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New Arithmetic-Geometric Indices

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Abstract. We introduce some new topological indices: second, third, fourth and fifth arithmetic-geometric indices of a molecular graph. A single number that can be computed from the molecular graph and used to characterize some property of the underlying molecule is said to be topological index or molecular structure descriptor. In this paper, we compute the general reformulated first Zagreb index and the fifth arithmetic-geometric index of triangular benzenoid T_n and hexagonal parallelogram $P(m,n)$ nanotube by using the line graphs of subdivision graphs of these chemical graphs.

Keywords: topological index, second, third, fourth and fifth arithmetic-geometric indices, triangular benzenoid, hexagonal parallelogram $P(m, n)$ nanotube.

AMS Mathematics Subject Classification (2010): 05C05, 05C12, 05C35

1. Introduction

We consider only finite, simple and connected graph with a vertex $V(G)$ and an edge set $E(G)$. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v. The edge connecting the vertices u and v will be denoted by uv. Let $d_G(e)$ denote the degree of an edge $e=uv$ in G, which is defined by $d_G(e)= d_G(u)+ d_G(v) – 2$. Let $S_G(v)$ denote the sum of degrees of all vertices adjacent to a vertex v. The line graph $L(G)$ of a graph G is the graph whose vertex set corresponds to the edges of G such that two vertices of $L(G)$ are adjacent if the corresponding edges of G are adjacent. The subdivision graph $S(G)$ of a graph G is the graph obtained from G by replacing each of its edges by a path of length two. We refer to [1, 2] for undefined term and notation.

We need the following existing results.

Lemma 1. [1] Let G be a (p, q) graph. Then $L(G)$ has q vertices and $\frac{1}{2}\sum_{i=1}^{p} d_G(u_i)^2 - q$ edges.

Lemma 2. [1] Let G be a (p, q) graph. Then $S(G)$ has $p+q$ vertices and $2q$ edges.

A molecular graph is a graph such that its vertices correspond to the atoms and the edges to the bonds. Chemical graph theory is a branch of Mathematical chemistry which has an important effect on the development of the chemical sciences. A single number that can be computed from the molecular graph and used to characterize some property of the underlying molecule is said to be a topological index or molecular structure descriptor. Numerous such descriptors have been considered in theoretical chemistry and have found some applications, especially in *QSPR*/Q*SAR* research, see [3]

In [4], Miličević et al. reformulated the first Zagreb index in terms of edge degrees instead of vertex degrees and defined the respective topological index as

$$EM_1(G)=\sum_{e\in E(G)} d_G(e)^2.$$

This topological index was also studied, for example, in [5, 6].

The *K*-edge index of a graph *G* is defined as

$$K_e(G)=\sum_{e\in E(G)} d_G(e)^3.$$

The *K*-edge index was introduced by Kulli in [7] and was studied, for example, in [8].

In [9], Kulli proposed the general reformulated Zagreb index of a graph *G* and defined it as

$$EM_1^a(G)=\sum_{e\in E(G)} d_G(e)^a$$

where *a* is a real number.

The arithmetic-geometric index [10] of a graph is defined as

$$AG_1(G)=\sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)d_G(v)}}.$$

Motivated by previous research on topological indices, we now propose the second, third, fourth and fifth arithmetic-geometric indices of a graph as follows:

The second arithmetic-geometric index of a graph *G* is defined as

$$AG_2(G)=\sum_{uv\in E(G)} \frac{n_u+n_v}{2\sqrt{n_u n_v}}$$

where the number n_u of vertices of *G* lying closer to the vertex *v* for the edge *uv* of a graph *G*.

The third arithmetic-geometric index of a graph *G* is defined as

$$AG_3(G)=\sum_{uv\in E(G)} \frac{m_u+m_v}{2\sqrt{m_u m_v}}$$

where the number m_u of edges of *G* lying closer to the vertex *v* for the edge *uv* of a graph *G*.

The fourth arithmetic-geometric index of a graph *G* is defined as

$$AG_4(G)=\sum_{uv\in E(G)} \frac{\varepsilon(u)+\varepsilon(v)}{2\sqrt{\varepsilon(u)\varepsilon(v)}}$$

where the number $\varepsilon(u)$ is the eccentricity of all vertices adjacent to a vertex *u*.

