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Degree-Based Entropy of Some Classes of Networks

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Abstract: A topological index is a number that is connected to a chemical composition in order to correlate a substance's chemical makeup with different physical characteristics, chemical reactivity, or biological activity. It is common to model drugs and other chemical substances as different forms, trees, and graphs. Certain physico-chemical features of chemical substances correlate better with degree-based topological invariants. Predictions concerning the dynamics of the continuing pandemic may be made with the use of the graphic theoretical approaches given here. In Networks, the degree entropy of the epidemic and related trees was computed. It highlights the essay's originality while also implying that this piece has improved upon prior literature-based realizations. In this paper, we study an important degree-based invariant known as the inverse sum indeg invariant for a variety of graphs of biological interest networks, including the corona product of some interesting classes of graphs and the pandemic tree network, curtain tree network, and Cayley tree network. We also examine the inverse sum indeg invariant features for the molecular graphs that represent the molecules in the bicyclic chemical graphs.

Keywords: mathematical chemistry; chemical graph theory; topological invariants; networks

MSC: 05C30; 05C90

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1. Introduction

Euler presented the graph theory, a subfield of discrete mathematics, for the first time in 1736. It has been utilized in a variety of other fields, including physics, biology, chemistry, etc. The chemical graph theory is the mathematical description of chemical events in conjunction with graph theory. It focuses on invariants that have a strong correlation to a molecule's or chemical compound's characteristics; see details in [1–4]. Ali et al. also presented the euler graph theory in [5–8]. In the QSAR/QSPR modeling [9,10], topological invariants are employed worldwide to forecast the physico-chemical and bioactivity features of a molecule or molecular compound. The topological invariant [11,12] is an original graph invariant of a chemical compound's topological structure. The physical characteristics of paraffin were determined using the Wiener invariant [13], which was initially made public in 1947.

A molecular graph [14,15] is a straightforward connected graph with atoms and chemical bonds acting as its vertices and edges, respectively; see more details in [16,17]. Many topological invariants have been generated as a result of extensive work on computing the invariants of various molecular graphs and networks. These indices are based on surface, degree, and distance [18–24]. The degree-based invariants(DBI) are more appealing to anticipate the characteristics of a molecule or a compound. Inverse sum indeg invariant (IS) is a prominent degree-based invariant that is defined for a molecular network Ω as

$IS(\Omega) = \sum\limits_{uv \in E(\Omega)} \frac{1}{\frac{1}{\lambda_\Omega(u)} + \frac{1}{\lambda_\Omega(v)}} = \sum\limits_{uv \in E(\Omega)} \frac{\lambda_\Omega(u)\lambda_\Omega(v)}{\lambda_\Omega(u)+\lambda_\Omega(v)}$, where $\lambda_\Omega(u)$ is a degree of a vertex u in Ω.

One of the discrete Adriatic TIs explored in [25] is the IS invariant, whose prediction abilities were assessed against the benchmark datasets of [15] from the International Academy of Mathematical Chemistry. In [26], extreme values of the IS were found for a variety of graph types, including linked graphs, chemical graphs, trees, and chemical trees. The boundaries of a descriptor are crucial data for a molecular graph since they define the descriptor's approximate range in terms of molecular structural characteristics. In [22], some precise constraints for the linked graphs' IS are provided. In [27], the IS of specific kinds of nanotubes is calculated. In [28–30], the relationship between the IS invariant and the vertex-edge corona product of graphs is found. For various graphs of biological interest networks, including pandemic tree networks, curtain tree networks, Cayley tree networks, and corona products of some interesting classes of graphs, we study one of the significant DBI in this work, known as the IS invariant. We also examine the IS invariant features for the molecular graphs that represent the molecules in the bicyclic chemical graphs.

2. Pandemic Tree Network

The reproduction number or S^0, evaluates the pandemic's intensity in epidemiology and is defined as the number of people who can become infected from a vulnerable population set. Figure 1 displays a pandemic tree for an epidemic with a S^0 (value of 4) epidemic.

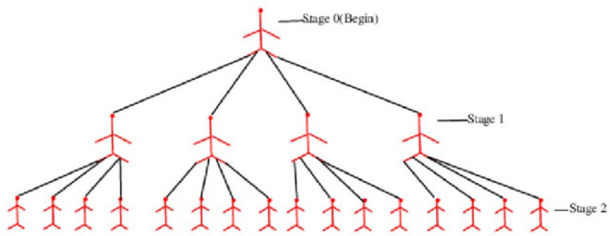

Figure 1. A pandemic tree with an eqidemiological R^0 value of 3.

The reproduction number of a pandemic, rounded to the closest integer, is S^0, and a pandemic tree is a full S^0-ary.

A rooted tree with no more than k offspring at each vertex is said to be k-ary. This vertex's descendants include all of a node's offspring. The height of a k-ary tree is defined as the greatest distance l from the leaf to the root vertex. Level 0 is referred to as the root vertex. According to induction, the offspring of vertices at level i are also at level $i+1$. If every internal vertex on a k-ary tree has precisely k descendants, the tree is said to be complete. A pandemic tree is a full k-ary tree that has the epidemiological S^0 value of k. rounded. This tree is represented by the letter Ω_l^k, where l indicates its height $k, l \geq 2$. Figure 2 depicts the pandemic tree levels 5 and 6.

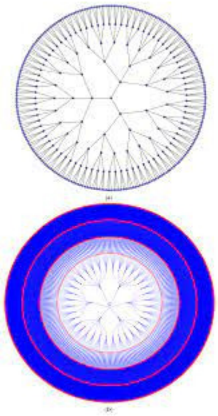

Figure 2. A 5-level pandemic tree Ω_5^3 and 6-level pandemic tree Ω_6^6.

Theorem 1. *Let Ω_l^k stand for an epidemic tree with l levels and k reproductions. Then,* $IS(\Omega_l^k) = \frac{k^2(k+1)}{2k+1} + \frac{k^l(k+1)}{k+2} + \sum_{i=1}^{l-2} \frac{k^{l-i}(k+1)}{2}$.

Proof. For i, $0 \leq i \leq 1$, the number of vertices of Ω_l^k with level i is k^i. Hence, we can easily calculate the total number of vertices and edges in Ω_l^k, that is, $\left|V(\Omega_l^k)\right| = \frac{k^{l+1}-1}{k-1}$ and $\left|E(\Omega_l^k)\right| = \frac{k^{l+1}-1}{k-1} - 1$. Now, we analyze the degree of any vertex x in Ω_l^k as follows;

(i) If x is a leaf of Ω_l^k, then $\lambda_{\Omega_l^k}(x) = 1$.
(ii) If x is a root of Ω_l^k, then $\lambda_{\Omega_l^k}(x) = k$.
(iii) If x is an internal vertex of Ω_l^k, then $\lambda_{\Omega_l^k}(x) = k+1$.

