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CLOSED-FORM EXPRESSIONS FOR DEGREE-BASED TOPOLOGICAL INDICES OF $K_m \odot S_n$

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Abstract:

We study degree-based topological indices for the corona product $K_m \circ S_n$, where K_m is a complete graph and S_n is a star graph. Using the degree partition induced by the vertex types (core vertices of K_m, the center of each star, and its leaves), we derive closed-form expressions for the first, second, and third Zagreb indices M_1, M_2, M_3; the Hyper-Zagreb index HM; the Sigma index σ; the Sombor index SO; the Forgotten index F; and the SK-type descriptors SK, SK_1, SK_2. Our approach relies on edge-class decompositions and exact counting of degree contributions across the corona's three interaction layers (within K_m, between K_m and star centers/leaves, and within stars). The resulting formulas reveal how parameters m and n govern connectivity, branching intensity, and degree heterogeneity in $K_m \circ S_n$. We discuss asymptotic behavior in m and n, identify dominant terms for large instances, and note consistencies with known special cases. The results provide analytically tractable descriptors for QSPR/QSAR applications and may guide the selection of indices suited to molecular structures exhibiting hub-leaf patterns.

MSC: 05C07, 05C09, 05C76.

Keywords: corona product, complete graph, star graph, degree-based topological indices, Zagreb indices, Hyper-Zagreb, Sigma, Sombor, Forgotten, SK-type indices.

1 Introduction

Graph theory is a fundamental branch of mathematics with wide-ranging applications in computer science, biology, and chemistry. In mathematical chemistry, molecules are often represented as molecular graphs, where vertices denote atoms and edges represent chemical bonds. This representation enables the application of graph-theoretical techniques to investigate molecular structures and predict their physical, chemical, and biological properties using discrete mathematical methods.

A central concept in this area is the topological index - a numerical invariant of a graph that remains unchanged under isomorphisms. Topological indices are crucial in Quantitative Structure-Property Relationships (QSPR) and Quantitative Structure-Activity Relationships (QSAR), where they help predict molecular characteristics such as boiling points, toxicity, and biological activity purely from structural information.

Among various classes, degree-based topological indices are particularly valued for their computational simplicity and structural expressiveness. Below, we recall several important indices along with their definitions and brief descriptions.

Gutman and Das [4] introduced the first Zagreb index, defined as

$$M_1(G) = \sum_{v \in V(G)} d_G^2(v).$$

This index is one of the earliest degree-based invariants in chemical graph theory. It measures the sum of the squares of vertex degrees and is useful in predicting molecular branching effects.
Gutman and Das [4] also presented the second Zagreb index, given by

$$M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v).$$

The second Zagreb index considers degree products over edges. It captures adjacency relationships and correlates with several physico-chemical properties.
Fath-Tabar [2] defined the third Zagreb index as

$$M_3(G) = \sum_{uv \in E(G)} |d_G(u) - d_G(v)|.$$

The third Zagreb index reflects degree differences between adjacent vertices and has applications in distinguishing irregular molecular structures.
Shirdel, Rezapour, and Sayadi [3] introduced the Hyper-Zagreb index, defined by

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

This is an extension of the first Zagreb index, giving greater weight to high-degree vertices. It is effective in analyzing complex and highly connected molecular graphs.
Gutman et al. [6] proposed the Sigma index, given as

$$\sigma(G) = \sum_{uv \in E(G)} (d_G(u) - d_G(v))^2.$$

The Sigma index measures squared degree differences over edges and can highlight irregularities and asymmetries in graph structures.
Gutman [5] introduced the Sombor index, defined as

