MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **62** (2009) 353-362

ISSN 0340 - 6253

The Vertex PI, Szeged and Omega Polynomials of Carbon Nanocones $CNC_4[n]$

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(Received May 24, 2008)

Abstract

A topological index of a graph G is a numeric quantity related to G which is invariant under automorphisms of G. A new counting polynomial, called the "Omega" W(G, x) polynomial, was recently proposed by Diudea on the ground of quasi-orthogonal cut "qoc" edge strips in a polycyclic graph. In this paper, the vertex PI, Szeged and omega polynomials of carbon nanocones $CNC_4[n]$ are computed.

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.[26] This theory had an important effect on the development of the chemical sciences.

We first describe some notations which will be kept throughout. 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. Suppose G is a connected molecular graph and x, y $\in$ V(G). The distance d(x,y) between x and y is defined as the length of a minimum path between x and y. Two edges e = ab and f = xy of G are called codistant, “e co f”, if and only if d(a,x) = d(b,y) = k and d(a,y) = d(b,x) = k+1 or vice versa, for a non-negative integer k. It is easy to see that the relation “co” is reflexive and symmetric but it is not necessary to be transitive.

Set C(e):= {f ∈ E(G) | f co e}. If the relation “co” is transitive on C(e) then C(e) is called an orthogonal cut “oc” of the graph G. The graph G is called co-graph if and only if the edge set E(G) a union of disjoint orthogonal cuts. If any two consecutive edges of an edge-cut sequence are *topologically parallel* within the same face of the covering, such a sequence is called a *quasi-orthogonal cut qoc* strip. The Omega polynomial Ω(G,x) for counting qoc strips in G was defined by Diudea as $\Omega(G,x)=\sum_c m(G,c)\cdot x^c$ with m(G,c) being the number of strips of length c. The summation runs up to the maximum length of *qoc* strips in *G*. If G is bipartite then a qoc starts and ends out of G and so $\Omega(G,1)=r/2$, in which r is the number of edges in out of G.[7-16]

A topological index of a graph G is a numeric quantity related to G. The oldest topological index is the Wiener index which introduced by Harold Wiener.[27] Padmakar Khadikar[22,23] defined a new topological index and named it Padmakar-Ivan (PI) index as $PI(G) = \sum_{e=uv\in E(G)}[m_u(e|G)+ m_v(e|G)]$, where $m_u(e|G)$ is the number of edges of G lying closer to u than to v and $m_v(e|G)$ is the number of edges of G lying closer to v than to u. Edges equidistant from both ends of the edge uv are not counted. Khalifeh et al[24] introduced a vertex version of PI index, named the vertex PI index and abbreviated by PI_v. This new index is defined as $PI_v(G) = \sum_{e=uv\in E(G)}[n_u(e|G)+ n_v(e|G)]$, where $n_u(e|G)$ is the number of vertices of G lying closer to u and $n_v(e|G)$ is the number of vertices of G lying closer to v.

The Szeged index is another topological index introduced by Ivan Gutman.[17,19] To define the Szeged index of a graph G, we consider the values $n_u(e|G)$ and $n_v(e|G)$ defined in last paragraph. Then the Szeged index of the graph G is defined as $Sz(G) = \sum_{e=uv\in E(G)}n_u(e|G)n_v(e|G)$. Notice that vertices equidistance from u and v are not taken into account.

The aim of this paper is to compute the vertex PI, Szeged polynomials and omega polynomial of carbon nanocones $CNC_4[n]$. Throughout this paper, our notation is standard. We encourage the reader to consult papers by Ashrafi et al[1-6] and Iranmanesh et al[20,21].

2. Main Result and Discussion

In this section the Vertex PI and Szeged polynomials and omega polynomial of one-tetragonal carbon nanocone $S = CNC_4[n]$ were computed.

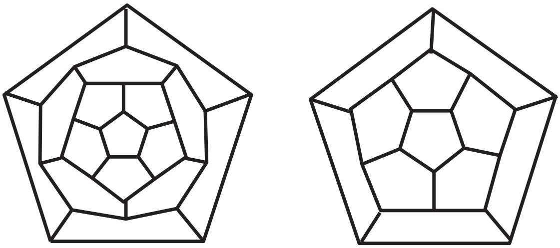

Figure 1. (a) The Fullerene Graph C_{30} .
(b) The Fullerene Graph C_{20}.

