Wiener Polarity Index of Tensor Product of Graphs

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Abstract

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. In theoretical chemistry, distance-based molecular structure descriptors are used for modeling physical, pharmacologic, biological and other properties of chemical compounds. The Wiener Polarity index of a graph $G$, denoted by $W_P(G)$, is the number of unordered pairs of vertices of distance 3. The Wiener polarity index is used to demonstrate quantitative structure-property relationships in a series of acyclic and cycle-containing hydrocarbons. Let $G$ and $H$ be two simple connected graphs, then the tensor product of them is denoted by $G \otimes H$ whose vertex set is $V(G \otimes H) = V(G) \times V(H)$ and edge set is $E(G \otimes H) = \{(a, b) (c, d) | ac \in E(G), bd \in E(H)\}$. In this paper, we aim to compute the Wiener polarity index of $G \otimes H$ which was computed wrongly in [J. Ma, Y. Shi and J. Yue, The Wiener polarity index of graph products, Ars Combin. 116 (2014) 235-244].

Keywords: Topological index, Wiener polarity index, tensor product, graph, distance.

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1. Introduction

In this section, we first describe some notations which will be kept throughout. A graph is a structure composed of points (vertices or nodes), connected by lines (edges or links).

A graph is called finite if both its vertex set and edge set are finite. If $e = uv$ is an edge of a graph, then we say that $e$ joins the pair vertices $u$ and $v$. Also

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the vertices $u$ and $v$ are named the end vertices of the edge $e$. An edge with identical end vertices is called a loop. We say that a graph is simple whenever it has no loop and no two of its edges join the same pair of vertices. The set of finite simple graphs is shown by $\Gamma$ and the set of finite graphs in which loops are admitted is denoted as $\Gamma_0$, so $\Gamma \subseteq \Gamma_0$ [13]. From now on, when we say that “$G$ is a graph” it means $G \in \Gamma$, otherwise $G \in \Gamma_0$. For a given graph $G$, we show the vertex and edge set of $G$ by $V(G)$ and $E(G)$, respectively. If $x$ is a vertex of the graph $G$, the degree of $x$ in $G$ is denoted by $\deg_G(x)$. In the other words, if for any vertex $x \in G$, $N_G(x)$ denotes the set of neighbors that $x \in G$, i.e. $N_G(x) = \{y \in V(G) | xy \in E(G)\}$, then $\deg_G(x) = |N_G(x)|$. The minimum and maximum degree of all vertices $x$ of a graph $G$ are denoted by $\delta(G)$ and $\Delta(G)$, respectively. A walk in $G$ is a sequence of (not necessarily distinct) vertices $v_1v_2 ... v_n$, such that $v_iv_{i+1} \in E(G)$ for $i = 1, 2, \ldots, n - 1$. We call such a walk a $(v_1, v_n)$-walk. A path in the graph is a walk without traversing any vertex twice. So, a path in the graph is a sequence of adjacent edges without traversing any vertex twice. The graph is called connected when there is a path between any pair of vertices in it, otherwise the graph is disconnected. For the vertices $u, v \in V(G)$, the distance between $u$ and $v$ in $G$ is denoted by $d_G(u, v)$ and it is the length of a shortest $(u, v)$-path in $G$. If $G$ is a disconnected graph, then we assume that the distance between any two vertices belonging to different components of $G$, is infinity. For a given vertex $x \in V(G)$, its eccentricity $ecc(x)$ is the largest distance between $x$ and any other vertex $y \in V(G)$, that is $ecc(x) = Max\{d_G(x, y) | y \in V(G)\}$. The maximum eccentricity over all vertices of $G$ is called the diameter of $G$ and denoted by $D(G)$. Also, the minimum eccentricity among the vertices of $G$ is called the radius of $G$ and denoted by $R(G)$. Let $G$ and $H$ be two graphs such that $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. Then we say that $H$ is a subgraph of $G$ and write $H \subseteq G$. Let us denote a cycle and a path on $n$ vertices by $C_n$ and $P_n$, respectively. For a graph $H$, a graph $G$ is called $H$-free if it has no subgraph isomorphic to $H$. So, a graph is called triangle free if it has no subgraph isomorphic to $C_3$. The adjacency matrix of a graph $G$, denoted by $A(G)$, is a $(0, 1)$–matrix whose rows and columns are indexed by $V(G)$ and the element $A(G)_{uv} = 1$ if and only if $uv \in E(G)$ for each $u, v \in V(G)$, otherwise $A(G)_{uv} = 0$.

