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# ARITHMETIC-COTRAHARMONIC AND CONTRAHARMONIC-ARITHMETIC INDICES

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***ABSTRACT***

*Topological indices are applied to measure the chemical characteristics of chemical compounds. In this paper, we introduce the arithmetic-contraharmonic (AC) and contraharmonic-arithmetic (CA) indices of a graph and compute the exact values for some standard graphs and some families of nanotubes.*

***Keywords:*** *arithmetic-contraharmonic index, contraharmonic-arithmetic index, graph, nanotube.*

***Mathematics Subject Classification:*** *05C05, 05C12, 05C35.*

## 1. INTRODUCTION

Let $G$ be a finite, simple, connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(u)$ of a vertex $u$ is the number of vertices adjacent to $u$. We refer [1], for other undefined notations and terminologies.

A molecular graph is a graph such that its vertices correspond to the atoms and edges to the bonds. Chemical Graph Theory is a branch of mathematical chemistry, which has an important effect on the development of Chemical Sciences. Several topological indices have been considered in Theoretical Chemistry and have found some applications.

The geometric-arithmetic index [2] of a graph $G$ was defined as

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

This index was studied, for example, in [3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16].

Motivated by the definition of geometric-arithmetic index of a graph $G$, we define the arithmetic-contraharmonic index as

$$AC(G)=\sum_{uv\in E(G)}\frac{(d_G(u)+d_G(v))/2}{(d_G(u)^2+d_G(v)^2)/(d_G(u)+d_G(v))}$$

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

This equation consists from arithmetic mean of end vertex degrees of an edge $uv$, $\left(d_G(u)+d_G(v)/2\right)$ as numerator and contraharmonic mean of end vertex degrees of the edge $uv$, $(d_G(u)^2+d_G(v)^2)/(d_G(u)+d_G(v))$ as denominator.

Also we introduce the contraharmonic-arithmetic index of a graph $G$ and defined it as

$$CA(G)=\sum_{uv\in E(G)}\frac{(d_G(u)^2+d_G(v)^2)/(d_G(u)+d_G(v))}{((d_G(u)+d_G(v))/2}$$

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

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Recently, some new indices were studied, for example, in [17, 18, 19, 20, 21, 22, 23, 24, 25].

In this paper, we compute these two newly defined novel graph indices for some standard graphs and certain families of nanotubes.. For nanotubes, see [26].

**2. RESULTS FOR SOME STENDARD GRAPHS**

**Proposition 1:** *Let $K_{r,s}$ be a complete bipartite graph with* $1 \leq r \leq s$ *and* $s \geq 2$ *vertices. Then*

$$AC\left(K_{r,s}\right)=\frac{rs(r+s)^2}{2(r^2+s^2)}.$$

**Proof:** Let $K_{r,s}$ be a complete bipartite graph with $r + s$ vertices and *rs edges* such that $|V_1|= r$, $|V_2| = s$, $V(K_{r,s}) = V_1 \cup V_2$ for $1 \leq r \leq s$, and $s \geq 2$. Every vertex of $V_1$ is incident with $s$ edges and every vertex of $V_2$ is incident with r edges.

$$AC\left(K_{r,s}\right)=\frac{rs(r+s)^2}{2(r^2+s^2)}.$$

**Corollary 1.1:** ***Let*** $K_{r,r}$ *be a complete bipartite graph with* $r \geq 2$. *Then*

$$AC\left(K_{r,r}\right)=r^2.$$

**Corollary 1.2:** *Let $K_{1,r-1}$ be a star with* $r \geq 2$. *Then*

$$AC\left(K_{1,r-1}\right)=\frac{(r-1)r^2}{2(r^2-2r+2)}.$$

**Proposition 2:** *If G is r-regular with n vertices and* $r \geq 2$, *then*

$$AC(G)=\frac{nr}{2}.$$

**Proof:** Let $G$ is $r$-regular with $n$ vertices and $r \geq 2$ and $\frac{nr}{2}$ edges. Then

$$AC(G)=\frac{nr}{2}\frac{(r+r)^2}{2(r^2+r^2)}=\frac{nr}{2}.$$

**Corollary 2.1:** *Let $C_n$ be a cycle with* $n \geq 3$ *vertices. Then*

$$AC\left(C_n\right)=n.$$

**Corollary 2.2:** *Let $K_n$ be a complete graph with* $n \geq 3$ *vertices. Then*

$$AC\left(K_n\right)=\frac{n(n-1)}{2}.$$

**Proposition 3:** *If G is a path with* $n \geq 3$ *vertices, then*

$$AC\left(P_n\right)=n-3+\frac{9}{5}.$$

**Proposition 4:** *Let $K_{r,s}$ be a complete bipartite graph with* $1 \leq r \leq s$ *and* $s \geq 2$ *vertices. Then*

