Iranian Journal of Mathematical Chemistry, Vol. 2, No. 2, December 2011, pp. 87 − 99 **IJMC**

PI, Szeged and Revised Szeged Indices of IPR Fullerenes

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(*Received August 12, 2011*)

ABSTRACT

In this paper PI, Szeged and revised Szeged indices of an infinite family of IPR fullerenes with exactly 60+12n carbon atoms are computed. A GAP program is also presented that is useful for our calculations.

Keywords: IPR fullerene, Szeged index, revised Szeged index, PI index.

1. INTRODUCTION

A (5,6)−fullerene is a cubic planar graph whose faces have sizes 5 or 6 having 12 pentagonal and (n/2 – 10) hexagonal faces, where 20 ≤ n (≠ 22) is an even integer. The discovery of the fullerene C_{60} in 1985 by Kroto and Smalley revealed a new form of existence of carbon element other than graphite, diamond and amorphous carbon [1,2]. We encourage the reader to consult [3−6] for more information on the mathematical properties of this important class of cubic graphs.

Throughout this paper the term "graph" means finite and simple graph. Chemical graphs are just graph-based descriptions of molecules, with vertices representing the atoms and edges representing the bonds. A numerical invariant associated with a chemical graph, if it is of chemical significance and/or applicability is called topological index. Between topological indices those are defined by distance function d(-,-) is called distance based topological index. Here, for arbitrary vertices u and v, the distance d(u,v) is defined as the length of a minimal path connecting u and v. The ***Wiener index,*** *W*, is the first topological index introduce by an American chemist Harold Wiener for investigating boiling points of

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alkanes [7]. After Wiener, many topological indices where proposed by chemist and also by mathematicians. The ***Padmakar-Ivan (PI) index*** was introduced by Padmakar-Khadikar. To explain, we assume that G is a graph and e = uv is and edge of G. Define $n_u(e)$ to be the number of edges of G lying closer to u than to v and $n_v(e)$ is defined analogously. The PI index is defined as PI(G) = $\sum_{e=uv}[n_u(e)+n_v(e)]$. The ***Szeged index*** is another topological indices was introduced by Ivan Gutman [8]. It is defined as Sz(G) = $\sum_{e=uv} n_u(e)n_v(e)$. We encourage the reader to consult paper [9] for more information about Szeged index.

Milan Randić [10] presented a modification of this topological index to find better applications in chemistry. Later [11] this modification was named the ***revised Szeged index***. It is defined as $Sz^*(G)=\sum_{e=uv}\left[n_u(e)+\frac{n_0(e)}{2}\right]\times\left[n_v(e)+\frac{n_0(e)}{2}\right]$, where $n_0(e)$ denotes the number of vertices equidistant from u and v. We refer the reader to papers [12−14] for mathematical properties, as well as chemical meaning of this topological index.

The aim of this paper is to compute these three indices for a class of IPR fullerenes with exactly 60 + 12n vertices. In papers [18−20] these three indices are computed for other IPR fullerenes with similar techniques.

2. COMPUTATIONAL DETAILS

In this section, a ***GAP*** program [21] is presented which is useful for computing the revised Szeged index of molecular graphs. The computer algebra system GAP is the most important group theoretical software for solving computational problems in group theory. Because of including GRAPE into GAP, this package is also useful for working with graphs. We apply this program to find some information about the problem and then prove our guess.

Suppose F is the molecular graph of an arbitrary n−vertex fullerene. The adjacency matrix of F is an n × n matrix A = $[a_{ij}]$ defined by a_{ij} = 1, if vertices i and j are connected by an edge and, a_{ij} = 0, otherwise. The distance matrix D = $[d_{ij}]$ of F is another n × n matrix in which d_{ij} is the length of a minimal path connecting vertices i and j, i ≠ j, and zero otherwise. To compute these three indices of F, we first draw F by ***HeperChem*** [22] and then apply ***TopoCluj*** software [23] of Diudea and his team to compute the distance matrices of this graph. Finally, we apply our GAP program to calculate these three indices of the fullerene graph F.

