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Modified Eccentric Connectivity polynomial of Circumcoronene Series of Benzenoid H_k

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ABSTRACT

Let *G=(V,E)* be a molecular graph, where *V(G)* is a non-empty set of vertices/atoms and *E(G)* is a set of edges/bonds. For $v\in V(G)$, defined d_v be degree of vertex/atom *v* and *S(v)* is the sum of the degrees of its neighborhoods. The modified eccentricity connectivity polynomial of a molecular graph *G* is defined as $\Lambda(G,x)=\sum_{v\in V(G)} S(v).x^{\varepsilon(v)}$, where *ε(v)* is defined as the length of a maximal path connecting *v* to another vertex of molecular graph *G*. In this paper we compute this polynomial for a famous molecular graph of Benzenoid family.

Indexing terms/Keywords

Molecular graph; Circumcoronene Series of benzenoid; Modified Eccentricity Connectivity polynomial.

SUBJECT CLASSIFICATION

E.g., Mathematics Subject Classification; 05C05, 05C12

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INTRODUCTION

Let G be a simple molecular graph without directed and multiple edges and without loops, in chemical graphs the vertex/atom set and edge/bond set of which are represented by $V(G)$ and $E(G)$, and the number of vertices and edges in a graph will be defined by $n=|V(G)|$ and $e=|E(G)|$, respectively. The vertices or atoms in the molecular graph G are connected by an edge or chemical bond. If there is an edge e connecting the vertices u and v in G $(u,v\in V(G))$, then we write $e=uv\in E(G)$ and say "u and v are adjacent". A connected graph is a graph such that there is a path between all pairs of vertices. For two vertices u and v of G, $d(u,v)$ denotes the length of a minimal path connecting u and v.
In chemical graphs, a *Topological Index* or *Molecular descriptors* of a molecular graph G is a numeric quantity related to G. The oldest nontrivial topological index is the *Wiener index* which was introduced by chemist *Harold Wiener* [1,2]. *John Platt* was the only person who immediately realized the importance of the Wiener's pioneering work and wrote papers analyzing and interpreting the physical meaning of the Wiener index. The name of topological index was introduced by *H. Hosoya*. Many topological indices have been defined and several applications of them have been found in physical, chemical and pharmaceutical models and other properties of molecules. Among topological descriptors, connectivity indices are very important and they have a prominent role in chemistry.
The *Eccentric Connectivity index* of the molecular graph G, $\xi(G)$ was proposed by *Sharma, Goswami* and *Madan*, in 1997 [3-8]. It is defined as

$$\xi(G)=\sum_{v\in V} d_v\times\varepsilon(v)$$

where d_v denotes the degree of vertex v of G and a eccentricity of vertex $u\in V(G)$ is the largest distance between u and any other vertex v of G. In other works,

$$\varepsilon(u)=Max\{d(u;v)\,|\,\forall v\in V(G)\}.$$

The radius and diameter of G are defined as the minimum and maximum eccentricity among vertices of G and denoted by $R(G)$ and $D(G)$, respectively [9,10]. And also, the *Eccentric Connectivity polynomial (ECP)* of G is equal to [11-15]

$$ECP(G;x)=\sum_{v\in V(G)} d_v x^{\varepsilon(v)}$$

The *Modified Eccentric Connectivity polynomial (MEC)* of G is defined as

$$\Lambda(G,x)=\sum_{v\in V(G)} S(v).x^{\varepsilon(v)}$$

where $S(v)$ is the sum of the degrees of its neighborhoods $S(v)=\sum_{u\in N_G(v)} d_u$ and $N_G(v)=\{u\in V(G)|uvE(G)\}$, see [15, 16].

The aim of this paper is to obtain a closed formula of the modified eccentric connectivity polynomial for *Circumcoronene Series of Benzenoid H_k ($k\geq1$).*

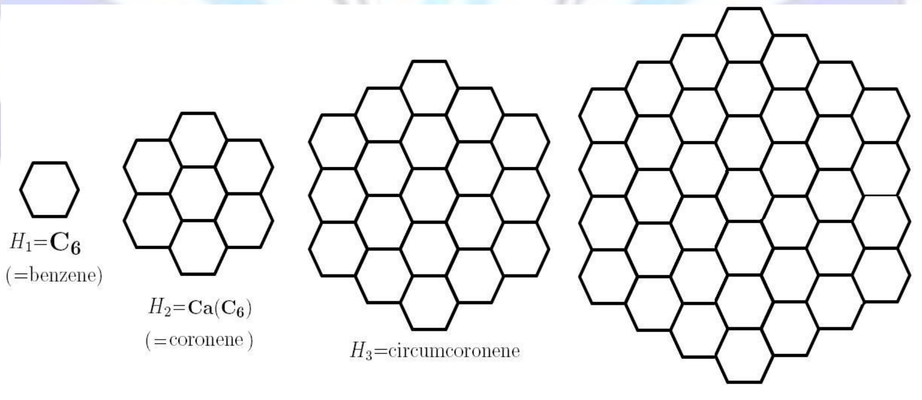

Fig 1. Some first members of *Circumcoronene Series of Benzenoid H_k ($k\geq1$).*

The Circumcoronene series of benzenoid is a famous family of molecular graph, which this family built solely from benzene C_6 (or hexagons) on circumference. For further study and more detail of this family of benzenoid molecular graph, see paper series [17-31] and following figures.

