Topological Indices and New Graph Structures

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Abstract
A topological representation of a molecule can be carried out through molecular graph. The descriptors are numerical values associated with chemical constitution for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. A topological index is the graph invariant number calculated from a graph representing a molecule. The most of the proposed topological indices are related either to a vertex adjacency relationship (atom-atom connectivity) in the graph G or to topological distances in G. In this paper we introduce an edge operation \( \hat{e} \) on the graphs \( G_1 \) and \( G_2 \) such that resulting graph \( G_1 \hat{e} G_2 \) has an edge introduced between arbitrary vertex of \( G_1 \) and an arbitrary vertex of \( G_2 \). We investigate few topological indices like Wiener index, Zagreb index, Zagreb coindex, Platt number, geometric – arithmetic index and reverse Wiener index for the graphs \( C_m \hat{e} C_n \) and \( (P_2 \times C_n) \hat{e} (P_2 \times C_n) \).

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1. Introduction

A representation of an object giving information only about the number of elements composing it and their connectivity is named as topological representation of an object. A topological representation of a molecule is called molecular graph. A molecular graph is a collection of points representing the atoms in the molecule and set of lines representing the covalent bonds. These points are named vertices and the lines are named edges in graph theory language. The advantage of topological indices is in that they may be used directly as simple numerical descriptors in a comparison with physical, chemical or biological parameters of molecules in Quantitative Structure Property Relationships (QSPR) and in Quantitative Structure Activity Relationships (QSAR). One of the most widely known topological descriptor is the Wiener index \([4]\) named after chemist Harold Wiener. Wiener index correlates well with many physico-chemical properties of organic compounds and as such has been well studied over the last quarter of a century.

Zagreb group indices \([4]\) \(M_1(G)\) and \(M_2(G)\) appeared in the topological formula for the \(\pi\)-electron energy of conjugated systems. Recently introduced Zagreb coindices \([1]\) are dependent on the degrees of non-adjacent vertices and thereby quantifying a possible influence of remote pairs of vertices to the molecule’s properties. For many physico chemical properties the predictive power of GA index \([6]\) is better than other connectivity indices. Platt number \([4]\) was used to predict the physical parameters of Alkanes. Reverse Wiener index \([7]\) is used to produce QSPR models for the alkane molar heat capacity.

2. Definitions

**Definition 2.1**: The Weiner index \([4]\) \(W(G)\) of a graph \(G\) is defined as the sum of half of the distances between every pair of vertices of \(G\).

\[
W(G) = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} d(v_i, v_j),
\]

where \(d(v_i, v_j)\) is the number of edges in a shortest path connecting the vertices \(v_i, v_j\). We have an equivalent definition of Wiener index

\[
W(G) = \frac{1}{2} \sum_{i < j} d(v_i, v_j).
\]
Wiener index of the 3-regular graph $P_2 \times C_N$, 

$$W(P_2 \times C_N) = \begin{cases} 
\frac{N(N^2 + 2N - 1)}{2}, & N \text{ is odd} \\
\frac{N^2(N + 2)}{2}, & N \text{ is even} 
\end{cases}$$

Wiener index of the cycle graph $C_N$, 

$$W(C_N) = \begin{cases} 
\frac{N(N^2 - 1)}{8}, & N \text{ is odd} \\
\frac{N^3}{8}, & N \text{ is even} 
\end{cases}$$

**Definition 2.2**: The Platt number $F(G)$ of a graph $G$ is defined as the total sum of degrees of edges in a graph, $F(G) = \sum_{i=1}^{M} D(e_i)$ where $D(e_i)$ denotes degree of the edge $e_i$, i.e., number of edges adjacent to $e_i$ and $M$ denotes the number of edges.

**Definition 2.3**: The Zagreb group indexes $M_1(G)$ (first Zagreb index) and $M_2(G)$ (second Zagreb index) are defined as

$$M_1(G) = \sum_{i} D_i^2, \quad M_2(G) = \sum_{(i,j)} D_i D_j$$

where $D_i$ stands for the degree of a vertex $i$. The sum in $M_1(G)$ is over all vertices of $G$, while the sum in $M_2(G)$ is over all edges of $G$.

**Definition 2.4**: The Zagreb group coindices $M_1(G)$ (first Zagreb co index) and $M_2(G)$ (second Zagreb coindex) are defined as

$$\overline{M_1}(G) = \sum_{(i,j)} \left( D_i + D_j \right), \quad \overline{M_2}(G) = \sum_{(i,j)} (D_i D_j)$$

where $D_i$ stands for the degree of the vertex $v_i$.

**Definition 2.5**: The geometric-arithmetic index $GA(G)$ of a graph $G$ is defined as
\[ GA(G) = \sum_{u \in V(G)} \sqrt{\frac{D_u D_v}{D_u + D_v}} \] where \( E(G) \) is the set of edges of the graph \( G \) and \( D_u \) denotes the degree of the vertex \( u \).

**Definition 2.6:** The reverse Wiener index [7] of a graph \( G \) denoted by \( \Lambda(G) \) is defined as \( \Lambda(G) = \sum_{i \neq j} r_{ij} \) where \( r_{ij} \) is defined as \( r_{ij} = \begin{cases} d - d_{ij} & \text{if } i \neq j \\ 0 & \text{otherwise} \end{cases} \), \( d \) is the diameter of the graph \( G \) and \( d_{ij} \) is the distance (i.e., the number of edges of a shortest path) between the vertices \( v_i \) and \( v_j \). The relation between Wiener index \( W(G) \) and reverse Wiener index \( \Lambda(G) \) is \( \Lambda(G) = \frac{1}{2} N (N - 1) d - W(G) \) where \( N \) denotes the number of vertices of the graph \( G \).

