

ON THE DISTANCE-BASED TOPOLOGICAL INDICES OF FULLERENE AND FULLERENYL ANIONS HAVING DENDRIMER UNITS

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The distance-based topological indices of fullerene and fullerenyl anions having dendrimer units have been calculated

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1. Introduction

A topological index is a real number related to a structural graph of a molecule. It does not depend on the labeling or pictorial representation of a graph. In recent years there has been considerable interest in the general problem of determining topological indices of nanotubes, nanotori and fullerenes. It has been established, for example, that the Wiener and hyper-Wiener indices of polyhex nanotubes and tori are computable from the molecular graph of these structures. Accordingly, some of the interest has been focused on computing topological indices of these nanostructures. Let G be an undirected connected graph without loops or multiple edges, with the vertex set $V(G)$ and the edge set $E(G)$. The distance between two vertices x and y is denoted by $d(x,y)$. The Winer index $W(G)$ of G , which is the oldest topological index, is a distance based topological index and is defined as the sum of distances between all vertices of the graph:

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

There are some other distance based topological indices. The Hyper Wiener index $WW(G)$ of G is defined as

$$WW(G) = \frac{1}{2}W(G) + \frac{1}{4} \sum_{\{u,v\} \subseteq V(G)} d(u,v)^2.$$

Haruo Hosoya¹ introduced a distance-based polynomial, which he called the Wiener polynomial, related to each connected graph G as:

$$H(G,y) = \sum_{k \geq 0} d(G,k)y^k$$

where $d(G,k)$ is the number of pair vertices of G that are at distance k of each other. However, today it is called the Hosoya polynomial^{2,3}. It is easy to see that it is equal to $H(G,y) = \sum_{\{u,v\} \subseteq V(G)} y^{d(u,v)}$.

Hosoya polynomial has many interesting properties such as⁴

1. the degree of this polynomial equals the diameter of graph G ,
2. the coefficient of y in this polynomial equals the number of edges of G ,
3. the first derivative of this polynomial at $y=1$ is equal to the Wiener index,
4. the second derivative of $\frac{1}{2}yH(G,y)$ at $y=1$ is equal to the hyper-Wiener index.

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The diameter d of a graph is the largest topological distance between any two vertices, i.e. the largest $d(u, v)$ value in the distance matrix. Balaban and co-authors introduced the reverse Wiener index⁵. They showed that starting from the distance matrix and subtracting from d each $d(u, v)$ value, one obtains a new symmetrical matrix which, like the distance matrix, has zeroes on the main diagonal and, in addition, at least a pair of zeroes off the main diagonal corresponding to the diameter in the distance matrix. They obtained a general formula for reverse Wiener index of a graph G with N vertices and the diameter d as (see [5])

$$\Lambda(G) = \frac{1}{2} N(N-1)d - W(G).$$

Among the modifications of the Wiener index the Schultz index (Molecular Topological Index) that proposed by Schultz in⁶, appears to be one of the most studied topological indices. It is defined as

$$S(G) = \frac{1}{2} \sum_{\{u,v\} \subset V(G)} (\deg(u) + \deg(v))d(u, v)$$

where $\deg(u)$ is the degree of the vertex u , i.e. the number of the vertices joining to the vertex u . In addition to the chemical applications, the Schultz index attracted some attention after it was discovered that in the case of trees it is closely related to the Wiener index⁷. Klavzar and Gutman in [8] defined the modified Schultz index as

$$S^*(G) = \frac{1}{2} \sum_{\{u,v\} \subset V(G)} (\deg(u) \deg(v))d(u, v).$$

Let u and v be two adjacent vertices of the graph G and $e=uv$ be the edge between them. The Balaban index of a molecular graph G was introduced by Balaban in 1982 as one of less degenerated topological indices. It calculate the average distance sum connectivity index according to the equation

$$J(G) = \frac{Q}{\mu + 1} \sum_{uv \in E(G)} [d(u)d(v)]^{-0.5}$$

where Q is the number of edges in G and μ is the cyclomatic number of G and

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

The Harary index, $H = H(G)$, of a molecular graph G is based on the concept of reciprocal distance and is defined

$$H(G) = \sum_{\substack{\{u,v\} \subset V(G) \\ u \neq v}} \frac{1}{d(u, v)}$$

in parallel to the Wiener index⁹⁻¹¹, as the half-sum of the off-diagonal elements of the reciprocal molecular distance matrix. The reciprocal distance matrix can be simply obtained by replacing all off-diagonal elements of the distance matrix by their reciprocals. It should be noted that diagonal elements of the reciprocal matrix are all equal to zero by definition. This matrix was first mentioned by Balaban *et al.*¹²

