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A new method for computing eccentric connectivity polynomial of an infinite family of linear polycene parallelogram benzenod

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Let G=(V,E) be a graph, where V(G) is a non-empty set of vertices and E(G) is a set of edges. For u ∈ V(G), defined d(u) be degree of vertex u. The eccentricity connectivity polynomial of a molecular graph G is defined as ECP(G,x) = $\sum_{u\in V(G)} \deg_G(u)x^{ecc(u)}$, where ecc(a) is defined as the length of a maximal path connecting a to another vertex of G. In this paper, we computing this polynomial for linear polycene parallalogram graph of benzenoid by a new method.

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1. Introduction

A graph G consists of a set of vertices $V(G)$ and a set of edges $E(G)$. The vertices in G are connected by an edge if there exists an edge $uv \in E(G)$ connecting the vertices u and v in G such that $u,v \in V(G)$. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds. The number of vertices and edges in a graph will be denoted by $|V(G)|$ and $|E(G)|$, respectively.

A topological index is a real number related to a molecular graph, which is a graph invariant. There are several topological indices already defined and many of them have found applications as means to model chemical, pharmaceutical and other properties of the molecules. The Wiener index is the first topological index proposed to be used in Chemistry. It was introduced in 1947 by Harold Wiener, as the path number for characterization of alkanes. It is defined as the sum of distances between all pairs of vertices in the graph under consideration. In the 1990s, a large number of other topological indices have been put forward, all being based on the distances between vertices of molecular graphs and all being closely related to W. The eccentric connectivity index of the molecular graph G, $\xi^c(G)$, was proposed by Sharma, Goswami and Madan [5]. It is defined as $\xi^c(G) = \sum_{u\in V(G)} \deg_G(u).ecc(u)$ where $deg_G(u)$ denotes the degree of the vertex u in G and $ecc(u)= Max\{d(x,u) \mid x \in V(G)\}$. The radius and diameter of G are defined as the minimum and maximum eccentricity among vertices of G, respectively [8-14].

We now define the eccentric connectivity polynomial of a graph G, ECP(G,x), as

$$\mathrm{ECP}(G,x)= \sum_{u\in V(G)} \deg_G(u)x^{ecc(u)} .$$

Then the eccentric connectivity index is the first derivative of $ECP(G, x)$ evaluated at $x = 1$.

2. Main results and discussion

In this section is to compute $ECP(G,x)$, for an infinite family of linear polycene parallalogram of benzenoid graph [2]. To do this we should to consider the following examples:

Example 1. Consider linear polycene parallalogram benzenoid graph $L_2[G]$ depicted in Fig. 1. This graph has *16* vertices and 19 edges. This graph has two vertices with eccentricity 4 and degree 3, two vertices with eccentricity 7 and degree 2, 8 vertices with eccentricity 5 such that four vertices with degree 2 and four vertices with degree 3. And four vertices of eccentricity 6 and degree 2. Then

$$ECP(L_2[G],x) =6x^4+20x^5+8x^6+4x^7$$

And $\xi^c(L_2[G])$ = $ECP(L_1[G],1)=200$

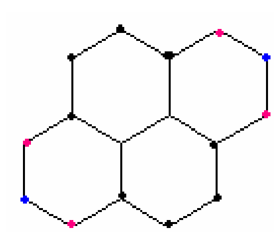

Fig. 1.

Example 2. Consider linear polycene parallelogram benzenoid graph $L_3[G]$ depicted in Fig. 2. This graph has *30* vertices and *38* edges. By computing eccentricity polynomial of $L_3[G]$ it is easy to check that

$$ECP(L_3[G],x)=4x^{11}+8x^{10}+12x^9+14x^8+26x^7+12x^6$$

and $\xi^c(L_3[G])=ECP'(L_3[G],1)=598$

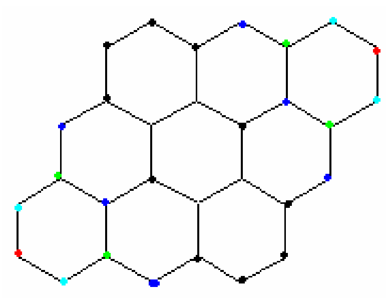

Fig. 2.

