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Edge harmonic index of carbon nanocones and an algorithm

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Edge harmonic index $H_e(G)$ of the (chemical) graph G is based on the end-vertex degrees of edges of the line graph $L(G)$. In this paper, the generalized formula and an algorithm (pseudocode) are given for edge harmonic index. The aim of this paper is to develop edge harmonic index for generalized carbon nanocones.

Keywords: Carbon nanocones, Edge harmonic index, Generalized formula, Graph theory.

INTRODUCTION

Graph theory has variety-applied fields, one of which is carbon nanostructure field. Carbon nanocones, which were firstly introduced by Ge and Sattler in 1994 [1], are well-founded devices in the nanostructures.

These are constructed from a graphene sheet by removing a 60° wedge and joining the edges to produce a cone with a single pentagonal defect at the apex [2]. A carbon nanocone is made up of one-polygonal and its center is surrounded by the layers of the polygonal. So, the carbon nanocones denoted by $CNC_m[n]$ consist of m-th polygonal and nth layer.

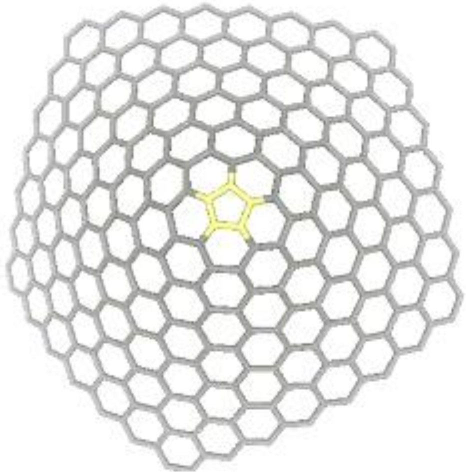
Fig. 1 illustrates the graph of one pentagonal carbon nanocone $CNC_5[6]$. In recent years, several useful research articles based on the topological indices have been studied on these structures [12-22].

A topological index is the numerical quantity attributed to a (chemical) graph G. The oldest topological index is the Wiener index, which was presented by the chemist Wiener [3]. It is defined as follows:

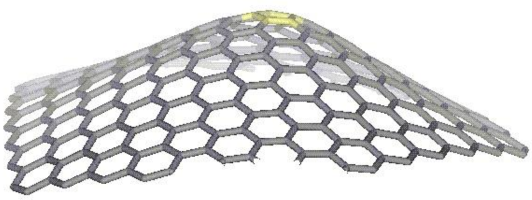
$$W(G)=\sum_{\{u,v\}\in V(G)} d(u,v),$$

where $d(u,v)$ is the distance between atoms u and v in the chemical graph G. The topological indices are graph invariants and are used to calculate quantitative structure-activity relationships (QSAR) and quantitative structure-property relationships (QSPR) [9,10]. For the QSAR and QSPR studies, the experimental numerical results have been shown in [11]. Yang and Hua [19] have established the explicit formula and mathematical properties of the harmonic index for general connected graphs and so they gained important results for QSAR and QSPR studies. In addition, the reader can refer to [12-22] for more information about topological indices and QSAR and QSPR.

Let us now give basic definitions. Let G be a chemical graph and its edge and vertex sets are represented by $E(G)$ and $V(G)$, respectively. In a chemical graph, the vertices of a graph are attributed to the atoms of the molecule and the edges represent the chemical bonds.



(a)



(b)

Fig. 1. (a), (b) The graph of one-pentagonal carbon nanocone CNC_5 [6] (top and side view) (color figure available online).

In 1987, the harmonic index $H(G)$ was presented by Fajtlowicz [4]. It is formulated as follows:

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$$H(G)=\sum_{uv\in E(G)}\frac{2}{d(u)+d(v)},$$

where $d(u)$ (or $d(v)$) represents the degree of the vertex u (or v) in G. Recently, the edge harmonic index has been introduced by Nazır *et al.* [5]. It is associated with the end-vertex degrees of the edges of their line graphs. It is formulated as follows:

$$H_e(G)=\sum_{ef\in E(L(G))}\frac{2}{d(e)+d(f)},$$

where $d(e)$ and $d(f)$ are the end-vertex degrees of vertices e and f in a line graph of G.

