RESEARCH PAPER

Application of Distance-Based Topological Indices of Corona Product Graphs in Drug Discovery and Pharmaceutical Network Analysis

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ABSTRACT
Topological indices are significant in chemical graph theory as they give numbers that describe the structural features of molecular networks. In this work, we study various topological indices of the corona product graphs $K_{m,n} \odot K_r$ and $K_{m,n} \odot \overline{K_r}$ based on distance. Each of the Wiener type indices is given explicitly by a closed-form formula. Systematic distance distribution analysis is carried out for the associated corona product structures to obtain the derivations. The results of this analysis provide useful computational tools for very large families of graphs, and contribute to the theory of graph invariants. Moreover, the indices obtained from these can also be applied in molecular drug drugability in pharmaceutical network analysis and drug development: the molecular structures can be represented as graphs, with chemical bonds as edges and atoms as vertices. The suggested corona product models can be applied to describe complex medicinal compounds that consist of an underlying molecular structure with a number of functional groups. Topological descriptors obtained can be used in Quantitative Structure–Activity Relationship (QSAR) and Quantitative Structure–Property Relationship (QSPR) studies to predict biological activity, molecular stability, toxicity, and pharmacological properties.
Additionally, drug-target interaction networks and drug delivery systems based on nanoparticles can be analysed using these graph models. The results of the study therefore provide valuable mathematical models for high-level drug design research, modeling of pharmaceutical networks, molecular screening and lead optimization.
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1. INTRODUCTION

Graph theory has evolved into a significant tool in mathematics for the modeling and analysis of complex structures in science, engineering and technology. Chemical graph theory particularly makes a significant link between the concepts of graphs and molecular structures, where vertices represent atoms and edges represent chemical bonds. Numerical measures obtained from these graph representations called topological indices, are useful for understanding the structure of molecules and have been used widely in fields such as chemistry, pharmacology, bioinformatics and network science.

Topological descriptors (TDS) have been the subject of considerable interest because they have been able to effectively describe the geometric and connectivity features of molecular structures. Among the different classes of topological descriptors, distance-based topological indices have gained much attention since they represent the most popular and effective tools for capturing the geometric and connectivity properties of molecular structures. These indices are widely used in quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) studies for the prediction of biological activity, toxicity, stability, boiling points, and other physical and chemical parameters of chemical compounds. One of the earliest and most influential distance-based descriptors is the Wiener index that was introduced by Wiener in 1947. Thereafter, several extensions of the Wiener index, such as Hyper-Wiener index, Harary index, Reciprocal Complementary Wiener index, Wiener Polarity index, Terminal Wiener index, Reverse Wiener index and Reciprocal Reverse Wiener index have been developed. These indices are

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complementary to each other and give information about the molecular branching, compactness, accessibility and communication efficiency in a graph.

Graph Operations are very important for building up more complex graph structures from simpler ones and for modelling large scale networks. A particular example of an operation is the corona product of graphs, which was proposed as an easily accessible tool for the construction of hierarchical and modular network structures. The corona product consists of multiple copies of a second graph attached to a base graph, resulting naturally in corona structures representing systems of a central graph, with several subsidiary units attached. These types of graph models find application in molecular structures, social networks, biological systems, and communication networks.

There has been a lot of research confirming the determination of the topological indices for some graph products and graph families in recent years. In fact, analytical expressions for these indices are of special interest since they not only save repeating calculations but also give efficient tools for the analysis of large classes of graphs. The above developments have led to the present work with a focus on the corona product graphs $K_{m,n} \odot K_r$ and $K_{m,n} \odot \overline{K_r}$, where $K_{m,n}$ is a complete bipartite graph, K_r is a complete graph and $\overline{K_r}$ is the complement of a complete graph. Such graph structures can model complex inter-connected systems, which have a bipartite central structure with peripheral subnetworks.

The main aim of this research is to find closed form expressions of some important distance based topological indices of the graphs $K_{m,n} \odot K_r$ and $K_{m,n} \odot \overline{K_r}$. In particular, we calculate Wiener index, Hyper-Wiener index, Harary index, Reciprocal Complementary Wiener index, Wiener Polarity index, Terminal Wiener index, Reverse Wiener index and Reciprocal Reverse Wiener index. Both the derivations follow a detailed analysis of the distance distributions of the vertices of the corona product structures.

The results obtained are not only mathematically significant but have also significant applications in drug discovery and pharmaceutical network analysis. Some possible corona product graphs can represent molecular scaffolds linked to functional groups, drug–target interaction systems, as well as drug delivery systems based on nanoparticles. The topological descriptors derived are quantitative measures which can help in molecular screening, lead optimization, prediction of biological activity and transport efficiency evaluation in pharmaceutical systems.

In this context, the results reported in this work are not only of a theoretical nature contributing to the development of chemical graph theory, but also offer a contribution to the field of practical applications such as in pharmaceutical research or drug design. The rest of the paper is organized as follows: Section 2 gives a derivation of the distance-based topological indices of the corona product graph $K_{m,n} \odot K_r$ and $K_{m,n} \odot \overline{K_r}$. The results obtained are discussed in the applications section in drug discovery and pharmaceutical network analysis (Part 3). Conclusions and suggestions for further research finally follow.

