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A GAP PROGRAM FOR COMPUTING THE HOSOYA POLYNOMIAL AND WIENER INDEX OF NANO STRUCTURES

A. R. ASHRAFI, MODJTABA GHORBANI•
Institute of Nanoscience and Nanotechnology, University of Kashan, Kashan 87317-51167, I. R. Iran

The Wiener index W(G) is defined as the sum of distances between all pairs of vertices of the G. In this paper, we present a GAP program to Computing the Hosoya polynomial and the Wiener index of every graph. We also run this program to compute the Hosoya polynomial and the Wiener index of carbon nanocone CNC_4 [n] for n=1,2,…,8.

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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 numeric quantity that is invariant under automorphisms of G. A 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 in G. Besides its purely graph-theoretic value, the Wiener index has interesting applications in chemistry. We quote[3], which gives an extensive summary on the various works, and refer to [4] for further information on the chemical applications. In connection with certain investigations in mathematical chemistry, Schultz [5] considered a graph invariant that he called “molecular topological index” and whose essential part is the Schultz index S,

•Author to whom correspondence should be addressed.(E-mail: Modjtaba.ghorbani@gmail. com)

$S(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} (\delta_u + \delta_v) d(u,v)$. The modified Schultz index is defined as: $S^*(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} (\delta_u . \delta_v) d(u,v)$. By above equations, it is easy to construct graph polynomials having the property that their first derivatives at $x = 1$ are equal to the Schultz and modified Schultz indices. These polynomials are $S(G,x) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} (\delta_u + \delta_v) x^{d(u,v)}$ and $S^*(G,x) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} (\delta_u . \delta_v) x^{d(u,v)}$ respectively.

The most important works on computing topological indices of nanostructures were done by Diudea and his co-authors.[6-11]. Ashrafi continued this program to calculate the Wiener index of some other nanostructures.[12-17]. In some research papers the Wiener, hyper Wiener and Szeged indices of nanotubes and nanotori are computed. We encourage the reader to consult[18-20] and references therein for background material as well as basic computational techniques. In this paper, we continue this program to compute the Hosoya Polynomial and the Wiener index of carbon nano cone $CNC_4[n]$, Figure 1. Our notation is standard and mainly taken from standard books of graph theory and the books of Trinajestic.

2. Main results and discussion

Let D_i ($D_i \in \{0,1,...\}$) be the number of paths of length i in wiener matrix. So, the Hosoya polynomial and the Wiener index are $H(G,x) = \sum_{i=1}^{n-1} D_i x^i$ and $W(G) = \frac{1}{2} \sum_{i=1}^{n-1} iD_i$, respectively. Now suppose S_n and K_n denoted the star graph and complete graph, respectively.

Theorem1. $W(G) \le |E| \frac{n(n-1)}{2}$, with equality if and only if $G \cong K_2$.

Proof. for every i $|E(G)| = D_1 \ge D_i$ and so, $\frac{1}{2} \sum_{i=1}^{n-1} iD_i \le \frac{1}{2} \sum_{i=1}^{n-1} iD_1$, which completes the first part of our theorem. For second part, $W(G) = |E| \frac{n(n-1)}{4}$ if and only if for every i and j ($1 \le i, j \le n-1$), $D_i = D_j$ if and only if $G \cong K_2$.

Theorem2. $W(G) \ge \frac{n^2 - n}{4}$, with equality if and only if $G \cong K_n$.

Proof. Because for every i, i ≥ 1, then $W(G) \ge \frac{n(n-1)}{4}$ and this complete first part of theorem. For second part, $W(G) = \frac{n(n-1)}{4}$ if and only if for every i, $D_i=1$ if and only if $G \cong K_n$.

Theorem3. Let G be a fullerene graph. The Schultz and polynomial of G are as follow:

$$1)\, S(G,x)=\frac{1}{2}\sum_{\{u,v\}\subseteq V(G)}(\delta_u+\delta_v)x^{d(u,v)}=3\sum_{\{u,v\}\subseteq V(G)}x^{d(u,v)}=6H(G,x),$$

$$2)\, S(G)=\frac{1}{2}\sum_{\{u,v\}\subseteq V(G)}(\delta_u+\delta_v)d(u,v)=3\sum_{\{u,v\}\subseteq V(G)}d(u,v)=6\,W(G),$$

$$3)\, S^*(G,x)=\frac{1}{2}\sum_{\{u,v\}\subseteq V(G)}(\delta_u.\delta_v)x^{d(u,v)}=\frac{9}{2}\sum_{\{u,v\}\subseteq V(G)}x^{d(u,v)}=9H(G,x),$$

$$4)\, S^*(G)=\frac{1}{2}\sum_{\{u,v\}\subseteq V(G)}(\delta_u.\delta_v)d(u,v)=\frac{9}{2}\sum_{\{u,v\}\subseteq V(G)}d(u,v)=9\,W(G).$$

Proof. We know fullerenes are 3- regular graphs. Thus, for $u \in V(G)$, $\delta_u = 3$ and this complete the proof.

