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THE EDGE VERSION OF GEOMETRIC– ARITHMETIC INDEX OF BENZENOID GRAPH

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The edge version of geometric–arithmetic index of graphs is introduced based on the end vertex degrees of edges of their line graphs; where the line graph L(G) of a graph G is defined to be the graph whose vertices are the edges of G, with two vertices being adjacent if the corresponding edges share a vertex in G. In this paper, formulas for calculating the above topological descriptors in Benzenoid Hk families are given.

Key words: Molecular graph, Benzenoid, Geometric–arithmetic index, Line graph, Degree (of a vertex).

INTRODUCTION

Let G is an arbitrary simple connected graph, with the vertex set $V(G)$ and edge set $E(G)$. In chemical graphs, the vertices of the graph correspond to the atoms of molecules while the edges represent chemical bonds[9,11,14]. Numbers encoding certain structural features of organic molecules and derived from the corresponding molecular graph, are called *graph invariants* or more commonly *topological indices*.

Topological indices have some applications in theoretical chemistry, especially in *QSPR/QSAR* research[11]. The oldest topological index which introduced by the chemist Harold Wiener in 1947 is ordinary (vertex) version of Wiener index[14] and defined as the sum of topological distances $d(u,v)$ between any two atoms in the molecular graph G. Also, the edge versions of Wiener index which were based on distance between edges introduced by *Iranmanesh et al.* in 2008[5]. These topological indices are formulated as follow:

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

$$W_e(G)=\sum_{\{e,f\}\in E(G)} d(e,f)$$

An important topological index introduced more than thirty years ago by *Milan Randic*[9] is the branching index and defined as the sum of certain bond contributions calculated from the vertex degree of the hydrogen suppressed molecular graphs.

In 2009, *D. Vukičević* and *B. Furtula*[12] introduced a topological index named the *Geometric-Arithmetic index GA(G)*

$$GA(G)=\sum_{e=uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v}$$

where d_u denotes the degree of the vertex u in G. The reader can find more information about the geometric-arithmetic index in[4, 12, 15].

Recently, *A. Iranmanesh et al* introduced[8] the *edge version of geometric-arithmetic index* on the ground of the end-vertex degree d_e and d_f of edges e and f in a line graph of G as follows

$$GA_e(G)=\sum_{ef\in E(L(G))} \frac{2\sqrt{d_e d_f}}{d_e+d_f}$$

where the line graph $L(G)$ of a graph G is defined to be the graph whose vertices are the edges of G, with two vertices being adjacent if the corresponding edges share a vertex in G.

In this paper, we focus our attention to the edge version of geometric-arithmetic index and obtain a closed formula of this index for a famous molecular graph that is *Circumcoronene Series of Benzenoid* H_k.

METHODS

In this section, we persent a computational method and by this method we can compute the edge GA index of Benzenoid H_k that k is positive integer number. Circumcoronene Homologous Series of Benzenoid is a family of molecular graphs, which are generalizations of benzene molecule and the *Benzene* molecule is a usual molecule in chemistry, physics and nano sciences and is very useful to synthesize aromatic compounds. In Figure 1, the general form of circumcoronene series of benzenoid is shown. For more information of benzenoid families, see the paper series[1, 2, 6, 7, 10, 13, 16]. Also, reader can see the vertex version of geometric-arithmetic index of H_k is equal to[3]:

$$GA(H_k) = 9k^2 + (\frac{24\sqrt{6}}{5} - 15)k + (12 - \frac{24\sqrt{6}}{5})$$

Now, we have following theorem for GA_e index of Benzenoid H_k, that is the main results in this paper.

Theorem 2.1. For the graphs from the circumcoronene series of benzenoid H_k $\forall$ $k\geq 1$.

$$GA_e(H_k) = 6k^2(3k-4) + \frac{48\sqrt{k-1}}{7} + \frac{24\sqrt{6}}{5}$$

Firstly, by introduce the following definition, we category the vertex set and edge set of a molecular graph G as follow.

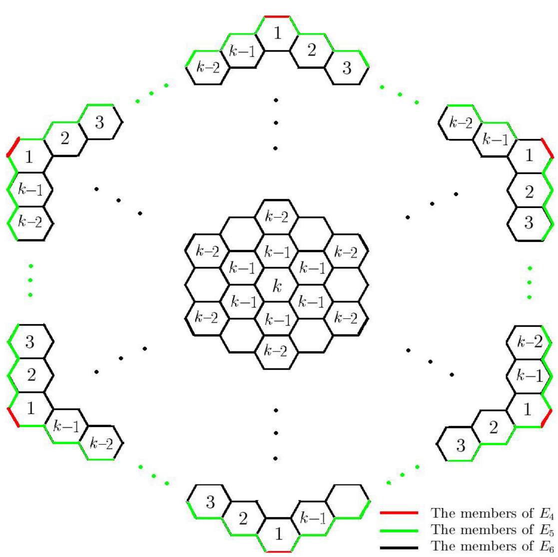

Fig. 1. The Circumcoronene Series of Benzenoid H_k $\forall$ $k\geq 1$ with edges marking.