In this paper, we consider only finite simple connected undirected graphs [3] and [4] . The eccentricity of a vertex u in a graph G is $e(u) = max\{d(u,v): v \in V(G)\}$. The radius (resp. diameter) of G is $r = rad(G) = min\{e(v): v \in V(G)\}$ (resp. $d = diam(G) = max\{e(v): v \in V(G)\}$). The Complement of a graph G is a graph $\overline{G}$ on the same set of vertices as of G such that there will be an edge between two vertices in $\overline{G}$ iff there is no edge in between in G. A graph G in which every pair of vertices is joined by exactly one edge is called complete graph. A complete graph on n vertices is denoted by K_n and complement of the complete graph on n vertices is denoted by $\overline{K}_n$. The Wiener index [5, 7, 20] is defind by the sum of distances between all unordered pairs of vertices of a graph G,

$$W(G) = \sum_{u,v \in V(G)} d\,(u,v).$$

The hyper-Wiener index is introduced by Milan Randić in 1993 [19] and is defind as follows :

$$WW(G) = \frac{1}{2} \sum_{u,v \in V(G)} [d(u,v) + d(u,v)^2].$$

In [17] Plavšić et. al., and in [12] Ivancine et. al., independently introduced the Harary index and denoted by

$$H(G) = \sum_{u,v \in V(G)} \frac{1}{d(u,v)}.$$

In [11, 13] Ivancine et. al., introduced the Reciprocal Complementary Wiener index, denoted by $RCW(G)$ and given by

$$RCW(G) = \sum_{u,v \in V(G)} \frac{1}{d + 1 - d(u,v)},$$

where d is the diameter of a graph G.

The Wiener polarity index W_P is introduced by Wiener in 1947 [6] and is defind as follows :

$$W_P(G) = |\{(u,v) \mid d(u,v) = 3, u, v \in V(G)\}|.$$

The terminal Wiener index of a graph G is defined by Gutman et.al., in[8] , as the sum of distance between all pairs of pendent vertices of G,

$$TW(G) = \sum_{u,v \in V(G), deg(u)=deg(v)=1} d\,(u,v).$$

The reverse Wiener index was proposed by Balaban et. al., in 2000 [2], is defined as follows

$$\wedge\,(G) = \frac{n(n-1)d}{2} - W(G),$$

where $n = |V(G)|$ and d is the diameter of G.

In [14], the Reciprocal Reverse Wiener (RRW) index $R \wedge (G)$ of a connected graph G is defined as

$$R \wedge (G) = \begin{cases} \sum_{u,v \in V(G)} \dfrac{1}{d - d(u,v)}, & \text{for } 0 < d(u,v) < d, 0, \quad \text{for otherwise.} \end{cases}$$

where d is the diameter of a graph G.

Various indices are studied by [10,15,16]. In this paper we calculate $W(G)$, $WW(G)$, $H(G)$, $RCW(G)$, $W_P(G)$, $TW(G)$, $\wedge\,(G)$ and $R \wedge (G)$ of $K_{m,n} \odot K_r$ and $K_{m,n} \odot \overline{K}_r$. In [1] the computation of distance-based topological indices have been studied for the corona product of two complete graphs.

Definition 1. *The corona product $G \odot H$ of two graphs G and H is defined as the graph obtained by taking one copy of G and $|V(G)|$ copies of H and by joining the i^{th} vertex of G to every vertex in the i^{th} copy of H.*

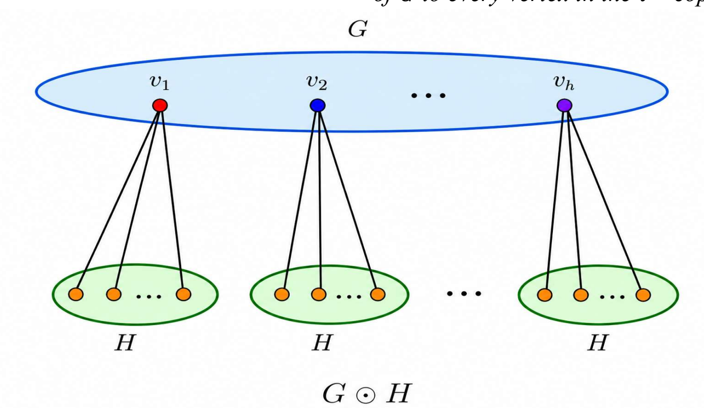

Figure 1. 1 *Corona Product of two graphs G and H*

Theorem 2. [9] *Let G_1 be a connected graph. Then* $W(G_1 \odot G_2) = (|G_2| + 1)^2 W(G_1) + |G_1|\,(|G_2|^2 - |E(G_2)|) + (|G_1|^2 - |G_1|)\,|G_2|\,(|G_2| + 1)$.