FullereneC₆₀ is a spherically π -conjugated all-carbon molecule¹³ which can accept six electrons successively in solution. Thus, it is considered as one of the most attractive units for incorporation as a functional core in dendrimers. Actually, a C₆₀ cage has been used as a core as well as branches of the dendrimers. In all the dendrimers having a fullerene cage as a core reported so far, the dendrons are connected to the C₆₀ cages by a formal [2+1] cycloaddition like pattern A shown in Figure 1, including carbon, nitrogen, and iridium elements directly attached to the C₆₀ cage. On the other hand, C₆₀-based dendrimers with the addition pattern B are quite intriguing because the electronic and chemical properties of the central C₆₀ cage should be dramatically changed by abstraction of the proton directly attached to the C₆₀ cage¹⁵. Synthesis and properties of novel fullerene derivatives having dendrimer units G_nC₆₀H, n=1-4 and the fullerenyl anions G_nC₆₀, n=1-4 generated therefrom discussed in [16]

In this work compute several topological indices of the first C₆₀-based dendrimers having various generations of dendrons with the addition pattern B.



Fig. 1.

Programs for computing some distance-based topological indices and polynomials of any graph

In this section we compute distance-matrix of arbitrary graph G. Iranmanesh and his team wrote GAP programs for computing the PI and Szeged index of any graph. We continue this work and write a MATHEMATICA program to compute distance matrix of any graph which we can easily add a few simple lines to our program to compute some topological indices of graphs. For this purpose, the following algorithm is presented:

Let G be a graph. First we do numbering the vertices of the graph G, then for every vertex i, the set of vertices that their distance to this vertex are equal to t is denoted by D(i)(t). If we denote the set of all adjacent vertices of a vertex i in the graph, with f(i), then we have¹⁷

$$D(i)(t+1) = \bigcup_{j \in D(i)(t)} (f(j) - (D(i)(t) \cup D(i)(t-1))), t \geq 1.$$

Using this fact we can write a simple MATHEMATICA program to generating the distance matrix of any graph. Let $|V(G)|=m$, then after numbering the vertices and defining the adjacent vertices of any vertex by a function f, we can write this program

```
Diam=Table[dia[i], {i,1,m}];
For[i=1,i≤m,
  u={i};
  x[i,1]=f[i];
  u=Union[u,x[i,1]];
  s=1;
  t=1;
```

```

While[1 ≤ s ≤ m ,
  x[i,t+1] = {};
  For[k=1, k ≤ Length[x[i,t]],
    Com = Complement[f[x[i,t][[k]]], u];
    For[l=1, l ≤ Length[Com],
      AppendTo[x[i,t+1], Com[[l]]];
      l++;
    k++;
  u = Union[u, x[i,t+1]];
  If[x[i,t+1] == {}, s=0, s=1];
  If[x[i,t+1] ⊆ {}, dia[i]=t];
  t=t+1;
];
i++;

```

Now we are ready to write a program to generate the distance matrix of any graph.

```

Dis = Table[d[i,j], {i, 1, m}, {j, 1, m}];
For[i=1, i ≤ m,
  For[j=1, j ≤ m,
    For[k=1, k ≤ dia[i],
      If[i ⊆ j, d[i,j]=0];
      If[MemberQ[x[i,k], j], d[i,j]=k];
      k++;
    j++;
  i++;

