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Delta Geometric-Arithmetic and Delta Arithmetic-Geometric Indices of Certain Nanotubes and Networks

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Abstract

In this study, we introduce the delta geometric-arithmetic index and the delta arithmetic-geometric index and their corresponding polynomials of a graph. Furthermore we present the computational formulas for calculating the delta geometric-arithmetic index and the delta arithmetic-geometric index and corresponding their polynomials of two families of nanotubes and two families of networks.

Keywords: 05C07, 05C09, 05C92.

2020 Mathematics Subject Classification: Delta geometric-arithmetic index; delta arithmetic-geometric index; nanotube; network.

1. Introduction

The graph $G=(V(G),E(G))$, where $V(G)$ vertex set and $E(G)$ edge set. Let $d_G(u)$ denote the degree of a vertex u. We refer [1], for other definitions. Topological indices are numerical values obtained from chemical structures. It is very important to determine topological indices of nanotubes and networks to compare physicochemical properties using QSAR models. The δ vertex degree was introduced in [2] and it is defined as

$$\delta_u = d_G(u) - \delta(G) + 1$$

The first and second δ-Banhatti indices [3] of a graph are defined as

$$\delta B_1(G) = \sum_{uv\in E(G)} (\delta_u + \delta_v)$$

$$\delta B_2(G) = \sum_{uv\in E(G)} \delta_u \delta_v$$

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Recently, some delta indices were studied in [4-11]. We introduce the delta geometric-arithmetic index of a graph G, defined it as

$$\delta GA\left(G\right)=\sum_{uv\in E(G)}\frac{2\sqrt{\delta_u\delta_v}}{\delta_u+\delta_v}$$

Considering the delta geometric-arithmetic index, we define the delta geometric-arithmetic polynomial of a graph G as

$$\delta GA\left(G,x\right)=\sum_{uv\in E(G)}x^{\frac{2\sqrt{\delta_u\delta_v}}{\delta_u+\delta_v}}$$

We also introduce the delta arithmetic-geometric index of a graph G, defined it as

$$\delta AG\left(G\right)=\sum_{uv\in E(G)}\frac{\delta_u+\delta_v}{2\sqrt{\delta_u\delta_v}}$$

Considering the delta arithmetic-geometric index, we define the delta arithmetic-geometric polynomial of a graph G as

$$\delta AG\left(G,x\right)=\sum_{uv\in E(G)}x^{\frac{\delta_u+\delta_v}{2\sqrt{\delta_u\delta_v}}}$$

The geometric-arithmetic and arithmetic-geometric indices have been researched in the past [12-19]. In this research work, we compute the delta geometric-arithmetic index and delta arithmetic-geometric index of certain nanotubes and networks.

2. Results for $HC_5C_7[p,q]$ Nanotubes

We focus on the family of nanotubes, denoted by $HC_5C_7[p,q]$, in which p is the number of heptagons in the first row and q rows of pentagons repeated alternately. Let G be the graph of a nanotube $HC_5C_7[p,q]$.

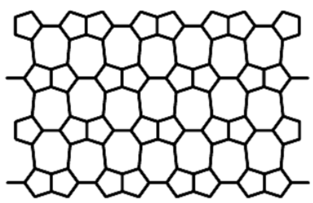

Figure 1: 2-D lattice ofnanotube $HC_5C_7[8,4]$

The 2-D lattice of nanotube $HC_5C_7[p,q]$ is shown in Figure 1. We obtain that G has $4pq$ vertices and $6pq-p$ edges. The graph G has two types of edges as follows:

$$E_1=\{uv\in E(G)|d_G(u)=2,d_G(v)=3\},\qquad |E_1|=4p$$
$$E_2=\{uv\in E(G)|d_G(u)=d_G(v)=3\},\qquad |E_2|=6pq-5p.$$

We have $\delta(G) = 2$. Therefore $\delta_u = d_G(u) - \delta(G) + 1 = d_G(u) - 1$. Thus there are two types of δ-edges as given in Table 1.