2. MAIN RESULTS

2.1. Indices of $K_{m,n} \odot K_r$

Definition 2. *The corona product $K_{m,n} \odot K_r$ is defined as the graph obtained by taking one copy of $K_{m,n}$ and $m + n$ copies of K_r and by joining the i^{th} vertex of $K_{m,n}$ to every vertex in the i^{th} copy of K_r, see Figure 2.1 for $K_{3,4} \odot K_2$.*

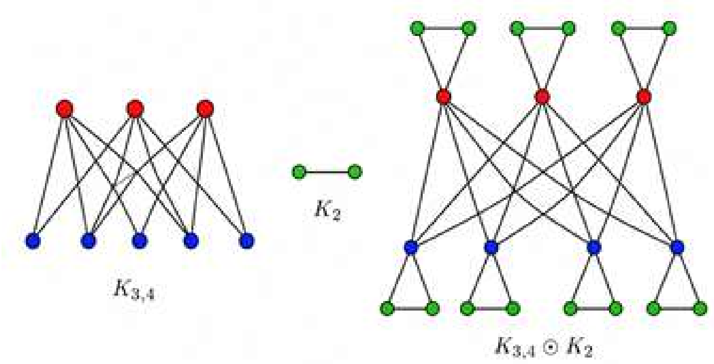

Figure 2.1 *Corona Product* $K_{3,4} \odot K_2$

Theorem 4. *For* $m, n \geq 2$ *and* $r \geq 1$, *we have*

(i) $W(K_{m,n} \odot K_r) = \frac{(r+1)}{2}[2mn(3r+1) + (m+n)r + 2[m(m-1) + n(n-1)](2r+1)]$.

(ii) $WW(K_{m,n} \odot K_r) = \frac{1}{2}\{2mn(6r^2 + 6r + 1) + (m+n)(3r-1) + [m(m-1) + n(n-1)](10r^2 + 12r + 3)\}$.

(iii) $H(K_{m,n} \odot K_r) = \frac{mn}{3}(r^2 + r + 1) + \frac{r}{2}(m+n)(r+1) + \frac{1}{24}[m(m-1) + n(n-1)](3r^2 + 8r + 6)$.

(iv) $RCW(K_{m,n} \odot K_r) = \frac{mn}{12}(6r^2 + 8r + 3) + \frac{1}{8}(m+n)r(r+1) + \frac{1}{6}[m(m-1) + n(n-1)](3r^2 + 3r + 1)$.

Proof. For $m, n \geq 2$ and $r \geq 1$, the $K_{m,n} \odot K_r$ is the corona product of $K_{m,n}$ and K_r. Let $V(K_{m,n} \odot K_r) = U_1 \cup U_2 \cup \cdots \cup U_m \cup V_1 \cup V_2 \cup \cdots \cup V_n$, where $U_i = \{u_{i,1}, u_{i,2}, \ldots, u_{i,r+1}\}$ and $V_j = \{v_{j,1}, v_{j,2}, \ldots, v_{j,r+1}\}$, $1 \leq i \leq m$ and $1 \leq j \leq n$. For $i, j = 1,2, \ldots, m$ and $p, q = 1,2, \ldots, n$ and $k, \ell = 2,3, \ldots, r+1$ the distance between any two vertices in $K_{m,n} \odot K_r$ are given by $d(u_{i,1}, v_{p,1}) = 1$, $d(u_{i,1}, u_{i,k}) = d(u_{i,k}, u_{i,\ell}) = 1$, for $k \neq \ell$, $d(v_{p,1}, v_{p,k}) = d(v_{p,k}, v_{p,\ell}) = 1$, for $k \neq \ell$, $d(u_{i,1}, u_{j,1}) = 2$ for $i \neq j$, $d(v_{p,1}, u_{q,1}) = 2$, for $p \neq q$, $d(u_{i,1}, v_{p,k}) = d(u_{i,k}, v_{p,1}) = 2$, $d(u_{i,k}, v_{p,\ell}) = 3$, $d(u_{i,1}, u_{j,k}) = 3$ for $i \neq j$, $d(v_{p,1}, v_{q,k}) = 3$, for $p \neq q$, $d(u_{i,k}, u_{j,\ell}) = 4$, for $i \neq j$, $d(v_{p,k}, v_{q,\ell}) = 4$, for $p \neq q$,