In graph theory, a line graph is obtained by using and converting the vertices and edges of any connected graph. In order to obtain a line graph from a graph G, the vertices of G are converted to edges; the edges of G are converted to vertices. However, the neighborhoods remain the same as in G. For example, in Fig. 2, the orange-colored vertices of nanocone (a) are converted to the orange-colored edges of the line graph (b) of the nanocone and the blue-colored edges of nanocone (a) are converted to the blue-colored vertices of the line graph (b) of the nanocone (similarly as in Figs 3 and 4).

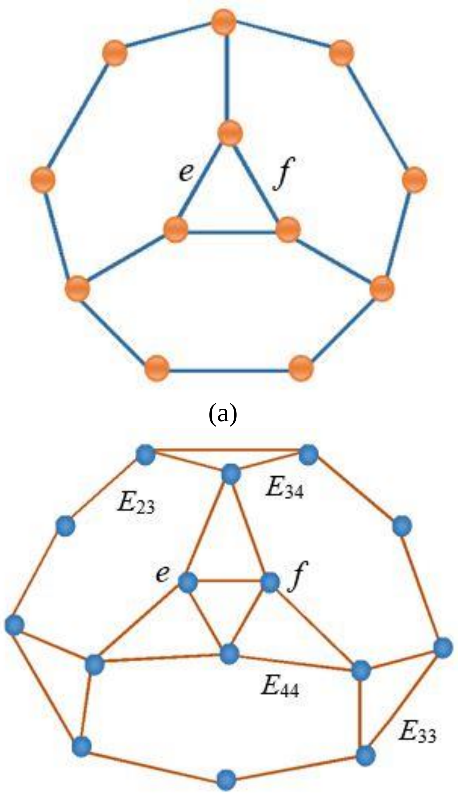

Fig. 2. The graph of carbon nanocone (a) $C_3[1]$ and its line graph (b) $L(C_3[1])$.

In this paper, we aim at developing the edge harmonic index for generalized carbon nanocones. Subsequently, we want to obtain a generalized formula for this index.

RESULTS AND DISCUSSION

Let $CNC_m[n]=C_m[n]$. Our notation is standard and mainly taken from standard books of graph theory [6-8]. Now, we give the required theorems and propositions to perform our aim.

Theorem 1. Consider the graph of carbon nanocone $C_3[n]$. Then we get

$$H_e(C_3[n])=\frac{12}{5}+(2n-1)+\frac{12n}{7}+\frac{9n^2}{4}.$$

Proof. Let us consider the graph $C_3[n]$ and $L(C_3[n])$. $L(C_3[n])$ has $(9n^2+12n+3)$ edges and $(9n^2+15n)/2+3$ vertices for the first $n=1,2,3\ldots$ layers. On the other hand, there are 6 edges of type ($d(e)=2$, $d(f)=3$), $(6n-3)$ edges of type ($d(e)=3$, $d(f)=3$), $(6n)$ edges of type ($d(e)=3$, $d(f)=4$) and $(9n^2)$ edges of type ($d(e)=4$, $d(f)=4$). For $C_3[n]$ $(n\geq 1)$, we get

$$H_e(C_3[n])=\frac{12}{5}+(2n-1)+\frac{12n}{7}+\frac{9n^2}{4}.$$

Theorem 2. Consider the graph of carbon nanocone $C_4[n]$. Then we get

$$H_e(C_4[n])=\frac{16}{5}+\frac{8n-4}{3}+\frac{16n}{7}+3n^2.$$

Proof. Let us consider the graph $C_4[n]$ and $L(C_4[n])$. $L(C_4[n])$ has $(12n^2+16n+4)$ edges and $(6n^2+10n+4)$ vertices for the first $n=1,2,3\ldots$ layers. On the other hand, there are 8 edges of type ($d(e)=2$, $d(f)=3$), $(8n-4)$ edges of type ($d(e)=3$, $d(f)=3$), $(8n)$ edges of type ($d(e)=3$, $d(f)=4$) and $(12n^2)$ edges of type ($d(e)=4$, $d(f)=4$). For $C_4[n]$ $(n\geq 1)$, we get

$$H_e(C_4[n])=\frac{16}{5}+\frac{8n-4}{3}+\frac{16n}{7}+3n^2.$$

Proposition 3. Consider the graph of carbon nanocone $C_3[1]$. Then we have

$$H_e(C_3[1])=\frac{12}{5}+1+\frac{12}{7}+\frac{9}{4}.$$

Proof. The graph $C_3[1]$ and its line graph $L(C_3[1])$ are illustrated in Fig. 2. The graph $L(C_3[1])$ has 24 edges and 15 vertices. If e and f be endpoints on any edge then there exist,

