

Wiener index for a square of some special graphs

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Abstract

The importance of the operations defined in graph theory is determined by finding applications for them in other sciences, including chemistry, for example: If we have a simple connected graph whose edge set is non-empty and we want to define an operation in graph theory, such as a square operation, then the resulting new graph will be more realistic in

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chemistry, this is done by connecting edges between two vertices whose distance is one or two.

In addition to the importance of finding the sum of the distances between vertices, which represents the "Wiener's index", our interest in this research was to find the Wiener's index for some special graphs after performing a squaring operation on it.

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1. Introduction:

A simple connected graph $\emptyset = (V(\emptyset), E(\emptyset))$ is known to an ordered pair of a set of object that is non-empty which denominated a set of vertex $V(\emptyset)$, and a set of unordered pairs of vertices is denominated the set of edges $E(\emptyset)$, such that the graph $\emptyset$ is consists of only one compound, [1]. "The distance, $d_{\emptyset}(u, v)$, between any two $u, v \in V(\emptyset)$ distinct vertices in $\emptyset$ is the shortest path between them" and a greatest distance of these distances is called the diameter of a graph $\emptyset$, $diam(\emptyset)$, [2]. Distance is of great importance in many cognitive sciences, for example, distance in mathematics, especially in graph theory-chemical applications, represents the bounds that connect between carbon atoms, as the number of bonds between carbon atoms has a significant impact on the structure of molecules and chemical compounds, [3]. The sum of distances in any connected graph $\emptyset$ is called "Wiener index", [4], that is,

$$WI(\emptyset) = \sum_{\{x,y\} \subseteq V(\emptyset)} d_{\emptyset}(x, y).$$

"The Wiener index of a single vertex, x " is defined as:

$$WI(x, \emptyset) = \sum_{y \in (V(\emptyset) - \{x\})} d_{\emptyset}(x, y).$$

Then,

$$WI(\emptyset) = 0.5 \sum_{x \in V(\emptyset)} WI(x, \emptyset).$$

The Wiener index was created in 1947, [4] by Wiener and had application in finding the boiling points of paraffin. It has received great attention from researchers in the mathematics, especially in graph theory, where many articles have been presented, ([5],[6],[7],[8]). Just as Wiener index was found for many of the special graphs and operations specified in graph theory by different methods ([9],[10],[11]), many topological indices were later found that had a major impact in determining many physical and chemical properties, ([12],[13],[14],[15]). Also, there are many relations between the topological indices and Wiener index due to its importance, ([16],[17],[18],[19]). It is worth noting here the recent research that has dealt with the calculation of the Wiener index as well as its development due to its great importance, where in 2024, both Meenakshi and Bramila found Wiener index for a special type of graphs called Abid-Waheed graph [20], while other researchers have found Wiener index for prime ideal sum graph [21], Subashini, Kannan and others also presented applied research on silicate networks by providing a definition exponential

Wiener index ,[22,23,24] and Hua and Liu also obtained some new results with respect to Wiener-type indices [25].

Therefore, our goal in this article to find a Wiener index for a knowledge operation (Square graph) on some graph related to the iterative formula method.

The **mean distance** $\mu(\phi)$ is defined as the following form:

$$\mu(\phi) = \frac{WI(\phi)}{\binom{p}{2}}, |V(\phi)| = p, \text{ see [26].}$$

Definition 1.1: If ϕ denotes to a non-trivial graph which is connected and simple. Then the square ϕ^2 of the graph ϕ is a graph has $V(\phi^2) = V(\phi)$ and $E(\phi^2) = \{e = \{u, v\} : 1 \leq (d_\phi(u, v)) \leq 2, u, v \in V(\phi)\}$. This idea was presented by both Harary and Ross in 1960, [24]. To clarify definition, we take the following example.

Assume that the graph ϕ has vertices set $V(\phi) = \{t_\alpha : \alpha = 1, 2, \dots, 6\}$ and $E(\phi) = \{e_\beta : \beta = 1, 2, \dots, 5\}$ such that $e_1 = t_1 t_2, e_2 = t_2 t_3, e_3 = t_3 t_4, e_4 = t_3 t_5, e_5 = t_5 t_6$ then the graph ϕ^2 has the edges set

$E(\phi^2) = E(\phi) \cup E_n$, where $E_n = \{e_6 = t_1 t_3, e_7 = t_2 t_4, e_8 = t_2 t_5, e_9 = t_3 t_6, e_{10} = t_4 t_5\}$. See Figure 1.