The fifth arithmetic-geometric index of a graph *G* is defined as

$$AG_5(G) = \sum_{uv \in E(G)} \frac{S_G(u) + S_G(v)}{2\sqrt{S_G(u) S_G(v)}}$$

where $S_G(u)$ is the sum of the degrees of all vertices adjacent to a vertex u.

In this paper, we compute the general reformulated first Zagreb index, reformulated first Zagreb index, K-edge index and fifth arithmetic-geometric index of triangular benzenoids T_n and hexagonal parallelogram $P(m, n)$ nanotubes by using the line graphs of the subdivision graphs of these chemical graphs.

2. Results for triangular Benzenoids T_n, $n \in N$

We consider triangular benzenoids which is a family of benzenoid molecular graphs. We denote the triangular benzenoid molecular graph by T_n in which n is the number of hexagons in the base of a graph, as shown in Figure 1(a). Clearly a triangular benzenoid T_n has $|V(T_n)| = n^2 + 4n + 1$ vertices and $\left|E(T_n)\right| = \frac{3}{2}n(n+3)$ edges.

The line graph of the subdivision graph of triangular benzenoid T_n is depicted in Figure 1(c).

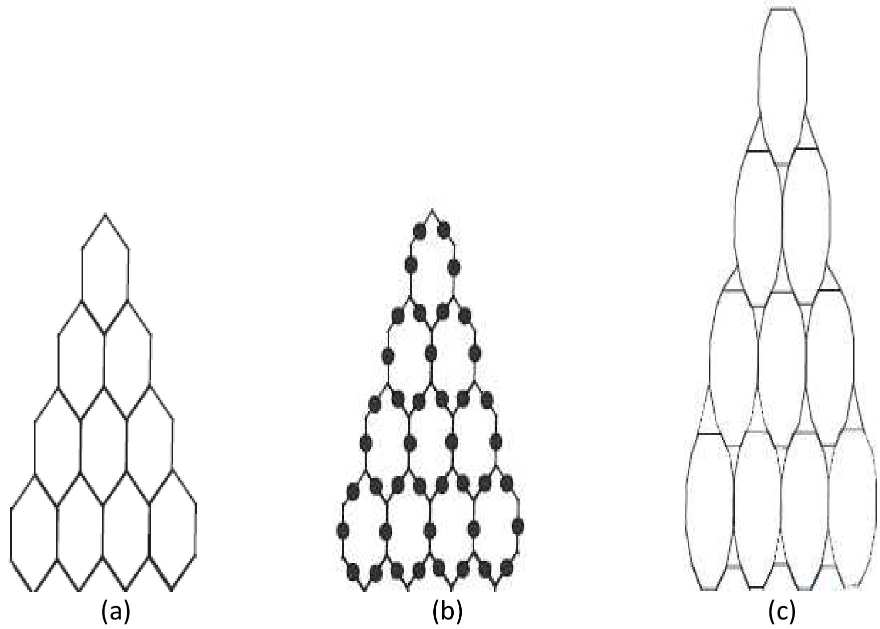

Figure 1: (a) triangular benzenoid T_4 (b) subdivision graph of T_4 (c) Line graph of the subdivision graph of T_4.

We now compute general reformulated Zagreb index, reformulated first Zagreb index and K-edge index of the line graph of the subdivision graph of a triangular benzenoid.

Theorem 1. Let G be the line graph of the subdivision graph of a triangular benzenoid T_n, $n \in \square N$. Then

$$EM_1^a(G) = 3(n+3)2^a + 6(n-1)3^a + \frac{3}{2}\left(3n^2 + n - 1\right)4^a. \qquad (1)$$

where a is a real number.

Proof: The triangular benzenoid is a graph with $n^2 + 4n + 1$ vertices and $\frac{3}{2}n(n+3)$ edges. By Lemma 2 and Lemma 1, the line graph of the subdivision graph G has $\frac{3}{2}\left(3n^2 + 7n - 2\right)$ edges. Father, the edge partition of G based on degree of end vertices of each edge is given in Table 1.