In this paper we introduce a new edge operation and construct new graph structures and investigate all the topological indices define above.

### 3. Motivation and Main Results

The main paradigm of medicinal chemistry is that biological activity, as well as physical, physicochemical and chemical properties of chemical compound depends on their molecular structure. Based on this paradigm Crum Brown and Fraser published the first quantitative structure activity relationship in 1868. This paradigm is guiding the discovery of new lead compounds. A lead compound is any chemical compound that shows the biological activity we are interested in. The role of topological indexes in drug discovery is analyzed and updated taking into account the most recent advances in lead discovery strategies. Consider the following sample reactions [5] as given in Fig.1, Fig.2 due to Rudolph Fittig and Fritz Ullmann. Here two haloarenes combine to form diphenyl. In graph terminology it is an edge introduced between arbitrary vertices of two graphs.

**Fittig reaction:** In this reaction two haloarenes combine with sodium metal in the presence of anhydrous ether. The resulting product is diphenyl.
Fittig reaction: is the synthesis of diphenyl from iodobenzene by heating aryl halides (ArX, where X = CI, Br, I) at 100°-360°C with powdered copper.

Above chemical reactions motivated us to introduce an edge operation $\hat{e}$ that is used to connect two graphs.

**Definition 3.1:** $G_1\hat{e}G_2$ is a connected graph obtained from $G_1$ and $G_2$ by introducing an edge between an arbitrary vertex of $G_1$ and an arbitrary vertex of $G_2$.

If $G_1(p_1, q_1)$ has $p_1$ vertices and $q_1$ edges and $G_2(p_2, q_2)$ has $p_2$ vertices and $q_2$ edges then $G_1\hat{e}G_2$ will have $(p_1 + p_2)$ vertices and $(q_1 + q_2 + 1)$ edges. If $G_1 = C_n$, $G_2 = C_n$ and $G_1 = P_2 \times C_n$, $G_2 = P_2 \times C_n$ interesting graph structures $G = C_n \hat{e}C_n$ and $G = (P_2 \times C_n)\hat{e}(P_2 \times C_n)$ are obtained respectively using our operation defined above and we prove the following results.

**Theorem 3.1:** The Wiener number of the graph $G = C_n \hat{e}C_n$,
\[ W(G) = \begin{cases} \frac{m(m^2 - 1)}{8} + \frac{n^3}{8} + \frac{n}{4} \left[ m(m + n + 4) - 1 \right], & \text{if } m \text{ is odd and } n \text{ is even} \\
\frac{m^3}{8} + \frac{n(n^2 - 1)}{8} + \frac{m}{4} \left[ n(m + n + 4) - 1 \right], & \text{if } m \text{ is even and } n \text{ is odd} \\
\frac{m^3}{8} + \frac{n^3}{8} + \frac{nm}{4} (m + n + 4), & \text{if } m \text{ is even and } n \text{ is even} \\
\frac{m(m^2 - 1)}{8} + \frac{n(n^2 - 1)}{8} + \frac{1}{4} \left[ nm(m + n + 4) - (m + n) \right], & \text{if } m \text{ is odd and } n \text{ is odd} \end{cases} \]

**Proof:** Let \( \{w_1, w_2, \ldots, w_m\} \) and \( \{v_1, v_2, \ldots, v_n\} \) be the vertex sets of the graphs \( C_m \) and \( C_n \) respectively. By the operation defined above we get the resulting graph \( G = C_m \cup \overline{C}_n \).

**Case (i):** When \( m \) is odd and \( n \) is even, Wiener number of the graph \( G \),

\[
W(G) = W(C_m) + W(C_n) + \sum_{i=1}^{m} \sum_{j=1}^{n} d(w_i, v_j)
\]

\[
= \frac{m(m^2 - 1)}{8} + \frac{n^3}{8} + \sum_{i=1}^{m} \sum_{j=1}^{n} d(w_i, v_j)
\]

where \( \sum_{i=1}^{m} \sum_{j=1}^{n} d(w_i, v_j) \) is the sum of the distance between the vertices of \( C_m \) to those of \( C_n \) in \( C_m \cup \overline{C}_n \) as given in Table 1. We calculate \( \sum_{i=1}^{m} \sum_{j=1}^{n} d(w_i, v_j) \) using the following procedure.

Adding the elements of 1st column from 2nd row up to \( m \)th row:

\[
2 \left[ \left( \frac{m+1}{2} \right) + \left( \frac{m+1}{2} - 1 \right) + \cdots + 2 \right]
\]  \hspace{1cm} (1)

Adding the elements of 2nd and 3rd columns, 3rd and \((n-1)\)th columns, ... from 2nd row up to \( m \)th row:

\[
4 \left[ \left( \frac{m}{2} + 1 \right) + \left( \frac{m}{2} - 1 \right) + \cdots + (2+1) \right] + \cdots + 4 \left[ \left( \frac{m}{2} + \left( \frac{n}{2} - 1 \right) \right) + \cdots + (2 + \left( \frac{n}{2} - 1 \right)) \right]
\]  \hspace{1cm} (2)

Adding the elements of 1st row:

\[
\left[ 1 + 2 \left( 1 + 1 \right) + \cdots + \left( 1 + \frac{n}{2} - 1 \right) \right] + \left[ 1 + \frac{n}{2} \right]
\]  \hspace{1cm} (3)
\[
\sum_{i=1}^{m} \sum_{j=1}^{n} d(w_i, v_j) = (1) + (2) + (3) = \frac{n}{4} [m(n+m+4) - 1]
\]

Hence \( W(G) = \frac{m^3}{8} + \frac{n(n^2-1)}{8} + \frac{n}{4} [m(n+m+4) - 1] \).