```

Now we can add some lines to the above program to compute many topological polynomials and related topological indices of any graph. Such as

```

h[y_] := 1/2 * Sum[Sum[y^d[i,j], {i, 1, m}], {j, 1, m}];
S[y_] := 1/2 * Sum[Sum[(Length[f[i]] + Length[f[j]]) * y^d[i,j], {i, 1, m}], {j, 1, m}];
M[y_] := 1/2 * Sum[Sum[(Length[f[i]] * Length[f[j]]) * y^d[i,j], {i, 1, m}], {j, 1, m}];
p[y_] := y * h[y];
h[y] // Simplify
S[y] // Simplify
M[y] // Simplify
W = Function[y, h'[y]][1]
WW = 1/2 * Function[y, p''[y]][1]
RW = 1/2 * (m)(m-1) * Max[Diam] - W
Sch = Function[y, S'[y]][1]
ModSch = Function[y, M'[y]][1]
Q = CoefficientList[h[y], y][[2]]

```

where $h[y]$, $S[y]$, $M[y]$, W , WW , RW , $\text{Max}[\text{Diam}]$, Sch , ModSch and Q are the Hosoya polynomial, Schultz polynomial, Modified Schultz polynomial, Wiener index, hyper-Wiener index, reverse-Wiener index, the diameter, Schultz, Modified Schultz indices and number of edges of graph G .

Moreover we can add simple below programs for computing the Balaban index, Harary index, Connectivity index:

```

J=0;
H=0;
R=0;
dd[i_] := Sum[d[i,j], {j, 1, m}];

```

```

For[i=1,i≤ m,
  For[j=1,j≤ m,
    If[d[i,j]□1,J=J+(dd[i]*dd[j])^-0.5];
    If[i<j,H=H+1/d[i,j]];
    If[d[i,j]□1,R=R+(Length[f[i]]*Length[f[j]])^-0.5];
    j++;
  i++];
J=(Q)/(Q-m+2)*J(*this is the balaban index of graph*)
H/N(*this is the Harray index of graph*)
R=1/2*R(*this is the connectivity index*)

```

Some distance-based topological indices and counting polynomials of fullerene

In this section, using the programs in the previous section, we compute some topological indices and polynomials of fullerene as follows.

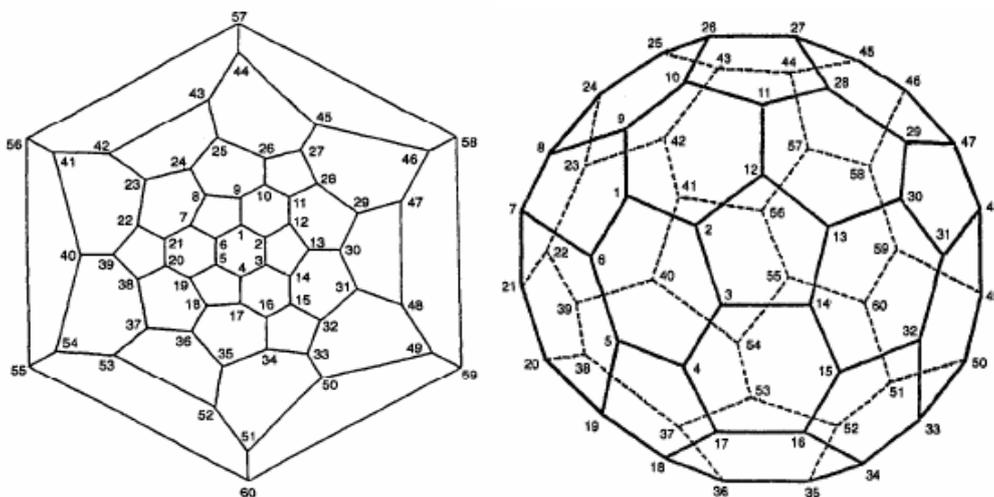


Fig. 2. Numbering for $[60-I_h]$ fullerene in 2D and 3D format (pictures taken from [18])