□

Let us consider the following edge partitions of a tree Ω_l^k based on its degrees of a edge. Let P_{ij} be the set of all edges with degree of end vertices i, j, that is, $P_{ij} = \{xy \in E(\Omega_l^k) | \lambda_{\Omega_l^k}(x) = i, \ \lambda_{\Omega_l^k}(y) = j\}$ and let p_{ij} be the number of edges in P_{ij}. From the structure of Ω_l^k, it is clear that $p_{k+1,k} = k$, $p_{1,k+1} = k^l$ and $p_{k+1,k+1} = \sum_{i=1}^{l-2} k^{l-i}$. Thus,

$$\begin{aligned}
IS(\Omega_l^k) &= \sum_{xy \in E(T_l^k)} \frac{\lambda_{\Omega_l^k}(x)\lambda_{\Omega_l^k}(y)}{\lambda_{\Omega_l^k}(x) + \lambda_{\Omega_l^k}(y)} \\
&= p_{k+1,k}\left(\frac{\lambda_{\Omega_l^k}(x)\lambda_{\Omega_l^k}(y)}{\lambda_{\Omega_l^k}(x) + \lambda_{\Omega_l^k}(y)}\right) + p_{1,k+1}\left(\frac{\lambda_{\Omega_l^k}(x)\lambda_{\Omega_l^k}(y)}{\lambda_{\Omega_l^k}(x) + \lambda_{\Omega_l^k}(y)}\right) + p_{k+1,k+1}\left(\frac{\lambda_{\Omega_l^k}(x)\lambda_{\Omega_l^k}(y)}{\lambda_{\Omega_l^k}(x) + \lambda_{\Omega_l^k}(y)}\right) \\
&= k\left(\frac{(k+1) \times k}{(k+1) + k}\right) + k^l\left(\frac{(k+1) \times 1}{(k+1) + 1}\right) + \sum_{i=1}^{l-2} k^{l-i} \times \left(\frac{(k+1) \times (k+1)}{(k+1) + (k+1)}\right) \\
&= \frac{k^2(k+1)}{2k+1} + \frac{k^l(k+1)}{k+2} + \sum_{i=1}^{l-2} \frac{k^{l-i}(k+1)}{2}.
\end{aligned}$$

3. Curtain Tree Network

Let C_i represent a branch of a tree Ω created by connecting i pendant paths of length 2 to the vertex x in such a way that x has degree $i+1$ in Ω. The curtain tree network, shown by $\Omega(r, C_k^s)$ in Figure 3, is created by joining s branches of C_k to each vertex of path P_r.

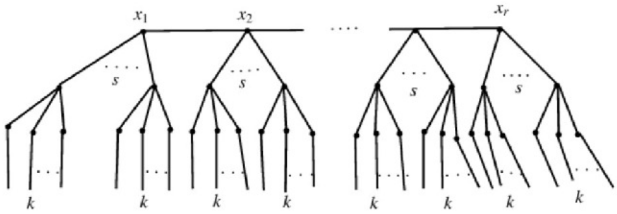

Figure 3. A 5-level pandemic tree Ω_5^3 and 6-level pandemic tree Ω_6^6.

Theorem 2. *Let r, s, k be three positive integers such that $r \geq 3, k \geq 2$ and $s \geq 1$. Then,* $IS(\Omega(r, C_k^s)) = \frac{4krs(2k+6)}{3(k+3)} + s(k+1)\left(\frac{2(s+1)}{s+k+2} + \frac{s(r-2)}{s+k+1}\right) + \frac{2(s+1)(s+2)}{2s+3} + \frac{(r-3)(s+2)^2}{2(s+2)}$.

Proof. We have rs of branches C_k based on the curtain tree network's $\Omega(r, C_k^s)$ structure. We shall first mark all of the branches' edges as follows:

(i) $2k$ edges make up the branch of C_k, and k of those edges have two vertices: the first of degree one, and the second of degree two. Two vertices can be found on other k edges as well, the first of degree two and the second of degree $k+1$.

(ii) The same is true for the rs edges connecting the vertices of the route and the branches of C_k, $2s$ of which include two vertices, the first of degree $s+1$ and the second of degree $k+1$. Two vertices are also present on the remaining $(r-2)s$ edges: one of degree $k+1$ and the other of degree $s+2$.

(iii) Only the path's edges are left at this point. This path has edges that are $r-1$. The first has a degree of $s+1$, and the second has a degree of $s+2$. Two of them have two vertices. Additionally, there are two vertices with the same degree $s+2$ on the remaining $r-3$ edges.

□

Let P'_{ij} be the set of all edges with the degree of end vertices i, j, that is, $P'_{ij} = \{xy \in E(\Omega(r, C_k^s)) | \lambda_{\Omega(r,C_k^s)}(x) = i, \ \lambda_{\Omega(r,C_k^s)}(y) = j\}$ and let p'_{ij} be the number of edges in P'_{ij}. From the structure of $\Omega(r, C_k^s)$, it is clear that $p'_{1,2} = krs$, $p'_{k+1,2} = krs$, $p'_{k+1,s+1} = 2s$, $p'_{k+1,s} = s(r-2)$, $p'_{s+1,s+2} = 2$ and $p'_{s+2,s+2} = r-3$. Thus

$$
\begin{aligned}
IS(\Omega(r, C_k^s)) &= \sum_{xy \in E(\Omega(r,C_k^s))} \frac{\lambda_{\Omega(r,C_k^s)}(x)\lambda_{\Omega(r,C_k^s)}(y)}{\lambda_{\Omega(r,C_k^s)}(x) + \lambda_{\Omega(r,C_k^s)}(y)} \\
&= p'_{1,2}\Big(\frac{\lambda_{\Omega(r,C_k^s)}(x)\lambda_{\Omega(r,C_k^s)}(y)}{\lambda_{\Omega(r,C_k^s)}(x) + \lambda_{\Omega(r,C_k^s)}(y)}\Big) + p'_{k+1,2}\Big(\frac{\lambda_{\Omega(r,C_k^s)}(x)\lambda_{\Omega(r,C_k^s)}(y)}{\lambda_{\Omega(r,C_k^s)}(x) + \lambda_{\Omega(r,C_k^s)}(y)}\Big) \\
&\quad + p'_{k+1,s+1}\Big(\frac{\lambda_{\Omega(r,C_k^s)}(x)\lambda_{\Omega(r,C_k^s)}(y)}{\lambda_{\Omega(r,C_k^s)}(x) + \lambda_{\Omega(r,C_k^s)}(y)}\Big) + p'_{k+1,s}\Big(\frac{\lambda_{\Omega(r,C_k^s)}(x)\lambda_{\Omega(r,C_k^s)}(y)}{\lambda_{\Omega(r,C_k^s)}(x) + \lambda_{\Omega(r,C_k^s)}(y)}\Big) \\
&\quad + p'_{s+1,s+2}\Big(\frac{\lambda_{\Omega(r,C_k^s)}(x)\lambda_{\Omega(r,C_k^s)}(y)}{\lambda_{\Omega(r,C_k^s)}(x) + \lambda_{\Omega(r,C_k^s)}(y)}\Big) + p'_{s+2,s+2}\Big(\frac{\lambda_{\Omega(r,C_k^s)}(x)\lambda_{\Omega(r,C_k^s)}(y)}{\lambda_{\Omega(r,C_k^s)}(x) + \lambda_{\Omega(r,C_k^s)}(y)}\Big) \\
&= krs\Big(\frac{1 \times 2}{1+2}\Big) + krs\Big(\frac{2 \times (k+1)}{(k+1)+2}\Big) + 2s\Big(\frac{(s+1)(k+1)}{(s+1)+(k+1)}\Big) \\
&\quad + s(r-2)\Big(\frac{s(k+1)}{s+(k+1)}\Big) + 2\Big(\frac{(s+1)(s+2)}{(s+1)+(s+2)}\Big) + r - 3\Big(\frac{(s+2)(s+2)}{(s+2)+(s+2)}\Big) \\
&= \frac{4krs(2k+6)}{3(k+3)} + s(k+1)\Big(\frac{2(s+1)}{s+k+2} + \frac{s(r-2)}{s+k+1}\Big) + \frac{2(s+1)(s+2)}{2s+3} + \frac{(r-3)(s+2)^2}{2(s+2)}.
\end{aligned}
$$

