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WIENER INDEX OF CHAIN GRAPHS

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ABSTRACT
The Wiener index W(G) is a distance-based topological invariant much used in the study of thestructure-property and the structure-activity relationships of various classes of biochemically interesting compounds introduced by Harold Wiener in 1947. It is defined by the sum of the distances between all (ordered) pairs of vertices of G. In this paper, we will give the wiener index of edge composition of finite number of graphs. Using this formula, we can easily find out the Wiener Index of some molecular structurehaving cut edges
Keywords: Distance sum, Bridge

1. INTRODUCTION

Molecular descriptor is a final result of a logic and mathematical procedure which transforms chemical information encoded with in a symbolic representation of a molecule into a useful number or the result of some standardized experiment.

The Wiener index **W(G)** is a distance-based topological invariant is also a molecular descriptor, it much used in the study of the structure-property and the structure-activity relationships of various classes of biochemically interesting compounds introduced by Harold Wiener [10] in 1947 for predicting boiling points ($\boldsymbol{b.p}$) of alkanes based on the formula

$$\boldsymbol{b.p = \alpha W + \beta w(3) + \gamma}$$

where$\boldsymbol{\alpha, \beta, \gamma}$ are empirical constants, and **w(3)** is called path number [7][8][10][11][12].

It is defined as the half sum of the distances between all pairs of vertices of G.

$$W(G) = \frac{1}{2}\sum_{u,v} d(u,v)$$

Notation:

$$W(G) = \frac{1}{2}\sum_{u,v} d(u,v) = \sum_{u<v} d(u,v) \quad = \sum_{i<j} d\left(u_i, u_j\right)$$

Definition

Our notation is standard and mainly taken from standard books of graph theory[9]. All graphs considered in this paper are simple and connected. The vertex and edge sets of a graph G are denoted by V(G) and E(G) respectively.

The **distance** d(u,v) between the vertices u and v of the graph G is equal to length of the shortest path that connects u and v.

Some Basic Results: [1], [2], [3], [15]

1. $W(P_n) = \frac{n(n^2-1)}{6}$

2. $W(C_n) = \begin{cases} \frac{1}{8}n^3 \text{ for n even} \\ \frac{1}{8}(n-1)n(n+1) \; for \; nodd \end{cases}$

3. $W(K_n) = \frac{n(n-1)}{2}$

Discussions around computing the Wiener Index of a generic chain-like polygonal systembegan from the late 1980's [13, 14]. Computing theWiener Index for such a chain was onceconsidered a very hard problem.N. PrabhakaraRao and co-authors have computed the wiener index of pentachainsand Ivan Gutman and at el, have discussed about the Generalized Wiener Indices of Zigzagging Pentachains.Sen-PengEu and at el, have determined about Generalized Wiener Indices in Hexagonal Chains.[4][5][6]

In this paper,we calculate the Wiener index of any graph,particularly having bridges. For our convenient, we modify the given graph into two or more graphs, which are connected by the cut edges.That is,if we modify the given graph G into $G_1,G_2\ldots G_k$, which are connected by the cut edges ,whose

$|V(G)| = |V(G_1)|+ |V(G_2)|+\ldots+|V(G_k)|$, $|E(G)| =|E(G_1)|+|E(G_2)|+\ldots+|E(G_k)|+k-1$

Hence we make a graph as a chain.

The following fig.1 illustrates above technique:

Let us consider graph G with 12 nodes, where G formed by G_1,G_2,G_3with3,4,5 vertices respectively and these are connected by the bridges

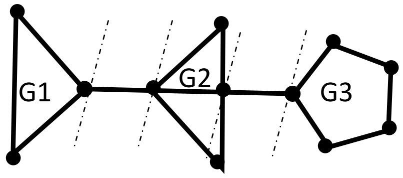


Fig:1

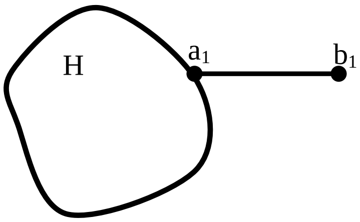
Main Result

Before proving our main results let us prove the following lemma

Lemma 1

Let**G** bea graph with n vertices. If it is formed by the graph H with n-1 vertices and it is connected to a vertex by an edge as shown in the fig.Where |V(G)|= |V(H)+1|then W(G) = W(H) + d(a_1| H) + n-1

Proof



G

Fig:2

$$W(G) = \sum_{u,v\in H} d\,(u,v) + \sum_{u\in H} d\,(u,b_1)$$

$$= W(H) + \sum_{u\in H} (d\,(u,a_1) + d(a_1,b_1))$$

$$= W(H) + \sum_{u\in H} d\,(u,\, a_1) + \sum_{u\in H} d\,(u,b_1)$$

$$= W(H) + d(a_1|\, H) + n-1$$

Hence the lemma

Lemma 2

Let **G** bea graph with n vertices. If it is formed by the graphs G_1 and $G_2$with $n_1$and $n_2$vertices and G_1, G_2 are connected by an edge as shown in the following fig.