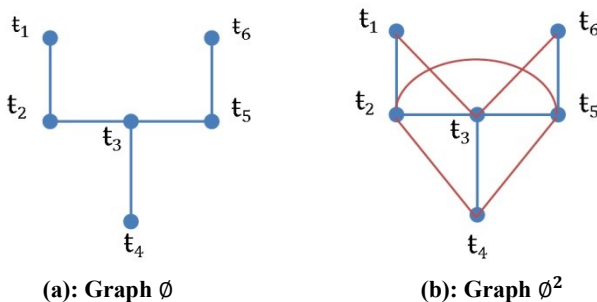


Figure 1
The Graph and Square Graph

Remark 1.2: From Definition 1.1, the square of each of the following graphs: complete, star, wheel and complete bipartite graphs are complete graphs K_p , and $WI(K_p) = \frac{1}{2}p(p-1)$, where $|V(K_p)| = p$.

2. Wiener index of the square path graph

Let P_p be the path graph which has $V(P_p) = \{v_1, v_2, \dots, v_p\}$, to explain the square path graph P_p^2 firstly, we divide $V(P_p)$ in to two subsets, V_1 and V_2 such that $v_\alpha \in V_1$, if $\alpha = 1, 3, 5, \dots, 2\left\lfloor \frac{p}{2} \right\rfloor - 1$ and $v_\alpha \in V_2$, if $\alpha = 2, 4, 6, \dots, 2\left\lfloor \frac{p}{2} \right\rfloor$, secondly, rename the vertices of V_1 and V_2 as, $V_1 = \{x_1, x_2, \dots, x_{\lfloor \frac{p}{2} \rfloor}\}$ and $V_2 = \{y_1, y_2, \dots, y_{\lfloor \frac{p}{2} \rfloor}\}$, Thus, $V(P_p^2) = V_1(P_p) \cup V_2(P_p)$ and $E(P_p^2) = \{x_\alpha x_{\alpha+1},$

$x_\alpha y_\alpha, y_\alpha x_{\alpha+1}, y_\alpha y_{\alpha+1}, \alpha = 1, 2, \dots, \frac{p}{2} - 1\} \cup \{x_{\frac{p}{2}} y_{\frac{p}{2}}\}$ when p be an even and $E(P_p^2) = \{x_\alpha x_{\alpha+1}, x_\alpha y_\alpha, y_\alpha x_{\alpha+1}, y_\alpha y_{\alpha+1}, \alpha = 1, 2, \dots, \frac{p-3}{2}\} \cup \{x_{\frac{p-1}{2}} x_{\frac{p+1}{2}}, x_{\frac{p-1}{2}} y_{\frac{p-1}{2}}, y_{\frac{p-1}{2}} x_{\frac{p+1}{2}}, y_{\frac{p-1}{2}} y_{\frac{p+1}{2}}\}$, when p be an odd, therefore p is the order of P_p^2 and its size is $2p - 3$, and has $\text{diam}(P_p^2) = \left\lfloor \frac{p}{2} \right\rfloor$. Figure 2 shows that

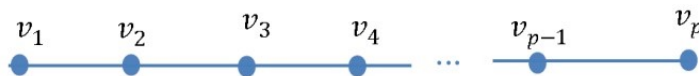
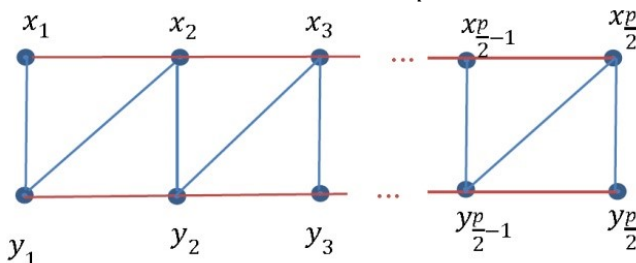
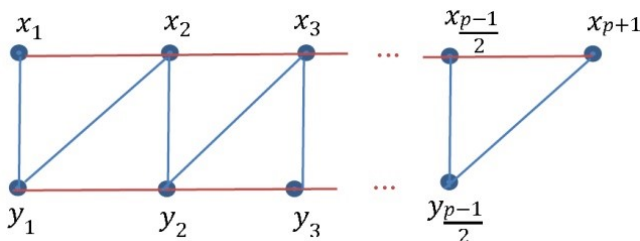
(a): Path Graph P_p (b): Graph P_p^2 when p is an even number(c): Graph P_p^2 when p is an odd number