**Case (ii):** When \( m \) is even and \( n \) is odd, Wiener number of the graph \( G \),

\[
W(G) = W(C_m) + W(C_n) + \sum_{i=1}^{m} \sum_{j=1}^{n} d(w_i, v_j)
\]

\[
= \frac{m^3}{8} + \frac{n(n^2-1)}{8} + \sum_{i=1}^{m} \sum_{j=1}^{n} d(w_i, v_j)
\]

By using the same procedure as in case (i) with the roles of \( m \) and \( n \) interchanged, we obtain:

\[
\sum_{i=1}^{m} \sum_{j=1}^{n} d(w_i, v_j) = \frac{m}{4} [n(n+m+4) - 1]
\]

Hence \( W(G) = \frac{m^3}{8} + \frac{n(n^2-1)}{8} + \frac{m}{4} [n(n+m+4) - 1] \).

**Case (iii):** When \( m \) is even and \( n \) is even, Wiener number of the graph \( G \),

\[
W(G) = W(C_m) + W(C_n) + \sum_{i=1}^{m} \sum_{j=1}^{n} d(w_i, v_j)
\]

\[
= \frac{m^3}{8} + \frac{n^3}{8} + \sum_{i=1}^{m} \sum_{j=1}^{n} d(w_i, v_j)
\]

By constructing the distance matrix \( D \) and using the similar procedure (as in case (i)) to evaluate \( \sum_{i=1}^{m} \sum_{j=1}^{n} d(w_i, v_j) \), we obtain:

\[
\sum_{i=1}^{m} \sum_{j=1}^{n} d(w_i, v_j) = 2 \left[ \sum_{k=1}^{m/2} \left( \frac{m}{2} - 1 \right) + \ldots + 2 \right] + 2 \left[ \sum_{k=1}^{m/2} \left( \frac{m}{2} - 1 \right) + \ldots + 2 \right] + \ldots + 2 \left[ \sum_{k=1}^{m/2} \left( \frac{m}{2} - 1 \right) + \ldots + 2 \right]
\]

\[
+ \ldots + 4 \left[ \sum_{k=1}^{n/2} \left( \frac{n}{2} - 1 \right) + \ldots + 2 + \left( \frac{n}{2} - 1 \right) \right] + \ldots + 4 \left[ \sum_{k=1}^{n/2} \left( \frac{n}{2} - 1 \right) + \ldots + 2 \right]
\]

\[
+ \ldots + 2 \left[ \sum_{k=1}^{n/2} \left( \frac{n}{2} - 1 \right) + \ldots + 2 \right] + \ldots + 2 \left[ \sum_{k=1}^{n/2} \left( \frac{n}{2} - 1 \right) + \ldots + 2 \right]
\]

\[
+ \left[ \sum_{k=1}^{m/2} \left( \frac{m}{2} - 1 \right) + \ldots + 2 \right] + \ldots + \left[ \sum_{k=1}^{m/2} \left( \frac{m}{2} - 1 \right) + \ldots + 2 \right]
\]

\[
+ \left[ \sum_{k=1}^{n/2} \left( \frac{n}{2} - 1 \right) + \ldots + 2 \right] + \ldots + \left[ \sum_{k=1}^{n/2} \left( \frac{n}{2} - 1 \right) + \ldots + 2 \right]
\]

\[
+ \left[ \sum_{k=1}^{m/2} \left( \frac{m}{2} - 1 \right) + \ldots + 2 \right] + \ldots + \left[ \sum_{k=1}^{m/2} \left( \frac{m}{2} - 1 \right) + \ldots + 2 \right]
\]
\[
\sum_{i=1}^{m} \sum_{j=1}^{n} d(w_i, v_j) = \frac{nm}{4}(m+n+4)
\]

Hence \( W(G) = \frac{m^3}{8} + \frac{n^3}{8} + \frac{nm}{4}(m+n+4) \).

Case (iv): When \( m \) is odd and \( n \) is odd, Wiener number of the graph \( G \),

\[
W(G) = W(C_m) + W(C_n) + \sum_{i=1}^{m} \sum_{j=1}^{n} d(w_i, v_j)
\]

\[
= \frac{m(m^2-1)}{8} + \frac{n(n^2-1)}{8} + \sum_{i=1}^{m} \sum_{j=1}^{n} d(w_i, v_j)
\]

\[
\sum_{i=1}^{m} \sum_{j=1}^{n} d(w_i, v_j) = 2 \left[ \left( \frac{m+1}{2} \right) + \left( \frac{m+1}{2} \right) + \ldots + 2 \right] + 4 \left[ \left( \frac{m+1}{2} \right) + \left( \frac{m+1}{2} \right) + \left( \frac{m+1}{2} \right) + \ldots + (2+1) \right]
\]

\[
+ \ldots + 4 \left[ \left( \frac{m}{2} \right) + \left( \frac{n}{2} - 1 \right) + \ldots + \left( 2 + \left( \frac{n}{2} - 1 \right) \right) \right]
\]

\[
\sum_{i=1}^{m} \sum_{j=1}^{n} d(w_i, v_j) = \frac{1}{4} \left[ nm(m+n+4) - (n+m) \right]
\]