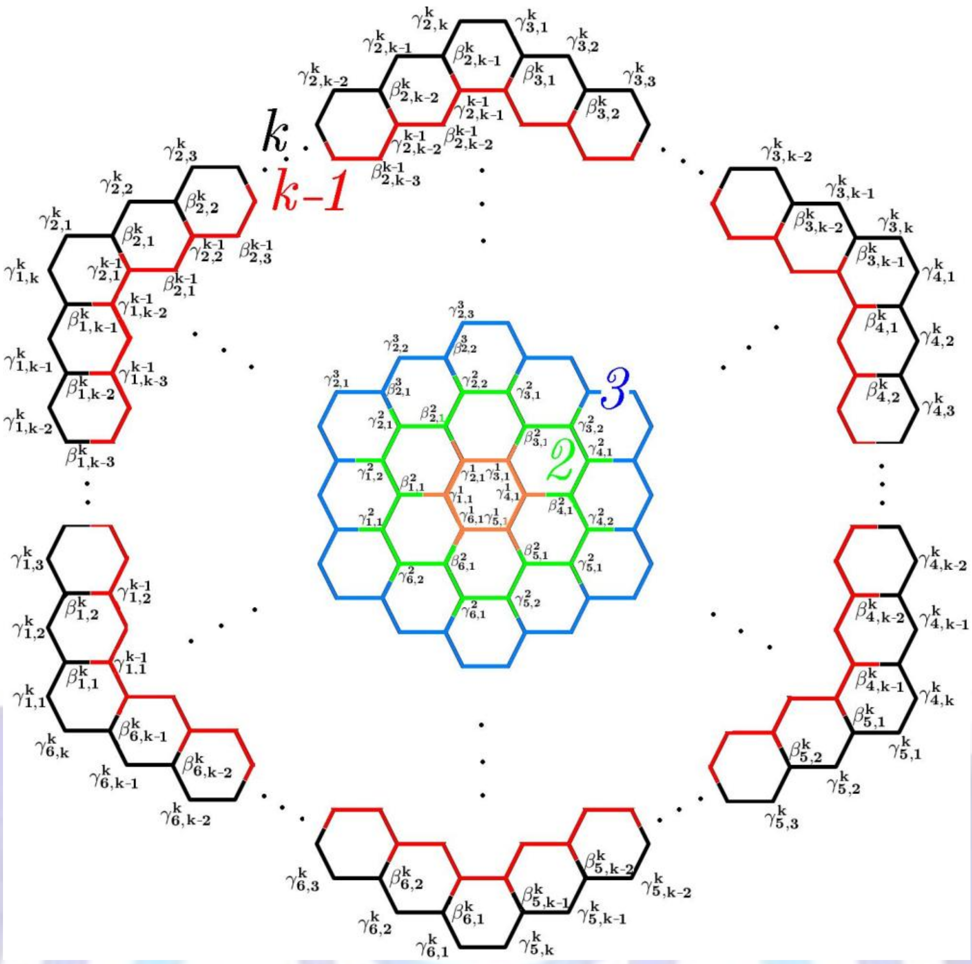

Fig 2. The notation of Circumcoronene Series, of Benzenoid H_k *(k≥1)*, together all ring-cuts [11].

Main Results and Discussions

In this section is to compute the modified eccentricity connectivity polynomial for a famous family of benzenoid graph, "*Circumcoronene Series of Benzenoid H_k* "*(k≥1)*, see Figure 2. To do this we should to consider the following denotation of all vertices of circumcoronene series of benzenoid H_k similar to Figure 2 and the vertex set and edge set of H_k will be

$$V(H_k) = \{\gamma^i_{z,j}, \beta^i_{z,l} \mid i=1,\dots,k,\ j\in\mathbb{Z}_i,\ l\in\mathbb{Z}_{i-1} and\ z\in\mathbb{Z}_6\}$$

$$E(H_k) = \{\beta^i_{z,j}\gamma^i_{z,j}, \beta^i_{z,j}\gamma^i_{z,j+1}, \beta^i_{z,j}\gamma^{i-1}_{z,j}\ and \gamma^i_{z,i}\gamma^i_{z+1,1} \mid i\in\mathbb{Z}_k\ j\in\mathbb{Z}_i, z\in\mathbb{Z}_6\}.$$

Then we have the following theorem by using the *Ring-cut Method*. Theorem 1 is the main result in this paper. The Ring-cut method is a modify version of the thoroughbred *Cut Method* that and the general form of this methods are presented in [30, 31].