$$CA\left(K_{r,s}\right)=\frac{rs2(r^2+s^2)}{(r+s)^2}.$$

**Proof:** Let $K_{r,s}$ be a complete bipartite graph with $r + s$ vertices and *rs edges* such that $|V_1|= r$ , $|V_2|= s$, $V(K_{r,s}) = V_1 \cup V_2$ for $1 \leq r \leq s$, and $s \geq 2$. Every vertex of $V_1$ is incident with $s$ edges and every vertex of $V_2$ is incident with r edges.

$$CA\left(K_{r,s}\right)=\frac{rs2(r^2+s^2)}{(r+s)^2}.$$

**Corollary 4.1:** ***Let*** $K_{r,r}$ *be a complete bipartite graph with* $r \geq 2$. *Then*

$$CA\left(K_{r,r}\right)=r^2.$$

 

**Corollary 4.2:** *Let $K_{1,r-1}$ be a star with $r \geq 2$. Then*

$$CA\left(K_{1,r-1}\right)=\frac{2(\mathrm{r}-1)(r^2-2r+2)}{r^2}.$$

**Proposition 5:** *If G is r-regular with n vertices and $r \geq 2$, then*

$$CA(G)=\frac{nr}{2}.$$

**Proof:** Let $G$ is $r$-regular with $n$ vertices and $r \geq 2$ and $\frac{nr}{2}$ edges. Then

$$CA(G)=\frac{nr}{2}\frac{2(r^2+r^2)}{(r+r)^2}=\frac{nr}{2}.$$

**Corollary 5.1:** *Let $C_n$ be a cycle with $n \geq 3$ vertices. Then*

$$CA\left(C_n\right)=n.$$

**Corollary 5.2:** *Let $K_n$ be a complete graph with $n \geq 3$ vertices. Then*

$$CA\left(K_n\right)=\frac{n\left(n-1\right)}{2}.$$

**Proposition 6:** If $G$ is a path with $n \geq 3$ vertices, then

$$CA\left(P_n\right)=n-3+\frac{20}{9}.$$

## 3. RESULTS FOR $HC_5C_7[p,q]$ NANOTUBES

In this section, 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 $HC_5C_7[p,q]$.

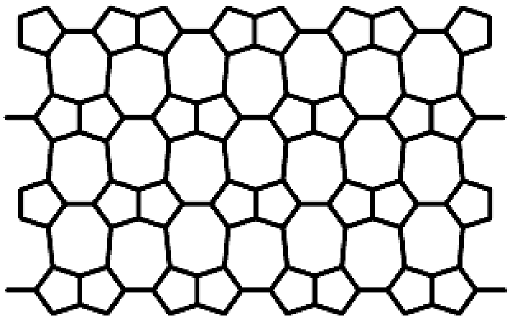

**Figure-1:** 2-*D* lattice of nanotube$HC_5C_7$ [8, 4]

The 2-D lattice of nanotube $HC_5C_7[p, q]$ is shown in Fig. 1.By calculation, we obtain that $G$ has $4pq$ vertices and $6pq - p$ edges. The graph $G$ has two types of edges based on the degree of end vertices of each edge as follows:

$E_1 = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_1| = 4p$.

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

**Theorem 1:** *Let G be the graph of a nanotube $HC_5C_7[p, q]$. Then*

$$AC\left(HC_5C_7\left[p,q\right]\right)=6pq-\frac{30}{26}.$$

**Proof:** From definition and by cardinalities of the edge partition of $HC_5C_7[p, q]$, we deduce

$$AC\left(HC_5C_7\left[p,q\right]\right)=\frac{4p(2+3)^2}{2(2^2+3^2)}+\frac{(6pq-5p)(3+3)^2}{2(3^2+3^2)}$$

$$=6pq-\frac{30}{26}.$$

**Theorem 2:** *Let G be the graph of a nanotube $HC_5C_7[p, q]$. Then*

$$CA\left(HC_5C_7\left[p,q\right]\right)=6pq-\frac{21}{25}.$$

**Proof:** From definitions and by cardinalities of the edge partition of $HC_5C_7[p, q]$, we deduce

$$CA\left(HC_5C_7\left[p,q\right]\right)=\frac{4p2(2^2+3^2)}{(2+3)^2}+\frac{(6pq-5p)2(3^2+3^2)}{(3+3)^2}$$

$$=6pq-\frac{21}{25}.$$

## 4. RESULTS FOR $SC_5C_7[p,q]$ NANOTUBES

In this section, 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 Fig. 2.