4. Cayley Tree Network

A k-Cayley tree $CN(k,l)$ with levels l is a tree where all vertices have the same degree k except the leaves. Figure 4 depicts the Cayley tree's structure, which has a degree of 3 and a level of 6.

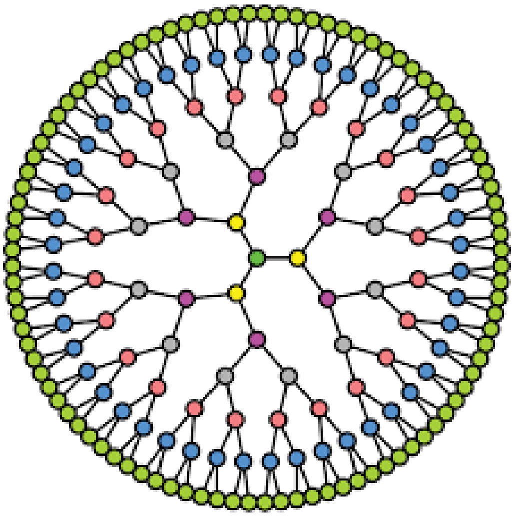

Figure 4. A 3-Cayley tree $CN(3,6)$ with 6 levels.

Theorem 3. *For a Cayley tree $CN(k,l)$, with $k,l \geq 3$, we have $IS(CN(k,l)) = \frac{k(k(k-1)^l-k+1)}{2(k^2-3k+2)} + \frac{k^2(k-1)^l}{(k+1)}$.*

Proof. Note that the number of vertices and edges in $CN(k,l)$ are, respectively, $\frac{k(k-1)^l-2}{k-2}$ and $\frac{k(k-1)^l-2}{k-2} - 1$. Let P''_{ij} be the set of all edges of $CN(k,l)$ with a degree of end vertices i, j and let p''_{ij} be its cardinality. Then, by the structure of $CN(k,l)$, we have $p''_{k,k} = \frac{k(k-1)^l-k+1}{k^2-3k+2}$ and $p''_{1,k} = k(k-1)^{l-1}$. Hence,

$$\begin{aligned}
IS(CN(k,l)) &= \sum_{xy \in E(CN(k,l))} \frac{\lambda_{CN(k,l)}(x)\lambda_{CN(k,l)}(y)}{\lambda_{CN(k,l)}(x) + \lambda_{CN(k,l)}(y)} \\
&= p''_{k,k} \frac{\lambda_{CN(k,l)}(x)\lambda_{CN(k,l)}(y)}{\lambda_{CN(k,l)}(x) + \lambda_{CN(k,l)}(y)} + p''_{1,k} \frac{\lambda_{CN(k,l)}(x)\lambda_{C(k,l)}(y)}{\lambda_{C(k,l)}(x) + \mu_{CN(k,l)}(y)} \\
&= \frac{k(k-1)^l - k + 1}{k^2 - 3k + 2} \times \left(\frac{k \times k}{k+k}\right) + k(k-1)^{l-1} \times \left(\frac{k \times 1}{k+1}\right) \\
&= \frac{k(k(k-1)^l - k + 1)}{2(k^2 - 3k + 2)} + \frac{k^2(k-1)^l}{(k+1)}.
\end{aligned}$$

□

5. Christmas Tree Network

If a graph can be created from a Meyniel graph by eliminating every edge between any two nodes, it is said to be slim graph. A tree, also known as a linked acyclic undirected graph, is an undirected graph in graph theory in which any two vertices are connected by precisely one route. Thus, we can gain a slim tree in graph theory. For $s \geq 2$, a Christmas tree $CTN(s)$ is composed of an s^{th} slim tree $ST(s) = (V_1, E_1, u_1, l_1, r_1)$ and an $(s+1)^{th}$ slim tree $ST(s+1) = (V_2, E_2, u_2, l_2, r_2)$ together with the edges u_1u_2,l_1r_2 and l_2r_1, where $ST(s) = (V, E, u, l, r)$, with V as the node set, E as the edge set, $u \in V$ as the root node, $l \in V$ as the left node, and $r \in V$ as the right node defined below:

(i) $ST(2)$ is the complete graph K_3 with its nodes labeled with u,l and r.

(ii) The s^{th} slim tree $ST(s)$, with $s \geq 3$ is composed of a root node u and two disjoint copies of $(s-1)^{th}$ slim trees as the left subtree and right subtree, denoted by $ST^l(s-1) = (V_1, E_1, u_1, l_1, r_1)$ and $ST^r(s-1) = (V_2, E_2, u_2, l_2, r_2)$, respectively, and $ST(s) = (V, E, u, l, r)$ is given by $V = V_1 \cup V_2 \cup \{u\}$,$E = E_1 \cup E_2 \cup \{(u, u_1), (u, u_2), (r_1, l_2)\}$,$l = l_1, r = r_2$. For illustration, the Christmas tree $CT(3)$ is shown in Figure 5.

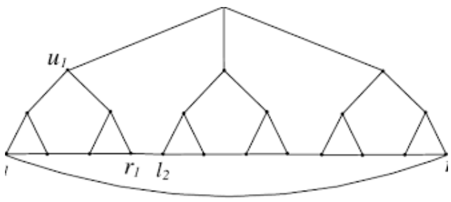

Figure 5. A Christmas tree $CTN(3)$ with 3 levels.