Theorem 1. The modified eccentricity connectivity polynomial of Circumcoronene Series of Benzenoid H_k *(k≥1)*, is equal to

$$\Lambda(H_k,x) = (6k+24)x^{4k-1} + 42(k-1)x^{4k-2} + 54(k-1)x^{2k-3} + 54\sum_{i=1}^{k-2} i\left(x^{2(k+i)} + x^{2(k+i)-1}\right)$$

Proof. Let G be the circumcoronene series of benzenoid H_k $\forall k≥1$. The ring-cut method divides all vertices of G into some partitions such that all members of any ring-cut have similar mathematical properties. Also every ring of H_k consists vertices $\gamma^i_{z,j}$ of set Γ and vertices $\beta^i_{z,l}$ of set B, $\forall i\in\mathbb{Z}_k$, $j\in\mathbb{Z}_i$, $l\in\mathbb{Z}_{i-1}$ and $z\in\mathbb{Z}_6$ (where $\mathbb{Z}_i$ *={1,2,…,i}* is the cycle finite group of order *i*).

Thus, by according to Figure 2 and using the Ring-cut method, one can see that the parameter *ε(v)* for all $v\in V(H_k)$ are equal to

$$\varepsilon\ \gamma_{z,j}^{i} = 2(k+i)-1$$

$$\varepsilon\ \beta_{z,j}^{i} = 2(k+i-1)$$

Obviously for $i=k$; $R(H_k)=2k+1$ and $D(H_k)=\varepsilon\ \gamma_{z,j}^{k}=4k-1$ are the radius number and diameter number of H_k.

By using above results, one can see the modified eccentricity connectivity polynomial for circumcoronene series of benzenoid H_k is as follows:

$$\Lambda(H_k,x)=\sum_{v\in V\ H_k} S\ v\ x^{\varepsilon(v)}$$

$$=\sum_{v\in\Gamma} S\ v\ x^{\varepsilon(v)}+\sum_{v\in B} S\ v\ x^{\varepsilon(v)}$$

$$=\sum_{i=1}^{k}\sum_{j=1}^{i}\sum_{z=1}^{6} S\ \gamma_{z,j}^{i}\ x^{\varepsilon(\gamma_{z,j}^{i})}+\sum_{i=2}^{k}\sum_{j=1}^{i-1}\sum_{z=1}^{6} S\ \beta_{z,j}^{i}\ x^{\varepsilon(\beta_{z,j}^{i})}$$

$$=6\sum_{i=1}^{k}\sum_{j=1}^{i} S\ \gamma_{1,j}^{i}\ x^{2\ k+i\ -1}+6\sum_{i=2}^{k}\sum_{j=1}^{i-1} S\ \beta_{1,j}^{i}\ x^{2\ k+i\ -2}$$

$$=6\ S\ \gamma_{1,1}^{k}+S\ \gamma_{1,k}^{k}\ \ x^{4k-1}+6\sum_{j=2}^{k-1} S\ \gamma_{1,j}^{k}\ x^{4k-1}+6\sum_{i=1}^{k-1}\sum_{j=1}^{i} S\ \gamma_{1,j}^{i}\ x^{2\ k+i\ -1}$$

$$+6\sum_{j=1}^{k-1} S\ \beta_{1,j}^{k}\ x^{4k-2}+6\sum_{i=2}^{k-1}\sum_{j=1}^{i-1} S\ \beta_{1,j}^{i}\ x^{2\ k+i\ -2}$$

From Figure 2, it is easy to see that $S\ \gamma_{z,1}^{k}=S\ \gamma_{z,k}^{k}$ =2+3, $S\ \gamma_{z,j}^{k}$ =3+3, $S\ \beta_{z,j}^{k}$ =2+2+3 and for all others $S\ \gamma_{z,j}^{i}=S\ \beta_{z,j}^{i}$ =3+3+3. By arrangement above formula, we have:

$$\Lambda(H_k,x)=12\ 5\ x^{4k-1}+6\sum_{j=2}^{k-1} 6x^{4k-1}+6\sum_{i=1}^{k-1}\sum_{j=1}^{i} 9x^{2\ k+i\ -1}+6\sum_{j=1}^{k-1} 7x^{4k-2}+6\sum_{i=2}^{k-1}\sum_{j=1}^{i-1} 9x^{2\ k+i\ -2}$$

$$=\ 6k+24\ x^{4k-1}+42\ k-1\ x^{4k-2}+54\ k-1\ x^{2k-3}+54\sum_{i=1}^{k-2} i\ \ x^{2\ k+i}\ +x^{2\ k+i\ -1}$$

And this compeled the proof of the main theorem.

For example the modified eccentricity connectivity polynomial of benzene C_6 is equal to $\Lambda(C_6,x)=12x^3$. Of course, *M.* Alaeiyan, *et al.* [15] proved the modified eccentricity connectivity polynomial of C_n (the cycle of length n) is equal to $\Lambda(C_n,x)=4nx\, x^{n/2}$, when n is even and $\Lambda(C_n,x)=4nx\, x^{n-1/2}$, when n is odd.

CONCLUSIONS

A family of Benzenoid built solely from Benzene C_6 (or hexagons), Circumcoronene Series of Benzenoid H_k $(k\geq 1)$, have been studied here and its *Modified Eccentric Connectivity polynomial (MEC)* have been counted.

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