$d_G(u), d_G(v)\backslash e = uv \in E(G)$	(2, 2)	(2, 3)	(3,3)
$d_G(e)$	2	3	4
Number of edges	$3(n+3)$	$6(n-1)$	$\frac{3}{2}\left(3n^2 + n - 1\right)$

Table 1: Edge degree partition of G

To compute $EM_1^a(G)$, we see that

$$EM_1^a(G) = \sum_{e \in E(G)} d_G(e)^a = \sum_{e \in E_4} d_G(e)^a + \sum_{e \in E_5} d_G(e)^a + \sum_{e \in E_6} d_G(e)^a$$

$$= 3(n+3)2^a + 6(n-1)3^a + \frac{3}{2}(3n^2 + n - 1)4^a.$$

An immediate result is the reformulated first Zagreb index of G.

Corollary 1.1. Let G be the line graph of the subdivision graph of a triangular benzenoid T_n, $n \in N$. Then

$EM_1(G) = 72n^2 + 90n + 42.$

Proof: Put $a = 2$ in equation (1), we get the required result.

Corollary 1.2. Let G be the line graph of the subdivision graph of a triangular benzonoid T_n, $n \in N$. Then

$K_e(G) = 288n^2 + 282n - 186.$

Prof: Put $a = 2$ in equation (1), we get the required result.

We compute fifth arithmetic-geometric index of the line graph of the subdivision graph of a triangular benzenoid.

Theorem 2. Let G be the line graph of the subdivision graph of a triangular benzenoid T_n, $n \in N$. Then

$$AG_5(G) = \frac{9}{2}n^2 + \left(\frac{39}{2\sqrt{10}} + \frac{17}{2\sqrt{2}} - \frac{3}{2}\right)n + \left(\frac{27}{2\sqrt{5}} - \frac{39}{2\sqrt{10}} - \frac{17}{2\sqrt{2}} + 6\right), \qquad \text{if } n \neq 1,$$

$$= 9, \qquad \text{if } n = 1.$$

Proof: The edge partition based on the degree sum of neighbor vertices of each edge of G is obtained as given in Table 2.

$S_G(u)$, $S_G(v)$ \ $uv \in E(G)$	(4,4)	(4,5)	(5,5)	(5, 8)	(8, 8)	(8, 9)	(9, 9)
Number of edges	9	6	$3(n-2)$	$6(n-1)$	$3(n-1)$	$6(n-1)$	$\frac{3}{2}(3n^2-5n+2)$

Table 2: Edge partition of G

Case 1. Suppose $n \neq 1$.

To compute $AG_5(G)$, we see that

$$AG_5(G) = \sum_{uv \in E(G)} \frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u)S_G(v)}}$$

$$= 9\left(\frac{4+4}{2\sqrt{4\times4}}\right) + \frac{6(4+5)}{2\sqrt{4\times5}} + 3(n-2)\left(\frac{5+5}{2\sqrt{5\times5}}\right) + 6(n-1)\left(\frac{5+8}{2\sqrt{5\times8}}\right) + 3(n-1)\left(\frac{8+8}{2\sqrt{8\times8}}\right)$$

$$+6(n-1)\frac{8+9}{2\sqrt{8\times9}} + \frac{3}{2}\left(3n^2-5n+2\right)\left(\frac{9+9}{2\sqrt{9\times9}}\right)$$

$$= 9+6\left(\frac{9}{4\sqrt{5}}\right) + 3(n-2) + 6(n-1)\left(\frac{13}{4\sqrt{10}}\right) + 3(n-1) + 6(n-1)\left(\frac{17}{12\sqrt{2}}\right)$$

$$+\frac{3}{2}\left(3n^2-5n+2\right)$$

$$= \frac{9}{2}n^2 + \left(\frac{39}{2\sqrt{10}} + \frac{17}{2\sqrt{2}} - \frac{3}{2}\right)n + \left(\frac{27}{2\sqrt{5}} - \frac{39}{2\sqrt{10}} - \frac{17}{2\sqrt{2}} + 6\right)$$