Firstly we number the fullerene vertices as shown in the Figure 2, and then we can write the following MATHEMATICA program

```

A=Table[a[i],{i,1,60}];
a[6]=1;
For[i=1,i≤5,
  If[EvenQ[i],a[i]=5*i/2+7,a[i]=5*(i-1)/2+9];
  i++];
For[i=7,i≤21,
  a[i]=Which[i□7,21,i□21,7,Mod[i,5]□4,2*(i-4)/5-1,Mod[i,5]□2,2*(i-2)/5-2,Mod[i,5]□3,6*(i-3)/5+18,Mod[i,5]□0,6*i/5+14,Mod[i,5]□1,6*(i-1)/5+16];
  i++];
For[i=22,i≤39,
  a[i]=Which[i□22,39,i□39,22,Mod[i,6]□5,5*(i-5)/6+27,Mod[i,6]□1,5*(i-1)/6+23,Mod[i,6]□3,5*(i-3)/6+25,Mod[i,6]□0,5*i/6-12,Mod[i,6]□2,5*(i-2)/6-10,Mod[i,6]□4,5*(i-4)/6-9];
  i++];
For[i=40,i≤54,
  a[i]=Which[i□40,54,i□54,40,Mod[i,5]□1,2*(i-6)/5+42,Mod[i,5]□4,2*(i-4)/5+41,Mod[i,5]□2,6*(i-2)/5-25,Mod[i,5]□0,6*i/5-27,Mod[i,5]□3,6*(i-3)/5-23];
  i++];
For[i=55,i≤60,

```

```

a[i]=Which[i□55,60,i□60,55,Mod[i,2]□0,5*i/2-99,Mod[i,2]□1,5*(i-1)/2-96];
i++;
f[i_]:=Which[i□1,{2,6,a[i]},i□60,{59,51,a[i]},2≤i≤59,{i-1,i+1,a[i]}];

```

Now we put $m=60$ in the programs of previous section, and run these programs. We summarized the outputs in the tables 1, 2.

Table 1. Counting polynomials of fullerene

Hosoya polynomial	$30(1+3y+6y^2+8y^3+10y^4+10y^5+10y^6+8y^7+3y^8+y^9)$
Schultz polynomial	$180(1+3y+6y^2+8y^3+10y^4+10y^5+10y^6+8y^7+3y^8+y^9)$
Modified Schultz polynomial	$270(1+3y+6y^2+8y^3+10y^4+10y^5+10y^6+8y^7+3y^8+y^9)$

Table 2. Topological indices of fullerene.

Wiener	Hyper-Wiener	Reverse-Wiener	Schultz	Modified Schultz	Balaban	Harray	Connectivity
8340	27180	7590	50040	75060	1.82104	493.869	30

Some distance-based topological indices and counting polynomials of G_nC_{60}

As another example, in this section, we compute some-topological indices and counting polynomials of fullerenyl anions having dendrimer units by use of our programs.

Note that in all the dendrimers having a fullerene cage as a core, the dendrons are connected to the C_{60} cages and it is easy to see that the number of all vertices of G_nC_{60} is $68+16(2^n-1)$.

First we do numbering all of vertices of G_nC_{60} . For this purpose we number the vertices of C_{60} cage as the same of previous section from 1 to 60 and since that the dendrimer units joint to the C_{60} cage at the vertex number 1, we label this vertex with $68+16(2^n-1)$. Now we continue the numbering from 61 to 67 as shown in the figure 3. Remaining vertices are separated in eight types A, B, C, D, E, F, G, and H. Note that the number of vertices of any above eight type is $2(2^n-1)$. We start with vertices of type A and label them, with numbers $68-67+2(2^n-1)$, of course $68-66+2^n$ for right hand and $67+2^n-67+2(2^n-1)$ for left hand vertices, and continue this numbering method respectively for vertices of other types as shown in the figure 5.

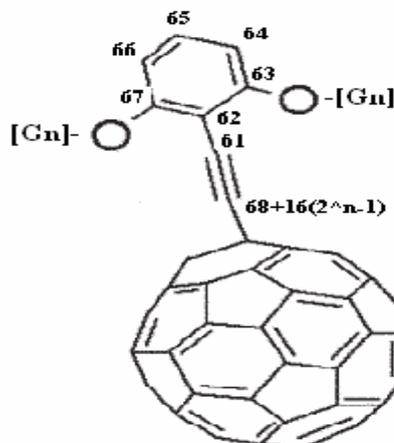


Fig. 3.

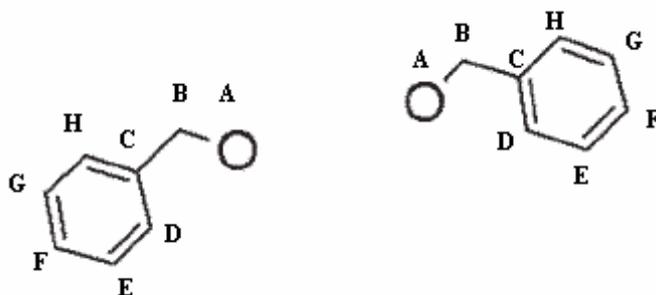


Fig. 4. Vertices of type A, B, C, D, E, F, G and H in the left and right hand dendrimer units.