$\delta_u, \delta_v \setminus uv \in E(G)$	Number of edges
(1, 1)	$4p$
(2, 2)	$6pq - 5p$

Table 1: δ-edge partition of $HC_5C_7[p, q]$

Theorem 2.1. *Let G be the graph of a nanotube $HC_5C_7[p, q]$. Then*

(i). $\delta GA\,(G) = 6pq + \left(\frac{8\sqrt{2}}{3} - 5\right)p.$

(ii). $\delta GA\,(G, x) = 4px^{\frac{2\sqrt{2}}{3}} + (6pq - 5p)\,x^1.$

Proof. From definitions and by using Table 1, we deduce

(i). $$\delta GA\,(G) = \sum_{uv \in E(G)} \frac{2\sqrt{\delta_u \delta_v}}{\delta_u + \delta_v}$$
$$= 4p\frac{2\sqrt{1 \times 2}}{1+2} + (6pq - 5p)\frac{2\sqrt{2 \times 2}}{2+2}$$
$$= 6pq + \left(\frac{8\sqrt{2}}{3} - 5\right)p.$$

(ii). $$\delta GA\,(G, x) = \sum_{uv \in E(G)} x^{\frac{2\sqrt{\delta_u \delta_v}}{\delta_u + \delta_v}}$$
$$= 4px^{\frac{2\sqrt{1\times 2}}{1+2}} + (6pq - 5p)\,x^{\frac{2\sqrt{2\times 2}}{2+2}}$$
$$= 4px^{\frac{2\sqrt{2}}{3}} + (6pq - 5p)\,x^1.$$

□

Theorem 2.2. *Let G be the graph of a nanotube $HC_5C_7[p, q]$. Then*

(i). $\delta AG\,(G) = 6pq + \left(\frac{6}{2\sqrt{2}} - 5\right)p.$

(ii). $\delta AG\,(G, x) = 4px^{\frac{3}{2\sqrt{2}}} + (6pq - 5p)\,x^1.$

Proof. From definitions and by using Table 1, we deduce

(i). $$\delta AG\,(G) = \sum_{uv \in E(G)} \frac{\delta_u + \delta_v}{2\sqrt{\delta_u \delta_v}}$$
$$= 4p\frac{1+2}{2\sqrt{1 \times 2}} + (6pq - 5p)\frac{2+2}{2\sqrt{2 \times 2}}$$
$$= 6pq + \left(\frac{6}{2\sqrt{2}} - 5\right)p$$

(ii). $$\delta AG\,(G, x) = \sum_{uv \in E(G)} x^{\frac{\delta_u + \delta_v}{2\sqrt{\delta_u \delta_v}}}$$
$$= 4px^{\frac{1+2}{2\sqrt{1\times 2}}} + (6pq - 5p)\,x^{\frac{2+2}{2\sqrt{2\times 2}}}$$
$$= 4px^{\frac{3}{2\sqrt{2}}} + (6pq - 5p)\,x^1$$

□

3. Results for $SC_5C_7[p,q]$ Nanotubes

We focus on the family of nanotubes, denoted by $SC_5C_7[p,q]$, in which p is the number of heptagons in the first row and q rows of vertices and edges are repeated alternately. The 2-D lattice of nanotube $SC_5C_7[p,q]$ is presented in Figure 2.

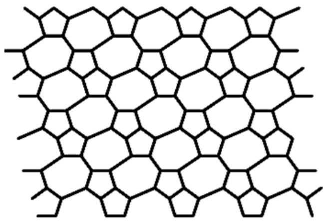

Figure 2: 2-D lattice of nanotube $SC_5C_7[p,q]$

Let G be the graph of $SC_5C_7[p,q]$. We obtain that G has $4pq$ vertices and $6pq-p$ edges. We get that G has three types of edges as follows:

$$E_1 = \{uv \in E(G) | d_G(u) = d_G(v) = 2\}, \qquad |E_1| = q.$$
$$E_2 = \{uv \in E(G) | d_G(u) = 2, d_G(v) = 3\}, \qquad |E_2| = 6q.$$
$$E_2 = \{uv \in E(G) | d_G(u) = d_G(v) = 3\}, \qquad |E_3| = 6pq - p - 7q.$$

We have $\delta(G) = 2$. Thus $\delta_u = d_G(u) - \delta(G) + 1 = d_G(u) - 1$. There are three types of δ-edges as given in Table 2.