Theorem 4. *For a Christmas tree $CTN(s)$, $IS(CTN(s)) = (9 \times 2^s - 6) \times \frac{3}{4}$.*

Proof. The number of vertices and edges of $CTN(s)$ are $(3 \times 2^s) - 2$ and $\frac{9 \times 2^s - 6}{2}$, respectively. As $CTN(s)$ is a 3-regular, $E_{3,3} = \{xy \in E(CTN(s)) | \lambda_{CTN(s)}(x) = 3 \ and \ \lambda_{CTN(s)}(y) = 3\}$ is a only edge partition of $CTN(s)$ and its number of edges is $\frac{9 \times 2^s - 6}{2}$. Hence,

$$\begin{aligned} IS(CTN(s)) &= \sum_{xy \in E(CTN(s))} \frac{\lambda_{CTN(s)}(x)\lambda_{CTN(s)}(y)}{\lambda_{CTN(s)}(x) + \lambda_{CTN(s)}(y)} \\ &= |E_{3,3}| \left(\frac{3 \times 3}{3+3}\right) = \frac{(9 \times 2^s - 6)}{2} \times \frac{9}{6} = (9 \times 2^s - 6) \times \frac{3}{4}. \end{aligned}$$

□

6. Corona Product of Graphs

Graph operations facilitate decomposition of a graph Ω into two or more isomorphic subgraphs. The corona product $\Omega_1 \oplus \Omega_2$ of two graphs Ω_1 and Ω_2 is defined as the graph obtained by taking a copy of Ω_1 and $|V(\Omega_1)|$ copies of Ω_2, and then joining the i^{th} vertex of Ω_1 with edges to every vertex in the i^{th} copy of Ω_2. It easily shows that $|V(\Omega_1 \oplus \Omega_2)| = |V(\Omega_1)| + |V(\Omega_1)||V(\Omega_2)|$ and $|E(\Omega_1 \oplus \Omega_2)| = |E(\Omega_1)| + |V(\Omega_1)||E(\Omega_2)| + |V(\Omega_1)||V(\Omega_2)|$. Now, we obtain the value for ISI of corona product of Christmas tree $CTN(S)$ and a path graph P_n.

Theorem 5. *If $CTN(S) \oplus P_n$ is a tree with $s, n \geq 2$, then $IS(CTN(S) \oplus P_n) = (3 \times 2^s - 2)\left(\frac{6n+22}{n+5} + \frac{3(n-2)(n+3)}{n+6} + \frac{9(n-1)}{4}\right)$.*

Proof. The number of vertices and edges of $CTN(S) \oplus P_n$ are $3 \times 2^s - 2 + (3 \times 2^s - 2)n$ and $\frac{9 \times 2^s - 6}{2} + ((3 \times 2^s) - 2)(2n - 1)$, respectively. From the structure of the corona product of $CTN(S)$ and P_n, we have the following five edge partitions based on degrees of vertices;
$P_{n+3,n+3} = \{xy \in E(CTN(S) \oplus P_n) | \lambda_{CTN(S) \oplus P_n}(x) = n+3 \ and \ \lambda_{CTN(S) \oplus P_n}(y) = n+3\}$,
$P_{n+3,2} = \{xy \in E(CTN(S) \oplus P_n) | \lambda_{CTN(S) \oplus P_n}(x) = n+3 \ and \ \lambda_{CTN(S) \oplus P_n}(y) = 2\}$,
$P_{n+3,3} = \{xy \in E(CTN(S) \oplus P_n) | \lambda_{CTN(S) \oplus P_n}(x) = n+3 \ and \ \lambda_{CTN(S) \oplus P_n}(y) = 3\}$,
$P_{2,3} = \{xy \in E(CTN(S) \oplus P_n) | \lambda_{CTN(S) \oplus P_n}(x) = 2 \ and \ \lambda_{CTN(S) \oplus P_n}(y) = 3\}$, and
$P_{3,3} = \{xy \in E(CTN(S) \oplus P_n) | \lambda_{CTN(S) \oplus P_n}(x) = 3 \ and \ \lambda_{CTN(S) \oplus P_n}(y) = 3\}$. □

One can observe that $p_{n+3,n+3} = \frac{9 \times 2^s - 6}{2}$,$p_{n+3,2} = 2(3 \times 2^s - 2)$, $p_{n+3,3} = (n-2)(3 \times 2^s - 2)$,$p_{2,3} = 2(3 \times 2^s - 2)$ and $p_{3,3} = (n-3)(3 \times 2^s - 2)$. Hence

$$\begin{aligned}
IS(CTN(S)\oplus P_n) &= \sum_{xy\in E(CTN(S)\oplus P_n)} \frac{\lambda_{CTN(S)\oplus P_n}(x)\lambda_{CTN(S)\oplus P_n}(y)}{\lambda_{CTN(S)\oplus P_n}(x)+\lambda_{CTN(S)\oplus P_n}(y)} \\
&= \frac{9\times 2^s-6}{2}\Big(\frac{(n+3)\times(n+3)}{(n+3)+(n+3)}\Big)+2(3\times 2^s-2)\Big(\frac{(n+3)\times 2}{(n+3)+2}\Big) \\
&\quad +(n-2)(3\times 2^s-2)\Big(\frac{(n+3)\times 3}{(n+3)+3}\Big)+2(3\times 2^s-2)\Big(\frac{2\times 2}{2+2}\Big)+(n-3)(3\times 2^s-2)\Big(\frac{3\times 3}{3+3}\Big) \\
&= \frac{3(3\times 2^s-2)}{2}\Big(\frac{(n+3)}{2}\Big)+2(3\times 2^s-2)\Big(\frac{2(n+3)}{n+5}\Big) \\
&\quad +(n-2)(3\times 2^s-2)\Big(\frac{3(n+3)}{n+6)}\Big)+2(3\times 2^s-2)+\frac{3(n-3)(3\times 2^s-2)}{2} \\
&= (3\times 2^s-2)\Big(\frac{6n+22}{n+5}+\frac{3(n-2)(n+3)}{n+6}+\frac{9(n-1)}{4}\Big).
\end{aligned}$$

Theorem 6. *The IS invariant of the corona product of two paths is* $IS(P_r\oplus P_s) = \frac{32(s+1)}{(s+3)} + \frac{24(s-2)(s+1)+16(r-2)(s+2)}{(s+4)} + \frac{2(s+1)+2(r-3)(s+2)+6r(s-3)}{2} + \frac{34r}{5} + \frac{4(s+1)(s+2)}{(2s+3)} + \frac{6(s+2)(s-2)(r-2)}{(s+5)}$.

Proof. One can observe that the number of vertices and edges of the graph $P_r\oplus P_s$ are, respectively, $r+rs$ and $2rs-1$. Let P_{ij} be the set of all edges with the degree of end vertices $i,\ j$, that is, $P_{ij}=\{xy\in E(P_r\oplus P_s)|\lambda_{P_r\oplus P_s}(x)=i,\lambda_{P_r\oplus P_s}(y)=j\}$. Let p_{ij} be the number of edges in P_{ij}. From the structure of $P_r\oplus P_s$, it is clear that

$p_{s+1,2} = 4$, $p_{s+1,3} = 2(s-2)$, $p_{s+1,s+1} = \begin{cases} 0 & \text{if } r>2 \\ 1 & \text{if } r=2 \end{cases}$, $p_{s+2,s+2} = \begin{cases} 0 & \text{if } r=2 \\ r-3 & \text{if } r>2 \end{cases}$, $p_{s+1,s+2} = \begin{cases} 0 & \text{if } r=2 \\ 2 & \text{if } r>2 \end{cases}$, $p_{s+2,2} = \begin{cases} 0 & \text{if } r=2 \\ 2(r-2) & \text{if } r>2 \end{cases}$, $p_{s+2,3} = \begin{cases} 0 & \text{if } r=2 \\ (r-2)(s-2) & \text{if } r>2 \end{cases}$, $p_{2,2} = \begin{cases} r & \text{if } s=2 \\ 0 & \text{if } s>2 \end{cases}$, $p_{2,3} = \begin{cases} 0 & \text{if } s=2 \\ 2r & \text{if } s>2 \end{cases}$ and $p_{3,3} = \begin{cases} 0 & \text{if } s=2 \\ r(s-3) & \text{if } s>2 \end{cases}$. $\square$

