Computing the MEC polynomial of an infinite family of the linear parallelogram P(n,n)

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Let G=(V,E) be a molecular graph, where V(G) is a non-empty set of vertices and E(G) is a set of edges. For u$\in$V(G), defined deg(u) be degree of vertex u, and n_G(u) is the sum of the degrees of its neighborhoods. The modified eccentricity connectivity polynomial of a molecular graph G is defined as Λ(G,x)= $\sum_{u\in V(G)}$ n_G(u). $x^{ecc(u)}$, where ecc(u) is defined as the length of a maximal path connecting u to another vertex of molecular graph G. In this paper, we computing this polynomial for an infinite family of linear polycene parallelogram P(n,n).

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1. Introduction

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. 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 so 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 defined by |V(G)| and |E(G)| respectively. In graph theory, a path of length n in a graph is a sequence of n + 1 vertices such that from each of its vertices there is an edge to the next vertex in the sequence. For two vertices u and v of G, d_G(u,v) denotes the length of a minimal path connecting u and v. A graph G is called connected, if there is a path connecting vertices u and v of G, for every u,v$\in$V(G). A topological index 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 Harold Wiener [4,5]. 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 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.

The eccentric connectivity index of the molecular graph G, $\xi^c(G)$, was proposed by Sharma, Goswami and Madan [7]. 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) | x $\in$V(G)}. The radius and diameter of G are defined as the minimum and maximum eccentricity among vertices of G, respectively [8,9].

The modified eccentric connectivity polynomial (MEC) of graph G is defined as

$$\Lambda(G,x)=\sum_{u\in V(G)}n_G(u)x^{ecc(u)},$$

where n_G(u) is the sum of the degrees of its neighborhoods, see[6].

For example, if C_n denotes the cycle graph on n vertices, then, for every v$\in$V(C_n), deg(v)=2.
One can see ecc(v)=n/2 when n is even and ecc(v)=(n-1)/2 when n is odd. Hence $\Lambda(C_n,x)=4nx^{\frac{n}{2}}$ when n is even and $\Lambda(C_n,x)=4nx^{\frac{n-1}{2}}$ when n is odd.

2. Main results and discussion

In this section is to compute the modified eccentricity connectivity polynomial for an infinite family of parallelogram P(n,n) of benzenoid graph, see [2]. To do this we should to consider the following examples:

Example 1. We consider the linear polycene parallelogram benzenoid graph P(2,2). 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

$$\Lambda\,(P(2,2),x) = 18x^4+48x^5+20x^6+8x^7$$

Example 2. We now determine the parallelogram benzenoid graph P(3,3). This graph has 30 vertices and 38 edges. By computing modified eccentricity connectivity polynomial of P(3,3) it is easy to check that

$$\Lambda\,(P(3,3),x)=8x^{11}+20x^{10}+28x^9+42x^8+66x^7+36x^6$$

Example 3. Consider the parallelogram benzenoid graph P(4,4) depicted in Fig. 1. This graph has 48 vertices and 63 edges. Then we have

$$\Lambda\,(P(4,4),x)=8x^{15}+20x^{14}+28x^{13}+42x^{12}+46x^{11}+80x^{10}+64x^9+54x^8$$

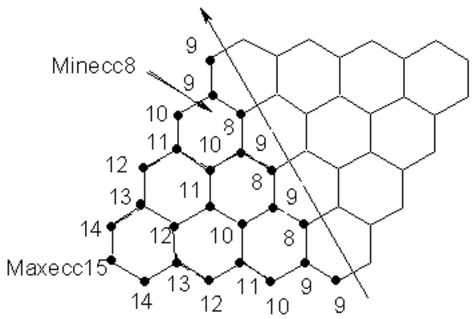

Fig. 1.

In generally consider the parallelogram benzenoid graph P(n,n) depicted in Fig. 2. This graph has 2n(n+2) vertices and $3n^2+4n-1$ edges. For computing the modified eccentric connectivity polynomial for P(n,n) 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 P(n,n). We have for $u \in V(P(n,n))$, Max ecc(u)=4n-1 and Min ecc(u)= 2n.

In Fig. 4, one can see the eccentric connectivity for every $u \in V(P(n,n))$ and in Fig. 3, one can see several deictic line for computing the eccentric connectivity. 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. 3,4 we have Table 1 , 2 and 3.