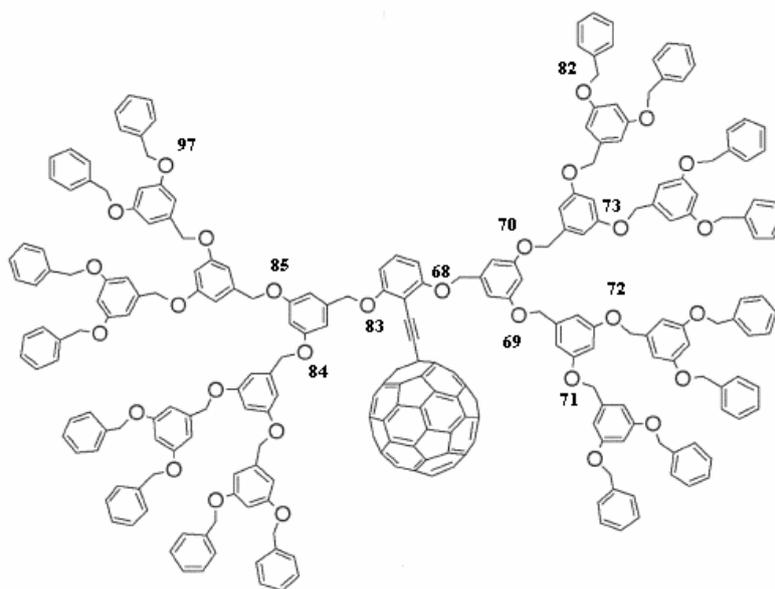


Fig. 5. G_4C_{60} and numbering of atoms.

Now we are ready to define the function $f[i]$ as follows.

```

A=Table[a[i],{i,1,60}];
a[6]=1;
For[i=1, i<=5,
  If[EvenQ[i],a[i]=5*i/2+7,a[i]=5*(i-1)/2+9];
  i++];
For[i=7, i<=21,
  a[i]=Which[i<=7, 21, i<=21, 7, Mod[i,5]<=4, 2*(i-4)/5-1, Mod[i,5]<=2, 2*(i-2)/5-2, Mod[i,5]<=3,
  6*(i-3)/5+18, Mod[i,5]<=0, 6*i/5+14, Mod[i,5]<=1, 6*(i-1)/5+16];
  i++];
For[i=22, i<=39,
  a[i]=Which[i<=22, 39, i<=39, 22, Mod[i,6]<=5, 5*(i-5)/6+27, Mod[i,6]<=1, 5*(i-1)/6+23,
  Mod[i,6]<=3, 5*(i-3)/6+25, Mod[i,6]<=0, 5*i/6-12, Mod[i,6]<=2, 5*(i-2)/6-10, Mod[i,6]<=4, 5*(i-4)/6-
  9];
  i++];
For[i=40, i<=54,
  a[i]=Which[i<=40, 54, i<=54, 40, Mod[i,5]<=1, 2*(i-6)/5+42, Mod[i,5]<=4, 2*(i-4)/5+41,
  Mod[i,5]<=2, 6*(i-2)/5-25, Mod[i,5]<=0, 6*i/5-27, Mod[i,5]<=3, 6*(i-3)/5-23];
  i++];
For[i=55, i<=60,
  a[i]=Which[i<=55, 60, i<=60, 55, Mod[i,2]<=0, 5*i/2-99, Mod[i,2]<=1, 5*(i-1)/2-96];