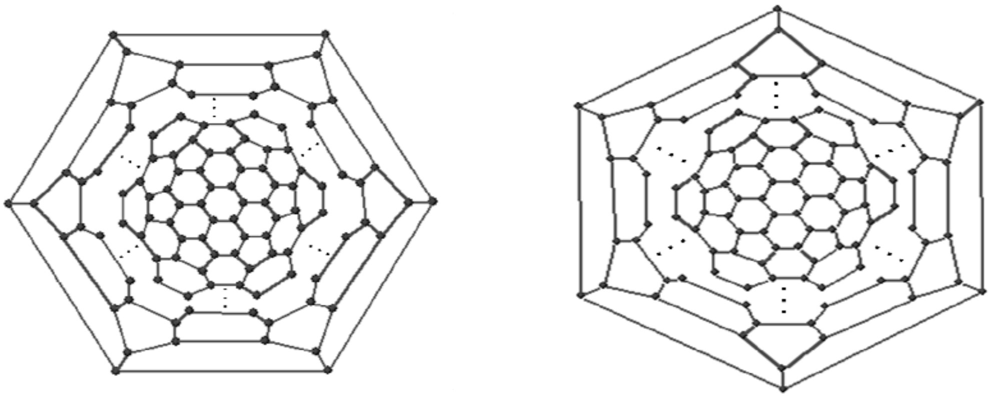
In what follows, we present a GAP program to compute PI, Szeged and revised Szeged indices.

A GAP Program for Computing Revised Szeged , Szeged and PI Index

```
f:=function(D)
local l,v,ss,s,t,k,e,w,x,ww,xx,a,i,j,ii,U,V,W;
l:=Length(D);v:=[];ss:=0;s:=[];t:=[];k:=[];e:=[];w:=[];x:=[];ww:=0;xx:=0;U:=[];V:=[];W:=[
];
 for i in[1..l]do
    for j in [i+1..l]do
         if D[i][j]=1 then
            Add(e,[i,j]);
         fi;
      od;
 od;
for a in e do
   for ii in [1..l]do
        if D[a[1]][ii]>D[a[2]][ii] then
            AddSet(s,ii);
         fi;
           if D[a[1]][ii]<D[a[2]][ii] then
             AddSet(t,ii);
           fi;
              if D[a[1]][ii]=D[a[2]][ii] then
                 AddSet(k,ii);
              fi;
       od;
          Add(U,Length(s));
          Add(V,Length(t));
          Add(W,Length(k));
          v:=(Length(t)+Length(k)/2)*(Length(s)+Length(k)/2);
          ss:=ss+v;
          w:=Length(t)*Length(s);
         ww:=ww+w;
         x:=Length(t)+Length(s);
       xx:=xx+x;
       s:=[];t:=[];k:=[];v:=[];x:=[];w:=[];
od;
Print("Revised Szeged INDEX is=",ss,"\n");Print("\n");
     Print("Szeged INDEX is=",ww,"\n");Print("\n");
         Print("Vertex PI INDEX is=",xx,"\n");Print("\n");
              Print("Number of vertex=",l,"\n");Print("\n");
                  Print("Number of edges=",Length(e),"\n");Print("\n");
                      Print("N1(e)=",U,"\n");Print("\n");
                          Print("N2(e)=",V,"\n");Print("\n");
                                Print("N0(e)=",W,"\n");
                                       Print("************************","\n");
end;
```

3. MAIN RESULTS AND DISCUSSION

Consider the fullerene C_{60+12n}, n ≥1, depicted in Figures 1 and 2. Apply our mentioned method for some small numbers of n. Using our program we obtain seven exceptional cases that n = 1, 2, 3, 4, 5, 6 and 7 for Szeged and revised Szeged indices and three exceptional cases that n = 1, 2 for PI index. Our method described in Section 2 is general and can be applied to compute these three of other molecular graphs.