Mathematical Chemistry is a branch of theoretical chemistry for studying the molecular structure using mathematical methods. Molecular Graphs or Chemical Graphs are models of molecules in which atoms are represented by vertices and chemical bonds by edges of a graph. The Chemical Graph Theory is a branch of mathematical chemistry concerned with the study of chemical graphs. In theoretical chemistry correlation of chemical structure with various physical properties, chemical reactivity or biological activity are often modeled by means of molecular-graph-based structure-descriptors, which are also referred to as topological indices. A topological index is a function $TOP$ from $\Gamma$ to the set of real numbers $\mathbb{R}$ with this property that $TOP(G) = TOP(H)$, whenever $G$ and $H$ are isomorphic.
There exist several types of such indices, especially those based on vertex and edge distances. The most well-known and successful topological indices with several applications in QSAR/QSPR studies in chemistry, was introduced by H. Wiener [27] for acyclic molecules. It is defined as the sum of distances between all pairs of vertices of the molecular graph. Let $G$ be a simple connected graph. Then the Wiener index of $G$ is defined as $W(G) = \frac{1}{2} \sum_{x,y \in V(G)} d(x,y)$. Let $\gamma(G, k)$ be the number of unordered vertex pairs of $G$ for which the distance of them is equal to $k$ and therefore one can write $W(G) = \sum_{k \geq 1} k \gamma(G, k)$. In the case $k = 3$, the number $\gamma(G, 3)$ is called the Wiener polarity index of $G$ and denoted by $W_P(G)$.

It is believed that the Wiener index was the first reported distance-based topological index. This topological index was used for modeling the shape of organic molecules and for calculating several of their physico-chemical properties [11]. For example, Wiener used a linear formula to calculate the boiling points of the paraffin (alkanes). More precisely, let $A$ be an alkane with the corresponding (Hydrogen suppressed) molecular graph $G$. Then the boiling point $t_B(A)$ of $A$ is estimated as follows

$$t_B(A) = aW(G) + bW_P(G) + c,$$

where $a$, $b$ and $c$ are constants for a given isomeric group.

and Sharafdini [1] computed maximum Wiener polarity index of bicyclic graphs.

Many graphs can be constructed from simpler graphs via certain operations called graph products [13, 17]. It is believed that the most difficult one in many aspects among standard products is the tensor product of graphs. The tensor product of graphs has been extensively studied in relation to the areas such as graph colorings, graph recognition, decompositions of graphs, graph embeddings, matching theory and design theory. For any two graphs $G, H \in \Gamma_0$, their tensor product (also known as direct product, Kronecker product, categorical product, cardinal product, relational product, weak direct product conjunction, ...) is denoted by $G \otimes H$ whose vertex set and edge set are as follows:

$$V(G \otimes H) = V(G) \times V(H)$$
$$E(G \otimes H) = \{ (a, b)(c, d) \mid ac \in E(G), bd \in E(H) \}.$$

The vertices $(a, b)$ and $(c, d)$ are adjacent in $G \otimes H$, whenever $ac$ is an edge in $G$ and $bd$ is an edge in $H$. From the definition, one can get immediately that

$$|V(G \otimes H)| = |V(G)||V(H)|$$

and if $(a, b)(c, d) \in E(G \otimes H)$, then also $(a, d)(c, b) \in E(G \otimes H)$ and hence

$$|E(G \otimes H)| = 2|E(G)||E(H)|.$$

Furthermore, we can see $deg_{G \otimes H}((a, b)) = deg_G(a)deg_H(b)$.