```

```

i++;
B=Table[b[i], {i,68,67+2*(2^n-1)}];
For[i=68, i<=67+2*(2^n-1),
b[i]=Which[i<=68, 63, i<=67+2^n, 67, n<=2&&69<=i<=66+2^n&&Mod[i,2]<=0, 67+12*(2^n-1)+(i-68)/2, n<=2&&69<=i<=66+2^n&&Mod[i,2]<=1, 67+8*(2^n-1)+(i-67)/2,
n<=2&&68+2^n<=i<=67+2*(2^n-1)&&Mod[i,2]<=0, 67+9*(2^n-1)+(i-(66+2^n))/2,
n<=2&&68+2^n<=i<=67+2*(2^n-1)&&Mod[i,2]<=1, 67+13*(2^n-1)+(i-(67+2^n))/2];
i++;
f[i_]:=Which[i<=68+16*(2^n-1), {1,61}, i<=1, {2,6,a[i], 68+16*(2^n-1), i<=60, {59,51,a[i]}, 2<=i<=59,
{i-1,i+1,a[i]}, i<=61, {68+16*(2^n-1), 62, 62<=i<=63, {i-1,i+1,i+5}, 64<=i<=66, {i-1,i+1}, i<=67, {62,66,68+2^n-1}, 68<=i<=67+2*(2^n-1), {b[i],i+2*(2^n-1)}, 68+2*(2^n-1)<=i<=67+4*(2^n-1)||68+6*(2^n-1)<=i<=67+8*(2^n-1), {i-2*(2^n-1),i+2*(2^n-1)}, 68+4*(2^n-1)<=i<=67+6*(2^n-1), {i-2*(2^n-1),i+2*(2^n-1),i+10*(2^n-1)}, n<=2&&68+8*(2^n-1)<=i<=67+9*(2^n-1)-2^(n-1), {i-2*(2^n-1), i+2*(2^n-1),2*(i-67-8*(2^n-1))+67}, 68+9*(2^n-1)-2^(n-1)<=i<=67+9*(2^n-1), {i-2*(2^n-1), i+2*(2^n-1), n<=2&&68+9*(2^n-1)<=i<=67+10*(2^n-1)-2^(n-1), {i-2*(2^n-1),i+2*(2^n-1),2*(i-67-9*(2^n-1))+66+2^n}, 68+10*(2^n-1)-2^(n-1)<=i<=67+10*(2^n-1)||68+10*(2^n-1)<=i<=67+12*(2^n-1), {i-2*(2^n-1),i+2*(2^n-1)}, n<=2&&68+12*(2^n-1)<=i<=67+13*(2^n-1)-2^(n-1), {i-2*(2^n-1),i+2*(2^n-1),2*(i-67-12*(2^n-1))+68}, 68+13*(2^n-1)-2^(n-1)<=i<=67+13*(2^n-1), {i-2*(2^n-1),i+2*(2^n-1), n<=2&&68+13*(2^n-1)<=i<=67+14*(2^n-1)-2^(n-1), {i-2*(2^n-1),i+2*(2^n-1),2*(i-67-13*(2^n-1))+67+2^n}, 68+14*(2^n-1)-2^(n-1)<=i<=67+14*(2^n-1), {i-2*(2^n-1), i+2*(2^n-1)}, 68+14*(2^n-1)<=i<=67+16*(2^n-1), {i-2*(2^n-1),i+10*(2^n-1)}];

```

Now if we put $m=68+16(2^n-1)$ in our programs then we have following results that summarized in tables 3-6.

Table3. Hosoya polynomial.

n=1	$42+117y+217y^2+283y^3+347y^4+361y^5+384y^6+351y^7+221y^8+177y^9+166y^{10}+182y^{11}+181y^{12}+158y^{13}+130y^{14}+101y^{15}+66y^{16}+32y^{17}+10y^{18}+2y^{19}$
n=2	$58+153y+265y^2+331y^3+393y^4+413y^5+442y^6+419y^7+295y^8+253y^9+246y^{10}+282y^{11}+309y^{12}+306y^{13}+312y^{14}+337y^{15}+362y^{16}+368y^{17}+338y^{18}+294y^{19}+240y^{20}+172y^{21}+96y^{22}+36y^{23}+8y^{24}$
n=3	$90+225y+361y^2+427y^3+485y^4+517y^5+558y^6+555y^7+435y^8+397y^9+398y^{10}+450y^{11}+501y^{12}+506y^{13}+516y^{14}+553y^{15}+626y^{16}+704y^{17}+722y^{18}+750y^{19}+808y^{20}+868y^{21}+880y^{22}+796y^{23}+696y^{24}+592y^{25}+472y^{26}+352y^{27}+248y^{28}+184y^{29}+160y^{30}+160y^{31}+128y^{32}+64y^{33}+16y^{34}$
n=4	$154+369y+553y^2+619y^3+669y^4+725y^5+790y^6+827y^7+715y^8+685y^9+702y^{10}+786y^{11}+885y^{12}+890y^{13}+908y^{14}+969y^{15}+1090y^{16}+1248y^{17}+1298y^{18}+1342y^{19}+1432y^{20}+1604y^{21}+1776y^{22}+1772y^{23}+1861y^{24}+1952y^{25}+2120y^{26}+2240y^{27}+2120y^{28}+1928y^{29}+1728y^{30}+1520y^{31}+1280y^{32}+976y^{33}+800y^{34}+768y^{35}+832y^{36}+896y^{37}+832y^{38}+704y^{39}+640y^{40}+640y^{41}+512y^{42}+256y^{43}+64y^{44}$

