WIENER INDEX OF SUM OF THE GRAPHS

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Abstract

In this paper we introduce the Wiener index for sum of the two graphs, particularly for Complete graph and Complete bipartite graph. A conjecture is obtained by proving many cases and also the Wiener index of the sum of the graphs has been tabulated.

Introduction

The ***Wiener index*** is one of the oldest molecular topological indices which has been introduced by Harry Wiener in 1947, while studying its correlations with boiling points of paraffin considering its molecular structure. The Wiener index also predicts the binding energy of a protein-ligand complex at a preliminary stage. The concept of the Wiener index is a frontier between algebraic graph theory and Chemistry [1,3]. Since then, it has been one of the most frequently used topological indices in Chemistry, as molecular structures are usually modeled as undirected graphs [2,6].

The ***Wiener index number*** reflects the index boiling points of alkane molecules. In chemical graph theory, the Wiener index or Path index is introduced by *Harry*. Wiener, is a *topological index* of a *molecule*, defined as the sum of the lengths of the *shortest paths* between all pairs of vertices in the *chemical graph* representing the non-*hydrogen* atoms in the molecule [7].

Definition:

The *Wiener index of a graph* invariant is the sum of the distance between all pairsof vertices in the graph [6]. For a connected graph G, the Wiener index is the sum of distances between all unordered pairs of vertices in the graph and is denoted by $W(G)$. If $d_G(u, v)$ denotes the distance from u to v that is, the minimum length of a path from u tov in the graph G, then

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

Definition:

Let G_1 and G_2 be the graph such that $V(G_1) \cap V(G_2) = \varphi$, then the *sum of the graphs* G_1 and G_2 is defined as the graph whose vertex set is $V(G_1)$ and $V(G_2)$ respectively and the edge set consisting those edges, which are in G_1 and in G_2 and the edges obtained, by joining each vertex of G_1 to each vertex of G_2 [5].

Wiener index of Complete graph:

Let K_n be a Complete graph and the vertex set is $V(K_n) = \{u_{1,} u_2 \dots u_m\}$. Then the Wiener index of Complete graph is given by,

$$W(K_n) = \sum_{\substack{i=1 \\ i<j}}^{n} d(u_{i,} u_j) = \frac{1}{2}\, n(n-1)$$

Wiener index of Complete bipartite graph:

Let $K_{m,n}$ be a Complete bipartite graph. Then the Wiener index of $K_{m,n}$ is

$$W(K_{m,n}) = (m+n)(m+n-1) - mn$$

Let $V_1 = \{u_{1,} u_2, u_3, \dots . u_m\}$ and $V_2 = \{v_1, v_2, v_3 \dots . . v_n\}$ be the vertex sets of $K_{m,n}$

Then the Wiener index of Complete bipartite graph, $K_{m,n}$ is calculated by

$$W(K_{m,n}) = W(V_1, V_2) = \sum_{i=1}^{m} \sum_{j=1}^{n} d(u_i, v_j) + \sum_{i<j}^{m} d(u_i, u_j) + \sum_{i<j}^{n} d(v_i, v_j)$$

Wiener index of sum of complete and complete bipartite graphs:

In this section the Wiener index for sum of the two graphs particularly for Complete graph and Complete bipartite graph has been introduced and a conjecture is obtained by proving many cases in the following theorem. Also the detailed calculated value of wiener index for the same has been represented in tabular form.

Theorem:

Let G_l be any complete graph and G_2 be any complete bipartite graph, then the Wiener indexof G_1 be $W(K_l)$ and G_2 be $W(K_{m,n})$. Then the sum of G_1 and G_2 are formulated by conjecture

$$W(K_l + K_{m,n}) = mn + lN + \frac{l(l-1)}{2} + 2\left[\binom{m}{2} + \binom{n}{2}\right]$$

Where $N = m + n$

Proof:

The sum of the graphs K_l and $K_{m,n}$ is drawn [4] by fixing K_l and taking the vertices m and n of $K_{m,n}$ in a manner such that it does not cross the vertices of K_l.

Hence, the sum of the graph $K_l + K_{m,n}$ is drawn with $l + m + n$ number of vertices.

Let $V_1 = \{u_1, u_2, u_3, \dots u_l\}$ be the vertex set of Complete graph, K_l with l number of vertices,

Let $V_2 = \{v_1, v_2, v_3 \dots v_m\}$ and $V_3 = \{w_1, w_2, w_3, \dots w_n\}$ be the vertex set of Complete bipartite graph , $K_{m,n}$ with m number of vertices and n number of vertices respectively.