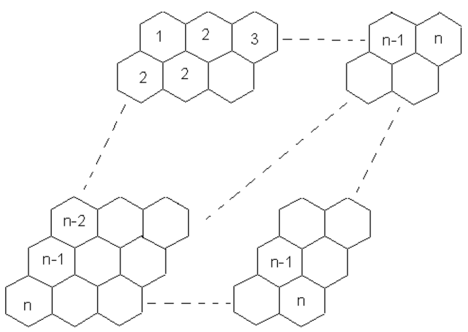

Fig. 2. The Parallelogram P(n,n).

Table 1. The eccentric connectivity for vertices P(n,n).

Line1	Line2	Line3	…	Line n-1	Line n
4n-1					
4n-2	4n-2				
4n-3	4n-3				
4n-4	4n-4	4n-4			
4n-5	4n-5	4n-5			
4n-6	4n-6	4n-6			
…	…	…	…		
2n+4	2n+4	2n+4			
2n+3	2n+3	2n+3			
2n+2	2n+2	2n+2		2n+2	
2n+1	2n+1	2n+1		2n+1	2n+1
2n+1	2n	2n		2n	

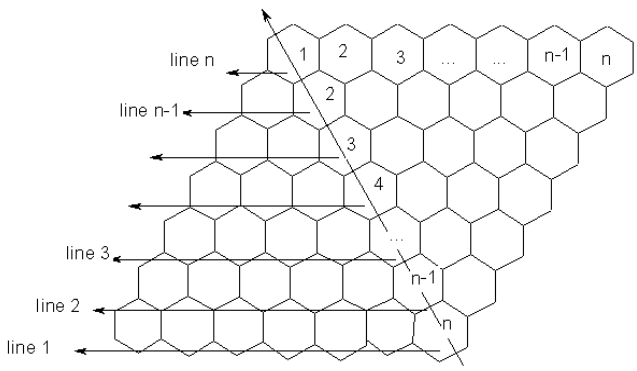

Fig. 3.

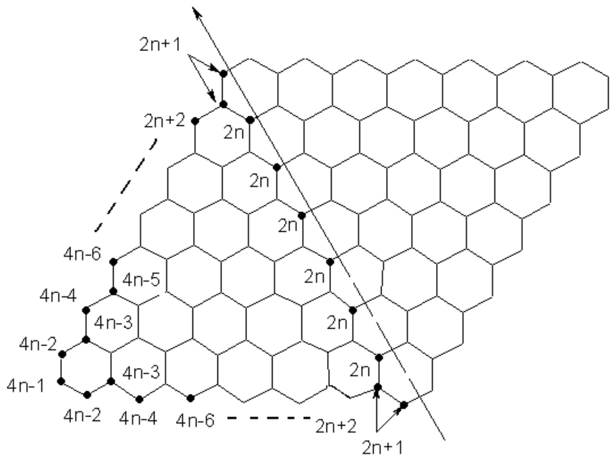

Fig. 4.

Table 2. Types of the eccentricity connectivity.

n	Types of ecc for P(n,n)
2	7 6 5 4
3	11 10 9 8 7 6
4	15 14 13 12 11 9 8
5	19 18 17 16 15 14 13 12 11 10
6	23 22 21 20 19 18 17 16 15 14 13 12
7	27 26 25 24 23 22 21 20 19 18 17 16 15 14
8	31 30 29 28 27 26 25 24 23 22 21 20 19 18 17 16
9	35 34 33 32 31 30 29 28 27 26 25 24 23 22 21 20 19 18
10	39 38 37 36 35 34 33 32 31 30 29 28 27 26 25 24 23 22 21 20
11	43 42 41 40 39 38 37 36 35 34 33 32 31 30 29 28 27 26 25 24 23 22
12	47 46 45 44 43 42 41 40 39 38 37 36 35 34 33 32 31 30 29 28 27 26 25 24
13	51 50 49 48 47 46 45 44 43 42 41 40 39 38 37 36 35 34 33 32 31 30 29 28 27 26
14	55 54 53 52 51 50 49 48 47 46 45 44 43 42 41 40 39 38 37 36 35 34 33 32 31 30 29 28
15	59 58 57 56 55 54 53 52 51 50 49 48 47 46 45 44 43 42 41 40 39 38 37 36 35 34 33 32 31 30

Table 3. The MEC Polynomial for every line in Fig. 3 and 4.