Table 4. Schultz polynomial.

n=1	$243+668y+1258y^2+1647y^3+2036y^4+2120y^5+2240y^6+2011y^7+1219y^8+925y^9+870y^{10}+941y^{11}+924y^{12}+808y^{13}+665y^{14}+511y^{15}+332y^{16}+160y^{17}+50y^{18}+10y^{19}$
n=2	$306+836y+1474y^2+1867y^3+2248y^4+2356y^5+2516y^6+2327y^7+1555y^8+1296y^9+1254y^{10}+1433y^{11}+1544y^{12}+1560y^{13}+1617y^{14}+1743y^{15}+1864y^{16}+1860y^{17}+1698y^{18}+1474y^{19}+1188y^{20}+832y^{21}+448y^{22}+164y^{23}+36y^{24}$
n=3	$450+1172y+1906y^2+2307y^3+2672y^4+2828y^5+3068y^6+2943y^7+2195y^8+1952y^9+1942y^{10}+2225y^{11}+2424y^{12}+2472y^{13}+2545y^{14}+2767y^{15}+3160y^{16}+3468y^{17}+3602y^{18}+3794y^{19}+4084y^{20}+4376y^{21}+4344y^{22}+3940y^{23}+3444y^{24}+2888y^{25}+2288y^{26}+1632y^{27}+1096y^{28}+808y^{29}+704y^{30}+672y^{31}+512y^{32}+256y^{33}+64y^{34}$
n=4	$738+1844y+2770y^2+3187y^3+3520y^4+3772y^5+4172y^6+4175y^7+3475y^8+3264y^9+3318y^{10}+3809y^{11}+4152y^{12}+4232y^{13}+4337y^{14}+4655y^{15}+5368y^{16}+5964y^{17}+6226y^{18}+6482y^{19}+6996y^{20}+7928y^{21}+8552y^{22}+8708y^{23}+9044y^{24}+9704y^{25}+10624y^{26}+10896y^{27}+10248y^{28}+9288y^{29}+8208y^{30}+7168y^{31}+5760y^{32}+4368y^{33}+3600y^{34}+3456y^{35}+3480y^{36}+3968y^{37}+3584y^{38}+3072y^{39}+2816y^{40}+2688y^{41}+2048y^{42}+1024y^{43}+256y^{44}$