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

The Sombor index uses the Euclidean norm of degree pairs. It is a recent addition and has shown promising results in molecular property prediction.
Furtula and Gutman [1] proposed the Forgotten index,

$$F(G) = \sum_{v \in V(G)} d_G^3(v).$$

The Forgotten index sums cubes of vertex degrees, emphasizing high-degree vertices. It can be applied in QSPR/QSAR models for molecular activity estimation.
Shegehalli and Kanabur [11] introduced the SK index,

$$SK(G) = \frac{1}{2} \sum_{uv \in E(G)} (d_G(u) + d_G(v)).$$

The SK index is a relatively new degree-sum based invariant that offers an alternative approach to analyzing vertex connectivity.
The same authors defined the $\mathbf{SK}_1$ index as

$$SK_1(G) = \frac{1}{2}\sum_{uv\in E(G)} d_G(u)d_G(v),$$

and the $\mathbf{SK}_2$ index as

$$SK_2(G) = \frac{1}{4}\sum_{uv\in E(G)} (d_G(u) + d_G(v))^2.$$

The SK_1 index provides insights into edge-based degree interactions, while the SK_2 index balances the influence of degree sums and connectivity patterns.

While these indices have been thoroughly investigated for standard graph families, their behavior under complex graph operations remains less explored. One such operation is the corona product $G \circ H$, obtained by taking one copy of G and $|V(G)|$ disjoint copies of H, then joining each vertex of G to every vertex of a corresponding copy of H.

In this paper, we examine the corona product $K_m \circ S_n$, where K_m is a complete graph and S_n is a star graph. We derive closed-form expressions for several degree-based topological indices of $K_m \circ S_n$, thereby shedding light on how structural properties influence index values. The results have potential applications in QSPR and QSAR modeling.

2 Basic Definitions

Throughout this work, all graphs are assumed to be finite, simple (no loops or multiple edges), connected, and undirected.

Definition 2.1. [9] A graph G can be represented as ($V(G), E(G), \chi_G$), where $V(G)$ is a finite, non-empty set of vertices, $E(G)$ is a set of edges with $E(G) \cap V(G) = \emptyset$, and the incidence function χ_G assigns to each edge an unordered pair of distinct vertices of G. If $\chi_G(e) = uv$, then u and v are called the endpoints of the edge e.

Definition 2.2. [9] The degree of a vertex v in a graph G, denoted $d_G(v)$, is the number of edges incident with v.

Definition 2.3. [9] A complete graph K_m is a simple undirected graph with m vertices in which every pair of distinct vertices is joined by an edge.

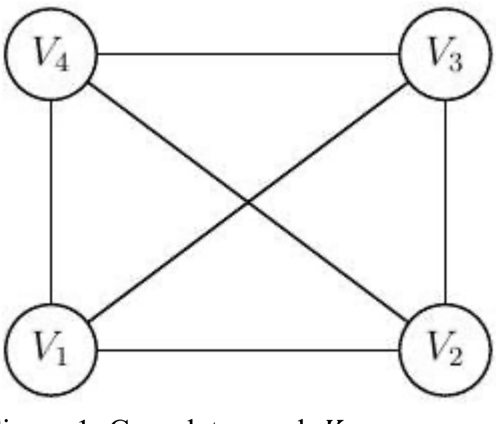

Figure 1: Complete graph K_4

Definition 2.4. [9] A star graph S_n is a tree with n vertices of degree 1 (leaves) and one vertex of degree n (center). Thus, S_n has $n + 1$ vertices in total and is isomorphic to $K_{1,n}$.

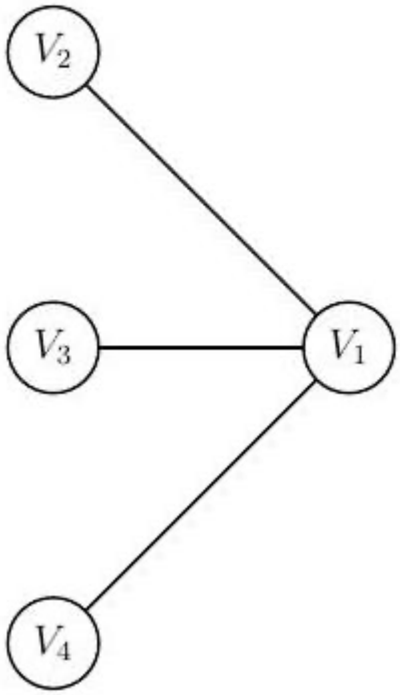

Figure 2: Star graph S_4

Definition 2.5 [10] The corona product of two graphs G and H, denoted $G \circ H$, is obtained by taking one copy of G together with $|V(G)|$ disjoint copies of H, and joining the i-th vertex of G to every vertex of the i-th copy of H.