(a) (b)

Figure 1. The Schlegel Graph of C_{60+12n} Fullerene, a) n is even; b) n is Odd.

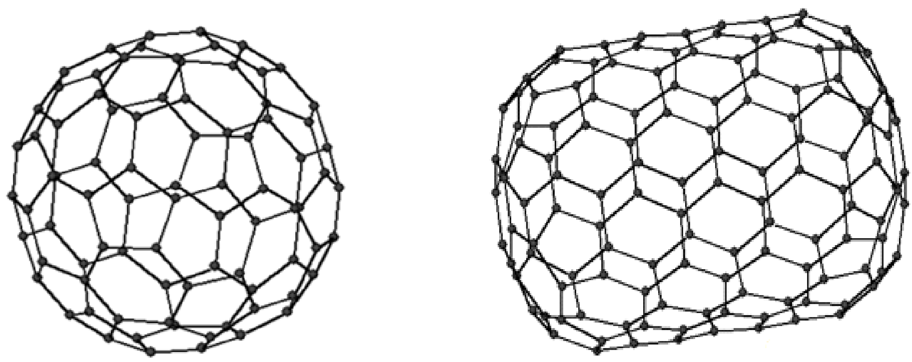


Figure 2. The Fullerene C_{72} (left) and C_{120} (right).

Suppose $G[n] = C_{60+12n}$, $1 \le n \le 7$. If e = uv is an edge of G[n] then the quantities $n_u(e)$, $n_v(e)$ and $n_0(e)$ are computed in Table 1. The eighth column of this table shows the number of edges of the given type.

To compute the revised Szeged index of G, we first consider the exceptional cases that n = 1, 2, 3, 4, 5, 6, 7. In Table 1, we apply our algorithm for every edge e of C_{72}, C_{84},

C_{96} ,C_{108}, C_{120}, C_{132} and C_{144} to compute the quantities $n_u(e)$, $n_v(e)$ and $n_0(e)$. In Figure 3, we partition edges of C_{72} fullerene into seven classes of edges such that $n_u(e)$, $n_v(e)$ and $n_0(e)$ are equal for edges of each class. The same is done in Figure 4, for the edges of C_{84} fullerene. We now apply definition of the revised Szeged index to compute this topological index for fullerenes C_{72}, C_{84}, C_{96}, C_{108}, C_{120}, C_{132} and C_{144}. We summarize our calculations in Table 1.

Table 1. The Values of N(e) for Different Types of Edges for $n \leq 7$.

C_{72}	C_{84}	C_{96}	C_{108}	C_{120}	C_{132}	C_{144}	No
34,34,4	-	46,46,4	-	58,58,4	-	-	12
-	42,42,0	-	-	-	-	-	30
-	-	-	54,54,0	-	-	-	36
-	-	-	-	-	66,66,0	-	42
-	-	-	-	-	-	70,70,4	24
25,35,12	30,38,16	33,43,20	38,46,24	41,51,28	46,54,32	49,59,36	12
24,32,16	34,34,16	36,34,26	46,34,28	48,34,38	58,34,40	60,34,50	24
-	-	40,40,16	-	52,52,16	58,58,16	64,64,16	12
28,28,16	-	-	-	-	-	-	24
-	30,30,24	-	42,42,24	-	54,54,24	-	12
-	36,34,14	-	-	-	-	-	48
32,32,8	-	-	-	-	-	-	12
-	-	44,44,8	-	-	-	-	24
-	-	-	-	56,56,8	-	-	48
28,32,12	-	-	-	-	-	-	24
-	-	-	-	64,44,12	76,44,12	88,44,12	24
-	-	38,42,16	-	-	-	-	48
-	-	42,42,12	-	-	-	-	12
-	-	-	54,40,14	66,40,14	78,40,14	90,40,14	24
-	-	-	48,50,10	-	-	-	24
-	-	-	46,46,16	-	-	-	6
-	-	-	52,42,14	-	-	-	24
-	-	-	-	-	66,60,6	-	24
-	-	-	-	-	54,72,6	54,84,6	24
-	-	-	-	-	-	78,62,4	24
-	-	-	-	-	-	68,68,8	48