Example 3. Consider linear polycene parallelogram benzenoid graph $L_4[G]$ depicted in Fig. 3. This graph has 48 vertices and 63 edges. By computing eccentricity polynomial of $L_4[G]$ we have $ECP(L_4[G],x)=2x^8(2x^7+4x^6+6x^5+7x^4+9x^3+10x^2+16x+9)$

and $\xi^c(L_4[G])=ECP'(L_4[G],1)=1326$

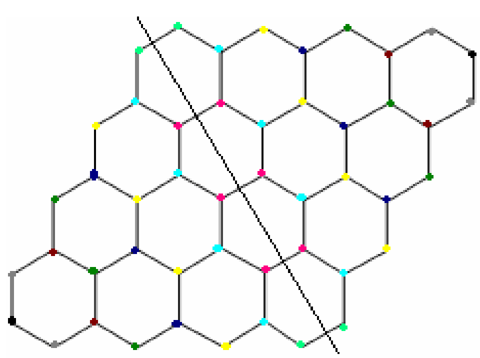

Fig. 3.

In generally consider linear polycene parallelogram benzenoid graph $L_n[G]$ depicted in Fig. 4. This graph has $2n(n+2)$ vertices and $3n^2+4n-1$ edges. For computing the eccentric connectivity index for $L_n[G]$ in total case, we using a new method.

In this method we compute maximum eccentric connectivity and minimum eccentric connectivity for linear polycene parallelogram benzenoid graph $L_n[G]$. We have for $u\in V(L_n[G])$

$$Max\ ecc(u)=4n-1 \quad \text{and} \quad Min\ ecc(u)=2n$$

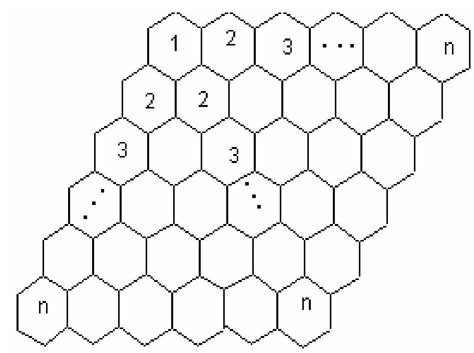

Fig. 4. Linear Polycene Parallelogram.

In Fig. 6, one can see the eccentric connectivity index for every $u\in V(L_n[G])$ and in Fig. 5, one can see several deictic line for computing the eccentric connectivity index. First line starting of Max $ecc(u)=4n-2$ and finally with $ecc(u)=2n+1$. and for secondly line, starting of $ecc(u)=4n-2$ and finally with $ecc(u)=2n$. Similarly for another lines we can computing eccentric connectivity index. Then by using of Fig. 5, 6 we have table (1).

Tabel 1. Eccentric connectivity index for vertices $L_n[G]$.

4n-1	4n-2	4n-3	4n-4	4n-5	…	2n+2	2n+1	2n+1
	4n-2	4n-3	4n-4	4n-5	…	2n+2	2n+1	2n
			4n-4	4n-5	…	2n+2	2n+1	2n
					…	2n+2	2n+1	2n
						.	.	.
						.	.	.
						.	.	.
						2n+2	2n+1	2n
							2n+1	

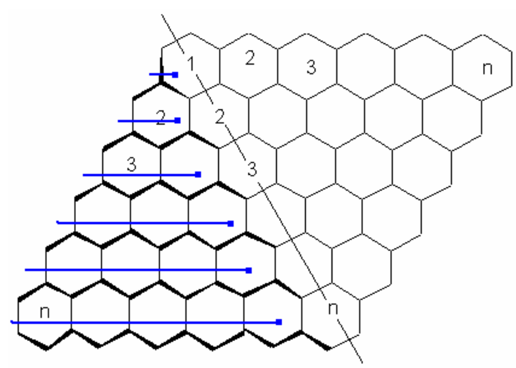

Fig. 5.