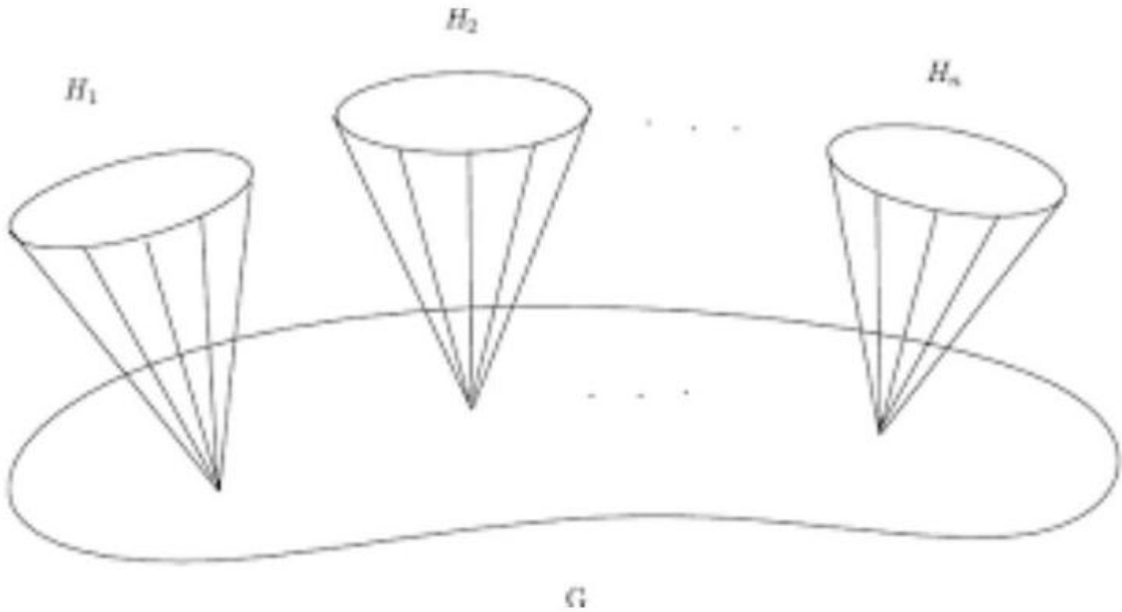

Figure 3: Corona Product of graphs G and H

3 Main Results

3.1 Indices of $K_m \circ S_n$

In this section, we present analytical derivations for several degree-based topological indices of the corona product $K_m \circ S_n$. This graph is constructed by attaching to each vertex of K_m a distinct copy of S_n, creating a composite structure whose degree distribution significantly influences the resulting index values.

Theorem 3.1. Let K_m and S_n be the complete and star graphs with $m \geq 2$ and $n \geq 1$ respectively. Then the corona product of K_m and S_n has
(i) $M_1(K_m \odot S_n) = m^2(m + 2(n-1)) + m(2n(n+1) - 3)$
(ii) $M_2(K_m \odot S_n) = \frac{m(m-1)}{2}[(m-1)^2 + n(2m+n-2)] + m^2[3n-2] + mn[7n-11] + 4m$.
(iii) $M_3(K_m \odot S_n) = m(n-1)[m+n-3] + m[m-1] + m(n-1)(n-2)$.
Proof. Consider the complete graph K_m with $m \geq 2$ and the star graph S_n with $n \geq 1$. From the definitions of M_1, M_2, and M_3, the corresponding formulas for $K_m \circ S_n$ are obtained as follows.