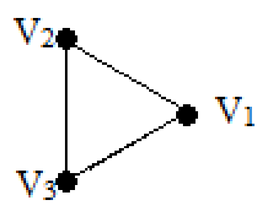
Then , the Weiner index of the sum of K_l and $K_{m,n}$ is calculated by ,

$$W(K_l + K_{m,n}) = \mathrm{W}(V_1 + V_2, V_3) = \sum_{i=1}^{l}\sum_{j=1}^{m} d(u_i, v_j) + \sum_{i=1}^{l}\sum_{j=1}^{n} d(u_i, w_j) + \sum_{i=1}^{m}\sum_{j=1}^{n} d(v_i, w_j) + \sum_{\substack{i,j=1\\ i<j}}^{l} d(u_i, u_j) + \sum_{\substack{i,j=1\\ i<j}}^{m} d(v_i, v_j) + \sum_{\substack{i,j=1\\ i<j}}^{n} d(w_i, w_j)$$

We shall prove the theorem by Mathematical Induction to find the Wiener Index for the sum of the graphs K_l and $K_{m,n}$

Case:A

Let $l = 1$



$K_1+K_{1,1}$

Case (i): When $m = 1$

Subcase (i): Let $n = 1$,

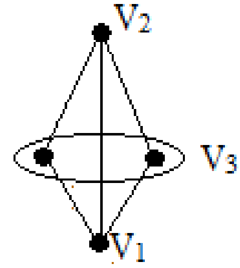
then the graph of $K_1 + K_{1,1}$ is formed with vertex sets

$$V_1 = \{u_1\}, V_2 = \{v_1\} \; and \; V_3 = \{w_1\}$$

Then, $W(K_1 + K_{1,1}) = d(u_1, v_1) + d(u_1, w_1) + d(v_1, w_1) = 3$

Subcase (ii): Let $n = 2$,

then the graph of $K_1 + K_{1,2}$ is formed with vertex sets



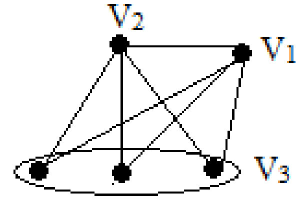
$K_1+K_{1,2}$

$V_1 = \{u_1\}, V_2 = \{v_1\}\ and\ V_3 = \{w_1, w_2\}$

$$W(K_1 + K_{1,2}) = d(u_1, v_1) + d(u_1, w_1) + d(u_1, w_2) + d(v_1, w_1) + d(v_1, w_2) + d(w_1, w_2) = 7$$

Subcase (iii): Let $n = 3$,

then the graph of $K_1 + K_{1,3}$ is formed with vertex sets



$K_1+K_{1,3}$

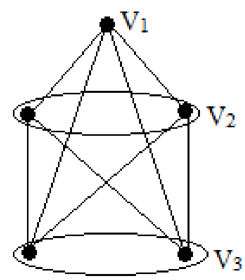
$V_1 = \{u_1\}, V_2 = \{v_1\}\ and\ V_3 = \{w_1, w_2, w_3\}$

$$W(K_1 + K_{1,3}) = d(u_1, v_1) + d(u_1, w_1) + d(u_1, w_2) + d(u_1, w_3) + d(v_1, w_1)$$
$$+ d(v_1, w_2) + d(v_1, w_3) + d(w_1, w_2) + d(w_1, w_3) + d(w_2, w_3) = 13$$

Case (ii): When $m = 2$,

Subcase (i): Let $n = 1$,

then the graph of $K_1 + K_{2,1}$ is formed with vertex sets



$K_1+K_{2,2}$

$V_1 = \{u_1\}, V_2 = \{v_1, v_2\} and\ V_3 = \{w_1\}$

From the above cases, it is clear that,

$$W(K_1 + K_{2,1}) = W(K_1 + K_{1,2}) = 7$$

Subcase (ii): Let $n = 2$ then the graph of $K_1 + K_{2,2}$ is formed with vertex sets

$V_1 = \{u_1\}, V_2 = \{v_1, v_2\}\ and\ V_3 = \{w_1, w_2\}$

$$W(K_1 + K_{2,2}) = d(u_1, v_1) + d(u_1, v_2) + d(u_1, w_1) + d(u_1, w_2) + d(v_1, w_1) + d(v_1, w_2)$$
$$+ d(v_2, w_1) + d(v_2, w_2) + d(v_1, v_2) + d(w_1, w_2) = 12$$

