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COMPUTATIONAL STUDY OF FULLERENES BY GAP

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The Wiener index W(G) is defined as the sum of distances between all pairs of vertices of the molecular graph G. In this paper, a GAP program is presented to compute the Hosoya polynomial, the Wiener and edge – Wiener indices G.

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1. Introduction

Mathematical calculations are absolutely necessary to explore important concepts in chemistry. Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is an important tool for studying molecular structures. This theory had an important effect on the development of the chemical sciences. In the past years, nanostructures involving carbon have been the focus of an intense research activity which is driven to a large extent by the quest for new materials with specific applications.

Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which are represented by V(G) and E(G), respectively. If x and y are two vertices of G then d(x,y) denotes the length of a minimal path connecting x and y. A topological index for G is a numerical quantity that is invariant under automorphisms of G. The Hosoya polynomial is the first distance-counting polynomial was introduced by Hosoya[1] as $H(G,x)=\sum_k d(G,k)\,x^k$. The Wiener index of a graph G, named after the chemist Harold Wiener[2], who considered it in connection with paraffin boiling points, is given by $W(G)=\sum_{\{x,y\}\subseteq V(G)} d_G(x,y)$, where d_G denotes the distance function in G. Besides its purely graph-theoretic value, the Wiener index has interesting applications in chemistry.[3-5]

Let G be a connected graph. Then the edge-Wiener index of G is defined as the sum of all distances (in the line graph) between all pairs of edges of G, i.e., $W_e(G)=\sum_{\{e,f\}\subseteq E(G)} d(e,f)$, where the distance between two edges is the distance between the corresponding vertices in the line graph of G.[6,7] Suppose $e=xy$ and $f=uv$. Then the first edge-Wiener number is defined as $W_{e,1}(G)=\sum_{\{e,f\}\subseteq E(G)} d_1(e,f)$, where $d_1(e,f)=\begin{cases} d_0(e,f)+1 & e\neq f \\ 0 & e=f \end{cases}$ and $d_0(e,f)=\min\{d(x,u),d(x,v),d(y,u),d(y,v)\}$. Obviously, $W_{e,0}(G)=W(L(G))$. The second

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edge-Wiener index of G is defined as $W_{e,1}(G) = \sum_{\{e,f\}\subseteq E(G)} d_2(e,f)$, where $d_2(e,f) = \begin{cases} d_3(e,f) & e \neq f \\ 0 & e = f \end{cases}$ and $d_3(e,f) = \max\{d(x,u), d(x,v), d(y,u), d(y,v)\}$.

The most important works on computing topological indices of nanostructures were done by Diudea and his co-authors.[8-13]. Ashrafi and his team continued this program to calculate the Wiener index of some other nanostructures.[14-22]. We encourage the reader to consult these papers and references therein for background material as well as basic computational techniques. Our notation is standard and mainly taken from standard books of graph theory and the books of Trinajestic.[5]

2. Main results and discussion

In this section, we first introduce a general method for computing the Hosoya polynomial, Wiener and edge Wiener indices of connected graphs. To do this, we first draw the molecule by HyperChem[23] and then compute the distance matrix of the molecular graph by TopoCluj.[24] Finally, we prepare a GAP[25] program for computing the line graph L(G), the Hosoya polynomial, Wiener and edge Wiener indices of any connected graph G. In Table 1, the Buckminster fullerene C_{60} is considered.

