The edge version of MEC index of linear polycene parallelogram benzenoid

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Let G be a molecular graph, the *edge modified eccentric connectivity index* of *G* is defined as $\Lambda_e(G)=\sum_{f\in E(G)} S_f \cdot ecc(f)$, where S_f is the sum of the degrees of neighborhoods of an edge *f* and *ecc*(*f*) is its eccentricity. In this paper an exact formula for the edge modified eccentric connectivity index of linear polycene parallelogram benzenoid was computed.

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1. Introduction

Molecular descriptors are playing significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place [15]. There are numerous of topological descriptors that have found some applications in theoretical chemistry, especially in QSPR/QSAR research.

More recently, a new topological index, *eccentric connectivity index*, has been investigated. This topological model has been shown to give a high degree of predictability of pharmaceutical properties, and may provide leads for the development of safe and potent anti-HIV compounds. We encourage the reader to consult papers [1–9] for some applications and papers [10–14] for the mathematical properties of this topological index.

Now, we introduce some notation and terminology. Let *G* be a graph with vertex set *V*(*G*) and edge set *E*(*G*). Let *deg*(*v*) denote the degree of the vertex *v* in *G*. If *deg*(*v*) = 1, then *v* is said to be a *pendent vertex*. An edge incident to a pendent vertex is said to be a *pendent edge*. For two vertices *u* and *v* in *V*(*G*), we denote by *d*(*u*,*v*) the distance between *u* and *v*, i.e., the length of the shortest path connecting *u* and *v*. The *eccentricity* of a vertex *v* in *V*(*G*), denoted by *ecc*(*v*), is defined to be

$$ecc(v)=\max\{d(u,v) \mid u\in V(G)\}$$

The *diameter* of a graph *G* is then defined to be max{*ecc*(*v*)|*v* ∈ *V*(*G*)}. The *eccentric connectivity index*, $\xi^c(G)$, of a graph *G* is defined as

$$\xi^c(G)=\sum_{v\in V(G)}\deg(v)\cdot ecc(v)$$

The *modified eccentric connectivity index* of *G* is defined as $\Lambda(G)=\sum_{v\in V(G)} S_v \cdot ecc(v)$, where S_v is the sum of the degrees of neighborhoods of an edge *f* and *ecc*(*f*) is its eccentricity.

Let $f = uv$ be an edge in *E*(*G*). Then the degree of the edge *f* is defined to be $\deg(u)+\deg(v)-2$. For two edges $f_1=u_1v_1$, $f_1=u_2v_2$ in *E*(*G*), the distance between f_1 and f_2, denoted by $d(f_1,f_2)$, is defined to be $d(f_1,f_2)=\min\{d(u_1,u_2),d(u_1,v_2),d(v_1,u_2),d(v_1,v_2)\}$ The *eccentricity* of an edge *f*, denoted by *ecc*(*f*), is defined as

$$ecc(f)=\max\{d(f,e) \mid e\in E(G)\}$$

The *edge eccentric connectivity index* of *G* [16], denoted by $\xi_e^{\,c}(G)$, is defined as

$$\xi_e^{\,c}(G)=\sum_{f\in E(G)}\deg(f)\cdot ecc(f)$$

Also the *edge modified eccentric connectivity index* of *G* is defined as $\Lambda_e(G)=\sum_{f\in E(G)} S_f \cdot ecc(f)$, where S_f is the sum of the degrees of neighborhoods of an edge *f* and *ecc*(*f*) is its eccentricity.

In this paper an exact formula for the edge modified eccentric connectivity index of linear polycene parallelogram benzenoid was computed.

2. Result and discussion

In generally consider linear polycene parallalogram benzenoid graph $L_n(G)$ depicted in Fig. 1.

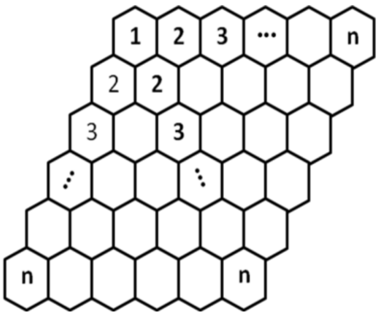

Fig. 1.