It is a well-known fact that for an acyclic graph T, Sz(T) = W(T). On the other hand, an acyclic graph T does not have cycles and so $n_u(e|G) + n_v(e|G) = |V(T)|$. Thus $PI_v(T) = |V(T)|.|E(T)|$. Since a fullerene graph F has 12 pentagonal faces, $PI_v(F) < |V(F)|.|E(F)|$. The aim of this section is computing vertex PI and Szeged polynomial (and then the vertex PI and Szeged indices) of some fullerene graphs, Figure 1.

Let G be a connected graph. The Szeged and PI_v polynomials of G are defined as $Sz(G;x) = \sum_{e=uv\in E(G)} x^{n_u(e|G)n_v(e|G)}$. and $PI_v(G;x) = \sum_{e=uv\in E(G)} x^{n_u(e|G)+n_v(e|G)}$, respectively. Obviously $PI_v'(G,1) = PI_v(G)$ and $PI_v(G,1) = |E(G)|$. Define $N(e) = |V| - (n_u(e|G)+n_v(e|G))$. Then $PI_v(G) = \sum_{e=uv}[|V| - N(e)] = |V||E| - \sum_{e=uv} N(e)$ and we have:

$$\begin{aligned} PI_v(G;x) &= \sum_{e=uv\in E(G)} x^{n_u(e|G)+n_v(e|G)} \\ &= \sum_{e=uv\in E(G)} x^{|V(G)|-N(e)} \\ &= x^{|V(G)|} \sum_{e=uv\in E(G)} x^{-N(e)}. \end{aligned} \tag{1}$$

Example 1. Suppose C_{30} denotes the fullerene graph on 30 vertices, see Figure 1(a). Then $PI_v(C_{30}, x) = 10x^{20} + 10x^{22} + 20x^{26} + 5x^{30}$ and so $PI_v(C_{30}) = 1090$. $Sz_v(C_{20}, x) = 10x^{100}+10x^{117}+20x^{168}+5x^{225}$ and so $Sz_v(C_{30})=6655$.

Example 2. Consider the carbon nanocones $G = CNC_4[n]$ with 16 vertices, Figure 2. Then $PI_v(G, x) = 20x^{16}$ and so $PI_v(G) = 320$. $Sz_v(G, x) = 12x^{55}+8x^{64}$ and so $Sz_v(G)=1172$.

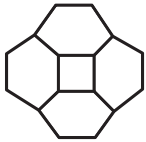

Figure 2. The Carbon Nanocone $CNC_4[1]$ with 16 vertices.

Example 3. Suppose H is the graph of carbon nanocones $CNC_4[n]$ with 36 vertices, see Figure 3. Then $PI_v(H, x) = 48x^{36}$ and so $PI_v(H) = 1728$. $Sz_v(H, x) = 16x^{203} + 8x^{315} + 12x^{320} + 12x^{324}$ and so $Sz_v(H)=13496$.

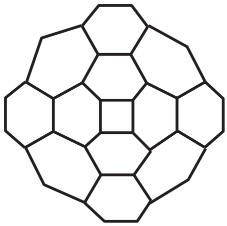

Figure 3. The Carbon Nanocone $CNC_4[2]$ with 36 vertices.

Now we compute the omega polynomial of the nanocone $CNC_4[n]$.

Theorem 1. Consider the nanocone $G = CNC_4[n]$ with $4(n+1)^2$ vertices. Then $\Omega(G, x) = 2x^{2m+2}+4(x^{2m+1}+x^{2m}+\ldots+x^{m+2})= 2x^{2m+2} + 4(x^{2m+2}-x^{m+2})/(x-1)$.

Proof. From Figure 4, one can see that there are m+1 type of edges of G. These are I_1, I_2,… and I_{m+1}. In Table 1, the number of equidistant edges of G are computed.

Table 1. The Number of Parallel Edges

Edges	Number of parallel edges	No
Type I_1 Edges	m+2	4
Type I_2 Edges	m+3	4
Type I_3 Edges	m+4	4
$\vdots$	$\vdots$	4
Type I_{m+1} Edges	2m+2	2

By using these calculations, the proof is completed.

