International Journal of Mathematical Archive-9(5), 2018, 164-167
Available online through www.ijma.info ISSN 2229 – 5046

VARIOUS TOPOLOGICAL INDEX OF DENDRIMER NANOSTARS AND SOME FULLERENE GRAPH

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(Received On: 11-04-18; Revised & Accepted On: 14-05-18)

ABSTRACT

In this study Wiener index, Harary index, first Zagreb index, second Zagreb index, first Zagreb coindex, and second Zagreb coindex of dendrimer nanostar and some fullerence graphs have been calculated using Matlab program.

Keywords: *distance sum, nanostar, fullerence graphs.*

2010 Mathematics Subject Classification: *68R10.*

1. INTRODUCTION

A Graph G is formally defined to be a pair [V(G,E(G)] where V(G) is a non empty finite set of elements called vertices and E(G) is a finite set of unordered pairs of elements of V(G) called edges. Molecular graphs represent the constitution of molecules [14]. They are generated using the following rule: Vertices stand for atoms and edges for bonds. A graph theoretical distance d(u, v) between the vertices u and v of the graph G is equal to the length of the shortest path that connects u and v. An invariant of a graph G is a number associated with G that has the same value for any graph isomorphic to G. If G is a molecular graph then the corresponding invariants are called molecular descriptor or topological indices and they are used in theoretical chemistry for the design of so called Quantitative Structure Property Relations (QSPR) and Quantitative Structure Activity Relations (QSAR). One of the oldest topological index is Wiener index and is defined as the half of the sum of all the distances between every pair of vertices of G.[15]
ie

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

The Harary index of a molecular graph G, denoted by H(G), has been introduced by Plavsic *et al*. [10] and by Ivanciuc *et al.* [8] in 1993 for the characterization of molecular graphs. It has been named by Plavsicetal. [10] the Harary index in honour of Professor Frank Harary on the occasion of his 70th birthday. Ivanciuc [8] called it initially the reciprocal distance sum index, but later they also adopted the suggested name [7]. Nowadays the name Harary index is generally accepted (e.g., [2]).The Harary index is defined as follows:

$$H(G)=\sum_{\substack{v_i,v_j\in V(G)\\ i\neq j}} 1/d(v_i,v_j)$$

where the summation goes over all unordered pairs of vertices of G.

An edge of G connecting the vertices x, y is denoted by xy. The degree of a vertex v denoted by deg(v) is the number of edges incident to v. A vertex of degree 1 is called a pendent vertex.

The Zagreb indices have been introduced more than forty years ago by Gutman and TrinajstIc [4, 5] which are the most known and widely studied topological indices [1, 6, 9, 16, 17, 18]. The first Zagreb index of G is defined as

$$M_1(G)=\sum_{u\in E(G)}\deg^2(u)$$

while the second Zagreb index of G is defined as

$$M_2(G)=\sum_{uv\in E(G)}\deg(u)\deg(v)$$

It should be pointed out that the Zagreb indices and their variants are useful molecular descriptors which found considerable use in QSPR and QSAR studies as summarized by Todeschini and Consonni [12, 13]. Several graph invariants based on vertex eccentricities attract some attention in chemistry and subject to large number of studies.

When the sum of the degrees of the vertices of G run over the edges of the complement of G, We get Zagreb coindices. These were introduced by Doslic in [3] in 2008 to express vertex-weighted Wiener polynomials of composite graphs and are defined by

$$\overline{M_1}(G) = \sum_{uv \notin E(G)} \deg(u) + \deg(v)$$

and

$$\overline{M_2}(G) = \sum_{uv \notin E(G)} \deg(u).\deg(v)$$

There is a common confusion that the Zagreb coindices of G are the Zagreb indices of the complement of G. Indeed the sums run over the edges of $\overline{G}$.

Among all these topological indices Wiener index and Harary index are distance based and other indices are degree based topological indices. Degree based topological indices can be calculated from the adjacency matrix and from the adjacency matrix, the distance based topological indices can be easily calculated by using the new distance matrix algorithm [11]. But the only complexity is that for graph G with more number of vertices it is hard to give the input adjacency list. To overcome this complexity we can define the general form of adjacency matrix of some graphs. By replacing adjacency matrix formation part of the program by this general form of adjacency matrix we can calculate the distance based and degree based topological indices of the corresponding graphs. In the following sections we define general form of adjacency matrix of dendrimer nanostar and fullerenes c_{12k+4} using MATLAB.

2. VARIOUS TOPOLOGICAL INDICES OF DENDRIMER NANOSTAR

Dendrimers are highly ordered branched macromolecules which have attracted much theoretical and experimental attention. The nanostar dendrimer is part of a new group of macromolecules that seem photon funnels just like artificial antennas and also, it is a great resistant of photo bleaching..General form of Adjacency matrix of dendrimer nanostar G[n] is explained in the following MATLAB program and is illustrated in figure 1.