Table5. Modified Schultz polynomial

n=1	$334+963y+1835y^2+2414y^3+3003y^4+3120y^5+3274y^6+2896y^7+1684y^8+1269y^9+1120y^{10}+1193y^{11}+1151y^{12}+1006y^{13}+826y^{14}+624y^{15}+402y^{16}+192y^{17}+60y^{18}+12y^{19}$
n=2	$418+1155y+2081y^2+2666y^3+3243y^4+3396y^5+3598y^6+3260y^7+2066y^8+1665y^9+1588y^{10}+1801y^{11}+1923y^{12}+1974y^{13}+2066y^{14}+2224y^{15}+2354y^{16}+2300y^{17}+2092y^{18}+1804y^{19}+1428y^{20}+980y^{21}+512y^{22}+184y^{23}+40y^{24}$
n=3	$586+1539y+2573y^2+3170y^3+3723y^4+3948y^5+4238y^6+3964y^7+2798y^8+2401y^9+2388y^{10}+2721y^{11}+2931y^{12}+3014y^{13}+3130y^{14}+3464y^{15}+3938y^{16}+4268y^{17}+4484y^{18}+4748y^{19}+5124y^{20}+5428y^{21}+5288y^{22}+4800y^{23}+4168y^{24}+3464y^{25}+2696y^{26}+1856y^{27}+1216y^{28}+880y^{29}+768y^{30}+704y^{31}+512y^{32}+256y^{33}+64y^{34}$
n=4	$922+2307y+3557y^2+4178y^3+4683y^4+5052y^5+5518y^6+5372y^7+4262y^8+3873y^9+3988y^{10}+4545y^{11}+4899y^{12}+5030y^{13}+5146y^{14}+567y^{15}+6514y^{16}+7132y^{17}+7476y^{18}+7804y^{19}+8596y^{20}+9684y^{21}+10344y^{22}+10688y^{23}+11144y^{24}+12072y^{25}+13064y^{26}+13104y^{27}+12272y^{28}+10922y^{29}+9680y^{30}+8272y^{31}+6464y^{32}+4896y^{33}+4000y^{34}+3968y^{35}+4352y^{36}+4352y^{37}+3904y^{38}+3328y^{39}+3072y^{40}+2816y^{41}+2048y^{42}+1024y^{43}+256y^{44}$

Topological indices of G_nC_{60} .

	Wiener	Hyper-Wiener	Reverse-Wiener	Schultz	Modified Schultz	Balaban	Harray	Connectivity
n=1	25756	136534	40478	139446	187437	1.36362	723.288	41.877
n=2	73468	559318	86612	377278	480193	1.01808	1024.45	57.6749
n=3	261436	2753270	286304	1280814	1559913	0.78897	1710.8	89.2709
n=4	1085628	15400950	994604	5120974	6024505	0.646783	3403.34	152.463
n=5	4928956	90898294	3644408	22682766	26075097	0.544036	7877.29	278.846
n=6	23182268	533474678	13832132	105254158	119440153	0.460527	20496.7	531.614

References

- [1] H. Hosoya, *Discr. Appl. Math.* **19**, 239 (1988)
- [2] I. Gutman, *Publ. Elektrotehn. Fak. (Beograd), Ser. Mat.* **10**, 53 (1999).
- [3] D. Stevanovic, *Discr. Math.* **235**, 237 (2001).
- [4] Bruce E. Sagan, Yeong-Nan Yeh, and Ping Zhang *Internat. J. of Quantum Chem.* **60**, 959 (1996).
- [5] A.T. Balaban, D. Mills, O. Ivanciuc and S.C. Basak, *Croat. Chem. Acta* **73**(4), 923 (2000).
- [6] H.P. Schultz, *J. Chem. Inf. Comput. Sci.* **29**, 227 (1989)
- [7] D. J. Klein, Z. Mihalic, D. Plavsic, N. Trinajstic, *J. Chem. Inf. Comput. Sci.*, **32**, 304 (1992).
- [8] S. Klavzar, I. Gutman. *Disc. Appl. Math.* **80**, 73 (1997).
- [9] H. Wiener, *J. Am. Chem. Soc.* **69**, 17 (1947).
- [10] H. Hosoya, *Bull. Chem. Soc. Jpn.* **44**, 2332 (1971).
- [11] S. Nikolic, N. Trinajstic, and Z. Mihalic, *Croat. Chem. Acta* **68**, 105 (1995).
- [12] T. S. Balaban, P. A. Filip, and O. Ivanciuc, *J. Math. Chem.* **11**, 79 (1992)
- [13] A. Hirsch, Thieme, New York, **1994**.
- [14] Q. Wie, E. Perez-Cordero and L. Echegoyen, *J. Am. Chem. Soc.*, **114**, 3978 (1992).
- [15] Y. Murata, K. Motoyama, K. Komatsu and T. S. M. Wan, *Tetrahedron*, **52**, 5077 (1996).
- [16] Yasujiro Murata, Miho Ito and Koichi Komatsu *J. Mater. Chem.*, **12**, 2009 (2002).
- [17] A. Iranmanesh, Y. Alizadeh and B. Taherkhani, *Int. J. Mol. Sci.* **9**, 131 (2008)
- [18] E. W. Godly and R. Taylor, *Pure & Appl. Chem.*, **69** (7), 1411 (1997).