COMPUTATION OF ZAGREB INDEX FOR COMPLEX GRAPH STRUCTURE

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Abstract : In this paper we present the first and second Zagreb topological indices of widely used Complex chemical structures. The results obtained in this paper have prospects for application in the chemical.

IndexTerms - Computation index; topological index; bipartite index;

I. INTRODUCTION

Chemical graph theory is a branch of Mathematical Chemistry in which different tools from graph theory are used to model Chemical phenomena mathematically. Molecules and molecular compounds are modelled as molecular graphs, in which the vertices correspond to the atoms and the edges correspond to the chemical bonds between the atoms. A topological index is a numeric value that is graph invariant and correlates the physico-chemical properties of a molecular graph. Topological indices are used for studying quantitative structure-activity relationships (QSAR) and quantitative structure property relationships (QSPR) for predicting different properties of chemical compounds and their biological activities. In chemistry, biochemistry and nanotechnology, different topological indices are found to be useful in isomer discrimination, QSAR, QSPR and pharmaceutical drug design. There are several studies regarding different topological indices of special molecular graphs, a few of which we mention [3-10].

These indices were introduced in a paper in 1972 [2] to study the structure-dependency of the total amount of p-electron energy in conjugated systems. It was found that the Zagreb indices provided a measure of the underlying molecules of carbon skeleton branching. For more information and recent results about Zagreb indices, see [11-15].

2. Definition:

2.1 The First Zagreb Index [1]:

The first Zagreb index of a graph G is defined by

$$M_1(G) = \sum_{v\in V(G)} d_G(v)^2 \text{ or } M_1(G) = \sum_{vu\in E(G)} \left| d_G(u) + d_G(v) \right|$$

where $d_G(v)$ is the degree of vertex v in G.

2.2 Theorem:

The first Zagreb index of the Cartesian product $K_{m,n} \times P_r$ is given by

$$M_1(K_{m,n} \times P_r) = 2[2m(m+1)^2] + (d-2)[(m+n)(m+2)^2]$$

Where d is number of copies of bipartite graphs and d>1

Proof:

When m=2, n=2,and d=2 we get $M_1(K_{2,2}\times P_2)=72$.
d=3 we get $M_1(K_{2,2}\times P_3)=136$.
d=4 we get $M_1(K_{2,2}\times P_4)=200$ and so on.
When m=3, n=3,and d=2 we get $M_1(K_{3,3}\times P_2)=192$.
d=3 we get $M_1(K_{3,3}\times P_3)=342$.
d=4 we get $M_1(K_{3,3}\times P_4)=492$ and so on.
When m=4, n=4,and d=2 we get $M_1(K_{4,4}\times P_2)=400$.
d=3 we get $M_1(K_{4,4}\times P_3)=688$.
d=4 we get $M_1(K_{4,4}\times P_4)=976$ and so on.
When m=5, n=5,and d=2 we get $M_1(K_{5,5}\times P_2)=720$.
d=3 we get $M_1(K_{5,5}\times P_3)=1210$.
d=4 we get $M_1(K_{5,5}\times P_4)=1700$ and so on.
Hence proceeding like this we get

$$M_1(K_{m,n} \times P_r) = 2[2m(m+1)^2] + (d-2)[(m+n)(m+2)^2]$$

2. 3 Python Program for First Zagreb index calculation of Cartesian Product $K_{m,n}\times P_r$

```
print("Enter M value : ")
m = int(input())
print("Enter D value : ")
d1 = int(input())
d1 = d1 + 1
n = m
```

```
M1G = 0
for d in range (2,d1):
  M1G = ((2*((2*m)*((m+1)*(m+1))))+((d-2)*(m+n)*((m+2)*(m+2))))
  print(M1G,end =",")
print("")
print("Final result is : ", M1G )
```

2.4 Table for First Zagreb Index of Cartesian Product $K_{9,9}\times P_r$:

S.No	Number of $K_{9,9}$	The Second Zagreb Index	Number of $K_{9,9}$	The Second Zagreb Index
1	d=2	$M_2(G)$=3600	d=7	$M_2(G)$=14490
2	d=3	$M_2(G)$=5778	d=8	$M_2(G)$=16668
3	d=4	$M_2(G)$=7956	d=9	$M_2(G)$=18846
4	d=5	$M_2(G)$=10134	d=10	$M_2(G)$=21024
5	d=6	$M_2(G)$=12312	d=11	$M_2(G)$=23202

3 The Second Zagreb Index [1]:

The Second Zagreb index of a graph G is defined by $M_2(G) = \sum_{uv\in E(G)} d_G(u)\, d_G(v)$ where $d_G(u)$ and $d_G(v)$ is the degree of vertex u and v in G.