Case 2. Suppose $n = 1$

To compute $AG_5(G)$, we see that

$$AG_5(G) = \sum_{uv \in E(G)} \frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u)S_G(v)}} = 9\left(\frac{4+4}{2\sqrt{4\times4}}\right) = 9$$

3. Results for hexagonal parallelogram $P(m, n)$ for any $m,n \in N$ nanotubes

We consider hexagonal parallelogram nanotubes. These nanotubes usually symbolized as $P(m, n)$ for any $m, n \in N$ in which m is the number of hexagons in any row and n is the number of hexagons in any column, see. Figure 2(a). A hexagonal parallelogram $P(m, n)$ has $2(m+n+mn)$ vertices and $3mn + 2m + 2n - 1$ edges.

The line graph of the subdivision graph of hexagonal parallelogram $P(m,n)$ is depicted in Figure 2(c).

We compute general reformulated Zagreb index, reformulated first Zagreb index and K-edge index of the line graph of the subdivision graph of a hexagonal parallelogram nanotube.

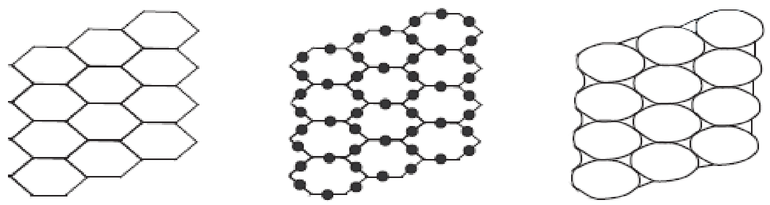

Figure 2: (a) hexagonal parallelogram $P(3,4)$ (b) subdivision graph of $P(3,4)$ (c) line graph of the subdivision graph of $P(3,4)$.

Theorem 3. Let G be the line graph of the subdivision graph of a hexagonal parallelogram $P(m, n)$ for any $m, n \in N$. Then

$$EM_1^{(a)}(G) = 2(m+n+4)2^a + 4(m+n-2)3^a + (9mn-2m-2n-5)4^a \quad (2)$$

where a is a real number.

Proof: The hexagonal parallelogram is a graph with $2(m+n+mn)$ vertices and $3mn+2m+2n-1$ edges. By Lemma 2 and Lemma 1, the line graph of the subdivision graph G has $2(3mn+2m+2n-1)$ vertices and $9mn+4m+4n$–5) edges. Further, the edge partition of G based on degree of end vertices of each edge is given in Table 3.

$d_G(u), d_G(v)\backslash e = uv \in E(G)$	(2, 2)	(2, 3)	(3,3)
$d_G(e)$	2	3	4
Number of edges	$2(m+n+4)$	$4(m+n-2)$	$9mn-2m-2n-5$

Table 3: Edge degree partition of G.

To compute $EM_1^{(a)}(G)$, we see that

$$EM_1^{(a)}(G) = \sum_{e \in E(G)} d_G(e)^a = \sum_{e \in E_4} d_G(e)^a + \sum_{e \in E_5} d_G(e)^a + \sum_{e \in E_6} d_G(e)^a$$

$$= 2(m+n+4)2^a + 4(m+n-2)3^a + (9mn-2m-2n-5)4^a.$$

An immediate result is the reformulated first Zagreb index of G.

Corollary 3.1. Let G be the line graph of the subdivision graph of a hexagonal parallelogram $P(m, n)$ for any $m,n \in N$. Then

$$EM_1(G) = 144mn + 12(m+n) - 120.$$

Proof: Put $a = 2$ in equation (2), we get the required result.

Another immediate result is the K-edge index of G.

Corollary 3.2. Let G be the line graph of the subdivision graph of a hexagonal parallelogram $P(m,n)$ for any $m, n \in N$. Then

$$K_e(G) = 576mn - 4(m+n) - 472.$$

Proof: Put $a = 3$ in equation (2), we get the required result.

We compute fifth arithmetic-geometric index of the line graph of the subdivision graph of a hexagonal parallelogram nanotube.