Figure 2
Graphs P_p and P_p^2

Theorem 2.1: Let p is an even number, then for all $p \geq 6$ we have :

$$WI(P_p^2) = \frac{1}{24} p(2p - 1)(p + 2) .$$

Proof:

$$WI(P_p^2) = \sum_{\alpha=1}^{\frac{p-1}{2}} \{d_{P_p^2}(x_\alpha, x_{\alpha+1}) + d_{P_p^2}(y_\alpha, y_{\alpha+1}) + d_{P_p^2}(y_\alpha, x_{\alpha+1}) + d_{P_p^2}(x_\alpha, y_\alpha)\} + d_{P_p^2}(x_{\frac{p}{2}}, y_{\frac{p}{2}}) + \sum_{\beta=2}^{\frac{p-1}{2}} \{ \sum_{\alpha=1}^{\frac{p-\beta}{2}} (d_{P_p^2}(x_\alpha, x_{\alpha+\beta}) +$$

$$\begin{aligned}
& d_{P_p^2}(y_\alpha, y_{\alpha+\beta})) + \sum_{\alpha=1}^{\frac{p}{2}+1-\beta} d_{P_p^2}(x_\alpha, y_{\alpha+\beta-1})\} + d_{P_p^2}(x_1, y_{\frac{p}{2}}) \\
& + \sum_{\beta=2}^{\frac{p}{2}-1} \sum_{\alpha=1}^{\frac{p}{2}-\beta} d_{P_p^2}(y_\alpha, x_{\alpha+\beta}) \\
& = \sum_{\alpha=1}^{\frac{p}{2}-1} \{1 + 1 + 1 + 1\} + 1 + \sum_{\beta=2}^{\frac{p}{2}-1} \{\sum_{\alpha=1}^{\frac{p}{2}-\beta} (\beta + \beta) + \sum_{\alpha=1}^{\frac{p}{2}+1-\beta} \beta\} \\
& + \frac{p}{2} + \sum_{\beta=2}^{\frac{p}{2}-1} \sum_{\alpha=1}^{\frac{p}{2}-\beta} \beta \\
& = 1 + \frac{p}{2} + \sum_{\alpha=1}^{\frac{p}{2}-1} 4 + \sum_{\beta=2}^{\frac{p}{2}-1} \{\sum_{\alpha=1}^{\frac{p}{2}-\beta} 2\beta + \sum_{\alpha=1}^{\frac{p}{2}+1-\beta} \beta\} + \sum_{\beta=2}^{\frac{p}{2}-1} \sum_{\alpha=1}^{\frac{p}{2}-\beta} \beta \\
& = 1 + \frac{p}{2} + 4(\frac{p}{2} - 1) + \sum_{\beta=2}^{\frac{p}{2}-1} \{2\beta (\frac{p}{2} - \beta) + \beta (\frac{p}{2} + 1 - \beta)\} \\
& + \sum_{\beta=2}^{\frac{p}{2}-1} \beta (\frac{p}{2} - \beta) \\
& = \frac{5p}{2} - 3 + \sum_{\beta=2}^{\frac{p}{2}-1} \{\beta p - 2\beta^2 + \frac{1}{2}\beta p + \beta - \beta^2\} + \sum_{\beta=2}^{\frac{p}{2}-1} (\frac{1}{2}p\beta - \beta^2) \\
& = \frac{5p}{2} - 3 + \sum_{\beta=2}^{\frac{p}{2}-1} \{2\beta p - 4\beta^2 + \beta\} \\
& = \frac{1}{24}(2p^3 + 3p^2 - 62p + 60p - 72 + 72) \\
& = \frac{1}{24}p(2p - 1)(p + 2) .
\end{aligned}$$

Remark 2.2: $WI(P_4^2) = 7$.