Hence \( W(G) = \frac{m(m^2-1)}{8} + \frac{n(n^2-1)}{8} + \frac{1}{4} \left[ nm(m+n+4) - (n+m) \right] \).
Topological indices and new graph structures

\[
\begin{pmatrix}
\text{v}_1 & \text{v}_2 & \cdots & \text{v}_{\left(\frac{n-1}{2}\right)} & \text{v}_{\left(\frac{n+3}{2}\right)} & \cdots & \text{v}_{\left(\frac{n}{2}\right)} & \text{v}_n
\end{pmatrix}
\begin{pmatrix}
1 & (1+1) & \cdots & \left(1+\left\lfloor \frac{n-1}{2} \right\rfloor\right) & \left(1+\left\lfloor \frac{n}{2} \right\rfloor\right) & \cdots & (1+2) & (1+1)
\end{pmatrix}
\]

<table>
<thead>
<tr>
<th>w_i</th>
<th>w_j</th>
<th>w_k</th>
<th>\cdots</th>
<th>w_m</th>
</tr>
</thead>
</table>
| 2 (2+1) & \cdots & \left(2+\left\lfloor \frac{n-1}{2} \right\rfloor\right) & \left(2+\left\lfloor \frac{n}{2} \right\rfloor\right) & \cdots & (2+2) & (2+1)
| \cdots | \cdots | \cdots | \cdots | \cdots | \cdots |
| \left(\frac{m+1-1}{2}\right) & \left(\frac{m+1-1}{2}\right) & \cdots & \left(\frac{m+1-1}{2}\right) & \left(\frac{m+1-1}{2}\right) & \cdots & \left(\frac{m+1-1}{2}\right) & \left(\frac{m+1-1}{2}\right)
| \left(\frac{m+1+1}{2}\right) & \left(\frac{m+1+1}{2}\right) & \cdots & \left(\frac{m+1+1}{2}\right) & \left(\frac{m+1+1}{2}\right) & \cdots & \left(\frac{m+1+1}{2}\right) & \left(\frac{m+1+1}{2}\right)
| \cdots | \cdots | \cdots | \cdots | \cdots | \cdots |
| 2 (2+1) & \cdots & \left(2+\left\lfloor \frac{n-1}{2} \right\rfloor\right) & \left(2+\left\lfloor \frac{n}{2} \right\rfloor\right) & \cdots & (2+2) & (2+1)

Table 1. Distance matrix - distance between the vertices \( w_i \) in \( C_n \) and \( v_j \) in \( C_n \) in the graph \( C_n \hat{e} C_n \)

**Theorem 3.2:** The Platt number of the graph \( G = C_m \hat{e} C_n \),
\[ F(G) = 2(m + n + 4) \]

**Proof:** The graph \( G \) has \((m+n+1)\) edges of which \((m+n-4)\) edges have degree 2, four edges have degree 3, and one edge has degree 4 and hence \( F(G) = 2(m + n + 4) \)

**Theorem 3.3:** First and second Zagreb indices of the graph \( G = C_m \hat{e} C_n \) are respectively, \( M_1(G) = 4(m + n) + 10 \) and \( M_2(G) = 4(m + n) + 17 \)

**Proof:** The graph \( G \) has \((m+n-2)\) vertices of degree 2 and two vertices of degree 3 and hence \( M_1(G) = 4(m + n) + 10 \). \( G \) has \((m+n-4)\) edges whose end vertices \( u \) and \( v \) have degrees 2 and 2 respectively, four edges have end vertices 2 and 3
respectively, one edge with end vertices 3 and 3 respectively, hence \( M_2(G) = 4(m+n) + 17 \).

**Theorem 3.4:** First and second Zagreb co-indices of \( C_m \hat{e} C_n \), are respectively, 
\[
\overline{M}_1(G) = 2(m+n)^2 - 4(m+n) - 12 \quad \text{and} \quad 
\overline{M}_2(G) = 2(m+n)(m+n-1) - 20
\]

**Proof:** Using \( \overline{M}_1(G) = 2m(n-1) - M_1(G), \quad \overline{M}_2(G) = 2m^2 - M_2(G) - \frac{1}{2}M_1(G) \) and Theorem 3.3, we get the results.

**Theorem 3.5:** The Geometric-Arithmetic index of \( G = C_m \hat{e} C_n \),
\[
\text{GA}(G) = (m+n) + \frac{8\sqrt{6}}{5} - 3
\]

**Proof:** By the similar reasoning of proof of Theorem 3.3 and by the definition of geometric-arithmetic index we get the result.