$\delta_u, \delta_v \setminus uv \in E(G)$	Number of edges
(1, 1)	q
(1, 2)	$6q$
(2, 2)	$6pq-p-7q$

Table 2: δ-edge partition of $SC_5C_7[p,q]$

Theorem 3.1. *Let Gbe the graph of a nanotube $HC_5C_7[p,q]$. Then*

(i). $\delta GA\,(G) = 6pq - p + \left(4\sqrt{2} - 6\right) q.$

(ii). $\delta GA\,(G,x) = 6qx^{\frac{2\sqrt{2}}{3}} + (6pq - p - 6q)\, x^1.$

Proof. From definitions and by using Table 2, we deduce

(i). $$\delta GA\,(G) = \sum_{uv \in E(G)} \frac{2\sqrt{\delta_u \delta_v}}{\delta_u + \delta_v}$$
$$= q\frac{2\sqrt{1\times 1}}{1+1} + 6q\frac{2\sqrt{1\times 2}}{1+2} + (6pq - p - 7q)\frac{2\sqrt{2\times 2}}{2+2}$$
$$= 6pq - p + \left(4\sqrt{2} - 6\right) q.$$

$$\begin{aligned}
\text{(ii). } \delta GA(G,x) &= \sum_{uv\in E(G)} x^{\frac{2\sqrt{\delta_u\delta_v}}{\delta_u+\delta_v}} \\
&= qx^{\frac{2\sqrt{1\times1}}{1+1}} + 6qx^{\frac{2\sqrt{1\times2}}{1+2}} + (6pq-p-7q)\,x^{\frac{2\sqrt{2\times2}}{2+2}} \\
&= 6qx^{\frac{2\sqrt{2}}{3}} + (6pq-p-6q)\,x^{1}.
\end{aligned}$$

□

Theorem 3.2. *Let Gbe the graph of a nanotube $HC_5C_7[p,q]$. Then*

(i). $\delta AG(G) = 6pq - p + \left(\frac{9}{\sqrt{2}} - 6\right) q.$

(ii). $\delta AG(G,x) = 6qx^{\frac{3}{2\sqrt{2}}} + (6pq-p-6q)\,x^{1}.$

Proof. From definitions and by using Table 2, we deduce

$$\begin{aligned}
\text{(i). } \delta AG(G) &= \sum_{uv\in E(G)} \frac{\delta_u+\delta_v}{2\sqrt{\delta_u\delta_v}} \\
&= q\frac{1+1}{2\sqrt{1\times1}} + 6q\frac{1+2}{2\sqrt{1\times2}} + (6pq-p-7q)\frac{2+2}{2\sqrt{1\times2}} \\
&= 6pq - p + \left(\frac{9}{\sqrt{2}} - 6\right) q.
\end{aligned}$$

$$\begin{aligned}
\text{(ii). } \delta AG(G,x) &= \sum_{uv\in E(G)} x^{\frac{\delta_u+\delta_v}{2\sqrt{\delta_u\delta_v}}} \\
&= qx^{\frac{1+1}{2\sqrt{1\times1}}} + 6qx^{\frac{1+2}{2\sqrt{1\times2}}} + (6pq-p-7q)\,x^{\frac{2+2}{2\sqrt{2\times2}}} \\
&= 6qx^{\frac{3}{2\sqrt{2}}} + (6pq-p-6q)\,x^{1}.
\end{aligned}$$

□

4. Results for Silicate Networks

Silicate networks are obtained by fusing metal oxide or metal carbonates with sand. A silicate network is denoted by SL_n. A 2-D silicate network is presented in Figure 3.

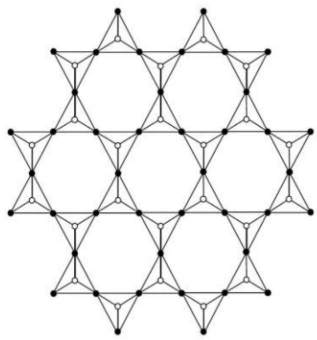

Figure 3: A 2-D silicate network

Let G be the graph of a silicate network SL_n. We obtain that G has $15n^2 + 3n$ vertices and $36n^2$ edges. In G, there are three types of edges as follows:

$$E_1 = \{uv \in E(G) | d_G(u) = d_G(v) = 3\}, \qquad |E_1| = 6n$$

$$E_2 = \{uv \in E(G)|d_G(u) = 3, d_G(v) = 6\}, \qquad |E_2| = 18n^2 + 6n$$
$$E_3 = \{uv \in E(G)|d_G(u) = d_G(v) = 6\}, \qquad |E_3| = 18n^2 - 12n$$

We have $\delta(G) = 3$ and hence $\delta_u = d_G(u) - \delta(G) + 1 = d_G(u) - 2$. Hence there are 3 types of δ-edges as given in Table 3.