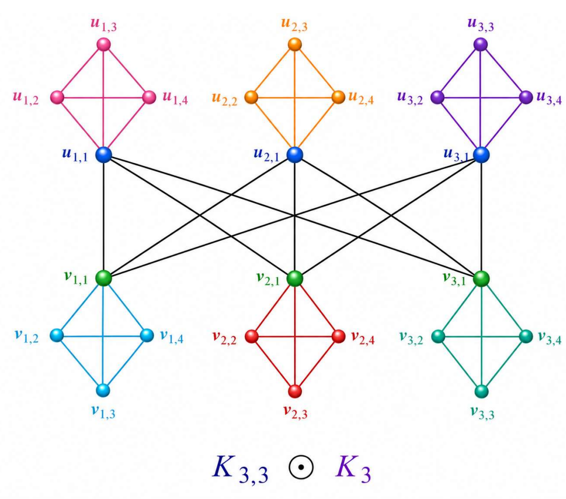

Figure 2.2. *Corona Product* $K_{m,n} \odot K_r$

Corona Product of $\boldsymbol{K_{m,n}}$ ***and*** $\boldsymbol{K_r}$

Here $diam(G) = 4$ and the distance between any pair of vertices varies from $1,2, \ldots, diam(G)$. The number of pair of vertices receives distance 1, 2, 3 and 4 are $mn + mr + nr + m\binom{r}{2} + n\binom{r}{2}$, $\binom{m}{2} + \binom{n}{2} + 2mnr$, $m(m-1)r + n(n-1)r + mnr^2$ and $r^2\binom{m}{2} + r^2\binom{n}{2}$ respectively. By using these we derive the following

$$\text{(i)}W(K_{m,n}\odot K_r) = mn+mr+nr+m\binom{r}{2}+n\binom{r}{2}+\left[\binom{m}{2}+\binom{n}{2}+2mnr\right]2$$
$$+[m(m-1)r+n(n-1)r+mnr^2]3+\left[r^2\binom{m}{2}+r^2\binom{n}{2}\right]4$$
$$=\frac{(r+1)}{2}[2mn(3r+1)+(m+n)r+2[m(m-1)+n(n-1)](2r+1)].$$

$$\text{(ii)}WW(K_{m,n}\odot K_r)$$
$$=\frac{1}{2}\left\{\left[mn+mr+nr+m\binom{r}{2}+n\binom{r}{2}\right](1+1^2)+\left[\binom{m}{2}+\binom{n}{2}+2mnr\right](2+2^2)\right.$$
$$\left.+[m(m-1)r+n(n-1)r+mnr^2](3+3^2)+\left[r^2\binom{m}{2}+r^2\binom{n}{2}\right](4+4^2)\right\}$$
$$=\frac{1}{2}\{2mn(6r^2+6r+1)+(m+n)(3r-1)+[m(m-1)+n(n-1)](10r^2+12r+3)\}.$$

$$\text{(iii)}H(K_{m,n}\odot K_r) = mn+mr+nr+m\binom{r}{2}+n\binom{r}{2}+\left[\binom{m}{2}+\binom{n}{2}+2mnr\right]\frac{1}{2}$$
$$+[m(m-1)r+n(n-1)r+mnr^2]\frac{1}{3}+\left[r^2\binom{m}{2}+r^2\binom{n}{2}\right]\frac{1}{4}$$
$$=\frac{mn}{3}(r^2+r+1)+\frac{r}{2}(m+n)(r+1)+\frac{1}{24}[m(m-1)$$
$$+n(n-1)](3r^2+8r+6).$$

$$\text{(iv)}RCW(K_{m,n}\odot K_r) = \left[mn+mr+nr+m\binom{r}{2}+n\binom{r}{2}\right]\frac{1}{4}+\left[\binom{m}{2}+\binom{n}{2}+2mnr\right]\frac{1}{3}$$
$$+[m(m-1)r+n(n-1)r+mnr^2]\frac{1}{2}+r^2\binom{m}{2}+r^2\binom{n}{2}$$
$$=\frac{mn}{12}(6r^2+8r+3)+\frac{1}{8}(m+n)r(r+1)+\frac{1}{6}[m(m-1)$$
$$+n(n-1)](3r^2+3r+1).$$

Remark 1. *In Theorem 4, when $m=n=1$, $K_{m,n}\odot K_r\cong K_2\odot K_r$, here the diameter of graph $K_{m,n}\odot K_r$ is 3 hence $RCW(K_{m,n}\odot K_r)$ is invalid but $W(K_{m,n}\odot K_r)$, $WW(K_{m,n}\odot K_r)$ and $H(K_{m,n}\odot K_r)$ are valid.*

Remark 2. *In Theorem 4, when either $m\geq 1$ or $n\geq 1$, $K_{m,n}\odot K_r\cong S_{m+n}\odot K_r$, here the diameter of graph $K_{m,n}\odot K_r$ is 4 and also the above Theorem 4 is valid.*

Corollary 5. *For $m,n\geq 1$ and $r\geq 1$,* $W_P(K_{m,n}\odot K_r)=r[m(m-1)+n(n-1)+mnr]$.

Proof. The number of 3 distance pair of vertices is $m(m-1)r+n(n-1)r+mnr^2$ by Theorem 4. So, $W_P(K_{m,n}\odot K_r)=r[m(m-1)+n(n-1)+mnr]$.

Corollary 6. *For $m,n\geq 1$ and $r=1$,* $TW(K_{m,n}\odot K_r)=r^2[3mn+2m(m-1)+2n(n-1)]$.

Proof. For $m,n\geq 1$ and $r=1$, by Theorem 4 we have $TW(K_{m,n}\odot K_r)=3mnr^2+\left[r^2\binom{m}{2}+r^2\binom{n}{2}\right]4=r^2[3mn+2m(m-1)+2n(n-1)]$.