**Note.** Since a connected graph $G$ is Eulerian if and only if it has no vertices of odd degree. Therefore, if $G \otimes H$ is a connected graph and one of the graphs $G$ or $H$ is Eulerian graph, then $G \otimes H$ is also an Eulerian graph.

We can consider the tensor product as a binary operation on the set $\Gamma_0$ [26]. It is known that, up to isomorphism, this product is commutative and associative in a natural way [24]. Also if the graph $I \in \Gamma_0$ denotes a vertex on which there is a loop, then $G \otimes I \cong G$ for any $G \in \Gamma_0$. Therefore $I$ is the identity element for tensor product as a binary operation.

**Note.** If we consider the tensor product of graphs as a binary operation on the set $\Gamma$, then this binary operation has no identity element.

By an appropriate ordering of $V(G) \times V(H)$, it follows that $A(G \otimes H) = A(G) \otimes A(H)$, where $A(G) \otimes A(H)$ is the Kronecker product of matrices $A(G)$ and $A(H)$ [25].

**Lemma 1.** ([4, 13]) Let $G$ and $H$ be two connected graphs. Then the graph $G \otimes H$ is connected if and only if any $G$ or $H$ contains an odd cycle if and only if at least $G$ or $H$ is non-bipartite. For example, Figures 1, 2 illustrate two examples of tensor products. Note that, in all Figures the vertex $(x, y)$ in the tensor product $G \otimes H$ is shown by $xy$.

As is depicted in Figure 2, $P_3 \otimes P_3$ is disconnected.
Moradi [22] computed Wiener type indices of the tensor product of graphs. In this article, we concerned about the Weiner polarity index of the tensor product of graphs. The Wiener polarity index of tensor product of graphs was wrongly computed in [21]. In order to show a counter example, we need to express the following lemma.

**Lemma 2.** For the positive integer $n \geq 3$,

$$W_P(C_n) = \begin{cases} 0, & n = 3, 4, 5; \\ 3, & n = 6; \\ n, & n \geq 7. \end{cases}$$

**Remark.** In [21] the authors (wrongly) stated in Theorem 4.1 that

$$W_P(G \square H) = 2W_P(G)W_P(H) + 2W_P(H)m(G) + 2W_P(G)m(H)$$

where $G$ and $H$ are two non-trivial connected graphs and at least one of them is non-bipartite, $m(G)$ and $m(H)$ are the number of edges of the graphs $G$ and $H$. 
respectively. Let us show that this formula is wrong as it is seen in Figure 1, for which \( P_2 \otimes C_5 \cong C_{10} \) and it follows from Lemma 3 that the left hand side of the equation in the above formula is \( W_P (P_2 \otimes C_5) = W_P (C_{10}) = 10 \), while the right hand side is zero.

In this article we aim to obtain Wiener polarity index of tensor product of graphs. Note that our technique is that of used in [22].

2. Main Results

Let \( G \) and \( H \) be two graphs. In this section, we consider the Wiener Polarity index of \( G \otimes H \). Since this topological index is defined on the connected graphs, it follows from Lemma 2 that we need to assume that at least one of the graph \( G \) or \( H \) is non-bipartite and thus in this case \( G \otimes H \) is connected.

Now, let us study some distance properties of the tensor product of graphs.

**Definition 3.** [22] Let \( G \) be a graph and \( x, y \in V(G) \). Define \( d'_G(x, y) \) as follows

1. If \( d_G(x, y) \) is an odd number, then \( d'_G(x, y) \) is defined as the length of a shortest even walk joining \( x \) and \( y \) in \( G \), and if there is no shortest even walk, then \( d'_G(x, y) = +\infty \).

2. If \( d_G(x, y) \) is an even number, then \( d'_G(x, y) \) is defined as the length of a shortest odd walk joining \( x \) and \( y \) in \( G \), and if there is no shortest odd walk, then \( d'_G(x, y) = +\infty \).