6 edges (E_{23}) of type $d(e)=2$ and $d(f)=3$,

3 edges (E_{33}) of type $d(e)=d(f)=3$,

6 edges (E_{34}) of type $d(e)=3$ and $d(f)=4$,

9 edges (E_{44}) of type $d(e)=d(f)=4$. Hence,

$$H_e(C_3[1])=\sum_{ef\in E(L(C_3[1]))}\frac{2}{d(e)+d(f)}=6\times\frac{2}{2+3}$$

$$+3\times\frac{2}{3+3}+6\times\frac{2}{3+4}+9\times\frac{2}{4+4}=\frac{12}{5}+1+\frac{12}{7}+\frac{9}{4}.$$

Proposition 4. Consider the graph of carbon nanocone $C_3[2]$. Then we have

$$H_e(C_3[2])=\frac{12}{5}+3+\frac{24}{7}+9.$$

Proof. The graph $C_3[2]$ and its line graph $L(C_3[2])$ are illustrated in Fig. 3. The graph $L(C_3[2])$ has 63 edges and 36 vertices. We have:

6 edges (E_{23}) of type $d(e)=2$ and $d(f)=3$,

9 edges (E_{33}) of type $d(e)=d(f)=3$,

12 edges (E_{34}) of type $d(e)=3$ and $d(f)=4$,

36 edges (E_{44}) of type $d(e)=d(f)=4$. Hence,

$$H_e(C_3[2])=6\times\frac{2}{2+3}+9\times\frac{2}{3+3}$$

$$+12\times\frac{2}{3+4}+36\times\frac{2}{4+4}=\frac{12}{5}+3+\frac{24}{7}+9.$$

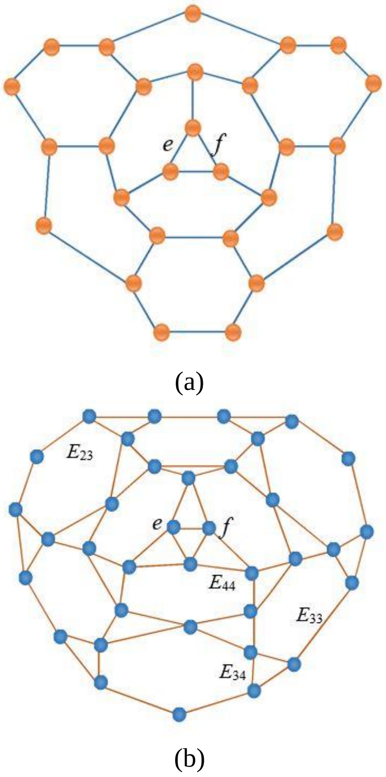

Fig. 3. The graph of carbon nanocone (a) $C_3[2]$ and its line graph (b) $L(C_3[2])$.

Proposition 5. Consider the graph of carbon nanocone $C_4[1]$. Then we have

$$H_e(C_4[1])=\frac{16}{5}+\frac{4}{3}+\frac{16}{7}+3.$$

Proof. The graph $C_4[1]$ and its line graph $L(C_4[1])$ are illustrated in Fig. 4. The graph $L(C_4[1])$ has 32 edges and 20 vertices. We get