$$
\begin{aligned}
(i) M_1(K_m \odot S_n) &= \sum_{v \in V(K_m \odot S_n)} d^2(v), \\
&= m((m-1)+n)^2 + m(n-1)(2)^2 + mn^2, \\
&= m((m-1)^2 + n^2 + 2n(m-1)) + 4m(n-1) + mn^2, \\
&= m^3 - 2m^2 + 2mn^2 + 2m^2 n + 2mn - 3m, \\
&= m^2(m + 2n - 2) + m(2n^2 + 2n - 3), \\
&= m^2(m + 2(n-1)) + m(2n(n+1) - 3).
\end{aligned}
$$

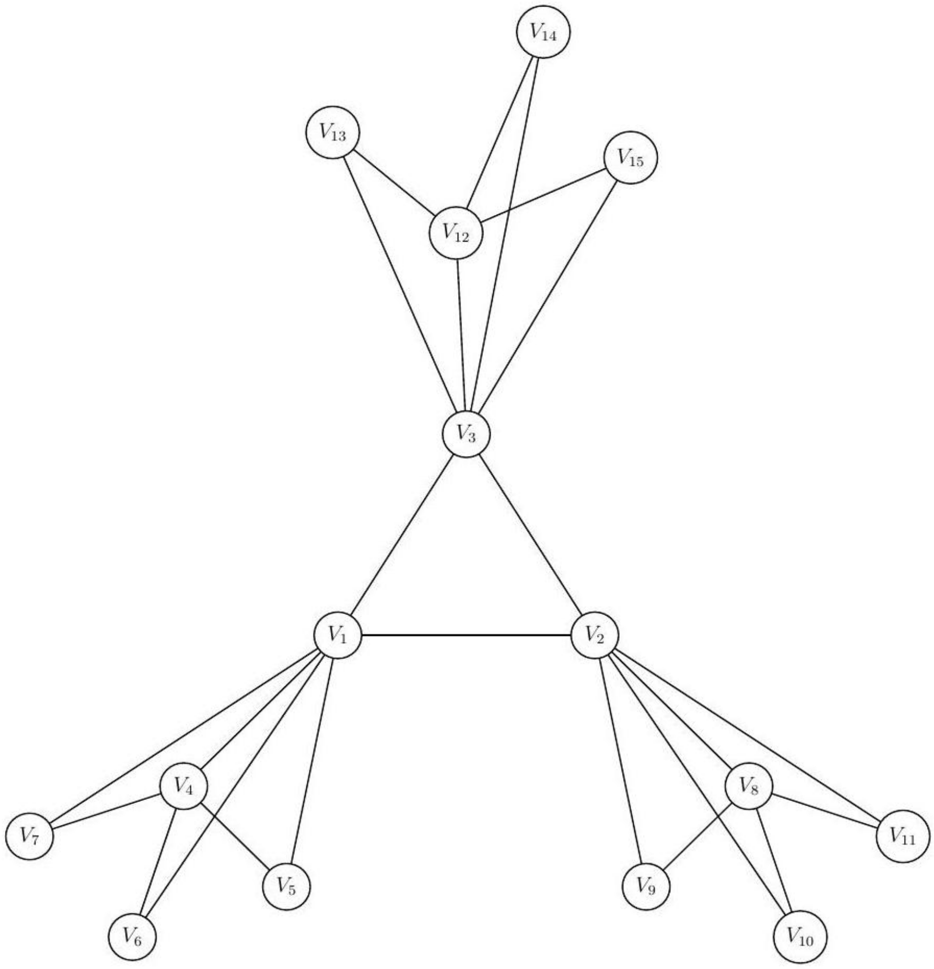

Figure 4: $K_3 \odot S_4$

$$(ii) M_2(K_m \odot S_n) = \sum_{u,v \in E(K_m \odot S_n)} (d(u)d(v)),$$
$$= \frac{m(m-1)}{2}(((m-1)+n)((m-1)+n))$$
$$+m(n-1)(2((m-1)+n)) + m(((m-1)+n)((n-1)+1))$$
$$+m(n-1)(2((n-1)+n)),$$
$$= \frac{m(m-1)}{2}[(m-1)^2 + 2mn - 2n + n^2]$$
$$+3m^2n - 11mn + 7mn^2 - 2m^2 + 4m,$$
$$= \frac{m(m-1)}{2}[(m-1)^2 + n(2m+n-2)] + m^2[3n-2]$$
$$+mn[7n-11] + 4m.$$
$$(\text{ iii }) M_3(K_m \odot S_n) = \sum_{u,v \in E(K_m \odot S_n)} |d(u) - d(v)|,$$
$$= \frac{m(m-1)}{2}|((m-1)+n) - ((m-1)+n)|$$
$$+m(n-1)|2 - ((m-1)+n)|$$
$$+m|((m-1)+n) - ((n-1)+1)|$$
$$+m(n-1)|2 - ((n-1)+n)|$$
$$= m(n-1)[m+n-3] + m[m-1] + m(n-1)(n-2)$$

Theorem 3.2. Let K_m and S_n be the complete and star graphs with $m \geq 2$ and $n \geq 1$ respectively. Then the corona product of K_m and S_n has
(i) $HM(K_m \odot S_n) = 2m^2[m^2 - 3m + 1] + mn^2[3 + 5n] + m^2n[5m - 4] + 4mn[mn - 1]$ -3 m