Where |V(G)|= |V(G_1)|+ |V(G_2)| and |E(G)| =|E(G_1)|+|E(G_2)|+1then

W(G) = W(G_1) +W(G_{2+}) +n_1 d(b_1| G_2) + n_2 d(a_1| G_1) +n_1n_2

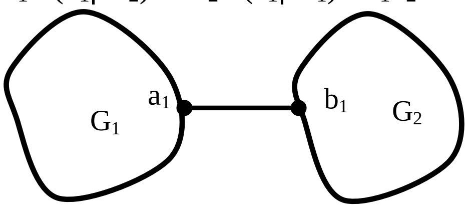


Fig.3

Proof:

$$W(G)= \sum_{u,v\in G1} d\,(u,v)+ \sum_{u\in G2} d\,(u,v)+ \sum_{\substack{u\in G1\\ v\in G2}} d\,(u,v)$$

$$= W(G_1) + W(G_2) + \sum_{u\in H} (d\,(u,a_1)+d(a_1,b_1) +d(b_1,v))$$

$$= W(G_1) +W(G_2) +n_1\, d(b_1|\, G_2) +n_2\, d(a_1|\, G_1) + n_1n_2$$

Hence the lemma.

Lemma 3

Let **G** bea chain graph with n vertices. If it is formed by the graphs G_1,G_2 and G_3 with n_1, n_2 and n_3 vertices, that are connected by the edges a_1b_1, a_2b_2 then

$$W(G) = W(G_1) +W(G_2) + W(G_3) + n_1[d(b_1|\, G_2) + d(b_1|\, G_3)]+n_2[d(a_1|\, G_1) +d(b_2|\, G_3) + n_3[d(a_1|G_1)+d(a_2|G_2)]+n_{1(}n_{2+}\, n_3)+ n_{3(}n_{1+}\, n_2)+d(b_1 , a_2)n_1n_3.$$

Proof:
This lemma follows immediately from the previous lemma.

For example W(G) =186 (seeFig.1)

Now we generalize the lemma 3,

Theorem1
Let **G** bea chain graph with n vertices. If it is formed by the graphs G_1,G_2 ….$G_k$with order n_1 , n_2 …. n_k respectively,that are connected by the edges a_1b_1, a_2b_2 , ……. $a_{k-1}b_{k-1}$ as shown in the following fig.

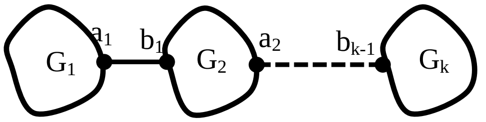


Fig.4

Where

$|V(G)|=|V(G_1)|+ |V(G_2)|+…+|V(G_k)|$, $|E(G)| =|E(G_1)|+|E(G_2)|+…+|E(G_k)|+k-1$then

$$W(G) =\sum_{i=1}^{k} W\,(G_i) + n_1[\sum_{i=1}^{k-1} d\,(bi|G_{i+1})]+n_2[d(a_1|G_1)+\sum_{i=2}^{k-1} d\,(bi|G_{i+1})]+$$

$$+\ldots\ldots+n_k[\sum_{i=1}^{k-1} d\,(a_i|G_i)]+\sum_{j=2}^{k-1} [n_{j-1}+(2+d(b_{j-2},a_{j-1})\, n_{j-2}++\ldots\ldots+$$

$$[(j-1)+d(b_1,a_2)+\ldots\ldots+ d(b_{j-2},a_{j-1})\, n_1]n_j$$

Proof:

$$W(G) = \sum_{i=1}^{k} W(G_i) + n_1[\sum_{i=1}^{k-1} d(bi|G_{i+1})] + n_2[d(a_1|G_1)+\sum_{i=2}^{k-1} d(bi|G_{i+1})]+$$

$$+\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots+n_k[\sum_{i=1}^{k-1} d(a_i|G_i)] +$$

$$+d(a_i,b_1)m_1m_2+\ldots\ldots+d(a_{n-1},b_{n-1})m_{n-1}m_n+$$

$$+d(a_i,b_2)m_1m_3+\ldots.+d(a_{n-2},b_{n-1})m_{n-2}m_n+$$

$$+\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots+$$

$$+d(a_1,b_{n-2})m_1m_{n-1}+d(a_2,b_{n-1})m_2m_n+$$

$$+d(a_1,b_{n-1})m_1m_n$$

$$= \sum_{i=1}^{k} W(G_i) + n_1[\sum_{i=1}^{k-1} d(bi|G_{i+1})]+n_2[d(a_1|G_1)+\sum_{i=2}^{k-1} d(bi|G_{i+1})]+\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots$$