Lemma 7. *For $m,n\geq 1$ and $r\geq 1$,* $\wedge(K_{m,n}\odot K_r)=2[(m+n)(r+1)][(m+n)(r+1)-1]-\frac{(r+1)}{2}[2mn(3r+1)+(m+n)r+2[m(m-1)+n(n-1)](2r+1)]$.

Proof. For $m,n\geq 1$ and $r\geq 1$, $|V(K_{m,n}\odot K_r)|=(m+n)(r+1)$, the diameter of $K_{m,n}\odot K_r$ is 4 (that is, $d=4$) by Theorem 4 and $W(K_{m,n}\odot K_r)=\frac{(r+1)}{2}[2mn(3r+1)+(m+n)r+2[m(m-1)+n(n-1)](2r+1)]$, hence $\wedge(K_{m,n}\odot K_r)=2[(m+n)(r+1)][(m+n)(r+1)-1]-\frac{(r+1)}{2}[2mn(3r+1)+(m+n)r+2[m(m-1)+n(n-1)](2r+1)]$.

Lemma 8. *For $m,n\geq 2$ and $r\geq 1$,* $R\wedge(K_{m,n}\odot K_r)=\frac{mn}{3}(3r^2+3r+1)+\frac{1}{6}(m+n)r(r+1)+\frac{1}{4}[m(m-1)+n(n-1)](4r+1)$.

Proof. For $m,n\geq 2$ and $r\geq 1$, the diameter of $K_{m,n}\odot K_r$ is 4 and the distance between any pair of vertices varies from $0<d(u,v)<d$. The number of pair of vertices receives distance 1, 2 and 3 are $mn+mr+nr+m\binom{r}{2}+n\binom{r}{2}$, $\binom{m}{2}+\binom{n}{2}+2mnr$ and $m(m-1)r+n(n-1)r+mnr^2$ respectively. Then we have

$$
\begin{aligned}
R \wedge \left(K_{m,n} \odot K_r\right) &= \left[mn + mr + nr + m\binom{r}{2} + n\binom{r}{2}\right]\frac{1}{3} + \left[\binom{m}{2} + \binom{n}{2} + 2mnr\right]\frac{1}{2} \\
&+m(m-1)r + n(n-1)r + mnr^2 \\
&= \frac{mn}{3}(3r^2 + 3r + 1) + \frac{1}{6}(m+n)r(r+1) \\
&+\frac{1}{4}[m(m-1) + n(n-1)](4r+1).
\end{aligned}
$$

2.2. Indices of $K_{m,n} \odot \overline{K}_r$

Theorem 5. *For* $m, n \geq 2$ *and* $r \geq 1$, *we have (i)* $W\left(K_{m,n} \odot \overline{K}_r\right) = mn(3r+1)(r+1) + (m+n)r^2 + [m(m-1) + n(n-1)](2r+1)(r+1)$. *(ii)* $WW\left(K_{m,n} \odot \overline{K}_r\right) = \frac{1}{2}\{2mn(6r^2 + 6r + 1) + (m+n)r(3r-1) + [m(m-1) + n(n-1)](10r^2 + 12r + 3)\}$. *(iii)* $H\left(K_{m,n} \odot \overline{K}_r\right) = \frac{mn}{3}(r^2 + 3r + 3) + \frac{1}{4}(m+n)r(r+3) + \frac{1}{24}[m(m-1) + n(n-1)](3r^2 + 8r + 6)$. *(iv)* $RCW\left(K_{m,n} \odot \overline{K}_r\right) = \frac{mn}{12}(6r^2 + 8r + 3) + \frac{1}{12}(m+n)r(2r+1) + \frac{1}{6}[m(m-1) + n(n-1)](3r^2 + 3r + 1)$.

Proof. For $m, n \geq 2$ and $r \geq 1$, the $K_{m,n} \odot \overline{K}_r$ is the corona product of $K_{m,n}$ and $\overline{K}_r$. Let $V\left(K_{m,n} \odot \overline{K}_r\right) = U_1 \cup U_2 \cup \cdots \cup U_m \cup V_1 \cup V_2 \cup \cdots \cup V_n$, where $U_i = \{u_{i,1}, u_{i,2}, \ldots, u_{i,r+1}\}$ and $V_j = \{v_{j,1}, v_{j,2}, \ldots, v_{j,r+1}\}$, $1 \leq i \leq m$ and $1 \leq j \leq n$.