Corollary 2.3: Let p is an even number, then the mean distance of a graph P_p^2 , $p \geq 6$ as:

$$\mu(P_p^2) = \frac{2p+5}{12} + \frac{1}{4(p-1)} .$$

Theorem 2.4: For all odd number $p \geq 7$ we have:

$$WI(P_p^2) = \frac{1}{24}(p^2 - 1)(2p + 3)$$

Proof:

$$\begin{aligned}
WI(P_p^2) &= \sum_{\alpha=1}^{\frac{p-1}{2}} \{d_{P_p^2}(x_\alpha, x_{\alpha+1}) + d_{P_p^2}(x_\alpha, y_\alpha)\} \\
&+ \sum_{\alpha=1}^{\frac{p-3}{2}} \{d_{P_p^2}(y_\alpha, y_{\alpha+1}) + d_{P_p^2}(y_\alpha, x_{\alpha+1})\} + d_{P_p^2}(y_{\frac{p-1}{2}}, x_{\frac{p+1}{2}}) \\
&+ \sum_{\beta=2}^{\frac{p-3}{2}} \{\sum_{\alpha=1}^{\frac{p+1}{2}-\beta} d_{P_p^2}(x_\alpha, x_{\alpha+\beta}) + \sum_{\alpha=1}^{\frac{p-1}{2}-\beta} d_{P_p^2}(y_\alpha, y_{\alpha+\beta})\}
\end{aligned}$$

$$\begin{aligned}
& + \sum_{\alpha=1}^{\frac{p+1}{2}-\beta} d_{P_p^2}(x_\alpha, y_{\alpha+\beta-1}) + \sum_{\alpha=1}^{\frac{p+1}{2}-\beta} d_{P_p^2}(y_\alpha, x_{\alpha+\beta}) \} \\
& + d_{P_p^2}(x_1, x_{\frac{p+1}{2}}) + d_{P_p^2}(x_1, y_{\frac{p-1}{2}}) + d_{P_p^2}(y_1, x_{\frac{p+1}{2}}) \\
& = 1 + \sum_{\alpha=1}^{\frac{p-1}{2}} \{1 + 1\} + \sum_{\alpha=1}^{\frac{p-3}{2}} \{1 + 1\} \\
& + \sum_{\beta=2}^{\frac{p-1}{2}} \left\{ \sum_{\alpha=1}^{\frac{p+1}{2}-\beta} \beta + \sum_{\alpha=1}^{\frac{p-1}{2}-\beta} \beta + \sum_{\alpha=1}^{\frac{p+1}{2}-\beta} \beta + \sum_{\alpha=1}^{\frac{p+1}{2}-\beta} \beta \right\} \\
& + \left\{ \frac{p-1}{2} + \frac{p-1}{2} + \frac{p-1}{2} \right\} \\
& = 1 + p - 1 + p - 3 + \sum_{\beta=2}^{\frac{p-3}{2}} \{3\beta(\frac{p+1}{2} - \beta) + \beta(\frac{p-1}{2} - \beta)\} \\
& + \frac{3}{2}(p - 1) \\
& = 2p - 3 + \frac{3}{2}(p - 1) + \sum_{\beta=2}^{\frac{p-3}{2}} \left\{ \frac{3\beta p + 3\beta}{2} - 3\beta^2 + \frac{\beta p - \beta}{2} - \beta^2 \right\} \\
& = \frac{4p-6+3p-3}{2} + \sum_{\beta=2}^{\frac{p-3}{2}} \{2\beta p - 4\beta^2 + \beta\} \\
& = \frac{7p-9}{2} + \frac{1}{24}(2p^3 + 3p^2 - 86p + 105) \\
& = \frac{1}{24}(p^2 - 1)(2p + 3) .
\end{aligned}$$

Remark 2.5:

1. $WI(P_3^2) = 3$.
2. $WI(P_5^2) = 13$.

Corollary 2.6: Let p is an odd number. The mean distance of a graph P_p^2 , $p \geq 7$ as:

$$\mu(P_p^2) = \frac{2p+5}{12} + \frac{1}{4p} .$$

3. Wiener index of the square cycle graphs

The order and the size of a square cycle graph C_p^2 of a cycle graph C_p , for all $p \geq 5$ are equal to p and $2p$ respectively. The diameter of C_p^2 depends to the value of p , that is, $\text{diam}(C_p^2) = \left\lfloor \frac{p}{2} \right\rfloor$, for all $p \geq 5$ except when p odd and $(p \equiv 1 \pmod{4})$ in this case $\text{diam}(C_p^2) = \left\lfloor \frac{p}{2} \right\rfloor$. Figure 3 shows that