This graph has $2n(n+2)$ vertices and $3n^2+4n-1$ edges. It is clear that the edge modified eccentric connectivity index of $L_1(G)$ is 48. For computing the eccentric connectivity index for $L_n(G)$ where $n \geq 2$, we using a new method. In this method we compute maximum edge eccentric connectivity and minimum edge eccentric connectivity for linear polycene parallalogram benzenoid graph $L_n(G)$. For $f \in E(L_n(G))$ *we have* $Max(ecc(f)) = 4n-3$ and $Min(ecc(f)) = 2n-2$.

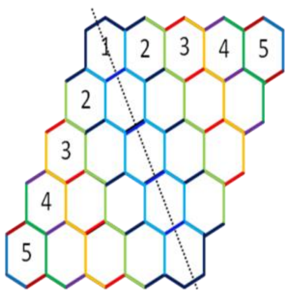

Fig. 2. The edges set with same eccentric connectivity in L5[G].

With respect to Fig. 2, it can be seen that we have 4 edges with the maximum edge eccentric connectivity 4n-3 such that the sum of the degrees of neighborhoods of them is 5 and we have 4 edges with the edge eccentric connectivity 4n-4 such that the sum of the degrees of neighborhoods of them is 9. Also we have n-1 edges with the minimum edge eccentric connectivity 2n-2 such that the sum of the degrees of neighborhoods of them is 16 and we have 4(n-1) edges with the edge eccentric connectivity 2n-1 such that the sum of the degrees of neighborhoods of 4 edges of them is 14 and the remaining edges of them is 16. On the other hand we have 2n+6 edges with the edge eccentric connectivity 2n such that the sum of the degrees of neighborhoods of them are 10, 9, 6 and 16. According to Table 1 we specify the number, edge eccentricity and the sum of the degrees of neighborhoods of another edges. Therefore we have:

$$\begin{aligned}
\Lambda_e\left(\mathrm{L_n}(G)\right) &= \sum\nolimits_{f\in E(G)} S_f \cdot ecc(f) = 4\times 5\times(4n-3) \\
&+4\times 9\times(4n-4)+4\times 10\times 2n+4\times 9\times 2n+32(n-2)\times 2n \\
&+2\times 6\times 2n+4\times 14\times(2\mathrm{n}-1)+(4\mathrm{n}-8)\times 16\times(2\mathrm{n}-1) \\
&+(\mathrm{n}-1)\times 16\times(2\mathrm{n}-2)+40\sum_{k=5}^{2n-1}(4\mathrm{n}-\mathrm{k})+56\sum_{k=2}^{n-1}(4\mathrm{n}-(2\mathrm{k}+1)) \\
&+16\sum_{k=2}^{n-1}(4\mathrm{n}-(2\mathrm{k}+1))(4\mathrm{k}-8)+16\sum_{k=3}^{n-1}(4\mathrm{n}-2\mathrm{k})(2\mathrm{k}-4)\cdot
\end{aligned}$$

Thus we have

$$\Lambda_e(L_n(G)) = 128\mathrm{n}^3 - 72\mathrm{n}^2 - 120\mathrm{n} + 140 .$$

Now we obtain the following theorem:

Theorem 1. The edge modified eccentric connectivity index of $L_n(G)$ is computed as

$$\Lambda_e(L_n(G)) = 128\mathrm{n}^3 - 72\mathrm{n}^2 - 120\mathrm{n} + 140 ,$$

where $n \geq 2$.

Tabel 1. Types of edges in $L_n(G)$.

Types of edges	num	ecc	S_f
1	4	4n-3	5
2	4	4n-4	9
3	4	4n-5	10
3	4	4n-5	14
3	0	4n-5	16
4	4	4n-6	10
4	2	4n-6	16
5	4	4n-7	10
5	4	4n-7	14
5	4	4n-7	16
6	4	4n-8	10
6	4	4n-8	16
7	4	4n-9	10
7	4	4n-9	14
7	8	4n-9	16
...	...	...	...
2n-3	4	2n+1	10
2n-3	4	2n+1	14
2n-3	4n-12	2n+1	16
2n-2	4	2n	10
2n-2	4	2n	9
2n-2	2	2n	6
2n-2	2(n-2)	2n	16
2n-1	4	2n-1	14
2n-1	4(n-2)	2n-1	16
2n	n-1	2n-2	16

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