(ii) $\sigma(K_m \odot S_n) = m^2n(m-8) + mn^2(5n-23) + mn(2mn+36) + m(4m-17)$.

Proof. Let $K_m (m \geq 2)$ and $S_n (n \geq 1)$ be as defined. Using vertex degrees in $K_m \circ S_n$, we evaluate the Hyper-Zagreb and Sigma indices.

$$(i) HM(K_m \odot S_n) = \sum_{u,v \in E(K_m \odot S_n)} (d(u) + d(v))^2$$
$$= \frac{m(m-1)}{2}(((m-1)+n) + ((m-1)+n))^2$$
$$+m(n-1)(2 + ((m-1)+n))^2$$
$$+m(((m-1)+n) + ((n-1)+1))^2$$
$$+m(n-1)(2 + ((n-1)+n))^2$$
$$= \frac{m(m-1)}{2}(2m+2n-2)^2 + m(n-1)(m+n+1)^2$$
$$+m(m+2n-1)^2 + m(n-1)(2n+1)^2$$
$$= 2m^2[m^2 - 3m + 1] + mn^2[3 + 5n]$$
$$+m^2n[5m-4] + 4mn[mn-1] - 3m$$

$$(ii)\sigma(K_m \odot S_n) = \sum_{u,v\in E((K_m\odot S_n)} (d(u) - d(v))^2,$$
$$= \frac{m(m-1)}{2}(((m-1)+n) - ((m-1)+n))^2$$
$$+m(n-1)(2 - ((m-1)+n))^2$$
$$+m(((m-1)+n) - ((n-1)+1))^2$$
$$+m(n-1)(2 - ((n-1)+n))^2,$$
$$= m(n-1)(m+n-3)^2 + m(m-1)^2 + m(n-1)(2n-3)^2, = m^3n + 5mn^3 -$$
$$= m^2n(m-8) + mn^2(5n-23) + mn(2mn+36) + m(4m-17)$$

Theorem 3.3. Let K_m and S_n be the complete and star graphs with $m \geq 2$ and $n \geq 1$ respectively. Then corona product of K_m and S_n has

(i) $SO(K_m \odot S_n) = \frac{m(m-1)}{2}[(m-1)+n]\sqrt{2} + m(n-1)\left[\sqrt{((m-1)+n)^2+4)} + \sqrt{((n-1)+1)^2+4)}\right] + m\left[\sqrt{((m-1)+n)^2+n^2}\right]$.

