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The edge version of MEC index of one-pentagonal carbon nanocones

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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 one-pentagonal carbon nanocones was computed.

Keywords: edge modified eccentric connectivity index, carbon nanocones, eccentricity

INTRODUCTION

Molecular descriptors are playing significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place [15]. There are numerous 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.

One-pentagonal carbon nanocones, Fig. 1, were originally discovered by Ge and Sattler in 1994 [17]. These are constructed from a graphene sheet by removing a 60° wedge and joining the edges thus producing a cone with a single pentagonal defect at the apex. One-pentagonal carbon nanocones consist of one pentagone, its core surrounded by layers of hexagons. If there are *n* layers, then the graph of this molecule is denoted by $G=\mathrm{CNC}_5[n]$.

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 as

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

The *diameter* of a graph *G* is then defined to be $\max\{ecc(v)\mid v\in V(G)\}$. 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 as $\deg(u)+\deg(v)-2$. 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

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ecc(*f*) is its eccentricity.

In this paper an exact formula for the edge modified eccentric connectivity index of one-pentagonal carbon nanocones was computed.

RESULTS AND DISCUSSION

Let C[n] = $CNC_5[n]$. In the following lemma, the maximum and minimum edge eccentric connectivity of C[n] is computed.

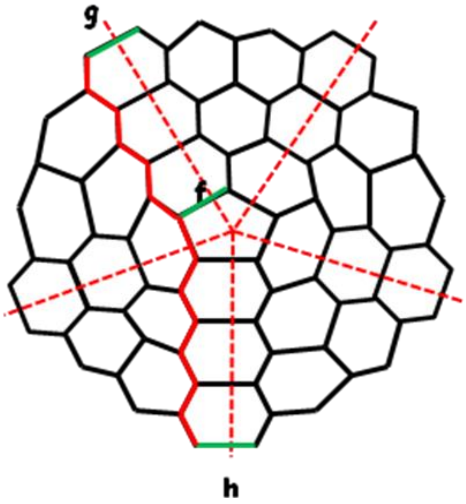

Fig. 1 A maximum and minimum path for computing eccentricity in CNC5[3]

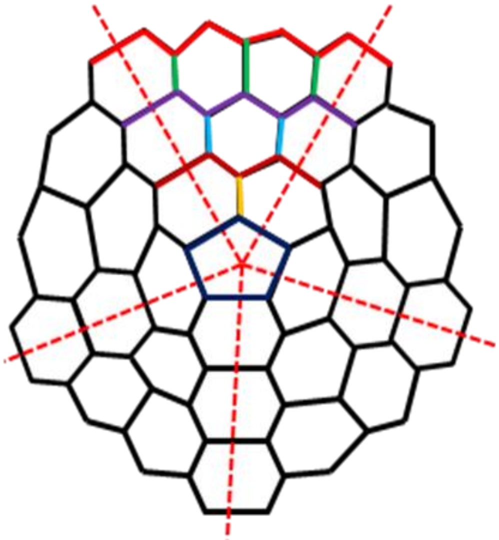

Fig. 2 The edges set with same eccentric connectivity for one section in CNC5[3]

Lemma 1. For any edge f in $E(C[n])$, we have

$$Max(ecc(f)) = 4n+1\ ,$$
$$Min(ecc(f)) = 2n+1.$$

Proof. Suppose f is an edge of the central pentagon of $C[n]$. Then from Fig. 1, one can see that there exists an edge g of degree 2 such that $d(f,g) = 2n$ and there exists another edge h of degree 2 such that $d(f,h) = 2n+1$. Therefore, the shortest path with maximum length is connecting two edges of degree 2 in $C[n]$ and thus the proof is completed.

In the following theorem we compute the edge eccentric connectivity index of $C[n]$.

Theorem 1. The edge modified eccentric connectivity index of $C[n]$ is computed as

$$\Lambda_e(C[n]) = 400n^3 + 520n^2 + 180n + 20.$$

Proof. Considering Figs. 1 and 2, it can be seen that we have 10n+5 numbers of edges with maximum eccentric connectivity, such as 5 numbers of edges type 1, 10 numbers of edges type 2 and 10n-10 numbers of edges type 3. Also 5n numbers of edges type 4 with eccentric connectivity of 4n, 10n-5 numbers of edges type 5 with eccentric connectivity of 4n-1, and so it continues until we have five edges of type 2n+2 with eccentric connectivity of 2n+2 and five edges of type 2n+3 with minimum eccentric connectivity of 2n+1. It is easy to check that the sum of the degrees of neighborhoods of five edges of maximum eccentric connectivity is 6. The sum of the degrees of neighborhoods of 10 edges of maximum eccentric connectivity is 9 and the sum of the degrees of neighborhoods of 10n-10 edges of maximum eccentric connectivity is 10. Also the sum of the degrees of neighborhoods of 5n edges of type 4 is 14. On the other hand, the sum of the degrees of neighborhoods of other types of edges is 16. (See Table 1).

Table 1. Types of edges for C[n]

Types of edges	Num	Ecc	S_f
1	5	4n+1	6
2	10	4n+1	9
3	10n-10	4n+1	10
4	5n	4n	14
5	10n-5	4n-1	16
6	5n-5	4n-2	16
7	10n-15	4n-3	16
8	5n-10	4n-4	16
9	10n-25	4n-5	16
...	...	...	...
2n	10	2n+4	16
2n+1	15	2n+3	16
2n+2	5	2n+2	16
2n+3	5	2n+1	16

This implies that

$$\Lambda_e(C[n]) = \sum_{f\in E(C[n])} S_f \cdot ecc(f)$$

$$=5\times 6\times(4n+1)+10\times 9\times(4n+1)$$
$$+(10n-10)\times 10\times(4n+1)+5n\times 14\times 4n$$
$$+16\sum_{k=1}^{n}(10n-10k+5)(4n-2k+1)$$
$$+16\sum_{k=1}^{n-1}(5n-5k)(4n-2k).$$

Therefore,

$$\Lambda_e(\mathrm{C}[n]) = 400\mathrm{n}^3 + 520\mathrm{n}^2 + 180\mathrm{n} + 20.$$

Thus, this proof is completed.

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РЕБРЕНО МОДИФИЦИРАН ИНДЕКС НА ЕКСЦЕНТРИЧНА СВЪРЗАНОСТ НА ЕДНО-ПЕНТАГОНАЛЕН НАНОКОНУС

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(Резюме)

Нека G е молекулярен граф. Ребрено модифицираният индекс на ексцентрична свързаност на G се дефинира с $\Lambda_e(G)=\sum_{f\in E(G)} S_f \cdot ecc(f)$, където S_f е сумата от степените на съседство на реброто f и ecc(f) е неговата ексцентричност. В тази статия е намерена точна формула за ребрено модифициран индекс на ексцентрична свързаност на едно-пентагонален въглероден наноконус.