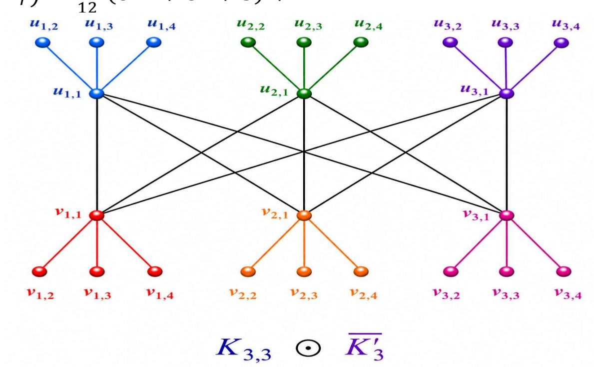

Figure 2.3. *Corona Product of* $K_{m,n}$ *and* $\overline{K}_r$

For $i, j = 1,2, \ldots, m$ and $p, q = 1,2, \ldots, n$ and $k, \ell = 2,3, \ldots, r+1$ the distance between any two vertices in $K_{m,n} \odot \overline{K}_r$ are given by $d\left(u_{i,1}, v_{p,1}\right) = d\left(u_{i,1}, u_{i,k}\right) = d\left(v_{p,1}, v_{p,k}\right) = 1$, $d\left(u_{i,1}, u_{j,1}\right) = 2$ for $i \neq j$, $d\left(v_{p,1}, u_{q,1}\right) = 2$, for $p \neq q$, $d\left(u_{i,k}, u_{i,\ell}\right) = d\left(v_{p,k}, v_{p,\ell}\right) = 2$, for $k \neq \ell$, $d\left(u_{i,1}, v_{p,k}\right) = d\left(u_{i,k}, v_{p,1}\right) = 2$, $d\left(u_{i,k}, v_{p,\ell}\right) = 3$, $d\left(u_{i,1}, u_{j,k}\right) = 3$ for $i \neq j$, $d\left(v_{p,1}, v_{q,k}\right) = 3$, for $p \neq q$, $d\left(u_{i,k}, u_{j,\ell}\right) = 4$, for $i \neq j$, $d\left(v_{p,k}, v_{q,\ell}\right) = 4$, for $p \neq q$, Here $diam(G) = 4$ and the distance between any pair of vertices varies from $1,2, \ldots, diam(G)$. The number of pair of vertices receives distance 1, 2, 3 and 4 are $mn + mr + nr$, $\binom{m}{2} + \binom{n}{2} + m\binom{r}{2} + n\binom{r}{2} + 2mnr$, $m(m-1)r + n(n-1)r + mnr^2$ and $r^2\binom{m}{2} + r^2\binom{n}{2}$ respectively. By using these we derive the following

$$
\begin{aligned}
\text{(i)}W(K_{m,n} \odot \overline{K}_r) &= mn + mr + nr + [\binom{m}{2} + \binom{n}{2} + m\binom{r}{2} + n\binom{r}{2} \\
&+2mnr]2 + [m(m-1)r + n(n-1)r + mnr^2]3 \\
&+ \left[r^2\binom{m}{2} + r^2\binom{n}{2}\right]4 \\
&= mn(3r+1)(r+1) + (m+n)r^2 \\
&+[m(m-1) + n(n-1)](2r+1)(r+1). \\
\text{(ii)}WW(K_{m,n} \odot \overline{K}_r) &= \frac{1}{2}\{[mn + mr + nr](1+1^2) \\
&+ \left[\binom{m}{2} + \binom{n}{2} + m\binom{r}{2} + n\binom{r}{2} + 2mnr\right](2+2^2) \\
&+[m(m-1)r + n(n-1)r + mnr^2](3+3^2) \\
&+ \left[r^2\binom{m}{2} + r^2\binom{n}{2}\right](4+4^2)\} \\
&= \frac{1}{2}\{2mn(6r^2+6r+1) + (m+n)r(3r-1) \\
&+[m(m-1) + n(n-1)](10r^2+12r+3)\}. \\
\text{(iii)}H(K_{m,n} \odot \overline{K}_r) &= mn + mr + nr + [\binom{m}{2} + \binom{n}{2} + m\binom{r}{2} + n\binom{r}{2} \\
&+2mnr]\frac{1}{2} + [m(m-1)r + n(n-1)r + mnr^2]\frac{1}{3} \\
&+ \left[r^2\binom{m}{2} + r^2\binom{n}{2}\right]\frac{1}{4} \\
&= \frac{mn}{3}(r^2+3r+3) + \frac{1}{4}(m+n)r(r+3) \\
&+ \frac{1}{24}[m(m-1) + n(n-1)](3r^2+8r+6). \\
\text{(iv)}RCW(K_{m,n} \odot \overline{K}_r) &= [mn + mr + nr]\frac{1}{4} + [\binom{m}{2} + \binom{n}{2} + m\binom{r}{2} \\
&+n\binom{r}{2} + 2mnr]\frac{1}{3} + [m(m-1)r + n(n-1)r \\
&+mnr^2]\frac{1}{2} + r^2\binom{m}{2} + r^2\binom{n}{2} \\
&= \frac{mn}{12}(6r^2+8r+3) + \frac{1}{12}(m+n)r(2r+1) \\
&+ \frac{1}{6}[m(m-1) + n(n-1)](3r^2+3r+1).
\end{aligned}
$$