- If $r=s=2$, then

$$\begin{aligned}
IS(P_r\oplus P_s) &= \sum_{xy\in E(G)} \frac{\lambda_{P_r\oplus P_s}(x)\lambda_{P_r\oplus P_s}(y)}{\lambda_{P_r\oplus P_s}(x)+\lambda_{P_r\oplus P_s}(y)} \\
&= 4\Big(\frac{2(s+1)}{(s+1)+2}\Big)+2(s-2)\Big(\frac{3(s+1)}{(s+1)+3}\Big)+\Big(\frac{(s+1)(s+1)}{(s+1)+(s+1)}\Big) \\
&\quad +2(r-2)\Big(\frac{2(s+2)}{(s+2)+2}\Big)+r\Big(\frac{2\times 2}{2+2}\Big) \\
&= \frac{8(s+1)}{(s+3)}+\frac{6(s-2)(s+1)}{(s+4)}+\frac{(s+1)}{2}+\frac{4(s+2)(r-2)}{(s+4)}+r \\
&= \Big(\frac{8(s+1)}{(s+3)}\Big)+\Big(\frac{(s+1)}{2}\Big)+r+\Big(\frac{6(s-2)(s+1)+4(r-2)(s+2)}{(s+4)}\Big).
\end{aligned}$$

- If $r=2$ and $s>2$, then

$$\begin{aligned}
IS(P_r \oplus P_s) &= 4\Big(\frac{2(s+1)}{(s+1)+2}\Big) + 2(s-2)\Big(\frac{3(s+1)}{(s+1)+3}\Big) + \Big(\frac{(s+1)(s+1)}{(s+1)+(s+1)}\Big) \\
&\quad +2(r-2)\Big(\frac{2(s+2)}{(s+2)+2}\Big) \\
&\quad +2r\Big(\frac{3\times 2}{3+2}\Big) + r(s-3)\Big(\frac{3\times 3}{3+3}\Big) \\
&= \frac{8(s+1)}{(s+3)} + \frac{6(s-2)(s+1)}{(s+4)} + \frac{(s+1)}{2} + \frac{4(s+2)(r-2)}{(s+4)} \\
&\quad + \frac{12r}{5} + \frac{3r(m-3)}{2}.
\end{aligned}$$

- If $r = s = 2$, then

$$\begin{aligned}
IS(P_r \oplus P_s) &= 4\Big(\frac{2(s+1)}{(s+1)+2}\Big) + 2(s-2)\Big(\frac{3(s+1)}{(s+1)+3}\Big) + 2\Big(\frac{(s+1)(s+2)}{(s+1)+(s+2)}\Big) \\
&\quad +(r-3)\Big(\frac{(s+2)(s+2)}{(s+2)+(s+2)}\Big) + 2(r-2)\Big(\frac{2(s+2)}{(s+2)+2}\Big) \\
&\quad +(r-2)(s-2)\Big(\frac{3(s+2)}{(s+2)+3}\Big) + r\Big(\frac{2\times 2}{2+2}\Big) \\
&= \frac{8(s+1)}{(s+3)} + \frac{6(s-2)(s+1)}{(s+4)} + \frac{2(s+1)(s+2)}{(2s+3)} + \frac{(r-3)(s+2)}{2} \\
&\quad + \frac{4(r-2)(s+2)}{(s+4)} + \frac{3(r-2)(s-2)(s+2)}{(s+5)} + r.
\end{aligned}$$

- If $r > 2$ and $s > 2$, then

$$\begin{aligned}
IS(P_r \oplus P_s) &= 4\Big(\frac{2(s+1)}{(s+1)+2}\Big) + 2(s-2)\Big(\frac{3(s+1)}{(s+1)+3}\Big) + 2\Big(\frac{(s+1)(s+2)}{(s+1)+(s+2)}\Big) \\
&\quad +(r-3)\Big(\frac{(s+2)(s+2)}{(s+2)+(s+2)}\Big) + 2(r-2)\Big(\frac{2(s+2)}{(s+2)+2}\Big) + (r-2)(s-2)\Big(\frac{3(s+2)}{(s+2)+3}\Big) \\
&\quad +2r\Big(\frac{3\times 2}{3+2}\Big) + r(s-3)\Big(\frac{3\times 3}{3+3}\Big) \\
&= \frac{8(s+1)}{(s+3)} + \frac{6(s-2)(s+1)}{(s+4)} + \frac{2(s+1)(s+2)}{(2s+3)} + \frac{(r-3)(s+2)}{2} \\
&\quad + \frac{4(r-2)(s+2)}{(s+4)} + \frac{3(r-2)(s-2)(s+2)}{(s+5)} + \frac{12r}{5} + \frac{3r(s-3)}{2}.
\end{aligned}$$

Theorem 7. *The IS invariant of the corona product of two cycles is* $IS(C_r \oplus C_s) = \frac{r(s+2)+3rs}{2} + \frac{3rs(s+2)}{(s+5)}$.

Proof. Clearly, the number of vertices and edges of the graph $C_r \oplus C_s$ are, respectively, $r + rs$ and $r + 2rs$ when $r, s > 2$. Let P_{ij} be the set of all edges with the degree of end vertices $i,\ j$, that is, $P_{ij} = \{xy \in E(C_r \oplus C_s) | d_{C_r \oplus C_s}(x) = i, d_{C_r \oplus C_s}(y) = j\}$. Let p_{ij} be the number of edges in P_{ij}. From the structure of $C_r \oplus C_s$, it is clear that $p_{s+2,s+2} = r$,$p_{s+2,3} = rs$ and $p_{3,3} = rs$. Thus,

$$\begin{aligned} IS(C_r \oplus C_s) &= \sum_{xy \in E(C_r \oplus C_s)} \frac{\lambda_{C_r \oplus C_s}(x) \lambda_{C_r \oplus C_s}(y)}{\lambda_{C_r \oplus C_s}(x) + \lambda_{C_r \oplus C_s}(y)} \\ &= r\Big(\frac{(s+2)(s+2)}{(s+2)+(s+2)}\Big) + rs\Big(\frac{3(s+2)}{(s+2)+3}\Big) + rs\Big(\frac{3 \times 3}{3+3}\Big) \\ &= \frac{r(s+2)^2}{2(s+2)} + \frac{3rs(s+2)}{(s+5)} + \frac{3sr}{2} \\ &= \frac{r(s+2)+3rs}{2} + \frac{3rs(s+2)}{(s+5)}. \end{aligned}$$