8 edges (E_{23}) of type $d(e)=2$ and $d(f)=3$,

4 edges (E_{33}) of type $d(e)=d(f)=3$,

8 edges (E_{34}) of type $d(e)=3$ and $d(f)=4$,

12 edges (E_{44}) of type $d(e)=d(f)=4$. Hence,

$$H_e(C_4[1])=8\times\frac{2}{2+3}+4\times\frac{2}{3+3}+8\times\frac{2}{3+4}$$

$$+12\times\frac{2}{4+4}=\frac{16}{5}+\frac{4}{3}+\frac{16}{7}+3.$$

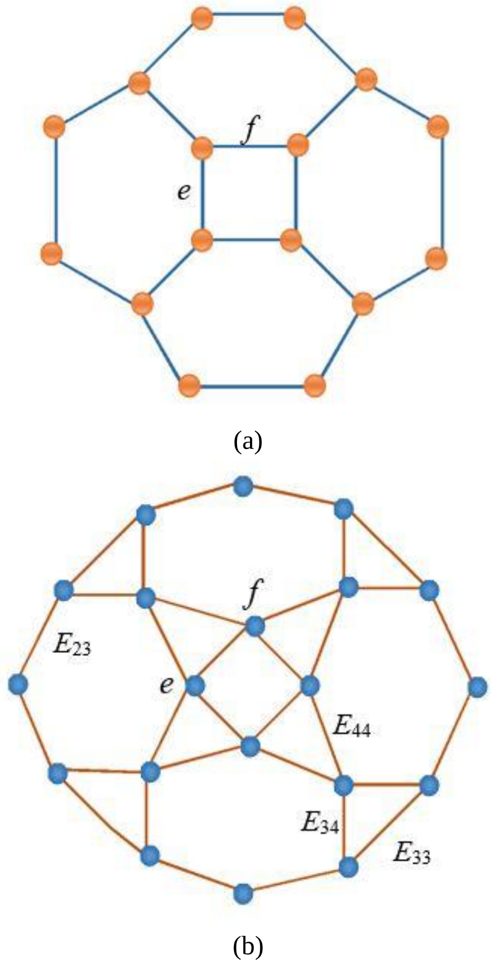

Fig. 4. The graph of carbon nanocone (a) $C_4[1]$ and its line graph (b) $L(C_4[1])$.

Proposition 6. Consider the graph of carbon nanocone $C_4[2]$. Then we have

$$H_e(C_4[2])=\frac{16}{5}+4+\frac{32}{7}+12.$$

Proof. The graph $L(C_4[2])$ has 84 edges and 48 vertices. Accordingly, 8 edges of type $d(e)=2$ and $d(f)=3$,

12 edges of type $d(e)=d(f)=3$,

16 edges of type $d(e)=3$ and $d(f)=4$,

48 edges of type $d(e)=d(f)=4$. Hence,

$$H_e(C_4[2]) = 8\times\frac{2}{2+3} + 12\times\frac{2}{3+3}$$

$$+16\times\frac{2}{3+4} + 48\times\frac{2}{4+4} = \frac{16}{5} + 4 + \frac{32}{7} + 12 .$$

We infer the following generalized formula from the above propositions and theorems.

Theorem 7. Let $m \geq 3$ and $n \geq 1$ be positive integers. Then, the generalized formula is of the form

$$H_e(C_m[n]) = 2m\times\frac{2}{2+3} + (2mn-m)\times\frac{2}{3+3}$$

$$+2mn\times\frac{2}{3+4} + 3mn^2\times\frac{2}{4+4}$$

$$= \frac{4m}{5} + \frac{m(2n-1)}{3} + \frac{4mn}{7} + \frac{3mn^2}{4} .$$

Proof. Let E_{23}, E_{33}, E_{34} and E_{44} orange-colored edges are subsets of $E(L(C_m[n]))$. Then, for every $E_{ij} = ef \in E(L(G))$, ($s(E_{23})$, $s(E_{33})$, $s(E_{34})$ and $s(E_{44})$ are the number of E_{23}, E_{33}, E_{34} and E_{44} orange-colored edges)

$$E_{23} = \{d(e)=2,\ d(f)=3\},\ \ s(E_{23}) = 2m,$$

$$E_{33} = \{d(e)=d(f)=3\},\ \ s(E_{33}) = m(2n-1),$$

$$E_{34} = \{d(e)=3,\ d(f)=4\},\ \ s(E_{34}) = 2mn,$$

$$E_{44} = \{d(e)=d(f)=4\},\ \ s(E_{44}) = 3mn^2.$$

Hence,

$$H_e(C_m[n]) = \frac{4m}{5} + \frac{m(2n-1)}{3} + \frac{4mn}{7} + \frac{3mn^2}{4} .$$

The proof is completed.

Yang and Hua [19] have introduced the generalized formula of harmonic index as the following theorem.

