)} \right) \\ &= n \left(\frac{n^2 + (q+1)^2}{n(q+1)} \right) \\ &+ nq \left(\frac{(q+1)^2 + 1}{q+1} \right). \end{split}$$

Hence the proof.



Fig. 8. Example of thorn multi-star $S_5(1,2,3)$.

Example: Consider the example of thorn multi-tar, $S_5(1,2,3)$, given in Fig. 8.

Here, the Sombor index of a thorn multi-tar, $S_5(1,2,3)$, is calculated as $5\sqrt{41} + 15\sqrt{17}$.

The harmonic index of a thorn multi-star, $S_5(1,2,3)$, is calculated as $\frac{10}{9}$ + 6.

The inverse sum index of a thorn multi-star, $S_5(1,2,3)$, is calculated as $\frac{100}{9}$ + 12.

The symmetric division deg index of a thorn multi-star, $S_5(1,2,3)$, is calculated as $\frac{41}{4} + \frac{255}{4}$.

IV. CONCLUSION

In this paper, the Sombor index, harmonic index, inverse sum index and symmetric division deg index of the thorn ring C_n^* , thorn path $P_{n,r,s}$, thorn star $S_{n,q,u}$ and also thorn multistar $S_n(r_1, r_2, \ldots, r_{q-1}, r_q)$ are estimated. The indices is predominantly used in Quantity Structure-Activity Relationship (QSAR) and Quantity Structure-Property Relationship (QSPR) studies. Though new topological indices arrive in the current era, the research can be extended to different graphs so that its applications can be brought to vast areas in the future.

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