Theorem 4. Let G be the line graph of the subdivision in graph of a hexagonal parallelogram $P(m,n)$ for any $m, n \in N$. Then

$$AG_5(G) = \left(5+\frac{13}{\sqrt{10}}+\frac{17}{3\sqrt{2}}\right)n+3+\frac{9}{\sqrt{5}}-\frac{13}{\sqrt{10}}-\frac{17}{3\sqrt{2}}, \quad \text{if } n\neq 1,\ m=1.$$

$$=9mn+\left(\frac{13}{\sqrt{10}}+\frac{17}{3\sqrt{2}}-4\right)(m+n)+3+\frac{18}{\sqrt{5}}-\frac{26}{\sqrt{10}}-\frac{34}{3\sqrt{2}}, \quad \text{if } n\neq 1,\ m>1.$$

Proof: Case 1. The edge partition based on the degree sum of neighbor vertices of each edge of $G = P(m,n)$ $n \neq 1$, $m = 1$ is obtained as given in Table 4.

$S_G(u)$, $S_G(v)\backslash uv \in E(G)$	(4,4)	(4,5)	(5,5)	(5, 8)	(8, 8)	(8, 9)	(9,9)
Number of edges	10	4	$2(n-2)$	$4(n-1)$	$2(n-1)$	$4(n-1)$	$n-1$

Table 4: Edge partition of $G = P(m, n)$, $n \neq 1$, $m = 1$

Suppose $n \neq 1$ and $m = 1$.
To compute $AG_5(G)$, we see that

$$AG_5(G) = \sum_{uv\in E(G)} \frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u)S_G(v)}}$$

$$=10\left(\frac{4+4}{2\sqrt{4\times 4}}\right)+4\left(\frac{4+5}{2\sqrt{4\times 5}}\right)+2(n-2)\left(\frac{5+5}{2\sqrt{5\times 5}}\right)+4(n-1)\left(\frac{5+8}{2\sqrt{5\times 8}}\right)$$

$$+2(n-1)\left(\frac{8+8}{2\sqrt{8\times 8}}\right)+4(n-1)\left(\frac{8+9}{2\sqrt{8\times 9}}\right)+(n-1)\left(\frac{9+9}{2\sqrt{9\times 9}}\right)$$

$$=\left(5+\frac{13}{\sqrt{10}}+\frac{17}{3\sqrt{2}}\right)n+3+\frac{9}{\sqrt{5}}-\frac{13}{\sqrt{10}}-\frac{17}{3\sqrt{2}}.$$

Case 2. The edge partition based on the degree sum of neighbor vertices of each edge of $G = P(m,n)$, $n \neq 1$, $m>1$ is obtained as given in Table 5.

$S_G(u)$, $S_G(v) \backslash uv\in E(G)$	(4,4)	(4,5)	(5,5)	(5, 8)	(8, 8)	(8, 9)	(9,9)
Number of edges	8	8	$2(m+n-4)$	$4(m+n-2)$	$2(m+n-2)$	$4(m+n-2)$	$9mn-8(m+n)+7$

Table 5: Edge partition of $G = P(m, n)$, $n \neq 1$, $m>1$.

Suppose $n \neq 1$, and $m>1$.
To compute $AG_5(G)$, we see that

$$AG_5(G) = \sum_{uv\in E(G)} \frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u)S_G(v)}}$$

$$=8\left(\frac{4+4}{2\sqrt{4\times 4}}\right)+8\left(\frac{4+5}{2\sqrt{4\times 5}}\right)+2(m+n-4)\left(\frac{5+5}{2\sqrt{5\times 5}}\right)+4(m+n-2)\left(\frac{5+8}{2\sqrt{5\times 8}}\right)$$

$$+2\left(m+n-2\right)\left(\frac{8+8}{2\sqrt{8\times 8}}\right)+4\left(m+n-2\right)\left(\frac{8+9}{2\sqrt{8\times 9}}\right)+\left(9mn-8m-8n+7\right)\left(\frac{9+9}{2\sqrt{9\times 9}}\right)$$

$$=9mn+\left(\frac{13}{\sqrt{10}}+\frac{17}{3\sqrt{2}}-4\right)\left(m+n\right)+3+\frac{18}{\sqrt{5}}-\frac{26}{\sqrt{10}}-\frac{34}{3\sqrt{2}}.$$

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