**Theorem 3.6:** The reverse Wiener index of the graph \( G = C_m \hat{e} C_n \),
\[
\Lambda(G) = \begin{cases} 
\frac{1}{4}(m+n)(m+n-1)(m+n+1) - W(G), & m \text{ is odd} \& n \text{ is even} \\
\frac{1}{4}(m+n)(m+n-1)(m+n+1) - W(G), & m \text{ is even} \& n \text{ is odd} \\
\frac{1}{4}(m+n)(m+n-1)(m+n+2) - W(G), & m \text{ is even} \& n \text{ is even} \\
\frac{1}{4}(m+n)(2m+2n-1)(m+n) - W(G), & m \text{ is odd} \& n \text{ is odd}
\end{cases}
\]

where \( W(G) = \begin{cases} 
m\left(\frac{m^2-1}{8}\right) + n\left(\frac{n^2-1}{8}\right) + \frac{1}{4}\left[m(m+n+4)-(m+n)\right], & m \text{ is odd} \& n \text{ is even} \\
m^3 + \frac{n}{8} + \frac{m}{4}\left[n(m+n+4)-(m+n)\right], & m \text{ is even} \& n \text{ is odd} \\
m\left(\frac{m^2-1}{8}\right) + n\left(\frac{n^2-1}{8}\right) + \frac{1}{4}\left[mn(m+n+4)-(m+n)\right], & m \text{ is odd} \& n \text{ is odd}
\end{cases} \)
Proof: Using the result \( \Lambda(G) = \sum_{i<j} n_i = \frac{1}{2} N(N-1)d - W(G) \) with the number of vertices

\[
N = m + n \quad \text{and the diameter} \quad d = \begin{cases} 
\left(\frac{m+1}{2} + \frac{n}{2}\right), & \text{if } m \text{ is odd and } n \text{ is even} \\
\left(\frac{m}{2} + \frac{n+1}{2}\right), & \text{if } m \text{ is even and } n \text{ is odd} \\
\left(\frac{m+1}{2} + \frac{n}{2}\right), & \text{if } m \text{ is even and } n \text{ is even} \\
\left(\frac{m}{2} + \frac{n-1}{2}\right), & \text{if } m \text{ is odd and } n \text{ is odd}
\end{cases}
\]

we get \( \Lambda(G) \).

Theorem 3.7: The Wiener number of the graph \( G = (P_2 \times C_m) \hat{\times} (P_2 \times C_n) \),

\[
W(G) = \begin{cases} 
\frac{m(m^2 + 2m - 1)}{2} + \frac{n(n^2 + 2n - 1)}{2} + mn(m+n) + 8mn - n, & \text{if } m \text{ is odd and } n \text{ is even} \\
\frac{m(m^2 + 2m - 1)}{2} + \frac{n(n^2 + 2n - 1)}{2} + mn(m+n) + 8mn - (m+n), & \text{if } m \text{ is odd and } n \text{ is odd} \\
\frac{m^2(m+2)}{2} + \frac{n^2(n+2)}{2} + mn(m+n) + 8mn - m, & \text{if } m \text{ is even and } n \text{ is odd} \\
\frac{m^2(m+2)}{2} + \frac{n^2(n+2)}{2} + mn(m+n) + 8mn, & \text{if } m \text{ is even and } n \text{ is even}
\end{cases}
\]

Proof: Let \( \{w_1, w_2, w_3, \ldots, w_m\} \) & \( \{v_1, v_2, v_3, \ldots, v_n\} \) be the vertex sets of the graphs \( P_2 \times C_m \) (3-regular) and \( P_2 \times C_n \) (3-regular) respectively. By using the operation defined above we get a resulting graph \( G = (P_2 \times C_m) \hat{\times} (P_2 \times C_n) \).

Case (i): When \( m \) is odd and \( n \) is even, Wiener number of the graph \( G \),

\[
W(G) = W(P_2 \times C_m) + W(P_2 \times C_n) + \sum_{i=1}^{2m} \sum_{j=1}^{2n} d(w_i, v_j)
\]

\[
W(G) = \frac{m(m^2 + 2m - 1)}{2} + \frac{n^2(n+2)}{2} + \sum_{i=1}^{2m} \sum_{j=1}^{2n} d(w_i, v_j)
\]
where $\sum_{i=1}^{2m} \sum_{j=1}^{2n} d(w_i, v_j)$ is the sum of the distance between the vertices of $P_2 \times C_m$ to those of $P_2 \times C_n$ in $(P_2 \times C_m) \times (P_2 \times C_n)$ as given in Table 2. We calculate $\sum_{i=1}^{2m} \sum_{j=1}^{2n} d(w_i, v_j)$ using the following procedure.

Adding the elements of $n^{th}$ column from $1^{st}$ row up to $(m-1)^{th}$ row:

$$2 \left[ \frac{m+1}{2} + \frac{m+1}{2} - 1 + \ldots + 2 \right]$$  \hspace{1cm} (1)

Adding the elements of $1^{st}$ and $(n-1)^{th}$ columns, $2^{nd}$ and $(n-2)^{th}$ columns, … from $1^{st}$ row up to $(m-1)^{th}$ row:

$$4 \left[ \frac{m+1}{2} + 1 + \frac{m+1}{2} + 1 + \ldots + (2+1) + \ldots + 4 \left[ \frac{m+1}{2} + \frac{n-1}{2} \right] + \ldots + \left( 2 + \frac{n-1}{2} \right) \right]$$ \hspace{1cm} (2)

Adding the elements of $\left( \frac{n}{2} \right)^{th}$ column from $1^{st}$ row up to $(m-1)^{th}$ row:

$$2 \left[ \frac{m+1}{2} + \frac{n}{2} + \ldots + 2 \left( \frac{n}{2} \right) \right]$$ \hspace{1cm} (3)