$\delta_u, \delta_v \backslash uv \in E(G)$	(1, 1)	(1, 4)	(4, 4)
Number of edges	$6n$	$18n^2 + 6n$	$18n^2 - 12n$

Table 3: δ-edge partition of SL_n

Theorem 4.1. *Let G be the graph of a silicate network SL_n. Then*

(i). $\delta GA\,(G) = \frac{162}{5}n^2 - \frac{6}{5}n$

(ii). $\delta GA\,(G,x) = (18n^2 + 6n)x^{\frac{4}{5}} + (18n^2 - 6n)x^1$

Proof. From definitions and by using Table 3, we deduce

$$\begin{aligned}
\text{(i). } \delta GA\,(G) &= \sum_{uv\in E(G)} \frac{2\sqrt{\delta_u\delta_v}}{\delta_u + \delta_v} \\
&= 6n\frac{2\sqrt{1\times 1}}{1+1} + (18n^2+6n)\frac{2\sqrt{1\times 4}}{1+4} + (18n^2-12n)\frac{2\sqrt{4\times 4}}{4+4} \\
&= \frac{162}{5}n^2 - \frac{6}{5}n.
\end{aligned}$$

$$\begin{aligned}
\text{(ii). } \delta GA\,(G,x) &= \sum_{uv\in E(G)} x^{\frac{2\sqrt{\delta_u\delta_v}}{\delta_u+\delta_v}} \\
&= 6nx^{\frac{2\sqrt{1\times1}}{1+1}} + (18n^2+6n)x^{\frac{2\sqrt{1\times4}}{1+4}} + (18n^2-12n)x^{\frac{2\sqrt{4\times4}}{4+4}} \\
&= (18n^2+6n)x^{\frac{4}{5}} + (18n^2-6n)x^1.
\end{aligned}$$

□

Theorem 4.2. *Let G be the graph of a silicate network SL_n. Then*

(i). $\delta AG\,(G) = \frac{81}{2}n^2 + \frac{3}{2}n$

(ii). $\delta AG\,(G,x) = (18n^2 + 6n)x^{\frac{5}{4}} + (18n^2 - 6n)x^1$

Proof. From definitions and by using Table 3, we deduce

$$\begin{aligned}
\text{(i). } \delta AG\,(G) &= \sum_{uv\in E(G)} \frac{\delta_u + \delta_v}{2\sqrt{\delta_u\delta_v}} \\
&= 6n\frac{1+1}{2\sqrt{1\times 1}} + (18n^2+6n)\frac{1+4}{2\sqrt{1\times 4}} + (18n^2-12n)\frac{4+4}{2\sqrt{4\times 4}} \\
&= \frac{81}{2}n^2 + \frac{3}{2}n
\end{aligned}$$

$$\begin{aligned}\text{(ii). } \delta AG(G,x) &= \sum_{uv\in E(G)} x^{\frac{\delta_u+\delta_v}{2\sqrt{\delta_u\delta_v}}}\\ &= 6nx^{\frac{1+1}{2\sqrt{1\times 1}}} + (18n^2+6n)x^{\frac{1+4}{2\sqrt{1\times 4}}} + (18n^2-12n)x^{\frac{4+4}{2\sqrt{4\times 4}}}\\ &= (18n^2+6n)x^{\frac{5}{4}} + (18n^2-6n)x^1\end{aligned}$$

□

5. Results for Honeycomb Networks

If we recursively use hexagonal tiling in particular pattern, honeycomb networks are formed. These networks are very useful in Chemistry and also in Computer Graphics. A honeycomb network of dimension n is denoted by HC_n. A honeycomb network of dimension four is shown in Figure 4.

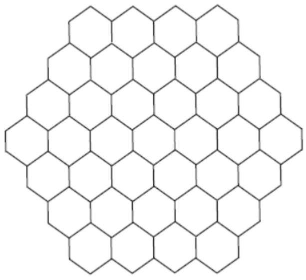

Figure 4: Honeycomb network of dimension four

Let G be the graph of a honeycomb network HC_n. We obtain that G has $6n^2$ vertices and $9n^2-3n$ edges. In G, there are three types of edges as follows:

$$\begin{aligned} E_1 &= \{uv\in E(G) | d_G(u)=d_G(v)=2\}, & |E_1| &= 6\\ E_2 &= \{uv\in E(G) | d_G(u)=2, d_G(v)=3\}, & |E_2| &= 12n-12\\ E_3 &= \{uv\in E(G) | d_G(u)=d_G(v)=3\}, & |E_3| &= 9n^2-15n+6\end{aligned}$$

We have $\delta(G)=2$ and hence $\delta_u = d_G(u)-\delta(G)+1 = d_G(u)-1$. Hence there are 3 types of δ-edges as given in Table 4.