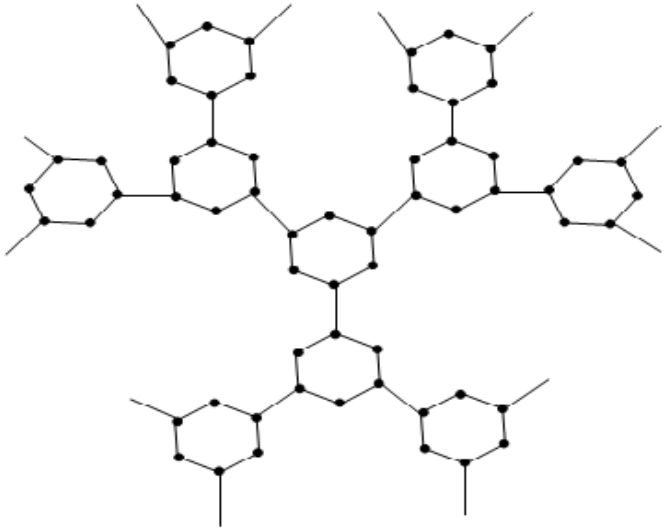

Figure-1: The dendrimer nanostar $G[n]$.

```
%PROGRAM TO CALCULATE THE ADJACENCY MATRIX OF DENDRIMER NANOSTAR
m=input('number of growth')
A=[];
n=18*2^(m-1)-12;
for i=1:18*2^(m-1)-12
   if rem(i,6)==0
      A(i,i-5)=1;A(i-5,i)=1;
   else
      A(i,i+1)=1;A(i+1,i)=1;
   end
end
```

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```
   count=-1;j=1;k=7;
   while j<18*2^(m-2)-12
      A(j,k)=1;A(k,j)=1;
      j=j+2;k=k+6;count=count+1;
      if count~=0&rem(count,2)==0
         j=j+2;
      end
   end
A
```

Illustration

n	W	H	M_1	M_2	$\overline{M_1}$	$\overline{M_2}$
3	14526	3.370948e+002	330	393	7812	8964
5	649890	3.218387e+003	1554	1869	174996	203436
8	87813234	9.422342e+004	12978	15645	12234708	14267724

Table-1

3. VARIOUS TOPOLOGICAL INDICES OF FULLERENES C_{12K+4}

General form of Adjacency matrix of an infinite family of fullerenes C_{12K+4} is explained in the following MATLAB program and is illustrated in figure 2.

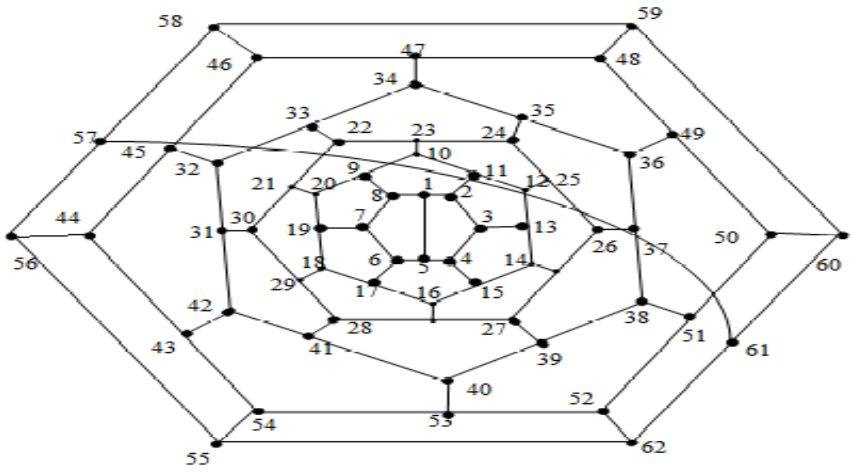

Figure-2: C_{12k+4}, $k = 6$

```
%%PROGRAM TO CALCULATE ADJACENCY MATRIX OF FULLERENES C12K+4
k=input('ENTER K VALUE')
n=12*k-8
A=[];
for i=1:12*k-9
   A(i,i+1)=1;A(i+1,i)=1;
      if i+1==8|i+1==12*k-8
         A(i+1,i-6)=1;A(i-6,i+1)=1;
      end
      if i==1|i==12*k-13
         A(i,i+4)=1;A(i+4,i)=1
      end
         if i>9&i<=12*k-30&rem(i,2)==0&rem(i,12)~=8
            A(i,i+13)=1;A(i+13,i)=1;
         end
            if ((rem(i,12)==9)|(i==4)|(i==6)|(i==12*k-22))&i<12*k-16
               A(i,i+11)=1;A(i+11,i)=1;
            end
            if i==7|i==12*k-24|i==12*k-26
               A(i,i+12)=1;A(i+12,i)=1;
            end
            if i==2
               A(i,i+9)=1;A(i+9,i)=1;
```

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```
        end
        if i==3|i==12*k-18|i==12*k-20
            A(i,i+10)=1;A(i+10,i)=1;
        end
end
```

Illustration

k	W	H	M_1	M_2	$\overline{M_1}$	$\overline{M_2}$
3	1198	1.513333e+002	252	378	2016	3024
5	5894	3.936508e+002	468	702	7488	11232
10	45206	1.242612e+003	1008	1512	36288	54432
15	151746	2.294823e+003	1548	2322	86688	130032
20	361486	3.475343e+003	2088	3132	158688	238032

Table-2

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Source of support: Nil, Conflict of interest: None Declared.

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