3. If \( d_G(x, y) = +\infty \), then \( d'_G(x, y) = +\infty \).

**Note.** We take \( d_G(x, y) = +\infty \), if there is no shortest odd walk and no shortest even walk between \( x \) and \( y \) in \( G \). Also, if \( d'_G(x, y) < +\infty \), then \( d'_G(x, y) \geq 2 \) and so \( d'_G(x, y) \neq 1 \).

**Definition 4.** [21, 22] Let \( G \) and \( H \) be two graphs and \( (a, b), (c, d) \in V(G \otimes H) \). The relation \( \sim \) on the vertex set \( V(G \otimes H) \) is defined as \( (a, b) \sim (c, d) \) whenever \( d_G(a, c), d_H(b, d) < +\infty \) and \( d_G(a, c) + d_H(b, d) \) is an even number, hence the parity of \( d_G(a, c) \) and \( d_H(b, d) \) are the same. Therefore \( (a, b) \sim (c, d) \) whenever \( d_G(a, c) = +\infty \) or \( d_H(b, d) = +\infty \) or \( d_G(a, c) + d_H(b, d) \) is an odd number.

**Lemma 5.** [21, 22] Let \( G \) and \( H \) be graphs and \( (a, b), (c, d) \in V(G \otimes H) \). Then

\[
d_{G \otimes H} ((a, b), (c, d)) = \begin{cases} 
  d_1 ((a, b), (c, d)) & \text{if } (a, b) \sim (c, d) \\
  d_2 ((a, b), (c, d)) & \text{if } (a, b) \not\sim (c, d)
\end{cases}
\]

where

\[
d_1 ((a, b), (c, d)) = Max \{ d_G(a, c), d_H(b, d) \}
\]

\[
d_2 ((a, b), (c, d)) = min \{ Max \{ d_G(a, c), d'_H(b, d) \}, Max \{ d'_G(a, c), d_H(b, d) \} \}
\]
Now let \((a, b), (c, d) \in V(G \otimes H)\) be arbitrary. Then one can see that the distance between them is depended on \((a, b) \sim (c, d)\) or \((a, b) \sim (c, d)\). Hence, if 
\[d_{G \otimes H}(a, b), (c, d) = 3\] 
then one may conclude that \(d_1(a, b)(c, d) = 3\) or \(d_2(a, b)(c, d) = 3\). So, we compute the distance between any two vertices in the graph \(G \otimes H\), in two cases. To proceed, let us discuss the first case as follows. 

**Proposition 6.** Suppose that 
\[
\mathcal{R}_1(G \otimes H) = \{(a, b), (c, d) \in V(G \otimes H) \mid (a, b) \sim (c, d) \& d_1((a, b), (c, d)) = 3\}.
\]
Then \(\mathcal{R}_1(G \otimes H) = 2\left|m_2W_P(G) + m_1W_P(H) + W_P(G)W_P(H)\right|\), where \(m_1 = |E(G)|\) and \(m_2 = |E(H)|\).

**Proof.** If \((a, b), (c, d) \in \mathcal{R}_1(G \otimes H)\), then can conclude that \(d_G(a, c) + d_H(b, d)\) is an even positive integer. Then only three cases occur as follows:

1. \(d_G(a, c) = 1\) and \(d_H(b, d) = 3\). In this case, the number of all unordered pairs that are satisfied in this case is equal to \(2m_1W_P(H)\).
2. \(d_G(a, c) = 3\) and \(d_H(b, d) = 1\). In this case, the number of all unordered pairs that are satisfied in this case is equal to \(2m_2W_P(G)\).
3. \(d_G(a, c) = 3\) and \(d_H(b, d) = 3\). In this case, the number of all unordered pairs that are satisfied in this case is equal to \(2W_P(G)W_P(H)\),

and our proof is complete. \(\square\)

**Note.** One can easily see that if \((a, b), (c, d)\) is satisfied in the condition of one part, then also \((a, d), (c, b)\) is satisfied.