$$+n_k[\sum_{i=1}^{k-1} d(a_i|G_i)] + n_1n_2+[n_2+(2+d(b_1,a_2)n_1]n_3+\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots+$$

$$+[n_{k-1}+n_{k-2}[2+ d(b_{k-2},a_{k-1})]+\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots+ [(n-1)+d(b_1,a_2)+\ldots\ldots\ldots+ d(b_{k-2},a_{k-1})n_1]n_j$$

$$= \sum_{i=1}^{k} W(G_i) + n_1[\sum_{i=1}^{k-1} d(bi|G_{i+1})]+n_2[d(a_1|G_1)+\sum_{i=2}^{k-1} d(bi|G_{i+1})]+$$

$$+\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots+n_k[\sum_{i=1}^{k-1} d(a_i|G_i)] +$$

$$+\sum_{j=2}^{k-1} [n_{j-1}+(2+d(b_{j-2},a_{j-1})\, n_{j-2} +\ldots\ldots\ldots+[(j-1)+d(b_1,a_2) + \ldots\ldots\ldots\ldots+ d(b_{j-2},a_{j-1})\, n_1]n_j$$

REMARK:

If we take k copies of the graph G then $G_1 = G_2 \ldots. = G_k$ with order $n_1 = n_2 \ldots.= n_k= t$(say) respectively, that are connected by the edges a_1b_1, a_2b_2 , ……. $a_{k-1}b_{k-1}$,where

$|V(G)| =k$, $|V(G_i)| = kt$for i=1 to k

$|E(G)| =k\ |E(G_i)|+k-1$,$d(b_i|G_{i+1}) = p$

$d(b_i,a_{i+1})= q$ then theorem 1, we have

$W(G)= kW(G_i)+tk(k-1)p + t^2[(k-1)+(k-2)(2+q)+(k-3)(3+2q)+\ldots\ldots+$

$[(k-1)+(k-2)q)]$

Proof:

Similar to theorem 1

The following Figure will provide better understanding of the above theorem.

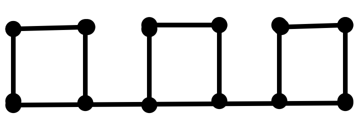


Fig.5

Here n =3, m =4 , p =4, q =1

W(G) = 200

CONCLUSION

In this paper, Wiener Index of chain graph is formulated. Using the above method,we can find the Wiener index of any graphs connected by means of edges one by one.

REFERENCES

[1] Ante Graovac, TomazPisanski,*On the Wiener index of a graph*, Journal of Mathematical Chemistry 8(1991)53-62

[2] Balakrishnan. R,.Sridharan. N, VishvanathanIyer.K, (2006), "*The Wiener index of odd graphs", J. Ind. Inst. Sci. 86(5)*

[3] Balakrishnan R. & Renganathan.K – A Text book of graph theory, springer – verlag New York, (2000)

[4] Ivan Gutman, Weigen Yan, Bo-YinYang, Yenong-Nan Yeh, Generalized Wiener indices of zigzagging pentachians, Journal of Mathematical Chemistry,Vol 42, No 2, Aug 2007, Springer

[5] PrabhakaraRao N, LaxmiPrasanna A, Wiener Indices of Pentachains, presented at National Conference on Discrete Mathematics and its applications, NCDMA 2007, Madurai,India

[6] Sen-PengEu, Bo-Yinang, Yeong-NanYeh Generalized Wiener Indices in Hexagonal Chains

[7] ***Gutman. I.; Yeh, Y.N.; Lee,*** S.L.; Luo, Y.L. *Some recent results in the theory of the Wiener number. Indian J. Chem*. 1993, 32A, 651–661

[8] Gutman. I, Polansky O. E., *Mathematical Concepts in Organic Chemistry, Springer-Verlag, Berlin, 1986*

[9] Harary. F, *Graph Theory* (Addison –Wesley, Reading MA , 1971).

[10] Wiener. H, *Structural determination of paraffin boiling points*- J.Amchem. Soc.69 (1947)17-20

[11] N. Trinajsti´c, *Chemical Graph Theory*, Vol. 2, CRC Press, Boca Raton (1983),

[12] F. Buckley and F. Harary, Distances in Graphs, Addison-Wesley (New York), 1990

[13] I. Gutman, *Wiener numbers of benzenoid hydrocarbons: Two theorems*, Chem. Phys. Letters, 136(1987) 134-136

[14] I. Gutman, J.W. Kennedy and L. V. Quintas, *Wiener numbers of random benzenoid chains*, Chemical Physics Letters, 173 (1990) 403–408.

[15] http://mathworld.wolfram.com/WienerIndex.