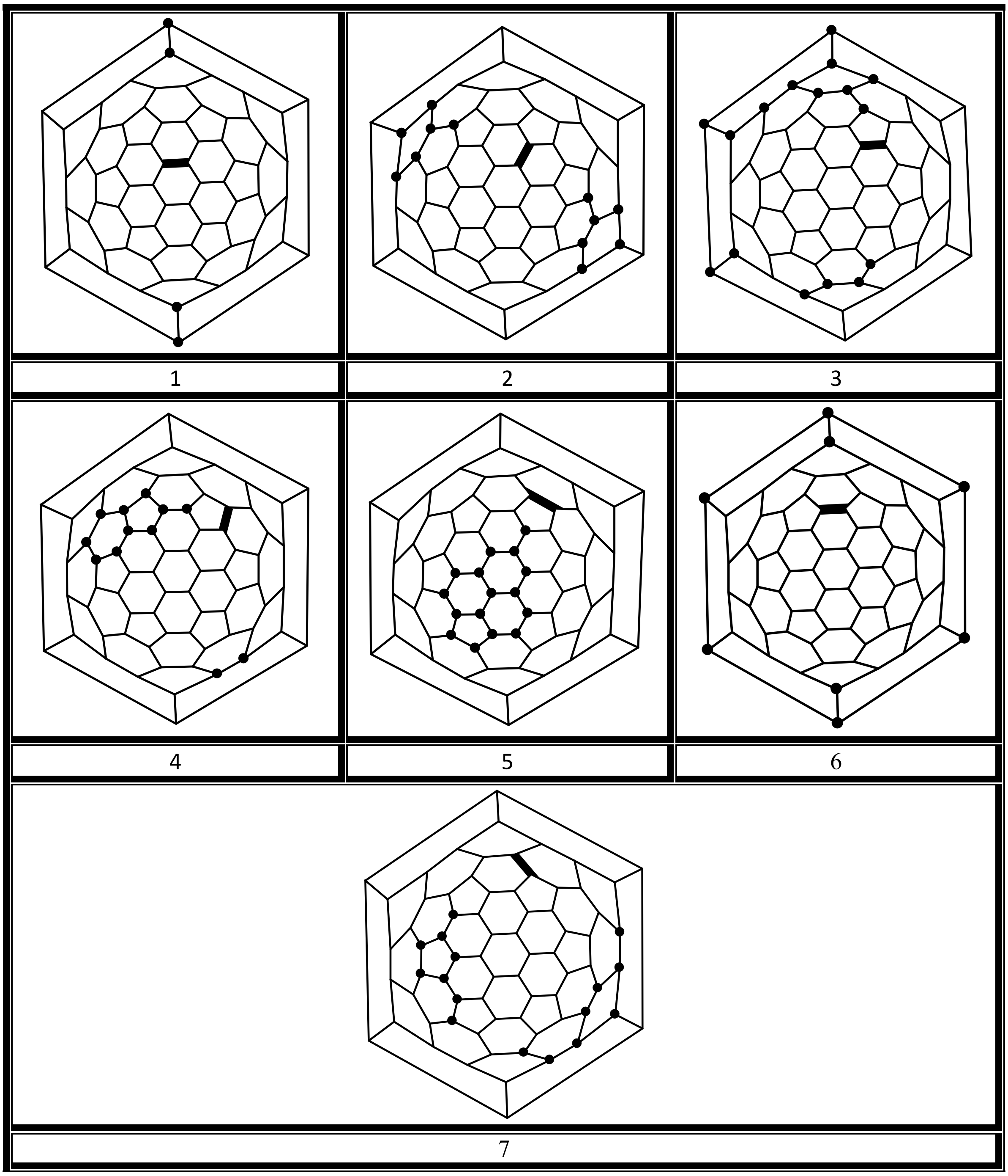


Figure 3. Seven Cases for the Vertices Equidistant from the Ends of an edge e $\in C_{72}$.