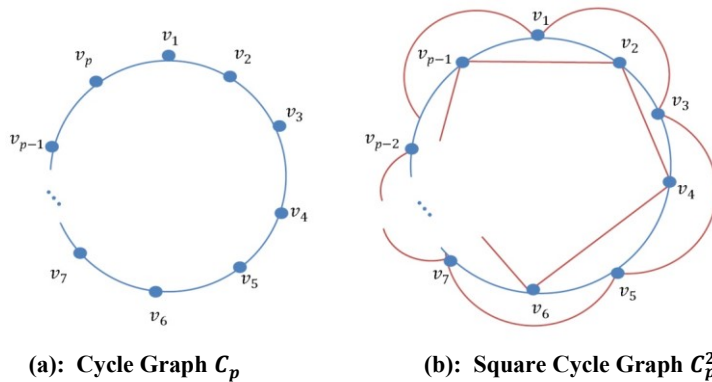


Figure 3
Cycle Graph and Square Cycle Graph

Theorem 3.1: For all $p \geq 5$, we have:

$$WI(C_p^2) = \frac{1}{16}p \begin{cases} (p-1)(p+3), & \text{if } \frac{(p-1)}{4} \in \mathbb{Z}^+, (p \text{ odd}), \\ (p+1)^2, & \text{if } \frac{(p-1)}{4} \notin \mathbb{Z}^+, (p \text{ odd}), \\ p(p+2), & p \text{ is an even.} \end{cases}$$

Proof: One must first we must determine the Wiener index for a vertex v_1 multiplied by the order of the graph C_p^2 and then divided by 2 due to symmetry. We take two statuses:

Status 1: If p is an odd, then there are two substatuses:

Substatus 1.1: If $\frac{(p-1)}{4} \in \mathbb{Z}^+$, then

$$\begin{aligned} WI(\xi_1, C_p^2) &= \sum_{\beta=1}^{\frac{p-1}{4}} \{d_{C_p^2}(\xi_1, \xi_{2\beta}) + d_{C_p^2}(\xi_1, \xi_{2\beta+1}) + d_{C_p^2}(\xi_1, \xi_{p-2\beta+2}) \\ &\quad + d_{C_p^2}(\xi_1, \xi_{p-2\beta+1})\} \\ &= 4 \sum_{\beta=1}^{\frac{p-1}{4}} \beta = \frac{1}{8}(p-1)(p+3) \end{aligned}$$

Substatus 1.2: If $\frac{(p-1)}{4} \notin \mathbb{Z}^+$, then

$$\begin{aligned} WI(\xi_1, C_p^2) &= \sum_{\beta=1}^{\frac{p-3}{4}} \{d_{C_p^2}(\xi_1, \xi_{2\beta}) + d_{C_p^2}(\xi_1, \xi_{2\beta+1}) + d_{C_p^2}(\xi_1, \xi_{p-2\beta+2}) \\ &\quad + d_{C_p^2}(\xi_1, \xi_{p-2\beta+1})\} + d_{C_p^2}(\xi_1, \xi_{\frac{p+1}{2}}) + d_{C_p^2}(\xi_1, \xi_{\frac{p+3}{2}}). \\ &= 4 \sum_{\beta=1}^{\frac{p-3}{4}} \beta + \frac{p+1}{4} + \frac{p+1}{4} \\ &= 4 \sum_{\beta=1}^{\frac{p-3}{4}} \beta + \frac{p+1}{2} = \frac{1}{8}(p+1)^2 \end{aligned}$$

Status 2 : If p is an even, then there are two substatuses:

Substatus 2.1 : If $p \equiv 0(mod\ 4)$, then

$$\begin{aligned} WI(\xi_1, C_p^2) &= \sum_{\beta=1}^{\frac{p-1}{4}} \{d_{C_p^2}(\xi_1, \xi_{2\beta}) + d_{C_p^2}(\xi_1, \xi_{2\beta+1}) + d_{C_p^2}(\xi_1, \xi_{p-2\beta+2}) \\ &\quad + d_{C_p^2}(\xi_1, \xi_{p-2\beta+1})\} + \sum_{\alpha=0}^2 d_{C_p^2}(\xi_1, \xi_{\frac{p}{2}+\alpha}) \\ &= 4 \sum_{\beta=1}^{\frac{p-1}{4}} \beta + \sum_{\alpha=0}^2 \frac{p}{4} \\ &= \frac{1}{8}p(p-4) + \frac{3p}{4} = \frac{1}{8}p(p+2) \end{aligned}$$