Line 1	$4x^{4n-1}+5x^{4n-2}+7x^{4n-3}+6x^{4n-4}+7x^{4n-5}+6x^{4n-6}+\ldots+6x^{2n+2}+7x^{2n+1}+5x^{2n+1}$
Line 2	$5x^{4n-2}+7x^{4n-3}+9x^{4n-4}+9x^{4n-5}+\ldots+9x^{2n}$
Line 3	$6x^{4n-4}+7x^{4n-5}+9x^{4n-6}+9x^{4n-7}+\ldots+9x^{2n}$
Line 4	$6x^{4n-6}+7x^{4n-7}+9x^{4n-8}+9x^{4n-9}+\ldots+9x^{2n}$
Line 5	$6x^{4n-8}+7x^{4n-9}+9x^{4n-10}+9x^{4n-11}+\ldots+9x^{2n}$
Line 6	$6x^{4n-10}+7x^{4n-11}+9x^{4n-12}+9x^{4n-13}+..+9x^{2n}$
….	………………………………………
Line n-2	$6x^{2n+4}+7x^{2n+3}+9x^{2n+2}+9x^{2n+1}+9x^{2n}$
Line n-1	$6x^{2n+2}+7x^{2n+1}+9x^{2n}$
Line n	$5x^{2n+1}$

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

$$\Lambda(P(n,n),x)= 4x^{4n-1}+5x^{4n-2}+7x^{4n-3}+6x^{4n-4}+7x^{4n-5}+6x^{4n-6}+\ldots+6x^{2n+2}+7x^{2n+1}+5x^{2n+1}+5x^{4n-2}+7x^{4n-3}+9\sum_{i=4}^{2n} x^{4n-i}+6x^{4n-4}+7x^{4n-5}+9\sum_{i=6}^{2n} x^{4n-i}+6x^{4n-6}+7x^{4n-7}+9\sum_{i=8}^{2n} x^{4n-i}+6x^{4n-8}+7x^{4n-9}+9\sum_{i=10}^{2n} x^{4n-i}+\ldots+6x^{2n+2}+7x^{2n+1}+9x^{2n}+5x^{2n+1}$$

By arrangement above formula, we have:

$$\Lambda(P(n,n),x)= 20x^{2n+1}+20x^{4n-2}+8x^{4n-1}+18\sum_{j=2}^{n}\sum_{i=2j}^{2n} x^{4n-i}+28\sum_{i=1}^{n-1} x^{4n-2i-1}+24\sum_{i=1}^{n-1} x^{4n-2i}.$$

Table 4. Some special types of MEC polynomial.

n	The MEC polynomial of P(n,n)
2	$8x^{7}+20x^{6}+48x^{5}+18x^{4}$
3	$8x^{11}+20x^{10}+28x^{9}+42x^{8}+66x^{7}+36x^{6}$
4	$8x^{15}+20x^{14}+28x^{13}+42x^{12}+46x^{11}+80x^{10}+64x^{9}+54x^{8}$
5	$8x^{19}+48x^{18}+28x^{17}+42x^{16}+46x^{15}+60^{14}+64x^{13}+48x^{12}+72x^{11}+24x^{10}$
6	$8x^{23}+48x^{22}+28x^{21}+42x^{20}+46x^{19}+60x^{18}+46x^{17}+78x^{16}+74x^{15}+96^{14}+100x^{13}+72x^{12}$

References

[1] A. A. Dobrynin, A. A. Kochetova, J. Chem., Inf. Comput. Sci, **34**, 1082 (1994).
[2] V. Padmakar Khadikar, Iranian Journal of Mathematical Chemistry **1**(1), 7 (2010).
[3] I. Gutman, N. Trinajstić, Chem. Phys. Lett. **17**, 535 (1972).
[4] H. Wiener, J. Am. Chem. Soc. **69**,17 (1947)
[5] H. Hosoya, Bull. Chem. Soc. Jpn., **44**, 2332 (1971).
[6] A.R. Ashrafi, M. Ghorbani, Electronic Materials Letters, **6**(2), 87 (2010).
[7] V. Sharma, R. Goswami, A. K. Madan, Eccentric connectivity index, J. Chem. Inf. Model., **37,** 273 (1997).
[8] H. Saheli, H. Saati, A.R. Asfrafi, Optoelectron. Adv. Mater. – Rapid Commun. **4**(6), 896 (2010).
[9] V. Kumar, A. K. Madan, J. Math. Chem. **42,** 925 (2007).

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