**Definition 7.** For a graph \(G\), the following notation is useful for the main results of this paper. Suppose that

\[
\begin{align*}
\mathcal{A}(G) &= \{uv \in E(G) \mid N_G(u) \cap N_G(v) = \emptyset\} = \{uv \in E(G) \mid \forall C_3 \subseteq G; uv \notin E(C_3)\}, \\
\mathcal{B}(G) &= \{x \in V(G) \mid \exists u, v \in N_G(x) ; uv \in E(G)\} = \{x \in V(G) \mid \exists C_3 \subseteq G; x \in V(C_3)\}, \\
\mathcal{C}(G) &= \{\{u, v\} \subseteq V(G) \mid d_G(u, v) = 2 \text{ and } \exists (u, v) - \text{walk of length 3}\}, \\
\text{also } A_G &= |\mathcal{A}(G)|, \quad B_G = |\mathcal{B}(G)| \quad \text{and } C_G = |\mathcal{C}(G)|.
\end{align*}
\]

**Proposition 8.** Suppose that 
\[
\mathcal{R}_2(G \otimes H) = \{(a, b)(c, d) \subseteq V(G \otimes H) \mid (a, b) \sim (c, d) \& d_2((a, b), (c, d)) = 3\}.
\]
Then \(\mathcal{R}_2(G \otimes H) = 2\left[C_H\varphi(G) + C_G\varphi(H)\right] + B_H\varphi(G) + B_G\varphi(H)\), where \(\varphi(G) = A_G + W_P(G)\) and \(\varphi(H) = A_H + W_P(H)\).

**Proof.** Let \((a, b)(c, d) \in \mathcal{R}_2(G \otimes H)\), then we can conclude that \(d_G(a, c) + d_H(b, d)\) is an odd natural number and

\[
\begin{align*}
\min\{\max\{d_G(a, c), d'_H(b, d)\}, \max\{d'_G(a, c), d_H(b, d)\}\} = 3.
\end{align*}
\]
Theorem 9. Let $G$ and $H$ be two graphs at least one of them is non-bipartite. Then

\[
\]

where $m_G$ and $m_H$ denote the number of edges of $G$ and $H$, respectively.

**Note.** Let $G$ be a simple connected graph. For any unordered vertex pair $\{u, v\} \in \mathcal{C}(G)$, either of the following holds:

**Case (1):**\[\max \{d_G(a, c), d'_H(b, d)\} = 3.\]

(i) $d_G(a, c) = 1, d'_H(b, d) = 3$;

(ii) $d_G(a, c) = 3, d'_H(b, d) = 3$.

Let us investigate each case as follows:

(i) In this case we have $d_G(a, c) = 1$ and $d'_H(b, d) = 3$. If $d_G(a, c) = 1$, then $\max \{d_G(a, c), d'_H(b, d)\} \leq \max \{d'_G(a, c), d_H(b, d)\}$ implies that the even number $d'_G(a, c) \neq 2$ and so $d'_G(a, c) \geq 4$. Also, $d'_H(b, d) = 3$ follows that $d_H(b, d) = 0$ or 2. Therefore we have two cases as follows:

If $d'_H(b, d) = 3$ and $d_H(b, d) = 0$, imply that $b = d$ and $b \in V(C_3)$ for some $C_3 \leq H$. If $d'_H(b, d) = 3$ and $d_H(b, d) = 2$, imply that $\{b, d\} \in \mathcal{C}(H)$. It follows that the number of all unordered vertex pairs $\{(a, b), (c, d)\} \subseteq V(G \otimes H)$ satisfying (i) is equal to $A_GB_H + 2A_GC_H$.