Adding the elements of $(2n)^{th}$ column from $1^{st}$ row up to $(m-1)^{th}$ row and that of $n^{th}$ column from $(m+1)^{th}$ row up to $(2m-1)^{th}$ row:

$$2 \times 2 \left[ \frac{m+1}{2} + \frac{m+1}{2} + \ldots + 3 \right]$$ \hspace{1cm} (4)

Adding the elements of $(n+1)^{th}$ and $(2n-1)^{th}$ columns, $(n+2)^{th}$ and $(2n-2)^{th}$ columns, … from $1^{st}$ row up to $(m-1)^{th}$ row & that of $1^{st}$ and $(n-1)^{th}$ columns, $2^{nd}$ and $(n-2)^{th}$ columns, … from $(m+1)^{th}$ row up to $(2m-1)^{th}$ row:

$$8 \left[ \frac{m+1}{2} + 1 + 3 + 1 + \ldots + 8 \left[ \frac{m+1}{2} + \frac{n-1}{2} \right] + \ldots + 3 + \left( \frac{n-1}{2} \right) \right]$$ \hspace{1cm} (5)

Adding the elements of $\left( \frac{n}{2} + \frac{n}{2} \right)^{th}$ column from $1^{st}$ row to $(m-1)^{th}$ row & that of $\left( \frac{n}{2} \right)^{th}$ column from $(m+1)^{th}$ row up to $(2m-1)^{th}$ row:

$$2 \times 2 \left[ \frac{m+1}{2} + \frac{n}{2} + \ldots + 3 \left( \frac{n}{2} \right) \right]$$ \hspace{1cm} (6)

Adding the elements of $(2n)^{th}$ column from $(m+1)^{th}$ row up to $(2m-1)^{th}$ row:
Adding the elements of 

\( \left( n+1 \right)^{th} \) and \( \left( 2n-1 \right)^{th} \) columns, \( \left( n+2 \right)^{th} \) and \( \left( 2n-2 \right)^{th} \) columns, \ldots \) from \( \left( m+1 \right)^{th} \) row up to \( \left( 2m-1 \right)^{th} \) row:

\[
4 \left[ \left( \frac{m+1}{2} + 2 \right) + \left( \frac{n}{2} + 1 \right) + \ldots + 4 \right]
\]

Adding the elements of \( \left( n+\frac{n}{2} \right)^{th} \) column from \( \left( m+1 \right)^{th} \) row up to \( \left( 2m-1 \right)^{th} \) row:

\[
2 \left[ \left( \frac{m+1}{2} + 2 \right) + \left( n \right) + \ldots + 4 \left( \frac{n}{2} \right) \right]
\]

Adding the elements of \( m^{th} \) row from \( 1^{st} \) column up to \( n^{th} \) column:

\[
2 \left( 2 + \left( \frac{m+1}{2} + 2 \right) + \left( \frac{n}{2} + 1 \right) \right) + 2 \left( \frac{n}{2} - 1 \right) + (2-1)
\]

Adding the elements of \( m^{th} \) row from \( \left( n+1 \right)^{th} \) column up to \( \left( 2n \right)^{th} \) column & that of \( \left( 2m \right)^{th} \) row from \( 1^{st} \) column up to \( n^{th} \) column:

\[
2 \times 2 \left[ 3 + \left( 3 + 1 \right) + \ldots + \left( \frac{n}{2} - 2 \right) \right] + 2 \left[ 3 + \left( \frac{n}{2} - 1 \right) \right] + 2(3-1)
\]

Adding the elements of \( \left( 2m \right)^{th} \) row from \( \left( n+1 \right)^{th} \) column up to \( \left( 2n \right)^{th} \) column:

\[
2 \left[ 4 + \left( 4 + 1 \right) + \ldots + \left( 4 + \frac{n}{2} - 2 \right) \right] + \left[ 4 + \frac{n}{2} - 1 \right] + (4-1)
\]

\[
\sum_{i=1}^{2m} \sum_{j=1}^{2n} d(w_i, v_j) = (1)+(2)+(3)+(4)+(5)+(6)+(7)+(8)+(9)+(10)+(11)+(12)
\]

\[
= mn(m+n) + 8mn - n
\]

Hence \( W(G) = \frac{m(m^2+2m-1)}{2} + \frac{n(n^2+n+2)}{2} + mn(m+n) + 8mn - n. \)

**Case (ii):** When \( m \) is odd and \( n \) is odd, Wiener number of the graph \( G \),

\[
W(G) = W(P_2 \times C_m) + W(P_2 \times C_n) + \sum_{i=1}^{2m} \sum_{j=1}^{2n} d(w_i, v_j)
\]

\[
= \frac{m(m^2+2m-1)}{2} + \frac{n(n^2+2n-1)}{2} + \sum_{i=1}^{2m} \sum_{j=1}^{2n} d(w_i, v_j)
\]
By constructing the distance matrix $D$ and using the similar procedure (as in case (i)) to evaluate $\sum_{i=1}^{2m} \sum_{j=1}^{2n} d(w_i, v_j)$, we obtain:

$$\sum_{i=1}^{2m} \sum_{j=1}^{2n} d(w_i, v_j) = 2\left[\left(\frac{m+1}{2}\right)+\left(\frac{m+1}{2}\right)+...+2\right] + 4\left[\left(\frac{m+1}{2}\right)+\left(\frac{m+1}{2}\right)+...+(2+1)\right]
+...+4\left[\left(\frac{m+1}{2}\right)+\left(\frac{n-1}{2}\right)+...\right] + 8\left[\left(\frac{m+1}{2}\right)+1\right]+\left(\frac{m+1}{2}\right)+...+(3+1)\right]
+...+8\left[\left(\frac{m+1}{2}\right)+\left(\frac{n-1}{2}\right)+...+\right]
+2\left[2+(2+1)+...+\left(2\left(\frac{n-1}{2}\right)\right)\right]+(2+1)+4\left[3+(3+1)+...+\left(3\left(\frac{n-1}{2}\right)\right)\right]
+2\left[4+(4+1)+...+\left(4\left(\frac{n-1}{2}\right)\right)\right]+(4-1) = mn(m+n)+8mn-(m+n)
$$

Hence $W(G) = \frac{m(m^2+2m-1)}{2} + \frac{n(n^2+2n-1)}{2} + mn(m+n)+8mn-(m+n)$.

Case (iii): When $m$ is even and $n$ is odd, Wiener number of the graph $G$,

$$W(G) = W(P_2 \times C_m) + W(P_2 \times C_n) + \sum_{i=1}^{2m} \sum_{j=1}^{2n} d(w_i, v_j)
= \frac{m^2(m+2)}{2} + \frac{n(n^2+2n-1)}{2} + \sum_{i=1}^{2m} \sum_{j=1}^{2n} d(w_i, v_j)
$$

By using the similar procedure as in case (i) with the roles of $m$ and $n$ interchanged, we obtain:

$$\sum_{i=1}^{2m} \sum_{j=1}^{2n} d(w_i, v_j) = mn(m+n)+8mn-m
$$

Hence $W(G) = \frac{m^2(m+2)}{2} + \frac{n(n^2+2n-1)}{2} + mn(m+n)+8mn-m$. 

Case (iv): When $m$ is even and $n$ is even, Weiner number of the graph

\[ G, W(G) = W(P_2 \times C_m) + W(P_2 \times C_n) + \sum_{i=1}^{2m} \sum_{j=1}^{2n} d(w_i, v_j) \]

\[ = \frac{m^2(m+2)}{2} + \frac{n^2(n+2)}{2} + \sum_{i=1}^{2m} \sum_{j=1}^{2n} d(w_i, v_j) \]

\[ \sum_{i=1}^{2m} \sum_{j=1}^{2n} d(w_i, v_j) \]

\[ = \left[ \left(\frac{m}{2}+1\right) + 2 \left(\left(\frac{m}{2}+1\right) + \left(\frac{m}{2}+1\right) + \ldots + \left(\frac{m}{2}+1\right) + \left(\frac{m}{2}+1\right) + \left(\frac{n}{2}+1\right) + \left(\frac{n}{2}+1\right) + \ldots \right) \right] \]

\[ + 2 \left[ \left(\frac{m}{2}+\left(\frac{n}{2}\right)-1\right) + \ldots + \left(\frac{m}{2}+\left(\frac{n}{2}\right)\right) \right] + 4 \left[ \left(\frac{m}{2}+1\right) + \ldots + (2+1) \right] + \ldots + 4 \left[ \left(\frac{m}{2}+\left(\frac{n}{2}\right)-1\right) + \ldots + \left(\frac{n}{2}-1\right) + \ldots \right] \]

\[ + 2 \left[ \left(\frac{m}{2}+\left(\frac{n}{2}\right)+\left(2+\frac{n}{2}\right)\right) + \left(2-1\right)+2 \left(2+0\right)+\left(2+1\right) + \ldots + \left(2+\left(\frac{n}{2}-2\right)\right) + \left(2+\left(\frac{n}{2}-1\right)\right) \right] \]

\[ + 4 \left[ \left(\frac{m}{2}+1\right) + \frac{m}{2} + \ldots + \frac{3}{2} \right] + 8 \left[ \left(\frac{m}{2}+1\right) + \ldots + \left(3+1\right) \right] + \ldots + 8 \left[ \left(\frac{m}{2}+1\right) + \frac{n}{2}-1 \right] + \ldots + 8 \left[ \left(\frac{m}{2}+1\right) + \frac{n}{2}-1 \right] \]

\[ + 8 \left[ \left(\frac{m}{2}+1\right) + \frac{n}{2} + \ldots + \left(3+\frac{n}{2}\right) \right] + 2 \left(3-1\right)+4 \left(3+0\right)+\left(3+1\right) + \ldots + \left(3+\left(\frac{n}{2}-2\right)\right) + 2 \left(3+\frac{n}{2}-1\right) \]

\[ + \left[ \left(\frac{m}{2}+3\right) + 2 \left(\left(\frac{m}{2}+3\right) + \left(\frac{m}{2}+3\right) + 2 \right) + \ldots + \left(\frac{m}{2}+3\right) + \left(\frac{n}{2}+3\right) + \left(\frac{n}{2}+3\right) + \ldots \right) \right] \]

\[ + 2 \left[ \left(\frac{m}{2}+2\right) + \ldots + \left(4+\frac{n}{2}\right) \right] + 4 \left[ \left(\frac{m}{2}+2\right) + \left(\frac{m}{2}+2\right) + \ldots + (4+1) \right] + \ldots + 4 \left[ \left(\frac{m}{2}+2\right) + \left(\frac{n}{2}-1\right) + \ldots + (4+\frac{n}{2}) \right] \]

\[ + 2 \left[ \left(\frac{m}{2}+2\right) + \frac{n}{2} + \ldots + \left(4+\frac{n}{2}\right) \right] \]

\[ = mn(m+n)+8mn \]

\[ W(G) = \frac{m^2(m+2)}{2} + \frac{n^2(n+2)}{2} + mn(m+n)+8mn. \]
Table 2. Distance matrix - distance between the vertices in $w_e P C$ and in $v_j P C$ in the graph $(P_e C) \mathcal{G}(P_e C)$