$\delta_u, \delta_v \setminus uv \in E(G)$	(1, 1)	(1, 2)	(2, 2)
Number of edges	6	$12n-12$	$9n^2-15n+6$

Table 4: δ-edge partition of HC_n

Theorem 5.1. *Let G be the graph of a honeycomb network HC_n. Then*

(i). $\delta GA(G) = 9n^2 + \left(8\sqrt{2}-15\right)n + 12 - 8\sqrt{2}$

(ii). $\delta GA(G,x) = (12n-12)x^{\frac{2\sqrt{2}}{3}} + (9n^2-15n+12)x^1$

Proof. From definitions and by using Table 4, we deduce

$$\begin{aligned}
\text{(i). } \delta GA\left(G\right) &= \sum_{uv\in E(G)} \frac{2\sqrt{\delta_u\delta_v}}{\delta_u+\delta_v} \\
&= 6\frac{2\sqrt{1\times 1}}{1+1} + (12n-12)\frac{2\sqrt{1\times 2}}{1+2} + (9n^2-15n+6)\frac{2\sqrt{2\times 2}}{2+2} \\
&= 9n^2 + \left(8\sqrt{2}-15\right)n + 12 - 8\sqrt{2}
\end{aligned}$$

$$\begin{aligned}
\text{(ii). } \delta GA\left(G,x\right) &= \sum_{uv\in E(G)} x^{\frac{2\sqrt{\delta_u\delta_v}}{\delta_u+\delta_v}} \\
&= 6x^{\frac{2\sqrt{1\times 1}}{1+1}} + (12n-12)x^{\frac{2\sqrt{1\times 2}}{1+2}} + (9n^2-15\,n+6)x^{\frac{2\sqrt{2\times 2}}{2+2}} \\
&= (12n-12)x^{\frac{2\sqrt{2}}{3}} + (9n^2-15\,n+12)x^1
\end{aligned}$$

□

Theorem 5.2. *Let G be the graph of a nanotube $HC_5C_7[p,q]$.Then*

(i). $\delta AG\left(G\right) = 9n^2 + \left(\frac{18}{\sqrt{2}}-15\right)n + 12 - \frac{18}{\sqrt{2}}$

(ii). $\delta AG\left(G,x\right) = (12n-12)x^{\frac{3}{2\sqrt{2}}} + (9n^2-15n+12)x^1$

Proof. From definitions and by using Table 4, we deduce

$$\begin{aligned}
\text{(i). } \delta AG\left(G\right) &= \sum_{uv\in E(G)} \frac{\delta_u+\delta_v}{2\sqrt{\delta_u\delta_v}} \\
&= 6\frac{1+1}{2\sqrt{1\times 1}} + (12n-12)\frac{1+2}{2\sqrt{1\times 2}} + (9n^2-15\,n+6)\frac{2+2}{2\sqrt{1\times 2}} \\
&= 9n^2 + \left(\frac{18}{\sqrt{2}}-15\right)n + 12 - \frac{18}{\sqrt{2}}
\end{aligned}$$

$$\begin{aligned}
\text{(ii). } \delta AG\left(G,x\right) &= \sum_{uv\in E(G)} x^{\frac{\delta_u+\delta_v}{2\sqrt{\delta_u\delta_v}}} \\
&= 6x^{\frac{1+1}{2\sqrt{1\times 1}}} + (12n-12)x^{\frac{1+2}{2\sqrt{1\times 2}}} + (9n^2-15\,n+6)x^{\frac{2+2}{2\sqrt{2\times 2}}} \\
&= (12n-12)x^{\frac{3}{2\sqrt{2}}} + (9n^2-15\,n+12)x^1
\end{aligned}$$

□

6. Conclusion

In this research work, we have introduced the delta geometric-arithmetic index and delta arithmetic-geometric index of a graph. The delta geometric-arithmetic index and delta arithmetic-geometric index of certain nanotubes and networks are determined. Also we have computed the delta geometric-arithmetic and delta arithmetic-geometric polynomials of certain nanotubes and networks.

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