(ii) Let $d_G(a, c) = 3$, furthermore the hypothesize $d'_H(b, d) = 3$ implies that $d_H(b, d) = 0$ or 2. If $d_H(b, d) = 0$, then we can conclude that $b = d$ and $b \in V(C_3)$ for some $C_3 \leq H$. If $d_H(b, d) = 2$, then $\{b, d\} \in \mathcal{C}(H)$. It follows that the number of all unordered vertex pairs $\{(a, b), (c, d)\} \subseteq V(G \otimes H)$ satisfying (ii) is equal to $B_HW_P(G) + 2C_HW_P(G)$.

Consequently, the number of all unordered vertex pairs $\{(a, b), (c, d)\} \subseteq V(G \otimes H)$ satisfying in Case (1) is equal to $A_GB_H + 2A_GC_H + B_HW_P(G) + 2C_HW_P(G)$.

**Case (2):**\[\max \{d'_G(a, c), d_H(b, d)\} = 3.\]

By a similar argument as Case (1), we can conclude that $|\mathcal{N}_2(G \otimes H)| = 2[C_H\varphi(G) + C_G\varphi(H)] + B_H\varphi(G) + B_G\varphi(H)$.

\[\square\]
i. The vertices $u$ and $v$ are two non-adjacent vertices of a cycle of length 5 of $G$.

ii. The vertices $u$ and $v$ are the vertices as depicted in Figure 3.

![Figure 3: Example of part ii of Note up to isomorphism.](image)

Therefore, if $G$ is a triangle free graph, then one can see that $A_G = |E(G)|$, $B_G = 0$. Also, $\{u, v\} \in C(G)$ if and only if $u, v$ are vertices of a cycle of length 5 of the graph $G$. Therefore, $C_G = 0$ whenever the graph $G$ is $C_5$-free.

**Corollary 10.** Let $G$ and $H$ be two simple connected $C_k$-free graphs for $k \in \{3, 5\}$. Then

$$W_P(G \odot H) = 2[m_HW_P(G) + m_GW_P(H)],$$

where $m_G$ and $m_H$ denote the number of edges of $G$ and $H$, respectively.

A graph is called **strongly triangular** if every pair of its vertices has a common neighbor.

**Corollary 11.** Let $G$ be a connected graph and $H$ be a strongly triangular graph. Then

$$W_P(G \odot H) = 2\left(\binom{n_H}{2}W_P(G) + A_G\left(\binom{n_H}{2} - m_H\right)\right) + n_H(A_G + W_P(G)),$$

where $m_H$ and $n_H$ denote the number of edges and the number of vertices of $H$, respectively.

**Proof.** Let $H$ be strongly triangular graph. Then each edge of $H$ belongs to a cycle of length 3, i.e. $C_3$. It follows that $A_H = 0, B_H = |V(G)|$. Let $u$ and $v$ be two arbitrary non-adjacent vertices of $H$. Since $H$ is strongly triangular, $u$ and $v$ have a common neighbor say $w$. Let $zv$ be common neighbor of vertices $u$ and $w$. In this case $uvw$ and $uzwv$ are paths of length 2 and 3, respectively. Therefore $C_G = \binom{n}{2} - m$. In the other hand, $W_P(H) = 0$ since every two arbitrary vertices of $H$ are adjacent or of distance 2. Hence the proof is done by Theorem 9. ∎
Let $P$ denote the Petersen graph. Now we apply our main theorem to $P \otimes G$, where $G$ is one of the following well-known graphs,

- $K_n =$ The complete graph on $n$ vertices;
- $W_n =$ The wheel on $n$ vertices;
- $S_n =$ The star graph on $n$ vertices;
- $K_{r,s} =$ The complete bipartite graph whose parts are of size $r$ and $s$;
- $Q_3 =$ The hyper cube graph on 8 vertices.

Our computations are summarized in the Table 1.

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<th>$G$</th>
<th>$n$</th>
<th>$m$</th>
<th>$D(G)$</th>
<th>$A_G$</th>
<th>$P_G$</th>
<th>$\lambda_G$</th>
<th>$W_P(G)$</th>
<th>$W_P(P \otimes G)$</th>
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</table>

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References


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