(ii) $F(K_m \odot S_n) = m^3[m+3n-3] + m^2[3n^2-6n+3] + m[2n^3-3n^2+11n-9]$

Proof. Let K_m and S_n be as above. We evaluate the Sombor and Forgotten indices for $K_m \circ S_n$.

$$(i)SO(K_m \odot S_n) = \sum_{u,v\in E(K_m\odot C_n)} \sqrt{(d(u)^2 + d(v)^2)}$$
$$= \frac{m(m-1)}{2}\left(\sqrt{((m-1)+n)^2 + ((m-1)+n)^2}\right.$$
$$+m(n-1)\left(2^2 + \sqrt{(m-1)+n)^2}\right.$$
$$+m\left(\sqrt{((m-1)+n)^2 + ((n-1)+1)^2}\right.$$
$$+m(n-1)\sqrt{(2^2 + ((n-1)+n))^2}$$
$$= \frac{m(m-1)}{2}[(m-1)+n]\sqrt{2} + m(n-1)\left[\sqrt{((m-1)+n)^2+4)}\right.$$
$$\left.+\sqrt{((n-1)+1)^2+4)}\right] + m\left[\sqrt{((m-1)+n)^2+n^2}\right].$$

$$(ii)F(K_m \odot S_n) = \sum_{v\in V(K_m\odot S_n)} d^3(v),$$
$$= m((m-1)+n)^3 + m(n-1)(2)^3 + mn^3,$$
$$= m^3[m+3n-3] + m^2[3n^2-6n+3] + m[2n^3-3n^2+11n-9].$$

Corollary 3.4. Let K_m and S_n be the complete and cycle graphs with $m \geq 2$ and $n \geq 1$ respectively. Then the corona product of K_m and S_n has $SK = \frac{1}{2}\{m(m^2-2m-2) + mn(2m+3n)\}$

Proof. Let $K_m(m \geq 2)$ and $C_n(n \geq 1)$ be the complete and cycle graphs. From the definition of the SK index and the degree structure of $K_m \circ S_n$, we compute:

$$SK(K_m \circ S_n) = \frac{1}{2}\{m(m^2-2m-2) + mn(2m+3n)\}$$

This follows directly by summing $(d(u) + d(v))$ over all edges and applying the degree values for each vertex type.

Corollary 3.5. Let K_m and S_n be the complete and star graphs with $m \geq 2$ and $n \geq 3$. Then

$$SK_1 = \frac{1}{2}\Big\{\frac{m(m-1)}{2}[(m-1)^2 + n(2m+n-2)] + m^2[3n-2]$$
$$+mn[7n-11] + 4m\}$$

Proof. Consider $K_m(m \geq 2)$ and $C_n(n \geq 3)$. Using the formula for $M_2(K_m \circ S_n)$ from Theorem ?? and the definition of SK_1, we find:

$$SK_1 = \frac{1}{2}\Big\{\frac{m(m-1)}{2}[(m-1)^2 + n(2m+n-2)] + m^2[3n-2]$$
$$+mn[7n-11] + 4m\}$$

Corollary 3.6. Let K_m and S_n be the complete and cycle graphs with $m \geq 2$ and $n \geq 1$ respectively. Then the corona product of K_m and S_n has

$$SK_2 = \frac{1}{2}\{2m^2[m^2 - 3m + 1] + mn^2[3 + 5n]$$
$$+m^2n[5m - 4] + 4mn[mn - 1] - 3m\}$$

Proof. Let K_m and S_n satisfy $m \geq 2$ and $n \geq 3$. By substituting the result of $HM(K_m \circ S_n)$ from Theorem ?? into the definition of SK_2, we obtain:

$$SK_2 = \frac{1}{2}\{2m^2[m^2 - 3m + 1] + mn^2[3 + 5n]$$
$$+m^2n[5m - 4] + 4mn[mn - 1] - 3m\}$$

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