Case (iii): When $m = 3$,

Subcase (i): Let $n = 2$ then the graph of $K_1 + K_{3,1}$ is formed with vertex sets

$V_1 = \{u_1\}, V_2 = \{v_1, v_2, v_3\}\ and\ V_3 = \{w_1\}$

From the above case, it is clear that,

$$W(K_1 + K_{3,1}) = W(K_1 + K_{1,3}) = 13$$

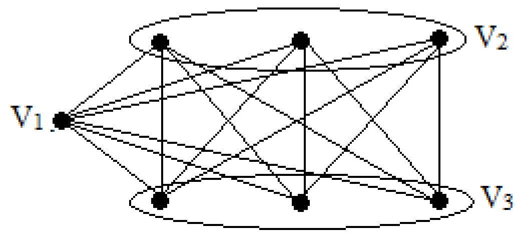
Subcase (ii): Let n=2, similarly from above cases,

$$W(K_1 + K_{3,2}) = W(K_1 + K_{2,3}) = 19$$

Subcase (iii): Let $n = 2$

then the graph of $K_1 + K_{3,3}$ is formed with vertex sets

$V_1 = \{u_1\}, V_2 = \{v_1, v_2, v_3\}$ *and* $V_3 = \{w_1, w_2, w_3\}$



K1+K3,3

$$W(K_1 + K_{3,3}) = d(u_1, v_1) + \cdots + d(u_1, v_3) + d(u_1, w_1) + \cdots + d(u_1, w_3)$$

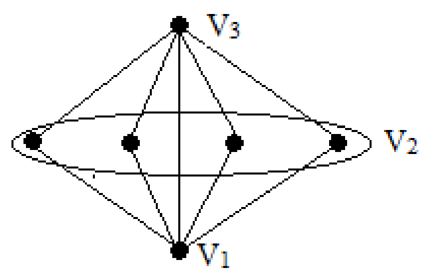
$$+ d(v_1, w_1) \ldots + d(v_1, w_3) + d(v_2, w_1) + \cdots + d(v_2, w_3) + d(v_3, w_1) + \cdots + d(v_3, w_3) = 27$$

Case (iv): When m=4

Subcase (i): Let $n = 1$

then the graph of $K_1 + K_{4,1}$ is formed with vertex sets

$V_1 = \{u_1\}, V_2 = \{v_1, v_2, v_3, v_4\}$*and* $V_3 = \{w_1\}$



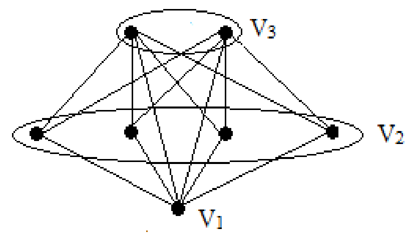
K1+K4,1

$$W(K_1 + K_{4,1}) = d(u_1, v_1) + d(u_1, w_1) + \cdots + d(u_1, w_4)$$
$$+ d(v_1, w_1) + \cdots + d(v_1, w_4) = 21$$

Subcase (ii): Let $n = 2$

then the graph of $K_1 + K_{4,2}$ is formed with vertex sets

$V_1 = \{u_1\}, V_2 = \{v_1, v_2, v_3, v_4\}$*and* $V_3 = \{w_1, w_2\}$



K1+K4,2

$$W(K_1 + K_{4,2}) = d(u_1, v_1) + d(u_1, v_2) + d(u_1, w_1) \ldots +$$
$$d(u_1, w_4) + d(v_1, w_1) + \cdots + d(v_1, w_4) + d(v_2, w_1) + \cdots + d(v_2, w_4) = 28$$

In general, $W(K_1 + K_{m,n})$ when $l = 1$ and $m, n = 1, 2, 3, \ldots$ is tabulated as follows:

$G=K_1+K_{1,n}$	W(G)	$G=K_1+K_{2,n}$	W(G)	$G=K_1+K_{3,n}$	W(G)	$G=K_1+K_{4,n}$	W(G)
$K_1+K_{1,1}$	**3**	$K_1+K_{2,1}$	**7**	$K_1+K_{3,1}$	**13**	$K_1+K_{4,1}$	**21**
$K_1+K_{1,2}$	**7**	$K_1+K_{2,2}$	**12**	$K_1+K_{3,2}$	**19**	$K_1+K_{4,2}$	**28**
$K_1+K_{1,3}$	**13**	$K_1+K_{2,3}$	**19**	$K_1+K_{3,3}$	**27**	$K_1+K_{4,3}$	**37**
$K_1+K_{1,4}$	**21**	$K_1+K_{2,4}$	**28**	$K_1+K_{3,4}$	**37**	$K_1+K_{4,4}$	**48**
$K_1+K_{1,5}$	**31**	$K_1+K_{2,5}$	**39**	$K_1+K_{3,5}$	**49**	$K_1+K_{4,5}$	**61**
$K_1+K_{1,6}$	**43**	$K_1+K_{2,6}$	**52**	$K_1+K_{3,6}$	**63**	$K_1+K_{4,6}$	**76**
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