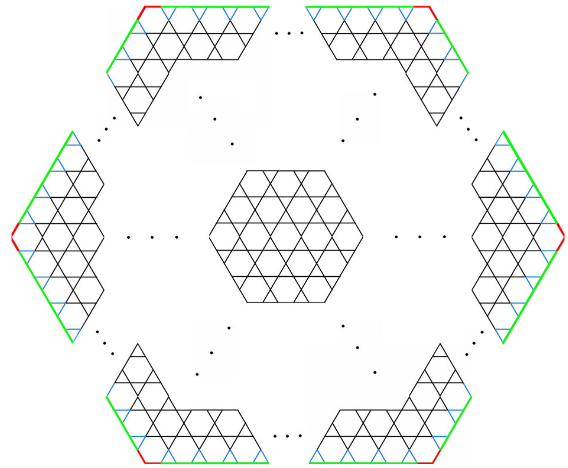

Fig. 2. The general representation of line graph of Circumcoronene Series of Benzenoid H_k $(k\geq 1)$ with edges marking.

Definition 2.2. Let G be the molecular graph and d_v is degree of vertex $v \in V(G)$ (Obviously $1\leq\delta\leq d_v\leq\Delta\leq n-1$, such that $\delta = Min\{d_v \mid v \in V(G)\}$ and $\Delta = Max\{d_v \mid v \in V(G)\}$). We divide edge set $E(G)$ and vertex set $V(G)$ of graph G to several partitions, as follow:

$$\forall k, \delta^2 \leq k \leq \Delta^2, V_k = \{v \in V(G) \mid d_u = k\}.$$
$$\forall j, \delta^2 \leq j \leq \Delta^2, E_j = \{e = uv \in E(G) \mid d_u \times d_v = j\}$$
$$\forall i, 2\delta \leq i \leq 2\Delta, E_i = \{e = uv \in E(G) \mid d_u + d_v = i\}$$

It's clear that we have two partitions $V_3 = \{v \in V(H_k) \mid d_v = 3\}$ and $V_2 = \{v \in V(H_k) \mid d_v = 2\}$ for circumcoronene series of benzenoid H_k $(k\geq 1)$ with size $6k(k-1)$ and $6k$, respectively. Obviously, there are three edge sets E_4, E_5 and E_6 as follow:

$$E_4 = \{e = uv \in E(G) \mid d_u = d_v = 2\} \Rightarrow |E_4| = 6$$
$$E_5 = \{e = uv \in E(G) \mid d_u = 2, d_v = 3\} \Rightarrow |E_5| = 12(k-1)$$
$$E_6 = \{e = uv \in E(G) \mid d_u = d_v = 3\} \Rightarrow |E_6| = 9k^2 - 15k + 6$$

We mark all edges belong to E_4 by red color, all edges belong to E_5 by green color and all edges of E_6 by black color in Figure 1, respectively.

Alternatively, we have three partitions $VL_4 = \{v \in V(L(H_k)) \text{ or } e \in E(H_k) \mid d_e = 4\}$, $VL_3 = \{e \in E(H_k) \mid d_e = 3\}$ and $VL_2 = \{e \in E(H_k) \mid d_e = 2\}$ for line graph of Circumcoronene series of benzenoid H_k $(k\geq 1)$. It's Obvious that these three vertex sets are equivalent respectively with three edge partitions E_4, E_5 and E_6.

On the other hands, we conclude $|V(L(H_k))| = 9k^2 - 3k$ from definition of line graph clearly and obtain

$$|E(L(H_k))| = \frac{4(9k^2 - 15k + 6) + 3 \times 12(k-1) + 2 \times 6}{2} = 18k^2 - 12k.$$

Now, consider the general representation of line graph of circumcoronene series of benzenoid in Figure 2. Thus, there exit four partitions EL_i *for* $i=5,\ldots,8$ as follow.