For vertices, with eccentric connectivity index *4n-1, 4n-2, 4n-4, 4n-6,…, 2n+2, 2n+1*, we have $deg(u)=2$ and for another vertices we have $deg(u)=3$, where $u\in V(L_n(G))$.

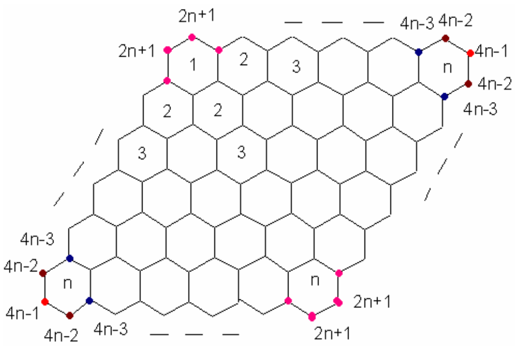

Fig. 6.

By using in this method one can see the eccentricity connectivity polynomial for an infinite family of linear polycene parallalogram benzenoid graph is as follows:

$$ECP(L_n[G],x)= 2[x^{4n-1}+2x^{4n-2}+x^{4n-3}+x^{4n-6}+\ldots+x^{2n+3}+x^{2n+2}+2x^{2n+1}] +6[(n-1)x^{2n}+nx^{2n+1}+(n-1)(1+x)x^2+(n-2)(1+x)x^4 +(n-3)(1+x)x^6+\ldots+3(1+x)x^{2n-6}+2(1+x)x^{2n-4}]$$

By arrangement above formula, we have:

$$ECP(L_n[G],x)= 4x^{2n+1}+4x^{4n-2} -6x^{2n} +6x^{2n}(1+x)\sum_{k=0}^{n-2}(n-k)x^{2k} +4x^{2n}\sum_{k=0}^{2n-2}x^{k+1}$$

Tabel 2. Namber eccentric connectivity index for linear polycene parallalogram for n=2,3,4,5,6,7,8.

7 6 5 4
11 10 9 8 7 6
15 14 13 12 11 9 8
19 18 17 16 15 14 13 12 11 10
23 22 21 20 19 18 17 16 15 14 13 12
27 26 25 24 23 22 21 20 19 18 17 16 15 14
31 30 29 28 27 26 25 24 23 22 21 20 19 18 17 16

Tabel 3. Eccentricity connectivity polynomial for linear polycene parallalogram for some values of n.

$n=2$	$4x^7+8x^6+20x^5+6x^4$
$n=3$	$4x^{11}+8x^{10}+12x^9+14x^8+26x^7+12x^6$
$n=4$	$4x^{15}+8x^{14}+12x^{13}+14x^{12}+18x^{11}+20x^{10}+32x^9+18x^8$
$n=5$	$4x^{19}+8x^{18}+16x^{17}+16x^{16}+22x^{15}+22x^{14}+28x^{13}+28x^{12}+38x^{11}+24x^{10}$
$n=6$	$4x^{23}+8x^{22}+16x^{21}+16x^{20}+32x^{19}+32x^{18}+28x^{17}+28x^{16}+34x^{15}+34x^{14}+44x^{13}+30x^{12}$
$n=7$	$4x^{27}+8x^{26}+16x^{25}+16x^{24}+22x^{23}+22x^{22}+28x^{21}+28x^{20}+34x^{19}+34x^{18}+40x^{17}+40x^{16}+46x^{15}+36x^{14}$

3. Conclusions

In this paper a method for computing eccentricity polynomial of linear polycene parallalogram benzenoid graph. This method is useful for working by all nanostructures and benzenoids. We applied our method on an infinite class of $L_n[G]$ benzenoids.

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