$G=K_1+K_{5,n}$	W(G)	$G=K_1+K_{6,n}$	W(G)	$G=K_1+K_{7,n}$	W(G)	$G=K_1+K_{8,n}$	W(G)
$K_1+K_{5,1}$	**31**	$K_1+K_{6,1}$	**43**	$K_1+K_{7,1}$	**57**	$K_1+K_{8,1}$	**73**
$K_1+K_{5,2}$	**39**	$K_1+K_{6,2}$	**52**	$K_1+K_{7,2}$	**67**	$K_1+K_{8,2}$	**84**
$K_1+K_{5,3}$	**49**	$K_1+K_{6,3}$	**63**	$K_1+K_{7,3}$	**79**	$K_1+K_{8,3}$	**97**
$K_1+K_{5,4}$	**61**	$K_1+K_{6,4}$	**76**	$K_1+K_{7,4}$	**93**	$K_1+K_{8,4}$	**112**
$K_1+K_{5,5}$	**75**	$K_1+K_{6,5}$	**91**	$K_1+K_{7,5}$	**109**	$K_1+K_{8,5}$	**129**
$K_1+K_{5,6}$	**91**	$K_1+K_{6,6}$	**108**	$K_1+K_{7,6}$	**127**	$K_1+K_{8,6}$	**148**
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

From the above tabulation, we obtain the following conjecture, for $l = 1$,

$$W(K_l + K_{m,n}) = mn + (m + n) + 2\left[\binom{m}{2} + \binom{n}{2}\right]$$

Similarly, $W(K_2 + K_{m,n})$ when $l = 2$ and $m, n = 1, 2, 3, \ldots$ is tabulated as follows:

$G=K_2+K_{1,n}$	W(G)	$G=K_2+K_{2,n}$	W(G)	$G=K_2+K_{3,n}$	W(G)	$G=K_2+K_{4,n}$	W(G)
$K_2+K_{1,1}$	**6**	$K_2+K_{2,1}$	**11**	$K_2+K_{3,1}$	**18**	$K_2+K_{4,1}$	**27**
$K_2+K_{1,2}$	**11**	$K_2+K_{2,2}$	**17**	$K_2+K_{3,2}$	**25**	$K_2+K_{4,2}$	**35**
$K_2+K_{1,3}$	**18**	$K_2+K_{2,3}$	**25**	$K_2+K_{3,3}$	**34**	$K_2+K_{4,3}$	**45**
$K_2+K_{1,4}$	**27**	$K_2+K_{2,4}$	**35**	$K_2+K_{3,4}$	**45**	$K_2+K_{4,4}$	**57**
$K_2+K_{1,5}$	**38**	$K_2+K_{2,5}$	**47**	$K_2+K_{3,5}$	**58**	$K_2+K_{4,5}$	**71**
$K_2+K_{1,6}$	**41**	$K_2+K_{2,6}$	**61**	$K_2+K_{3,6}$	**73**	$K_2+K_{4,6}$	**87**
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

$G=K_2+K_{5,n}$	W(G)	$G=K_2+K_{6,n}$	W(G)	$G=K_2+K_{7,n}$	W(G)	$G=K_2+K_{8,n}$	W(G)
$K_2+K_{5,1}$	**38**	$K_2+K_{6,1}$	**41**	$K_2+K_{7,1}$	**66**	$K_2+K_{8,1}$	**83**
$K_2+K_{5,2}$	**47**	$K_2+K_{6,2}$	**61**	$K_2+K_{7,2}$	**77**	$K_2+K_{8,2}$	**95**
$K_2+K_{5,3}$	**58**	$K_2+K_{6,3}$	**73**	$K_2+K_{7,3}$	**90**	$K_2+K_{8,3}$	**109**
$K_2+K_{5,4}$	**71**	$K_2+K_{6,4}$	**87**	$K_2+K_{7,4}$	**105**	$K_2+K_{8,4}$	**125**
$K_2+K_{5,5}$	**86**	$K_2+K_{6,5}$	**103**	$K_2+K_{7,5}$	**122**	$K_2+K_{8,5}$	**143**
$K_2+K_{5,6}$	**103**	$K_2+K_{6,6}$	**121**	$K_2+K_{7,6}$	**141**	$K_2+K_{8,6}$	**163**
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