Theorem 8. [19] The formula of the harmonic index for the generalized carbon nanocones is

$$H(C_m[n]) = \frac{m}{2} + \frac{17nm}{30} + \frac{mn^2}{2} .$$

In Tables 1 and 2, the numbers of edges of type ($d(e)$=2, $d(f)$=3), ($d(e)$=3, $d(f)$=3), ($d(e)$=3, $d(f)$=4) and ($d(e)$=4, $d(f)$=4) have been illustrated, respectively. The values of H_e index have been calculated for some $C_3[n]$, $C_4[n]$, $C_5[n]$ and $C_7[n]$. In addition, we make comparison between the edge harmonic and harmonic indices in Table 3.

Table 1. The values of H_e index for some $C_3[n]$ and $C_4[n]$

Types of nanocones	Number of edges of type $d(e)$=2, $d(f)$=3	Number of edges of type $d(e)$=3, $d(f)$=3	Number of edges of type $d(e)$=3, $d(f)$=4	Number of edges of type $d(e)$=4, $d(f)$=4	H_e index values
$C_3[1]$	6	3	6	9	7.37
$C_3[2]$	6	9	12	36	17.83
$C_3[3]$	6	15	18	81	32.79
$C_3[4]$	6	21	24	144	52.26
$C_4[1]$	8	4	8	12	9.82
$C_4[2]$	8	12	16	48	23.77
$C_4[3]$	8	20	24	108	43.72
$C_4[4]$	8	28	32	192	69.68

Table 2. The values of H_e index for some $C_5[n]$ and $C_7[n]$

Types of nanocones	Number of edges of type $d(e)$=2, $d(f)$=3	Number of edges of type $d(e)$=3, $d(f)$=3	Number of edges of type $d(e)$=3, $d(f)$=4	Number of edges of type $d(e)$=4, $d(f)$=4	H_e index values
$C_5[1]$	10	5	10	15	12.27
$C_5[2]$	10	15	20	60	29.72
$C_5[3]$	10	25	30	135	54.66
$C_5[4]$	10	35	40	240	87.10
$C_7[1]$	14	7	14	21	17.18
$C_7[2]$	14	21	28	84	41.60
$C_7[3]$	14	35	42	189	76.52

Table 3. A comparison between H_e and H for some $C_3[n]$, $C_5[n]$ and $C_7[n]$

Nanocones	$C_3[1]$	$C_3[2]$	$C_3[3]$	$C_4[4]$	$C_5[1]$	$C_5[2]$	$C_5[3]$	$C_7[1]$	$C_7[2]$	$C_7[4]$
H_e index	7.37	17.83	32.79	69.68	12.27	29.72	54.66	17.18	41.60	121.93
H index [19]	4.7	10.9	20.1	43.07	7.83	18.17	33.5	10.97	25.43	75.37

AN ALGORITHM FOR H_e INDEX

In this section, an algorithm (pseudocode) is given.

m is the number of edges of the line graph,

$h_1, h_2, \ldots, h_m$ (h=ef) are edges of the line graph,

Sum is the sum of H_e index for each edge.

Step 0. Start.

Step 1. Take *Sum*=0, i=0.

Step 2. i=i+1.

Step 3. Determine the degrees of $d(e)$ and $d(f)$ for h_i.

Step 4. *Sum*=*Sum* $+2/\left(d(e)+d(f)\right)$.

Step 5. If i<m then, return to *Step 2*.

Step 6. Else, write the *Sum.*

Step 7. Stop.

CONCLUSIONS

Many topological indices have been established in the physco-chemical, pharmaceutical, toxicologic, biological models and other structure analyzing.

In this paper, we have obtained a generalized formula of edge harmonic index of carbon nanocones by using propositions and theorems.

The numerical results in Table 3 can be easily used and evaluated for QSAR and QSPR studies in [11]. For further studies, it would be interesting to use the line graphs of carbon nanocones in the investigation of their mathematical properties, QSAR, QSPR studies and other topological indices.

In addition, Theorem 7 can be easily applied to the other carbon nanocones.

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РЪБОВ ХАРМОНИЧЕН ИНДЕКС НА ВЪГЛЕРОДНИ НАНОКОНУСИ И АЛГОРИТЪМ

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(Резюме)

Ръбовият хармоничен индекс $H_e(G)$ на (химичната) графа G се основава на крайните степени на ръбовете на линейната графа $L(G)$. В настоящата статия се предлага обобщена формула и алгоритъм (псевдокод) за ръбовия хармоничен индекс. Целта на статията е да се разработи ръбов хармоничен индекс за въглеродни наноконуси.