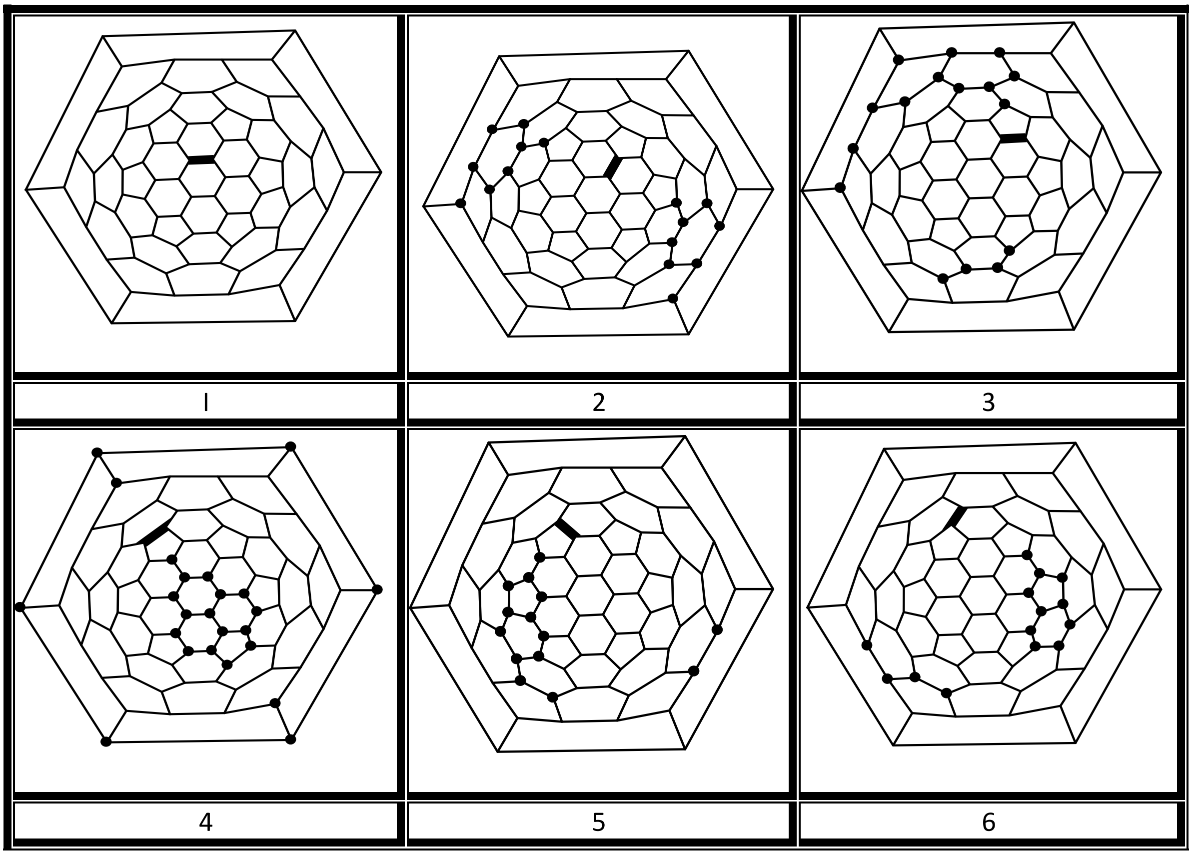


Figure 4. Six Cases for an Edge e and Vertices Equidistant from the Ends of e in C_{84}.

