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Numerical Computation of Wiener Index for Bridge molecular structure in Medicines

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Abstract: — In this paper, we study Wiener Topological index for Bridge molecular graphs using Python Program.

Keywords: ***Bridge graph, Bridge molecular graph, Computational medical, topological index***

I. INTRODUCTION

The methods on topological index computation are very suitable for to test all biological properties of drugs without much lab facility .

A fast development of medicine production, a large amount of new medicines have been developed each day. Hence it demands a huge amount of research to determine pharmacological, chemical characteristics of new medicines, and such works become more and more huddle. It requires tools and supporter to test the performances and the side effects of existing new drugs[5]. Nevertheless, in undeveloped countries, there is no sufficient money to pay equipment which can be employed to calculate the biochemical properties. Providentially, many previous studies have pointed that compound and pharmacodynamics characteristics of drugs as well as their molecular structures are closely linked[6].

In Molecular graph, vertices are compounds and edges are bonds between compounds. It is undirected graph. Molecular structure of chemical compound is called molecular graph[5].

In this paper, we use Python program to compute the Wiener index of a bridge molecular graph**.** The interested readers can check https://repl.it/MoYv/2 and https://repl.it/LmwA/9 for further information.

A. Wiener Index[1]:

The Wiener index of a graph G is defined by

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

where $d_G(u, v)$ is the distance between vertices u and v of G.

B. Bridge Molecular Graph[5] :

Let $\{G_i\}^d$ be a set of finite Molecular graphs with vertices v_i. The Bridge Molecular graph $B(G_1 ,G_2....G_d,v_1,v_2,....v_d)$ of $\{G_i\}^d$ with respect to the vertices $\{v_i\}^d$, from the Molecular graphs $G_1 ,G_2....G_d$ in which the vertices v_i and v_{i+1} are connected by an edge for i=1,2...d-1.

C. Theorem:

For the bridge molecular graph $G_d(K_3,v)$ the Wiener index is given by

$W(G_d(K_3,v))=E+(S+X)$

Where n=n*3

E=(n/3)-1+n

S=2((((n/3)-1)*5)-1)

X=C*(b-i)+X , i=(0 to m),

b=(n/3)+1,

m=(n/3)-1,X=1,c=4

c=c+8 if i=0

c=c+9 otherwise.

Then finally $W(G)= W(G_d(K_3,v))-1$

Here i ranges from 0 to m. E – Number of edges. Let K_3 be a complete graph of n vertices. Then it has (n/3)-1+n edges. Here we find Wiener Index for bridge graph, in which main part is complete graph with 3 vertices.

1.4 Program:

The following is the **Python** program to calculate Wiener for bridge molecular graph $\mathbf{G_d(K_3,v)}$**:**

```
Print("Enter number of  Triangle:")
N=int(input())
n=n*3
E=(n/3)-1+n
```

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```
S=2*((((n//3)-1)*5)-1)
 If(S<0):
   S=0
M=(n//3)-1
B=(n//3)+1
C=4
X=1
For i in range (0,m):
   X=C*(b-i)+X
   If (i==0):
      C=C+8
   Else:
      C=C+9
Temp=e+(S+X)
Print("Number of vertex : ",n)
Print("Number of Edges :",e)
Print("Wiener index      : ",temp-1)
```

Theorem 1.5:

For the bridge molecular graph $G_d(K_3,v)$ the Wiener index is given by

$W(G_d(K_3,v))=$

$$3d+(d-1)a+\sum_{i=1}^{l}(d-(i+1))(a+ib),(d>2)$$

where a=21, b=9, l=|E|-|V|

Where d is the number of complete graphs with 3 vertices (K_3). |E| is the number of edges. If number of vertices 3 of a bridge molecular graph then d difference between number of edges and number of vertices is 0. Hence $W(G_d(K_3,V)= |E|$. That is 3.

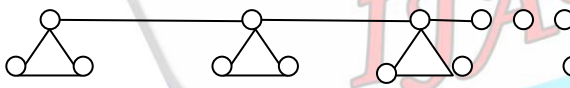

Figure 1: Bridge Molecular Graph $G_d(K_3,v)$

1.6 Table for Wiener Index of Bridge molecular graph $G_d(K_3,v)$:

S.No	Number of vertices n	Number of edges |E|	Wiener Index W(G)
1	n=3	|E|=3	W(G)=3
2	n=6	|E|=7	W(G)=27
3	n=9	|E|=11	W(G)=81
4	n=12	|E|=15	W(G)=174
5	n=15	|E|=19	W(G)=315
6	n=18	|E|=23	W(G)=513
7	n=21	|E|=27	W(G)=777
8	n=24	|E|=31	W(G)=1116
9	n=27	|E|=35	W(G)=1539
10	n=30	|E|=39	W(G)=2055

2.1 Bridge Cyclic Molecular graph $G_d(C_n,v)$[5]:

Let C_n be the cycle with n vertices. Then $G_d(C_n,v)$ is a bridge molecular graph in which d copies of C_n are present in such a way that successive C_n 's are connected by an edge.

2.2 Theorem :

For the bridge molecular graph $G_d(C_4,v)$ the Wiener index is given by

$W(G_d(C_4,v))$

$$=8d+(d-1)a+\sum_{i=1}^{l}(d-(i+1))(a+ib),(d>2)$$

where a=48, b=16, l=|E|-|V|

2.3 Program:

Python program to calculate Wiener index for bridge molecular graph $G_d(C_4,v)$.

```
a=48``````
res=0
n=int(input())
if(n>1):
  for I in range(n,1,-1):
  res=((i-1)*a)+res
  a=a+16
res=res+(n*8)
print(res)
```

2.3 Theorem :

For the bridge molecular graph $G_d(C_6,v)$ the Wiener index is given by

$W(G_d(C_6,v))=$

$$27d+(d-1)a+\sum_{i=1}^{l}(d-(i+1))(a+ib),(d>2)$$

where a=144, b=36, l=|E|-|V|

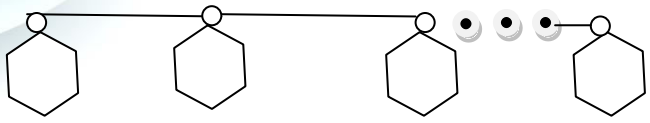

Figure 2: Bridge Cyclic Molecular Graph $G_d(C_6,v)$

2.3 Program:

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Python program to calculate Wiener index for bridge molecular graph $G_d(C_6,v)$.

```
a=144
res=0
n=int(input())
if(n>1):
  for i in range(n,1,-1):
  res=((i-1)*a)+res
  a=a+36
res=res+(n*27)
print(res)
```

2.4 Table for Wiener Indices of Bridge molecular graph:

S.No	Number of Hexagon	Wiener Index	Number of Hexagon	Wiener Index
1	n=1	W(G)=27	n=6	W(G)=3042
2	n=2	W(G)=198	n=7	W(G)=4473
3	n=3	W(G)=549	n=8	W(G)=6264
4	n=4	W(G)=1116	n=9	W(G)=8451
5	n=5	W(G)=19	n=10	W(G)=110
		35		70

Conclusion:

The Wiener Topological index is established to the complete graphs with three vertices, cyclic graph with four vertices and cyclic graph with six vertices respectively.

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