**Theorem 3.8:** The Platt number of the graph $G = (P_2 C_\infty) \mathcal{G}(P_2 C_\infty)$, 
\[ F(G) = 12(m + n + 1) \]
**Proof:** The graph $G$ has $(3m+3n+1)$ edges of which $3(m+n-2)$ edges have degree 4, six edges have degree 5, and one edge has degree 6 and hence $F(G)=12(m+n+1)$.

**Theorem 3.9:** First and second Zagreb indices of the graph $G = (P_2 \times C_m) \hat{e}(P_2 \times C_n)$ are respectively, $M_1(G) = 18(m+n)+14$ and $M_2(G) = 27(m+n)+34$

**Proof:** The graph $G$ has $2(m+n-1)$ vertices of degree 3 and two vertices of degree 4 and hence $M_1(G) = 18(m+n)+14$. $G$ has $3(m+n-2)$ edges whose end vertices $u$ and $v$ have degrees 3 and 3 respectively, six edges have end vertices 3 and 4 respectively, one edge with end vertices 4 and 4 respectively, hence $M_2(G) = 27(m+n)+34$.

**Theorem 3.10:** First and second Zagreb co-indices of $(P_2 \times C_m) \hat{e}(P_2 \times C_n)$, are respectively, $\overline{M}_1(G) = 12(m+n)^2 - 20(m+n) - 16$ and $\overline{M}_2(G) = 18(m+n)^2 - 24(m+n) - 39$

**Proof:** Using $\overline{M}_1(G) = 2m(n-1) - M_1(G)$, $\overline{M}_2(G) = 2m^2 - M_2(G) - \frac{1}{2} M_1(G)$ and Theorem 3.3, we get the results.

**Theorem 3.11:** The Geometric-Arithmetic index of $G = (P_2 \times C_m) \hat{e}(P_2 \times C_n)$,

$GA(G) = 3(m+n) + \frac{24\sqrt{3}}{7} - 5$

**Proof:** By the similar reasoning of proof of Theorem 3.3 we get the result.

**Theorem 3.12:** The reverse Wiener index of the graph $G = (P_2 \times C_m) \hat{e}(P_2 \times C_n)$,

$$\Lambda(G) = \begin{cases} 
\frac{1}{2}(m+n)(2m+2n-1)(m+n+5) - W(G), & m \text{ is odd} \& n \text{ is even} \\
\frac{1}{2}(m+n)(2m+2n-1)(m+n+4) - W(G), & m \text{ is odd} \& n \text{ is odd} \\
\frac{1}{2}(m+n)(2m+2n-1)(m+n+5) - W(G), & m \text{ is even} \& n \text{ is odd} \\
\frac{1}{2}(m+n)(2m+2n-1)(m+n+4) - W(G), & m \text{ is even} \& n \text{ is even}
\end{cases}$$
where
\[
W(G) = \begin{cases} 
\frac{m(m^2 + 2m - 1)}{2} + \frac{n(2n + 2)}{2} + mn(m + n) + 8mn - n, & \text{m is odd and n is even} \\
\frac{m(m^2 + 2m - 1)}{2} + \frac{n(2n + 2)}{2} + mn(m + n) + 8mn - (m + n), & \text{m is odd and n is odd} \\
\frac{m^2(m + 2)}{2} + \frac{n(n^2 + 2n - 1)}{2} + mn(m + n) + 8mn - m, & \text{m is even and n is odd} \\
\frac{m^2(m + 2)}{2} + \frac{n(n^2 + 2n - 1)}{2} + mn(m + n) + 8mn, & \text{m is even and n is even}
\end{cases}
\]

**Proof:** Using the result \( \Lambda(G) = \sum_{i,j} r_{ij} = \frac{1}{2}N(N-1)d - W(G) \) with the number of vertices \( N = 2m + 2n \) and the diameter \( d = \begin{cases} 
\left(\frac{m+1}{2} + \frac{n}{2}\right), & \text{m is odd & n is even} \\
\left(\frac{m+1}{2} + \frac{n-1}{2}\right), & \text{m is odd & n is odd} \\
\left(\frac{m}{2} + \frac{n+1}{2} + 2\right), & \text{m is even & n is odd} \\
\left(\frac{m}{2} + 2 + \frac{n}{2}\right), & \text{m is even & n is even}
\end{cases} \)

we get \( \Lambda(G) \).

### 4. Conclusion

An effort is made to calculate some of the topological indices of the graphs \( C_w \ast C_n \) and \( (P_2 \times C_n) \ast (P_2 \times C_n) \). The graphs obtained in this manner may or may not represent a stable chemical compound in reality, but it is the interest of the chemist to check the so obtained structure of the resulting graph.

### References


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