Theorem 2. Suppose T = $CNC_4[n]$. Then $PI_v(T, x) = x^{4(n+1)^2(16n+4)}$.

Proof. It is clear that T has exactly $4(n+1)^2$ vertices and 16n+4 edges. Since T is bipartite, by Lemma 1 of Ref. 24, the proof is complete.

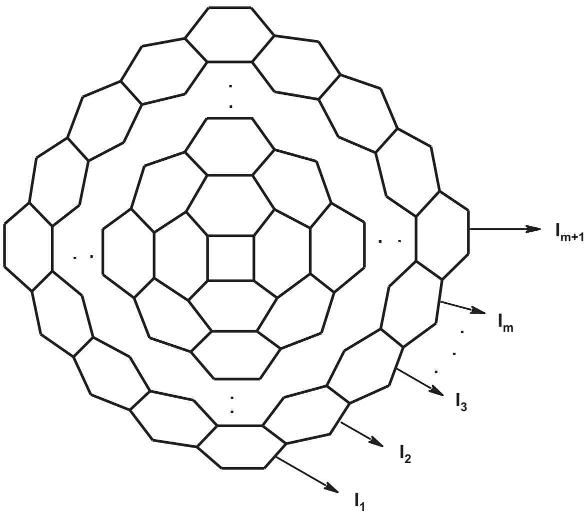

Figure 4. The graph of Carbon Nanocones $CNC_4[n]$.

Theorem 3. Suppose T = $CNC_4[n]$. Then the Szeged polynomial of T is as follows:

$$Sz(T,x)=\begin{cases} 8\sum_{i=1}^{n/2}(n\text{-}2i+1)x^{4(n+1)^4-9i^4}+4(n+1)x^{4(n+1)^4}+\sum_{i=1}^{n}4(n\text{-}i+1)x^{(2ni+i^2+2i)(4(n+1)^2\text{-}2ni\text{-}i^2\text{-}2i)} \\ +8\sum_{i=1}^{n/2}ix^{(2ni+i^2+2i)(4(n+1)^2\text{-}2ni\text{-}i^2\text{-}2i)}+8\sum_{i=n/2+1}^{n}(n\text{-}i+1)x^{(2ni+i^2+2i)(4(n+1)^2\text{-}2ni\text{-}i^2\text{-}2i)} & \text{n is even} \\ 8\sum_{i=1}^{n/2}(n\text{-}2i+1)x^{4(n+1)^4-9i^4}+4(n+1)x^{4(n+1)^4}+\sum_{i=1}^{n}4(n\text{-}i+1)x^{(2ni+i^2+2i)(4(n+1)^2\text{-}2ni\text{-}i^2\text{-}2i)} \\ +8\sum_{i=1}^{n\text{-}1/2}ix^{(2ni+i^2+2i)(4(n+1)^2\text{-}2ni\text{-}i^2\text{-}2i)}+8\sum_{i=n+3/2}^{n}(n\text{-}i+1)x^{(2ni+i^2+2i)(4(n+1)^2\text{-}2ni\text{-}i^2\text{-}2i)}+ \\ 8((n+1)/2)x^{(2n(n+1)/2+(n+1/2)^2+2(n+1/2)(4(n+1)^2\text{-}2n(n+1/2)\text{-}(n+1/2)^2\text{-}2(n+1/2))} & \text{n is odd} \end{cases}$$

Proof. From Figures 4 and 5, one can see that there are four types of edges of fullerene graph T. These are the horizontal edges (I), the first and second types of oblique edges (II, III) and the vertical edges (IV). In Table 2, n_u, n_v and N(e) are computed for each case.

Table 2. Computing $n_u(e)$ and $n_v(e)$ for Different Edges.