Remark 3. *In Theorem 9, when $m = n = 1$, $K_{m,n} \odot \overline{K}_r \cong K_2 \odot \overline{K}_r$, here the diameter of graph $K_{m,n} \odot \overline{K}_r$ is 3 hence $RCW(K_{m,n} \odot \overline{K}_r)$ is invalid but $W(K_{m,n} \odot \overline{K}_r)$, $WW(K_{m,n} \odot \overline{K}_r)$ and $H(K_{m,n} \odot \overline{K}_r)$ are valid.*

Remark 4. *In Theorem 9, when either $m \geq 1$ or $n \geq 1$, $K_{m,n} \odot \overline{K}_r \cong S_{m+n} \odot \overline{K}_r$, here the diameter of graph $K_{m,n} \odot \overline{K}_r$ is 4 and also the above Theorem 9 is valid.*

Corollary 10. *For $m, n \geq 1$ and $r \geq 1$, $W_P(K_{m,n} \odot \overline{K}_r) = r[m(m-1) + n(n-1) + mnr]$.*

Proof. The number of 3 distance pair of vertices is $m(m-1)r + n(n-1)r + mnr^2$ by Theorem 9. So, $W_P(K_{m,n} \odot \overline{K}_r) = r[m(m-1) + n(n-1) + mnr]$.

Corollary 11. *For $m, n \geq 1$ and $r \geq 1$, $TW(K_{m,n} \odot \overline{K}_r) = 2r^2[m(m-1) + n(n-1)] + (m+n)r(r-1) + 3mnr^2$.*

Proof. For $m, n \geq 1$ and $r \geq 1$, by Theorem 9 we have $TW(K_{m,n} \odot \overline{K}_r) = [m\binom{r}{2} + n\binom{r}{2}]2 + 3mnr^2 + [r^2\binom{m}{2} + r^2\binom{n}{2}]4 = 2r^2[m(m-1) + n(n-1)] + (m+n)r(r-1) + 3mnr^2$.

Lemma 12. *For $m, n \geq 1$ and $r \geq 1$, $\wedge(K_{m,n} \odot \overline{K}_r) = 2[(m+n)(r+1)][(m+n)(r+1) - 1] - [mn(3r+1)(r+1) + (m+n)r^2 + [m(m-1) + n(n-1)](2r+1)(r+1)]$.*

Proof. For $m, n \geq 1$ and $r \geq 1$, $\mid V(K_{m,n} \odot \overline{K}_r) \mid = (m+n)(r+1)$, the diameter of $K_{m,n} \odot \overline{K}_r$ is 4 (i.e., $d = 4$) by Theorem 9 and $W(K_{m,n} \odot \overline{K}_r) = mn(3r+1)(r+1) + (m+n)r^2 + [m(m-1) + n(n-1)](2r+1)(r+1)$, hence $\wedge(K_{m,n} \odot \overline{K}_r) = 2[(m+n)(r+1)][(m+n)(r+1) - 1] - [mn(3r+1)(r+1) + (m+n)r^2 +$

$[m(m-1)+n(n-1)](2r+1)(r+1)]$.

Lemma 13. *For* $m,n \geq 2$ *and* $r \geq 1$, $R \wedge (K_{m,n} \odot \overline{K}_r) = \frac{mn}{3}(3r^2+3r+1)+\frac{1}{12}(m+n)r(3r+1)+\frac{1}{4}[m(m-1)+n(n-1)](4r+1)$.

Proof. For $m,n \geq 2$ and $r \geq 1$, the diameter of $K_{m,n} \odot \overline{K}_r$ is 4 and the distance between any pair of vertices varies from $0 < d(u,v) < d$. The number of pair of vertices receives distance 1, 2 and 3 are $mn+mr+nr$, $\binom{m}{2}+\binom{n}{2}+m\binom{r}{2}+n\binom{r}{2}+2mnr$ and $m(m-1)r+n(n-1)r+mnr^2$ respectively. Then we have

$$\begin{aligned} R \wedge (K_{m,n} \odot \overline{K}_r) &= [mn+mr+nr]\frac{1}{3}+[\binom{m}{2}+\binom{n}{2}+m\binom{r}{2}+n\binom{r}{2} \\ &+2mnr]\frac{1}{2}+m(m-1)r+n(n-1)r+mnr^2 \\ &= \frac{mn}{3}(3r^2+3r+1)+\frac{1}{12}(m+n)r(3r+1) \\ &+\frac{1}{4}[m(m-1)+n(n-1)](4r+1). \end{aligned}$$

3. APPLICATION IN DRUG DISCOVERY AND PHARMACEUTICAL NETWORK ANALYSIS

The distance-based topological indices derived for the corona product graphs $K_{m,n} \odot K_r$ and $K_{m,n} \odot \overline{K}_r$ have promising applications in drug discovery and pharmaceutical network analysis. In chemical graph theory, a molecular structure is represented as a graph where vertices correspond to atoms and edges correspond to chemical bonds. Topological indices such as the Wiener, Hyper-Wiener, Harary, Reciprocal Complementary Wiener, and Reverse Wiener indices serve as numerical descriptors that capture the structural characteristics of molecules. These descriptors are widely employed in Quantitative Structure–Activity Relationship (QSAR) and Quantitative Structure–Property Relationship (QSPR) studies to predict biological activity, toxicity, stability, and physicochemical properties of drug compounds.