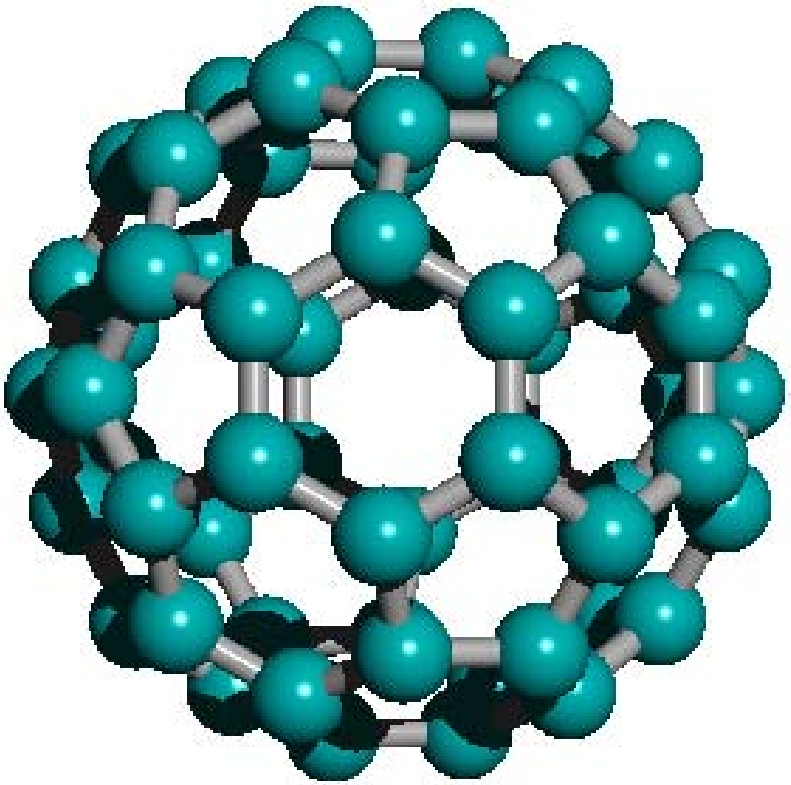

Fig. 1. Fullerene graph C_{60}.

Table1. The Values of the First Edge - Wiener Number, Second Edge - Wiener Number, W(L(G)) and W(G) for Fullerene C_{60}.

Fullerene	First Edge Wiener Number	Second Edge Wiener Number	W(L(G))	W(G)
C_{60}	39150	43650	39150	8340
	Hosoya Polynomial			
	$60+180x+360x^2+480x^3+560x^4+570x^5+480x^6+340x^7+260x^8+160x^9+100x^{10}+50x^{11}$			

A GAP Program for Computing The Hosoya Polynomial And Wiener Index

```
f:=function(M)
    local h,i,j,g,gg,a;
       h:=[];g:=[];gg:=[];
          for i in M do
              for j in i do
                  Add(h,j);
              od;
          od;
             Sort(h);
                 for i in h do
                     for j in h do
                             if j=i then
                                   Add(g,j);
                             fi;
                      od;
                       AddSet(gg,g);g:=[];
                 od;
                      for i in [1..Length(gg)-1] do
                            Print(Length(gg[i]),"x");
                                 Print(gg[i][1]);Print("+");
                      od;
                            a:=Length(gg);
                               Print(Length(gg[a]),"x");
                                  Print(gg[a][1],"\n");
                                     Print("**************************","\n");
                   Print("\n");
          return;
end;
```

A GAP Program for Computing the first and second edge-Wiener numbers and Wiener Index of L(G)

```
f:=function(M)
local l,s,ss,e,MM,MMM,w,sq,ssq,I,j,k,a,b,b1,b2,bb1,bb2,bbb1,bbb2,x,y;
l:=Length(M);s:=[];ss:=[];e:=[];MM:=[];MMM:=[];w:=0;sq:=0;ssq:=0;
for i in [1..l]do
for j in[i+1..l] do
                    if M[i][j]=1 then
                                Add(e,[i,j]);
                    fi;
```

```
            od;
od;
for a in e do
     for b in e do
          if a<> b then
  sq:=sq+Minimum(M[a[1]][b[1]],M[a[1]][b[2]],M[a[2]][b[1]],M[a[2]][b[2]])+1;
             ssq:=ssq+Maximum(M[a[1]][b[1]],M[a[1]][b[2]],M[a[2]][b[1]],M[a[2]][b[2]]);
         fi;
     od;
od;
Print("The first edge - Wiener number is: ", sq);Print("\n");Print("\n");
Print("The second edge - Wiener number is: ", ssq);Print("\n");
for a in e do
for b in e do
if a=b then Add(MM,0);
fi;
if  a<>b and ((Minimum(M[a[1]][b[1]],M[a[1]][b[2]])=0) or
(Minimum(M[a[2]][b[1]],M[a[2]][b[2]])=0)) then Add(MM,1);
                    fi;
if a<>b and ((M[a[1]][b[1]]>0) and (M[a[1]][b[2]]>0) and  (M[a[2]][b[1]]>0) and
(M[a[2]][b[2]]>0)) then Add(MM,0); fi;
           od;
     Add(MMM,MM);MM:=[];
od;
Print("The adjacency matrix of L(G) is: ");Print("\n");Print("\n");
Print(MMM);Print("\n");Print("\n");
l:=Length(MMM);
b2:=[];bb2:=[];bbb2:=[];b1:=[];bb1:=[];bbb1:=[];
           for x in [1..l] do
                    for y in [1..l] do
                              for k in [1..l] do
B2:=MMM^k;
                                        if B2[x][y]<>0 then
AddSet(b2,k);break;
fi;
                                od;
if y<=x then Add(bb2,0);
else
Add(bb2,b2[1]);
fi;
                         b2:=[];
od;
     Add(bbb2,bb2);bb2:=[];
od;
for i in bbb2 do
for j in i do
w:=w+j;
od;
od;
Print("\n");
Print("The W( L(G)) =: ", 2*w);Print("\n");Print("\n");
```

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