The following result is a direct consequence of our calculations given in Table 1:

Proposition 1:

a) The PI index of G[n] fullerene, $n \geq 3$, are computed as follows:

$$PI(G[n]) = \begin{cases} 216n^2 + 1920n + 4104 & , \ n \text{ is even} \\ 216n^2 + 1920n + 3612 & , \ n \text{ is odd} \end{cases},$$

b) The Szeged and revised Szeged indices of G[n] fullerene, $n \geq 8$, are computed as follows:

$$RSz(G[n]) = \begin{cases} 504n^3 + 8640n^2 + 62568n + 46368 & n \text{ is even} \\ 504n^3 + 8640n^2 + 62856n + 45588 & n \text{ is odd} \end{cases},$$

$$Sz(G[n]) = \begin{cases} 504n^3 + 7464n^2 + 48264n + 11496 & n \text{ is even} \\ 504n^3 + 7464n^2 + 47592n + 4812 & n \text{ is odd} \end{cases}.$$

Proof. We first assume that n ≥ 8 is even. In Figure 5, eleven separate cases for the edges of G[n] are depicted and in Table 2 the values of quantities n_u, n_v and n_0 are given. By calculations given this table, one can compute the Szeged and the revised Szeged indices of G[n], for even n. Next we assume that n ≥ 8 is odd. In Figure 6, twelve separate cases for the edges of G[n] are depicted and in Tables 3, the values of quantities n_u, n_v and n_0 are given. By these calculations, we can obtain the formulas given this result for the Szeged and revised Szeged indices of G[n] fullerenes. ♦

Proposition 2:

a)The PI index of G[n] fullerene, n =1,2, are computed as follows:

$$PI(G[n]) = \begin{cases} 6432 & n=1 \\ 9048 & n=2 \end{cases},$$

b) The Szeged and revised Szeged indices of G[n] fullerene, 1≤ n ≤7, are computed as follows:

$$RSz(G[n]) = \begin{cases} 139188 & n=1 \\ 222024 & n=2 \\ 331260 & n=3 \\ 469536 & n=4 \\ 639634 & n=5 \\ 841872 & n=6 \\ 1081836 & n=7 \end{cases} \quad \& \quad Sz(G[n]) = \begin{cases} 95412 & n=1 \\ 163896 & n=2 \\ 235236 & n=3 \\ 359208 & n=4 \\ 493428 & n=5 \\ 678936 & n=6 \\ 876612 & n=7 \end{cases}.$$

Table 2. The Values of N(e) for Different Types of Edges, when n is even & n ≥ 8.

Edges	**The Number of vertices Closer to u than to v, The Number of vertices Closer to v than to u and Equidistant Vertices**	***No***
1	6(n+5), 6(n+5),0	3(n+8)
2	4n+22,4n+30,4n+8	*12*
3	6n+22,34,6n+4	*24*
4	12n+6,40,14	*24*
5	6n+18,6n+18,24	*12*
6	6n+22,6n+22,16	*3(n-2)*
7	12n+4,44,12	*24*
8	12n,54,6	*24*
9	12n-6,62,4	*24*
10	12n-14,72,2	*24*
11	12(n – i),12(5 + i),0 n≥6 + 2i, i=2,3,…	*24*

