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

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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 \( n=1,2,\ldots,8 \). 

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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 \( H(G,x) = \sum d(G,k)x^k \). 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 
\( W(G) = \sum_{(x,y) \in V(G)} d_G(x,y) \), 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 \( S \),

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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

$$S'(G, x) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} (\delta_u \cdot \delta_v) x^{d(u,v)}$$

respectively.

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

$$H(G, x) = \sum_{i=0}^{n-1} D_i x^i$$

and

$$W(G) = \frac{1}{2} \sum_{i=1}^{n-1} i D_i,$$

respectively. Now suppose $S_n$ and $K_n$ denoted the star graph and complete graph, respectively.

**Theorem 1.** $W(G) \leq E \left| \frac{n(n-1)}{2} \right|$, with equality if and only if $G \cong K_2$.

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

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

**Proof.** Because for every $i, i \geq 1$, then $W(G) \geq \frac{n(n-1)}{4}$ 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 $G \cong K_n$.

**Theorem 3.** Let $G$ be a fullerene graph. The Schultz and polynomial of $G$ are as follow:

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

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

**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 $\text{CNC}_4[n]$ for $n=1,2,\ldots,8$.

### Table 1. Values of $W(\text{CNC}_4[n])$ and $H(\text{CNC}_4[n])$, for $1 \leq n \leq 8$.

<table>
<thead>
<tr>
<th>n</th>
<th>Hosoya Polynomial of $\text{CNC}_4[n]$</th>
<th>Wiener Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$4+8x+4x^2$</td>
<td>20</td>
</tr>
<tr>
<td>2</td>
<td>$16+40x+60x^2+44x^3+24x^4+8x^5$</td>
<td>384</td>
</tr>
<tr>
<td>3</td>
<td>$36+96x+164x^2+208x^3+160x^4+112x^5+60x^6+24x^7+8x^8$</td>
<td>2744</td>
</tr>
<tr>
<td>4</td>
<td>$64+176x+316x^2+424x^3+528x^4+520x^5+480x^6+388x^7+296x^8+196x^{10}+120x^{11}+64x^{12}+24x^{13}+8x^{14}$</td>
<td>11704</td>
</tr>
<tr>
<td>5</td>
<td>$100+280x+516x^2+712x^3+860x^4+968x^5+1024x^6+996x^7+912x^8+764x^{10}+616x^{11}+456x^{12}+328x^{13}+212x^{14}+120x^{15}+64x^{16}+24x^{17}+8x^{18}$</td>
<td>35912</td>
</tr>
<tr>
<td>6</td>
<td>$144+408x+764x^2+1072x^3+1324x^4+1528x^5+1672x^6+1768x^7+1796x^8+1776x^9+1684x^{10}+1544x^{11}+1328x^{12}+1112x^{13}+876x^{14}+680x^{15}+492x^{16}+336x^{17}+216x^{18}+120x^{19}+64x^{20}+24x^{21}+8x^{22}$</td>
<td>89620</td>
</tr>
<tr>
<td>7</td>
<td>$256+736x+1404x^2+2008x^3+2540x^4+3008x^5+3400x^6+3728x^7+3972x^8+4152x^9+4244x^{10}+4272x^{11}+4208x^{12}+4080x^{13}+3852x^{14}+3560x^{15}+3164x^{16}+2768x^{17}+2344x^{18}+1976x^{19}+1604x^{20}+1280x^{21}+980x^{22}+720x^{23}+512x^{24}+336x^{25}+216x^{26}+120x^{27}+64x^{28}+24x^{29}+8x^{30}$</td>
<td>378736</td>
</tr>
<tr>
<td>8</td>
<td>$324+936x+1796x^2+2584x^3+3292x^4+3928x^5+4480x^6+5348x^7+5664x^8+5884x^{10}+6032x^{11}+6080x^{12}+6056x^{13}+5924x^{14}+5720x^{15}+5404x^{16}+5016x^{17}+4512x^{18}+4008x^{19}+3468x^{20}+2992x^{21}+2508x^{22}+2080x^{23}+1672x^{24}+1312x^{25}+996x^{26}+720x^{27}+512x^{28}+336x^{29}+216x^{30}+120x^{31}+64x^{32}+24x^{33}+8x^{34}$</td>
<td>683016</td>
</tr>
</tbody>
</table>
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:=[ ]); 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("************************");
    Print("n");
    return;
end;
References