Now we compute the Hosoya polynomial and the Wiener Index of any Connected graph. To do this, we first draw the molecule by HyperChem[21] and then compute the distance matrix of the molecular graph by TopoCluj.[22] Finally, we prepare a GAP[23] program for computing the Hosoya polynomial and the Wiener Index of any graph. In Table 1 we compute the Hosoya polynomial and the Wiener Index of Carbon nanocones $CNC_4[n]$ for n=1,2,…,8.

Table 1. Values of $W(CNC_4[n])$ and $H(CNC_4[n])$, for $1 \le n \le 8$.

n	Hosoya Polynomial of $CNC_4[n]$	Wiener Index
1	$4+8x+4x^2$	20
2	$16+40x+60x^2+64x^3+44x^4+24x^5+8x^6$	384
3	$36+96x+164x^2+208x^3+220x^4+208x^5+160x^6+112x^7+60x^8+24x^9+8x^{10}$	2744
4	$64+176x+316x^2+424x^3+492x^4+528x^5+520x^6+480x^7+388x^8+296x^9+196x^{10}+120x^{11}+64x^{12}+24x^{13}+8x^{14}$	11704
5	$100+280x+516x^2+712x^3+860x^4+968x^5+1024x^6+1040x^7+996x^8+912x^9+764x^{10}+616x^{11}+456x^{12}+328x^{13}+212x^{14}+120x^{15}+64x^{16}+24x^{17}+8x^{18}$	35912
6	$144+408x+764x^2+1072x^3+1324x^4+1528x^5+1672x^6+1768x^7+1796x^8+1776x^9+1684x^{10}+1544x^{11}+1328x^{12}+1112x^{13}+876x^{14}+680x^{15}+492x^{16}+336x^{17}+216x^{18}+120x^{19}+64x^{20}+24x^{21}+8x^{22}$	89620
7	$256+736x+1404x^2+2008x^3+2540x^4+3008x^5+3400x^6+3728x^7+3972x^8+4152x^9+4244x^{10}+4272x^{11}+4208x^{12}+4080x^{13}+3852x^{14}+3560x^{15}+3164x^{16}+2768x^{17}+2344x^{18}+1976x^{19}+1604x^{20}+1280x^{21}+980x^{22}+720x^{23}+512x^{24}+336x^{25}+216x^{26}+120x^{27}+64x^{28}+24x^{29}+8x^{30}$	378736
8	$324+936x+1796x^2+2584x^3+3292x^4+3928x^5+4480x^6+4960x^7+5348x^8+5664x^9+5884x^{10}+6032x^{11}+6080x^{12}+6056x^{13}+5924x^{14}+5720x^{15}+5404x^{16}+5016x^{17}+4512x^{18}+4008x^{19}+3468x^{20}+2992x^{21}+2508x^{22}+2080x^{23}+1672x^{24}+1312x^{25}+996x^{26}+720x^{27}+512x^{28}+336x^{29}+216x^{30}+120x^{31}+64x^{32}+24x^{33}+8x^{34}$	683016

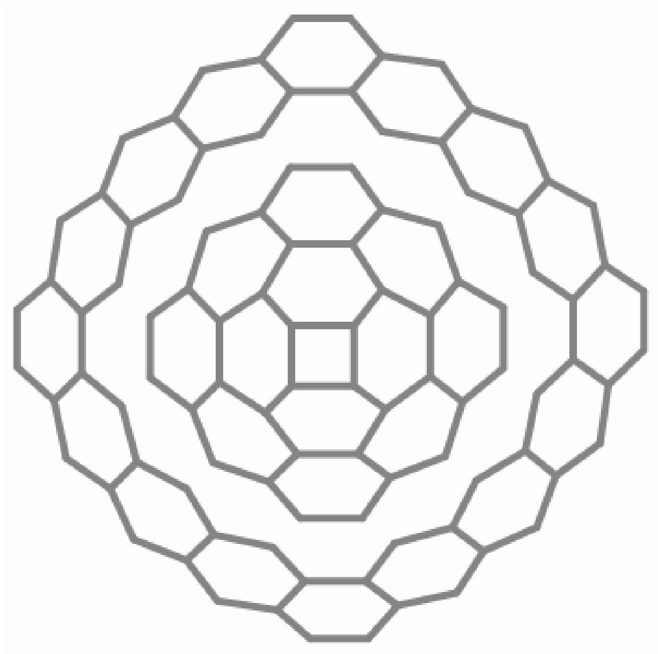

Fig. 1. The graph of Carbon Nanocones $CNC_4[n]$.

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;
```

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