Vertex	The number of vertices closer to u than to v, the number of vertices closer to v than to u and equidistant vertices	No
Type I Edges	$2(n+1)^2$, $2(n+1)^2$, 0	$4(n+1)^4$
Type II Edges	$2n^2+4n-3i^2+2$, $2n^2+4n+3i^2+2$, 0 i=1..[n/2]	n-2i+1
Type III Edges (n is even)	$2ni+i^2+2i$, $4(n+1)^2-(2ni+i^2+2i)$, 0 i=1..n/2 . . $2ni+i^2+2i$, $4(n+1)^2-(2ni+i^2+2i)$, 0 i=n/2+1..n	1 2 . n/2 n/2 . 2 1
Type III Edges (n is odd)	$2ni+i^2+2i$, $4(n+1)^2-(2ni+i^2+2i)$, 0 i=1..n-1/2 . . $2ni+i^2+2i$, $4(n+1)^2-(2ni+i^2+2i)$, 0 i=n+1/2..n	1 2 . n/2-1 n/2 n/2-1 . 2 1
Type IV Edges	$2ni+i^2+2i$, $4(n+1)^2-(2ni+i^2+2i)$, 0 i=1..n	4(n-i+1) i=1..n

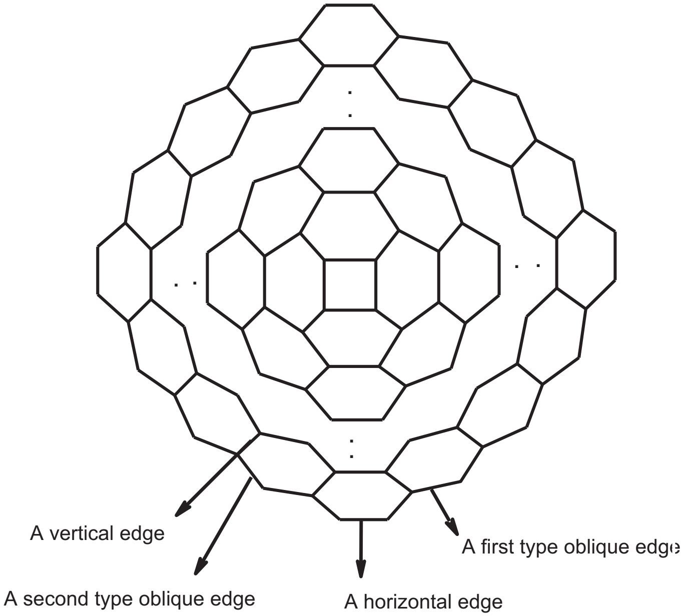

Figure 5. The graph of Carbon Nanocones $CNC_4[n]$.

A GAP Program for Computing Vertex PI and Szeged Indices of Molecular Graphs

```
f:=function(A,M)
    local l,ss,S,v,e,T,tt,I,j,;
    l:=Length(M); v:=0; ss:=0; S:=[]; T:=[]; e:=[]; tt:=0; dd:=[]; g:=[]; gg:=[];
    ddd:=[]; gg1:=[];g1:=[];
        for i in [1..l]do
            for j in[i+1..l] do
                if A[i][j]=1 then
                    Add(e,[i,j]);
                fi;
            od;
        od;
for a in e do
    for i in [1..l] do
        if M[a[1]][i]>M[a[2]][i]  then
```

```
            AddSet(S,i);
        fi;
        if M[a[1]][i]<M[a[2]][i]  then
             AddSet(T,i);
        fi;
    od;
    ss:=ss+Length(S)+Length(T);Add(dd,Length(S)+Length(T));
    tt:=tt+Length(S)*Length(T);Add(ddd,Length(S)*Length(T));
    T:=[];S:=[];
od;
Sort(dd);
    for i in dd do
        for j in dd do
            if j=i then
                Add(g,j);
            fi;
        od;
        AddSet(gg,g);g:=[];
    od;
Sort(ddd);
    for i in ddd do
        for j in ddd do
            if j=i then
                Add(g1,j);
            fi;
        od;
        AddSet(gg1,g1);g1:=[];
    od;
Print("**********************************","\n");
Print("Vertex PI Polynomial=");
    for i in [1..Size(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("Szeged Polynomial=");
    for i in [1..Size(gg1)-1] do
        Print(Length(gg1[i]),"x^");Print(gg1[i][1]);Print("+");
    od;
a1:=Length(gg1);
```

```
Print(Length(gg1[a1]),"x^");Print(gg1[a1][1],"\n"); Print("\n");
Print("Vertex PI Index=",ss,"\n");
Print("\n");
Print("Szeged Index=",tt,"\n");
Print("***********************************","\n");
Return;
end;
```

Acknowledgement. This research was in part supported by a grant from the Center of Excellence of Algebraic Methods and Applications of Isfahan University of Technology.

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