□

Theorem 8. *The IS invariant of the corona product of a complete graph K_r and a path graph P_s is $IS(K_r \oplus P_s) = \frac{r(r-1)(r+s-1)}{2} + \frac{8r(r+s-1)}{(r+s+1)} + \frac{6r(s-2)(r+s-1)}{(r+s+2)} + \frac{3r(s-3)}{2} + \frac{17r}{5}$.*

Proof. One can observe that the number of vertices and edges of the graph $K_r \oplus P_s$ are, respectively, $r + rs$ and $rs + r(s-1) + \frac{r(r-1)}{2}$. Let P_{ij} be the set of all edges with the degree of end vertices $i,\ j$, that is, $P_{ij} = \{xy \in E(K_r \oplus P_s) | d_{K_r \oplus P_s}(x) = i, d_{K_r \oplus P_s}(y) = j\}$. Let p_{ij} be the number of edges in P_{ij}. From the structure of $P_r \oplus P_s$, it is clear that $p_{r+s-1,r+s-1} = \frac{r(r-1)}{2}$,$p_{r+s-1,2} = 2r$,$p_{r+s-1,3} = r(s-2)$,$p_{2,2} = \begin{cases} 0 & \text{if } s > 2 \\ r & \text{if } s = 2 \end{cases}$,
$p_{2,3} = \begin{cases} 0 & \text{if } s = 2 \\ 2r & \text{if } s > 2 \end{cases}$ and $p_{3,3} = \begin{cases} 0 & \text{if } s = 2 \\ r(s-3) & \text{if } s > 2 \end{cases}$. Hence

- If $r \geq 2$ and $s = 2$, then

$$\begin{aligned} IS(K_r \oplus P_s) &= \sum_{xy \in E(K_r \oplus P_s)} \frac{\lambda_{K_r \oplus P_s}(x) \lambda_{K_r \oplus P_s}(y)}{\lambda_{K_r \oplus P_s}(x) + \lambda_{K_r \oplus P_s}(y)} \\ &= \frac{r(r-1)}{2}\Big(\frac{(r+s-1)(r+s-1)}{(r+s-1)+(r+s-1)}\Big) + 2r\Big(\frac{2(r+s-1)}{(r+s-1)+2}\Big) \\ &\quad + r(s-2)\Big(\frac{3(r+s-1)}{(r+s-1)+3}\Big) + r\Big(\frac{2 \times 2}{2+2}\Big) \\ &= \frac{r(r-1)(r+s-1)}{4} + \frac{4r(r+s-1)}{(r+s+1)} + \frac{3r(s-2)(r+s-1)}{(r+s+2)} + r. \end{aligned}$$

- If $r \geq 2$ and $s > 2$, then

$$\begin{aligned} IS(K_r \oplus P_s) &= \frac{r(r-1)}{2}\Big(\frac{(r+s-1)(r+s-1)}{(r+s-1)+(r+s-1)}\Big) + 2r\Big(\frac{2(r+s-1)}{(r+s-1)+2}\Big) \\ &\quad + r(s-2)\Big(\frac{3(r+s-1)}{(r+s-1)+3}\Big) + 2r\Big(\frac{3 \times 2}{3+2}\Big) + r(s-3)\Big(\frac{3 \times 3}{3+3}\Big) \\ &= \frac{r(r-1)(r+s-1)}{4} + \frac{4r(r+s-1)}{r+s+1} + \frac{3r(s-2)(r+s-1)}{r+s+2} + \frac{12r}{5} + \frac{3r(s-3)}{2}. \end{aligned}$$

□

It is easy to see that $\Omega_1 \oplus \Omega_2$ is not in general isomorphic to $\Omega_2 \oplus \Omega_1$. Thus, the following theorem gives the value for ISI of $P_r \oplus K_s$.

Theorem 9. $IS(P_r \oplus K_s) = \frac{4r^2(r+1)}{2r+1} + \frac{2r^2(r+1)+2(r+1)+(s+2)(s-3)}{2} + \frac{2(r+1)(r+2)}{2r+3} + \frac{r^2(r+2)(s-2)}{2(r+1)}$.

Proof. One can observe that the number of vertices and edges of the graph $P_r \oplus K_s$ are, respectively, $r + rs$ and $rs + (s-1) + \frac{sr(r-1)}{2}$. Let P_{ij} be the set of all edges with the degree of end vertices $i,\ j$, that is, $P_{ij} = \{xy \in E(P_r \oplus K_s) | d_{P_r \oplus K_s}(x) = i, d_{P_r \oplus K_s}(y) = j\}$. Let p_{ij} be the number of edges in P_{ij}. From the structure of $P_r \oplus K_s$, it is clear that

$p_{r,r} = \frac{sr(r-1)}{2}$,$p_{r,r+1} = 2r$,$p_{r+1,r+1} = \begin{cases} 0 & \text{if } s > 2 \\ 1 & \text{if } s = 2 \end{cases}$, $p_{r+1,r+2} = \begin{cases} 0 & \text{if } s = 2 \\ 2 & \text{if } s > 2 \end{cases}$,

$p_{r+2,r} = \begin{cases} 0 & \text{if } s = 2 \\ r(s-2) & \text{if } s > 2 \end{cases}$ and $p_{r+2,r+2} = \begin{cases} 0 & \text{if } s = 2 \\ (s-3) & \text{if } m > 2 \end{cases}$. Hence

- If $r \geq 2$ and $s = 2$, then

$$\begin{aligned} IS(P_r \oplus K_s) &= \sum_{xy \in E(P_r \oplus K_s)} \frac{\lambda_{P_r \oplus K_s}(x) \lambda_{P_r \oplus K_s}(y)}{\lambda_{P_r \oplus K_s}(x) + \lambda_{P_r \oplus K_s}(y)} \\ &= \frac{(r+1)(r+1)}{(r+1)+(r+1)} + \frac{sr(r-1)}{2}\Big(\frac{r \times r}{r+r}\Big) + 2r\Big(\frac{r(r+1)}{r+(r+1)}\Big) \\ &= (r+1) + \frac{r^2(r-1)}{2} + \frac{2r^2(r+1)}{2r+1}. \end{aligned}$$

- If $r \geq 2$ and $s = 2$, then

$$\begin{aligned} IS(P_r \oplus K_s) &= \frac{sr(r-1)}{2}\Big(\frac{r \times r}{r+r}\Big) + 2r\Big(\frac{r(r+1)}{r+(r+1)}\Big) + 2\Big(\frac{(r+1)(r+2)}{(r+1)+(r+2)}\Big) \\ &\quad + (s-3)\Big(\frac{(r+2)(r+2)}{(r+2)+(r+2)}\Big) + r(s-2)\Big(\frac{r(r+2)}{r+(r+2)}\Big) \\ &= \frac{r^2(r-1)}{2} + \frac{2r^2(r+1)}{2r+1} + \frac{2(r+1)(r+2)}{2r+3} + \frac{(s-3)(r+2)}{2} + \frac{r^2(s-2)(r+2)}{2r+2}. \end{aligned}$$

□

Theorem 10. *The value of IS of the corona product of two complete graphs is* $IS(K_r \oplus K_s) = \frac{s^2(s-1)}{2} + \frac{rs^2(r+s-1)}{r+2s-1} + \frac{r(r-1)(r+s-1)}{4}$.