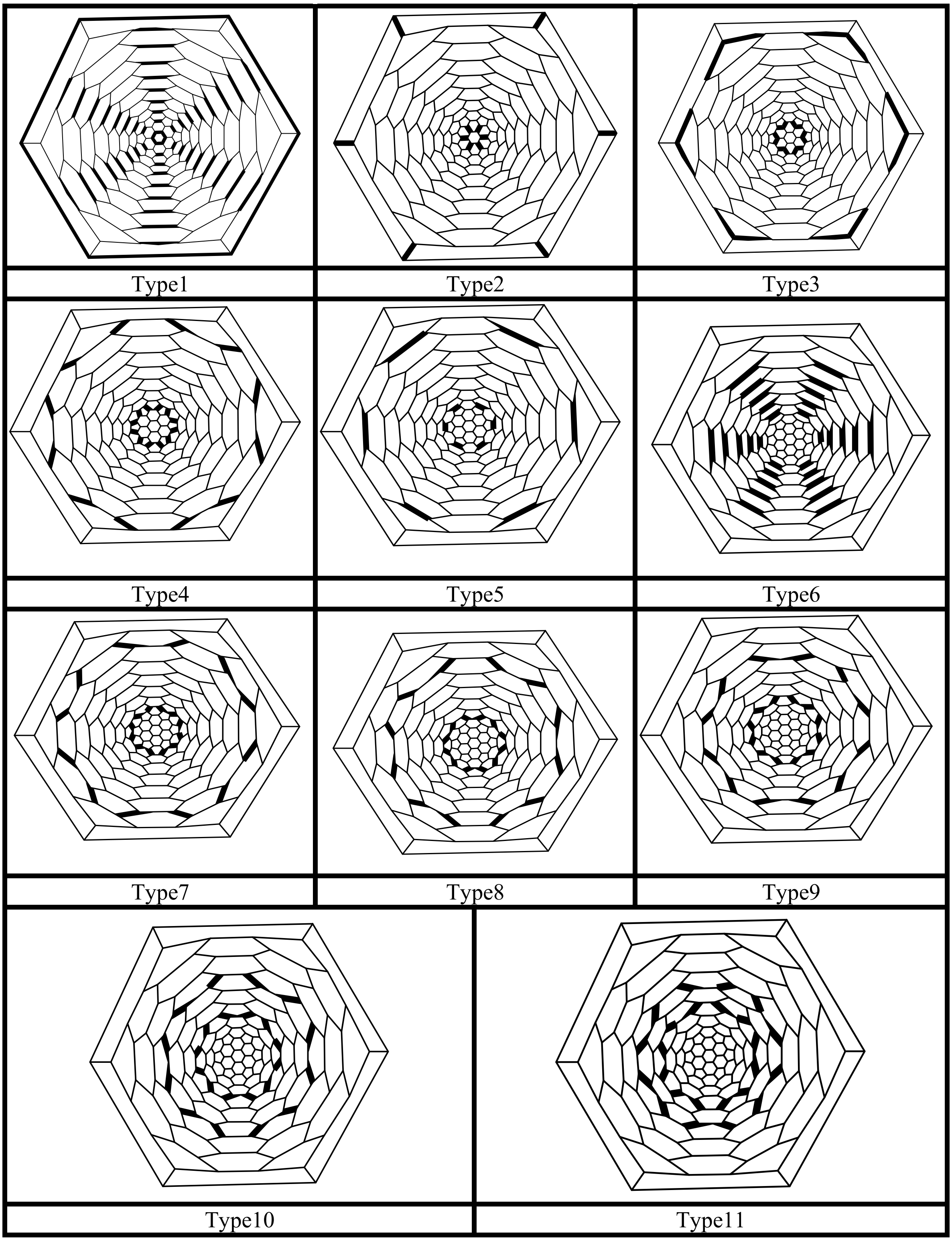


Figure 5. Eleven Different Types of Edges in C_{60+12n}Fullerene, 2|n.