Substatus 2.2 : If $p \not\equiv 0(mod\ 4)$, then

$$\begin{aligned} WI(\xi_1, C_p^2) &= \sum_{\beta=1}^{\frac{p-2}{4}} \{d_{C_p^2}(\xi_1, \xi_{2\beta}) + d_{C_p^2}(\xi_1, \xi_{2\beta+1}) + d_{C_p^2}(\xi_1, \xi_{p-2\beta+2}) \\ &\quad + d_{C_p^2}(\xi_1, \xi_{p-2\beta+1})\} + d_{C_p^2}(\xi_1, \xi_{\frac{p+2}{2}}). \\ &= 4 \sum_{\beta=1}^{\frac{p-2}{4}} \beta + \frac{p+2}{4} \\ &= \frac{1}{8}(p^2 - 4) + \frac{p+2}{4} = \frac{1}{8}p(p+2). \end{aligned}$$

Hence

$$WI(\xi_1, C_p^2) = \begin{cases} \frac{1}{8}(p-1)(p+3), & \text{if } \frac{(p-1)}{4} \in Z^+, (p \text{ odd}), \\ \frac{1}{8}(p+1)^2, & \text{if } \frac{(p-1)}{4} \notin Z^+, (p \text{ odd}), \\ \frac{1}{8}p(p+2), & \text{if } p \text{ is an even.} \end{cases}$$

$$\text{Then, } WI(C_p^2) = \frac{1}{16}p \begin{cases} (p-1)(p+3), & \text{if } \frac{(p-1)}{4} \in Z^+, (p \text{ odd}), \\ (p+1)^2, & \text{if } \frac{(p-1)}{4} \notin Z^+, (p \text{ odd}), \\ p(p+2), & \text{if } p \text{ is an even.} \end{cases}$$

Remark 3.2:

1. $WI(C_4^2) = WI(K_4) = 6$.
2. $WI(C_5^2) = 10$.
3. $WI(C_6^2) = 18$.
4. $WI(C_7^2) = 28$.

Corollary 3.3: The mean distance of a graph C_p^2 , $p \geq 5$ is

$$\mu(C_p^2) = \frac{1}{8(p-1)} \begin{cases} (p-1)(p+3), & \text{if } \frac{(p-1)}{4} \in Z^+, (p \text{ odd}), \\ (p+1)^2, & \text{if } \frac{(p-1)}{4} \notin Z^+, (p \text{ odd}), \\ p(p+2), & \text{if } p \text{ is an even.} \end{cases}$$

4. Conclusion

Through our study of this research and the results we obtained, we conclude that, the Wiener index for a path and a cycle graphs is larger than the Wiener index for a square path graph and a square cycle graph, respectively. The following Table 1 explains that

Table 1
Wiener Indices for Path and Cycle Graphs with their Square

Graph $\emptyset$	The Wiener index for a graph G	The Wiener index for a square graph $\emptyset^2$
$P_p, p \geq 8$	$WI(P_p) = \binom{p+1}{3}$	$WI(P_p^2) = \begin{cases} \frac{1}{24}(p^2-1)(2p+3), & \text{when } p \text{ an odd} \\ \frac{1}{24}p(2p-1)(p+2), & \text{when } p \text{ an even} \end{cases}$
$C_p, p \geq 5$	$WI(C_p) = \begin{cases} \frac{1}{8}p^3, & \text{when } p \text{ an odd} \\ \frac{1}{8}p(p^2-1), & \text{when } p \text{ an even} \end{cases}$	$WI(C_p^2) = \frac{1}{16}p \begin{cases} (p-1)(p+3), & \text{if } p \equiv 1 \pmod{4}, \\ & p \text{ is an odd,} \\ (p+1)^2, & \text{if } p \not\equiv 1 \pmod{4}, \\ & p \text{ is an odd,} \\ p(p+2), & \text{if } p \text{ is an even.} \end{cases}$

Finally, the importance of the results we have reached in this paper is indicated by the fact that Wiener indices for this special graphs under the square operation of graphs is more in touch with reality for chemical applications to know many properties such as boiling point, melting point, etc. ... through this operation defined in graph theory.

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