Proof. One can observe that the number of vertices and edges of the graph $K_r \oplus K_s$ are, respectively, $r + rs$ and $rs + (s-1) + \frac{sr(r-1)}{2}$. Let P_{ij} be the set of all edges with degree of end vertices $i,\ j$, that is, $P_{ij} = \{xy \in E(K_r \oplus K_s) | \lambda_{K_r \oplus K_s}(x) = i, \lambda_{K_r \oplus K_s}(y) = j\}$. Let p_{ij} be the number of edges in P_{ij}. From the structure of $K_r \oplus K_s$, it is clear that $p_{s,s} = \frac{rs(s-1)}{2}$,$p_{s,r+s-1} = rs$ and $p_{r+s-1,r+s-1} = \frac{r(r-1)}{2}$. Hence,

$$\begin{aligned} IS(K_r \oplus K_s) &= \sum_{xy \in E(K_r \oplus K_s)} \frac{\lambda_{K_r \oplus K_s}(x) \lambda_{K_r \oplus K_s}(y)}{\lambda_{K_r \oplus K_s}(x) + \lambda_{K_r \oplus K_s}(y)} \\ &= s(s-1)\frac{s.s}{s+s} + rs\Big(\frac{s(r+s-1)}{s+(r+s-1)}\Big) + \frac{r(r-1)}{2}\Big(\frac{(r+s-1)(r+s-1)}{(r+s-1)+(r+s-1)}\Big) \\ &= \frac{s^2(s-1)}{2} + \frac{rs^2(r+s-1)}{r+2s-1} + \frac{r(r-1)(r+s-1)}{4}. \end{aligned}$$

□

Corona products occasionally appear in chemical literature as plerographs of the typical hydrogen-suppressed molecular graphs known as Kneographs. For example, for a path P_s, the graph $K_2 \oplus P_s$ is called the bottleneck graph of P_s. Let C_t be the cycle with t vertices and define the molecular graph $T_{r,3} = G_r(C_3, v_1)$, which is the corona product of P_r and K_2. The fan graph $F_{s+1} = K_1 \oplus P_s$. By using above theorems, we obtain the following:

(i) $ISI(K_2 \oplus P_s) = \frac{(s+1)(s+19)}{s+3} + \frac{12(s-2)(s+1)}{s+4} + \frac{15s-11}{5}$,

(ii) $ISI(K_1 \oplus P_s) = \frac{8s}{s+2} + \frac{6s(s-2)}{s+3} + \frac{15s-11}{10}$ and
(iii) $ISI(P_r \oplus K_2) = \frac{4r^2(r+1)}{2r+1} + \frac{2(r+1)(r+2)}{2r+3} + (r+1)(r^2+1) - 2$.

7. Bicyclic Graphs

The generic formula for the IS invariant of various bicyclic graphs is given in this section. To start, we have the following assumption related to the jellyfish graph $\Omega^{C_k}(r,s,t)$. A linked graph is said to be bicyclic if there are one more edges than vertices in the graph. The Jellyfish graph is created by connecting two cycles of length r and s by a path of length t, then adding branches of length Ck to each vertex in the two cycles and path (except from the terminal vertices in the path where we add one of Ck), as illustrated in Figure 6.

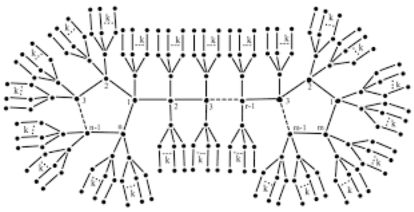

Figure 6. The graph $\Omega^{C_k}(r,s,t)$.

Theorem 11. *Let r,s,k be positive integers such that $r \geq 3$, $k \geq 2$ and $s \geq 1$. Then,* $IS(\Omega^{C_k}(r,s,t)) = 2(n+m+r-3)\left(\frac{2k(k+1)}{k+3} + \frac{4(k+1)}{k+5} + \frac{2k}{3}\right) + 2(n+m+r-1)$.

Proof. We have $2(r+s+t-3)$ of branches Ck based on the $\Omega^{C_k}(r,s,t)$ structure of the Jellyfish graph. We shall first mark all of the branches' edges as follows:

(i) $2k$ edges make up the branch of Ck, and k of those edges have two vertices: the first of degree one, and the second of degree two. Two vertices, the first of degree two and the second of degree $k+1$, may be found on another k edge of them.
(ii) Additionally, there are $2(r+s+t-3)$ edges connecting branches of Ck that each contain two vertices, the first of degree 4 and the second of degree $k+1$.
(iii) We also have $r+s+t-1$ edges with degree 4 vertices in them.

□

Let Q'_{ij} be the set of all edges with the degree of end vertices $i,\ j$, that is, $Q_{ij} = \{xy \in E(\Omega(r, C_k^s)) | \lambda_{\Omega^{C_k}(r,s,t)}(x) = i,\ \ \lambda_{\Omega^{C_k}(r,s,t)}(y) = j\}$. Let q_{ij} be the number of edges in Q_{ij}. From the structure of $\Omega^{C_k}(r,s,t)$, it is clear that $q_{1,2} = 2k(r+s+t-3)$, $q_{k+1,2} = 2k(r+s+t-3)$, $q_{k+1,4} = 2(r+s+t-3)$ and $q_{4,4} = r+s+t-1$. Thus,

$$\begin{aligned}
IS(\Omega^{C_k}(r,s,t)) &= \sum_{xy \in E(\Omega^{C_k}(r,s,t))} \frac{\lambda_{\Omega^{C_k}(r,s,t)}(x)\lambda_{\Omega^{C_k}(r,s,t)}(y)}{\lambda_{\Omega^{C_k}(r,s,t)}(x) + \lambda_{\Omega^{C_k}(r,s,t)}(y)} \\
&= q_{1,2}\Big(\frac{1 \times 2}{1+2}\Big) + q_{k+1,2}\Big(\frac{(k+1) \times 2}{(k+1)+2}\Big) + q_{4,k+1}\Big(\frac{4 \times (k+1)}{(k+1)+4}\Big) + p_{4,4}\Big(\frac{4 \times 4}{4+4}\Big) \\
&= 2k(r+s+t-3)\Big(\frac{2}{3}\Big) + 2k(r+s+t-3)\Big(\frac{2(k+1)}{(k+3)}\Big) \\
&\quad +2(r+s+t-3)\Big(\frac{4(k+1)}{(k+5)}\Big) + 2(r+s+t-1) \\
&= 2(r+s+t-3)\Big(\frac{2k(k+1)}{k+3} + \frac{4(k+1)}{k+5} + \frac{2k}{3}\Big) + 2(r+s+t-1).
\end{aligned}$$

In order to discover a generic formula for IS, we will now examine applications of the bicyclic graph in chemistry, such as polycyclic alkanes, as seen in Figure 7. In order to produce numerous rings, two or more cycloalkanes are linked together to form polycyclic alkanes, which are molecules. The carbons of cycloalkanes are organized in the shape of a ring, making them cyclic hydrocarbons. Additionally, saturated cycloalkanes have single bonds between all of the carbon atoms that make up the ring (no double or triple bonds).