3.1 Theorem:

The second Zagreb index of the Cartesian product $K_{m,n}\times P_r$ is given by

$$M_2(K_{m,n}\times P_r) = 2mn(m+1)^2 + [(d-2)mn + (d-3)2n](m+n)^2 + 2(m+n)(m+1)(m+2)$$

Where d is number of copies of bipartite graphs.

Proof:

When m=2, n=2,and d=2 we get $M_2(K_{2,2}\times P_2)$=108.
d=3 we get $M_2(K_{2,2}\times P_3)$=232.
d=4 we get $M_2(K_{2,2}\times P_4)$=360 and so on.

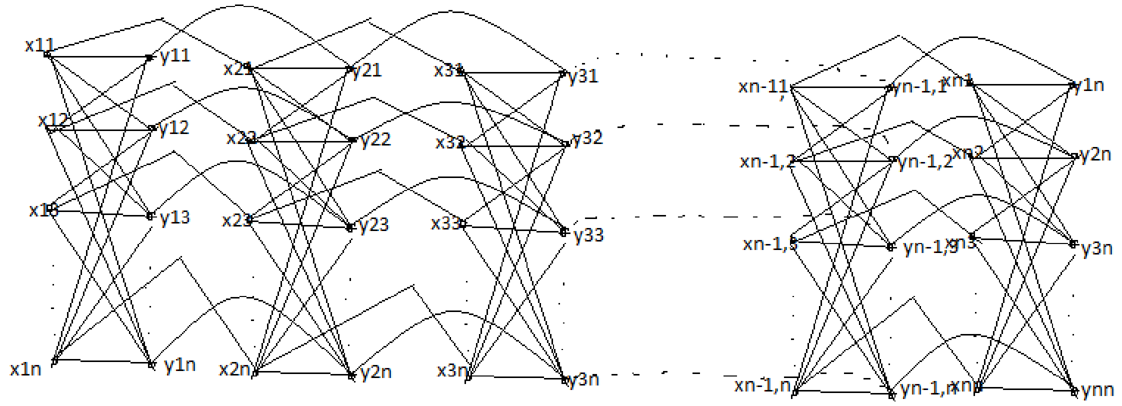
When m=3, n=3,and d=2 we get $M_2(K_{3,3}\times P_2)$=384.
d=3 we get $M_2(K_{3,3}\times P_3)$=753.
d=4 we get $M_2(K_{3,3}\times P_4)$=1128 and so on.

When m=4, n=4,and d=2 we get $M_2(K_{4,4}\times P_2)$=1000.
d=3 we get $M_2(K_{4,4}\times P_3)$=1856.
d=4 we get $M_2(K_{4,4}\times P_4)$=2720 and so on.

When m=5, n=5,and d=2 we get $M_2(K_{5,5}\times P_2)$=2640.
d=3 we get $M_2(K_{5,5}\times P_3)$=3865.
d=4 we get $M_2(K_{5,5}\times P_4)$=5580 and so on.

Hence proceeding like this we get

$$M_2(K_{m,n}\times P_r) = 2mn(m+1)^2 + [(d-2)mn + (d-3)2n](m+n)^2 + 2(m+n)(m+1)(m+2)$$



Cartesian Product Kn,n *Pr

3.2 Python Program for Second Zagreb index calculation of Cartesian Product $K_{m,n}\times P_r$

```
print("Enter M value : ")
m = int(input())
print("Enter D value : ")
d1 = int(input())
```

```
d1 = d1 + 1
n = m
M2G = 0
for d in range (2,d1):
  M2G = (((2*m*n)*((m+1)*(m+1)))+ ((((d-2)*m*n)+((d-3)*2*n))*((m+2)*(m+2))) + (2*(m+n)*(m+1)*(m+2)))
  if(d==2):
    M2G = M2G + m + n
  print(M2G,end =",")
print("")
print("Final result is : ", M2G )
```

3.3 Table for Second Zagreb Index of Cartesian Product $K_{4,4}\times P_r$:

S.No	Number of $K_{4,4}$	The Second ZagrebIndex	Number of $K_{4,4}$	The Second ZagrebIndex
1	d=2	$M_2(G)$=1000	d=7	$M_2(G)$=5312
2	d=3	$M_2(G)$=1856	d=8	$M_2(G)$=6176
3	d=4	$M_2(G)$=2720	d=9	$M_2(G)$=7040
4	d=5	$M_2(G)$=3584	d=10	$M_2(G)$=7904
5	d=6	$M_2(G)$=4448	d=11	$M_2(G)$=8768

Conclusion:

The First and Second Zagreb Topological index is established to the complex structure graph, that is Cartesian product of complete bipartite graph and path graph with two vertices, three vertices, four vertices and any number of vertices.

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