From the above tabulation, we obtain the following conjecture, for $l = 2$,

$$W(K_l + K_{m,n}) = mn + (m+n) + (m+n+1) + 2\left[\binom{m}{2} + \binom{n}{2}\right]$$

Proceeding as above we set a sequence of conjectures, as

When $l = 1$, $W(K_l + K_{m,n}) = mn + (m+n) + 2\left[\binom{m}{2} + \binom{n}{2}\right]$

When $l = 2$, $W(K_l + K_{m,n}) = mn + (m+n) + (m+n+1) + 2\left[\binom{m}{2} + \binom{n}{2}\right]$

When $l = 3$, $W(K_l + K_{m,n}) = mn + (m+n) + (m+n+1) + (m+n+2) + 2\left[\binom{m}{2} + \binom{n}{2}\right]$

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$$W(K_l + K_{m,n}) = mn + (m+n) + (m+n+1) + \cdots + (m+n+\overline{l-1}) + 2\left[\binom{m}{2} + \binom{n}{2}\right]$$

Let $N = m + n$,

$$= mn + N + (N+1) + (N+2) + \cdots \ldots\ldots + (N+\overline{l-1}) + 2\left[\binom{m}{2} + \binom{n}{2}\right]$$

$$= mn + lN + (1+2+3+\cdots.+\overline{l-1}) + 2\left[\binom{m}{2} + \binom{n}{2}\right]$$

Hence, $W(K_l + K_{m,n}) = mn + lN + \frac{l(l-1)}{2} + 2\left[\binom{m}{2} + \binom{n}{2}\right]$, where $N = m + n$

Hence the proof.

Remark:

Since, $K_{m,n}$ and $K_{n,m}$ has same number of vertices, hence $K_{m,n} \cong K_{n,m}$ which implies that

$$K_1 + K_{m,n} \cong K_1 + K_{n,m}$$

$$K_2 + K_{m,n} \cong K_2 + K_{n,m}$$

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$$K_l + K_{m,n} \cong K_l + K_{n,m}$$

Also, $W(K_1 + K_{m,n}) = 3n^2 , if\ m = n$

Where l, m, n are any positive integers

We infer that the calculated value of Wiener index of the sum of the graphs canbe represented in the matrix form, in which Row represents complete graph and Column represents complete bipartite graph.

+	$K_{1,n}$	$K_{2,n}$	$K_{3,n}$	$K_{4,n}$	$K_{5,n}$	$K_{6,n}$	…
K_1	**3**	**7**	13	21	31	43	…
	7	**12**	**19**	28	39	52	…
	13	**19**	**27**	**37**	49	63	….
	21	28	**37**	**48**	**61**	76	…
	31	39	49	**61**	**75**	**91**	…
	43	52	63	76	**91**	**108**	…
	⋮	⋮	⋮	⋮	⋮	⋮	⋮
K_2	**6**	**11**	18	27	38	41	…
	11	**17**	**25**	35	47	61	…
	18	**25**	**34**	**45**	58	73	…
	27	35	**45**	**57**	**71**	87	…
	38	47	58	**71**	**86**	**103**	…
	41	61	73	87	**103**	**121**	…
	⋮	⋮	⋮	⋮	⋮	⋮	⋮
K_n							

Conclusion:

This paper deals on analyzing the Wiener index for sum of the graphs. Presently many research on Wiener index is going on, but this paper enables to calculate the Wiener index for sum of two graphs.

It may be concluded that studying distance based or Wiener number of chemical theory solves many problems in analyzing the structural properties of molecules which is an effective tool of molecular topology, polymer science and crystal research. Since the properties and the interaction of the vertices in a molecule are taken into account, a similar graph structure for combination of many graphs can be framed.

This paper can be extended to find sum of more than two graphs, cartesian product and wiener index for K- partite graphs. Also, wiener index for sum of complete and complete K- partite graphs can be analyzed.

Acknowledgement:

The author is very thankful to the managing trustee, Nerhu Civic Charitable trust (Registered NGO) under Saradha Gangadharan Research fund Scheme, for their support through financial assistance for the minor project.

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