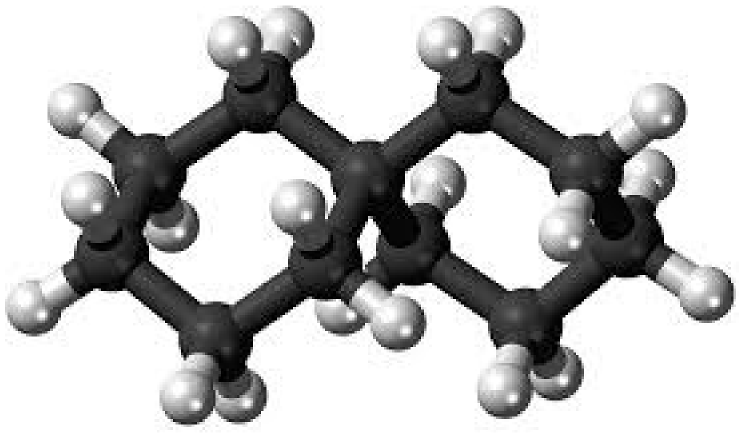

Figure 7. Molecular graph of polycyclic alkane.

Classes of alkanes with one hydrogen atom removed are referred to as the group of alkyl or branches of alkyl. Its main equation is C_nH_{2n+1}. It will include the branches of alkyl if n is larger than or equal to 1. A novel kind of bicyclic chemical graph is created when two separate chemical compounds are joined as cycloalkanes by an alkyl branch.

The molecular graph for the bicyclic chemical graphs is given by the symbol $C_{n,m}^{R_i}$, where n, m and r are the number of carbon atoms. The IS invariant connected to bicyclic chemical networks $C_{n,m}^{R_i}$ is given by the following theorem.

Theorem 12. *Let n, m, r be a positive integer such that $n, m \geq 3, r \geq 1$. Then $IS(C_{n,m}^{R_i}) = \frac{18(n+m+r-1)}{5}$.*

Proof. There are two different kinds of edges in the bicyclic chemical graphs $C_{n,m}^{R_i}$. In this graph, we will first mark each edge as follows:

(i) In the first kind, there are two vertices with the same degree of four on each of $n + m + r - 1$ edges.
(ii) In the second kind, there are two vertices of degree one and degree four that are incident on edges with the value $2(n + m + r - 1)$.

□

Let Q'_{ij} be the set of all edges with the degree of end vertices $i,\ j$, that is, $Q'_{ij} = \{xy \in E(C_{n,m}^{R_i}) | \lambda_{C_{n,m}^{R_i}}(x) = i,\ \ \lambda_{C_{n,m}^{R_i}}(y) = j\}$. Let q'_{ij} be the number of edges in Q'_{ij}. From the structure of $C_{n,m}^{R_i}$, it is clear that $q'_{4,4} = n + m + r - 1$ and $q'_{1,4} = 2(n + m + r - 1)$. Thus,

$$\begin{aligned} IS(C_{n,m}^{R_i}) &= \sum_{xy \in E(C_{n,m}^{R_i})} \frac{\lambda_{C_{n,m}^{R_i}}(x)\lambda_{C_{n,m}^{R_i}}(y)}{\lambda_{C_{n,m}^{R_i}}(x) + \lambda_{C_{n,m}^{R_i}}(y)} \\ &= q'_{4,4}\Big(\frac{4 \times 4}{4+4}\Big) + q'_{1,4}\Big(\frac{1 \times 4}{1+4}\Big) \\ &= \frac{18(n+m+r-1)}{5}. \end{aligned}$$

Let $C_{n,r,m}^{R_s}$ be a bicyclic graph connected to a certain class of chemical compound's molecular graph. This class's molecular structure is created by combining two distinct cycloalkanes of lengths n and m with an alkyl branch of length r. We create a new class of bicyclic chemical graphs and the molecular graph $C_{n,r,m}^{R_s}$ that represents them by adding branches of alkyl Rs to each hydrogen atom.

Theorem 13. *Let r and s be positive integers such that $r \geq 3$ and $s \geq 1$. Then, $IS(C_{n,r,m}^{R_s}) = \frac{2(2s+1)}{5}\Big(9(n+m+r) - 10s + 1\Big)$.*

Proof. We have $2(n+m+r-1)$ branches in the bicyclic graph CRs when we consider its structure. First, we shall designate each branch's margin as follows:

(i) The branch of R_s has $3s$ edges, $2s+1$ of which have two vertices, the first of degree 1 and the second of degree 4. Two vertices of degree 4 are also present in the remaining $s-1$ edges.
(ii) We also have branches of Rs with vertices of two cycles and a connecting route, each with two vertices of the same degree 4, and $2(n+r+m-1)$ edges linking those branches.
(iii) The connecting path for all of the edges in this instance has two vertices of the same degree 4. We also have $n+m+r+1$ of edges that formed two cycles.

□

Let Q''_{ij} be the set of all edges with the degree of end vertices $i,\ j$, that is, $Q''_{ij} = \{xy \in E(C_{n,r,m}^{R_s}) | \lambda_{C_{n,r,m}^{R_s}}(x) = i,\ \ \lambda_{C_{n,r,m}^{R_s}}(y) = j\}$. Let q''_{ij} be the number of edges in Q''_{ij}. From the structure of $C_{n,m}^{R_i}$, it is clear that $q''_{1,4} = (4s+2)(n+m+r-1)$ and $q''_{4,4} = (2s+1)(n+m+r) - 2s + 1$. Thus,

$$
\begin{aligned}
IS(C_{n,r,m}^{R_s}) &= \sum_{xy \in E(C_{n,r,m}^{R_s})} \frac{\lambda_{C_{n,r,m}^{R_s}}(x)\lambda_{C_{n,r,m}^{R_s}}(y)}{\lambda_{C_{n,r,m}^{R_s}}(x) + \lambda_{C_{n,r,m}^{R_s}}(y)} \\
&= q'_{1,4}\Big(\frac{1 \times 4}{1+4}\Big) + q'_{4,4}\Big(\frac{4 \times 4}{4+4}\Big) \\
&= \frac{8(2s+1)(n+m+r-1)}{5} + 2(2s+1)(n+m+r) - 4s + 2 \\
&= \frac{2(2s+1)}{5}\Big(9(n+m+r) - 10s + 1\Big).
\end{aligned}
$$

8. Conclusions

To create quantitative structure–activity relationships (QSAR), quantitative structure–property relationships (QSPR), and quantitative structure–toxicity relationships, topological indices (TI) are often utilized as molecular descriptors (QSTR). We have demonstrated in the present study that the TIs created are crucial for assessing the network data present in pandemic trees. The graph theoretical methods described here can also help with a variety of predictions about the dynamics of the ongoing epidemic. Last but not least, we calculated the degree-based entropy of the pandemic trees and the associated networks. These results significantly increased our understanding of how serious the continuing COVID-19 pandemic scenario is.

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