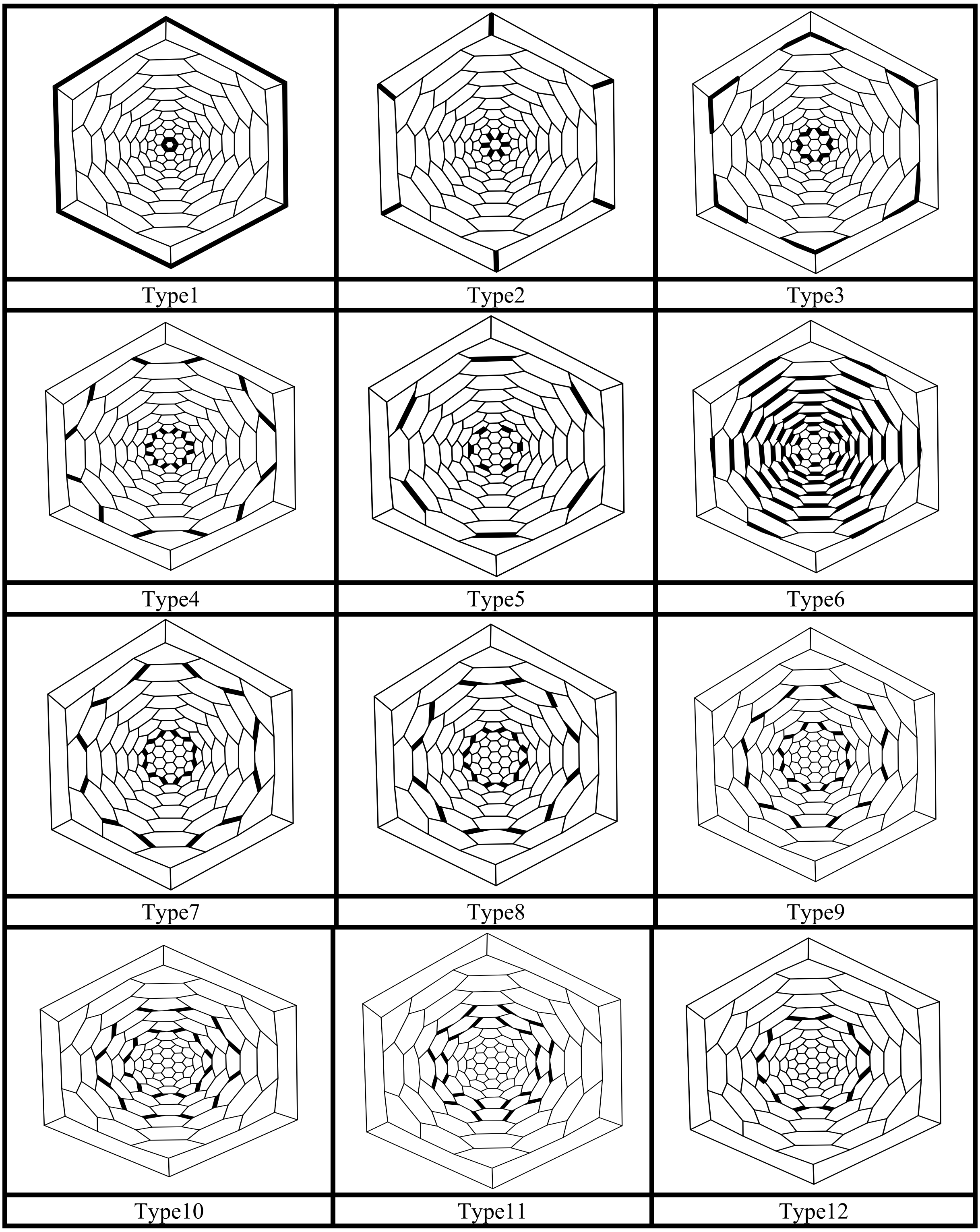


Figure 6. Twelve Different Types of Edges in C_{60+12n}Fullerene, 2łn.

Table 3. The Values of N(e) for Different Types of Edges, when n is odd & n ≥ 8.

Edges	**The Number of vertices Closer to u than to v, The Number of vertices Closer to v than to u and Equidistant Vertices**	*No*
1	6n + 18, 6n + 18, 4	12
2	4n + 21, 4n + 31, 4n + 8	12
3	6n + 18, 34, 6n + 8	24
4	12n + 6, 40, 14	24
5	6n + 22, 6n + 22, 16	12
6	6n + 26, 6n + 26, 8	6(n+1)
7	12n + 4, 44, 12	24
8	12n, 54, 6	24
9	12n – 6, 62, 4	24
10	12n – 14, 72, 2	24
11	12(n – i),12(5 + i),0.., n ≥ 6 + 2i , i = 2,3,…	24
12	6n + 30, 6n + 30, 0	12

4. CONCLUDING REMARKS

In this paper a new method for computing revised Szeged index of fullerene graphs is presented. Our results suggest that the fullerene graphs can be characterized by these numbers, up to isomorphism. So it is worth studying to think for a classification of fullerene graphs by these numbers.

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