The corona product structure considered in this work can model complex pharmaceutical compounds consisting of a central molecular scaffold connected to several functional groups. The complete bipartite graph $K_{m,n}$ represents the core framework of a drug molecule, while the attached copies of K_r or $\overline{K}_r$ represent substituent groups or molecular fragments that influence biological activity.The obtained closed-form expressions reduce computational complexity in molecular screening procedures by enabling quick computation of topological descriptors for vast families of structurally related molecules without the need to build individual molecular graphs.

Additionally, these graph models can be used for drug-target interaction networks, in which biological targets are represented by the center vertices and interacting drug molecules or functional domains are represented by the associated subgraphs. increased binding affinity and increased pharmacological efficacy may be correlated with higher values of connectivity-based indices, which show effective communication channels within the molecular network. Thus, the insights can help researchers find viable lead compounds and optimize molecular structures while designing drugs. Furthermore, the suggested graph topologies can simulate drug delivery systems based on nanoparticles, where the associated subgraphs represent encapsulated drug molecules and the core framework serves as the carrier platform. Quantitative measurements of structure compactness, accessibility, and transport efficiency are provided by the computed topological indices. These elements are crucial for focused therapeutic delivery and regulated drug release. As a result, this study's mathematical findings provide useful theoretical tools for enhanced drug delivery research, virtual screening, lead optimization, and pharmaceutical modeling.

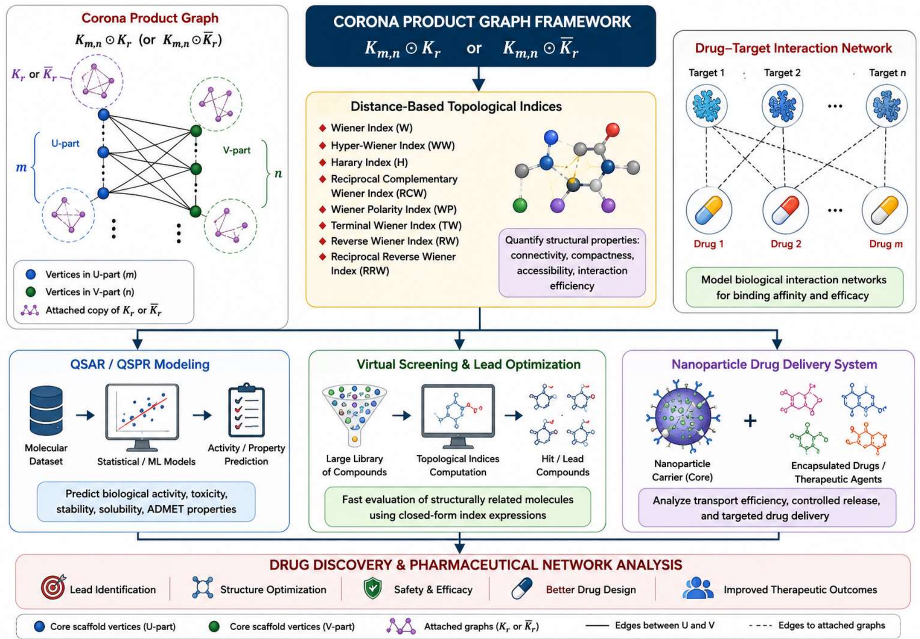

Figure 3. 1 *Corona Product Graph-Based Framework for Drug Discovery, QSAR Modeling, Drug–Target Interaction Analysis, and Nanoparticle Drug Delivery Systems*

4. CONCLUSION

Explicit closed-form expressions for a number of distance-based topological indices of the corona product graphs $K_{m,n} \odot K_r$ and $K_{m,n} \odot \overline{K}_r$ are presented in this study. These include the Wiener, Hyper-Wiener, Harary, Reciprocal Complementary Wiener, Wiener Polarity, Terminal Wiener, Reverse Wiener, and Reciprocal Reverse Wiener indices. The resulting formulas enhance the theoretical framework of Chemical Graph Theory and graph product research by offering effective analytical tools for assessing huge graph families without the need for repeated distance computations. These indices have important uses in pharmacological and biochemical network analysis because they capture key structural features like connectedness, compactness, accessibility, and interaction efficiency. Specifically, the corona product graphs under consideration can be used to describe biological interaction systems and molecular scaffolds, with attached graph copies representing functional groups, drug fragments, or biomolecular components. As a result, QSAR/QSPR research, molecular screening, lead optimization, drug–target interaction prediction, and nanoparticle-based drug delivery design can all benefit from the descriptors that were collected. Graph-theoretical modeling and contemporary drug development are closely associated because the availability of precise mathematical expressions lowers computational complexity and speeds up the evaluation of structurally related substances. These studies could be expanded in the future to include weighted, fuzzy, and dynamic graph models, as well as their integration with AI methods for cutting-edge medicinal and pharmaceutical applications.

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