$$EL_5 = \{\mu = ef \in E(L(H_k)) \mid d_e = 2, d_f = 3\}$$
$$\Rightarrow |EL_5| = 2|VL_2| = 12$$

$$EL_6=\{\mu=ef\in E(L(H_k))\mid d_e=d_f=3\}$$
$$\Rightarrow |EL_6|=|VL_3|-|VL_2|=6(2k-3)$$
$$EL_7=\{\mu=ef\in E(L(H_k))\mid d_e=3, d_f=4\}$$
$$\Rightarrow |EL_6|=|VL_3|=12(k-1)$$
$$EL_8=\{\mu=ef\in E(L(H_k))\mid d_e=d_f=4\}$$
$$\Rightarrow |EL_8|=|E(L(H_k))|-|EL_7|-|EL_6|-|EL_5|$$
$$=18k^2-36k+18=18(k-1)^2.$$

Example 2.3. The edge GA index of benzenoid H_3 is

$$GA_e(H_3)=GA(L(H_3))=\frac{24\sqrt{6}}{5}+\frac{96\sqrt{3}}{7}+90=125.5114.$$

Proof. Consider the Circumcoronene H_3 and line graph of Circumcoronene $L(H_3)$ that shown in Figure 3. The number of edges of line graph of H_3 is *126*. The number of edges e_5, e_6 and e_7 in line graph H_3 are equal to *12, 18, 24* which belong to EL_5, EL_6 and EL_7, respectively. Also, the number of other edges which have the vertices with degrees *4* in $L(H_3)$ is *72*. We mark all members of EL_5, EL_6, EL_7 and EL_8 by red, green, blue and black color in Figure 3, respectively. Therefore, the desire result can be concluded.

RESULTS AND DISCUSSIONS

By using above mentions in the above section (Section 2. The method), we can compute the edge vertion of geometric-arithmetic index of Circumcoronene Homologous Series of Benzenoid H_k that k is positive integer number. Thus, we have the desire result can be concluded and we will prove the main theorem (Theorem 2.1) of this work as follow.

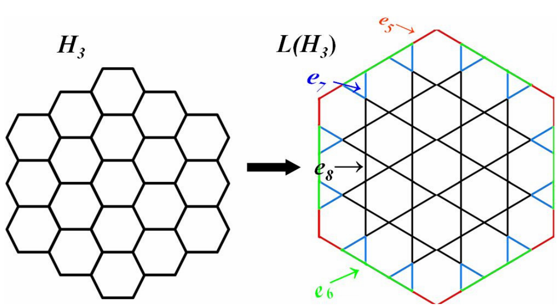

Fig. 3. The representation of Circumcoronene H_3 and its line graph $[L(H_3)]$.

Proof of Theorem 2.1. Consider the general case of Circumcoronene series of Benzenoid H_k for every integer number k. This molecular graph have $n_k=6k^2$ vertices and $m_k=9k^2-3k$ edges. By refer to definition of line graph of a graph G, we can compute the edge version of geometric-arithmetic index of H_k as follow. Of course by using the above argument, it's clear that $GA_e(G)$ is equivalent with geometric-arithmetic index of line graph of G. Thus,

$$GA_e(H_k)=\sum_{ef\in E(L(H_k))}\frac{2d_ed_f}{\sqrt{d_e+d_f}}$$
$$=\sum_{ef\in EL_5}\frac{2\sqrt{3\times 2}}{3+2}+\sum_{ef\in EL_6}\frac{2\sqrt{3\times 3}}{3+3}$$
$$+\sum_{ef\in EL_7}\frac{2\sqrt{4\times 3}}{4+3}+\sum_{ef\in EL_8}\frac{2\sqrt{4\times 4}}{4+4}$$
$$=\sum_{ef\in EL_5}\frac{2\sqrt{6}}{5}+\sum_{ef\in EL_6}1+\sum_{ef\in EL_7}\frac{4\sqrt{3}}{7}+\sum_{ef\in EL_8}1$$
$$=12\times\frac{2\sqrt{6}}{5}+6(2k-3)$$
$$+12(k-1)\times\frac{4\sqrt{3}}{7}+18(k-1)^2$$
$$=6k^2(3k-4)+\frac{48\sqrt{k-1}}{7}+\frac{24\sqrt{6}}{5}.$$

Here, proof of 2.1 Theorem is completed.

CONCLUSIONS

In Theoretical Chemistry, the topological indices and molecular structure descriptors are used for modeling physico-chemical, toxicologic, biological and other properties of chemical compounds and nano steucture analizing.

In this paper, we were counting one of new connectivity indices of the line graph of molecular graph Circumcoronene series of Benzenoids. This new topological connectivity index is useful to surveying the structure of molecular graphs, which called in molecular graphs. The *edge version of geometric-arithmetic index* recently introduced by *A. Iranmanesh et al.* on the ground of the end-vertex degree d_e and d_f of edges e and f in a line graph of G, where the line graph L(G) of a graph G is defined to be the graph whose vertices are the edges of G, with two vertices being adjacent if the corresponding edges share a vertex in G.

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