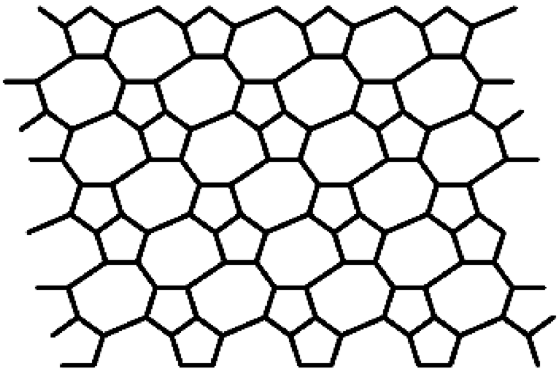

**Figure-2:** 2-*D* lattice of nanotube $SC_5C_7[p,q]$

Let $G$ be the graph of $SC_5C_7[p,q]$. By calculation, we obtain that $G$ has $4pq$ vertices and $6pq - p$ edges. Also by calculation, we get that $G$ has three types of edges based on the degree of end vertices of each edge as follows:

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

**Theorem 3:** *Let G be the graph of a nanotube $SC_5C_7[p, q]$. Then*

$$AC\left(SC_5C_7\left[p,q\right]\right)=6pq-p-\frac{3}{13}q.$$

**Proof:** From definition and by cardinalities of the edge partition of $SC_5C_7[p, q]$, we deduce

$$AC\left(SC_5C_7[p,q]\right)=\frac{q(2+2)^2}{2(2^2+2^2)}+\frac{6q(2+3)^2}{2(2^2+3^2)}+\frac{(6pq-p-7q)(3+3)^2}{2(3^2+3^2)}$$

$$=6pq-p-\frac{3}{13}q.$$

**Theorem 4:** *Let G be the graph of a nanotube $SC_5C_7[p, q]$. Then*

$$CA\left(SC_5C_7\left[p,q\right]\right)=6pq-p-\frac{6}{25}q.$$

**Proof:** From definitions and by cardinalities of the edge partition of $SC_5C_7[p, q]$, we deduce

$$CA\left(SC_5C_7[p,q]\right)=\frac{q2(2^2+2^2)}{(2+2)^2}+\frac{6q2(2^2+3^2)}{(2+3)^2}+\frac{(6pq-p-7q)2(3^2+3^2)}{(3+3)^2}$$

$$=6pq-p-\frac{6}{25}q$$

## 5. RESULTS FOR ARMCHAIR POLYHEX NANOTUBES

Carbon polyhex nanotubes are the nanotubes whose cylindrical surface is made up of entirely hexagons. These carbon nanotubes exist in nature with remarkable stability and possess very interesting electrical, thermal and mechanical properties, The armchair polyhex nanotube is denoted by $TUAC_6$ $[p, q]$ is shown in Fig. 3.

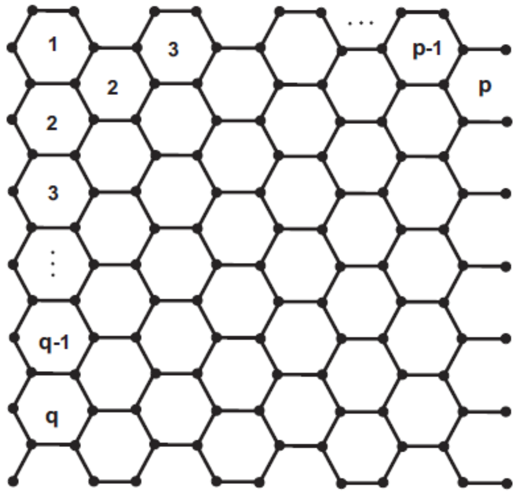


**Figure-3:** A 2-dimensional networks of $TUAC_6[p, q]$.

Let $G = TUAC_6$ $[p, q]$. By calculation, $G$ has $2p(q+1)$ vertices and $3pq + 2p$ edges. There are three types of edges based on degrees of end vertices of each edge. We present that the edge partition of $G$ is given in Table 3.

| $d_G(u), d_G(v) \setminus uv \in E(G)$ | (2, 2) | (2, 3) | (3, 3) |
|---|---|---|---|
| Number of edges | $p$ | $2p$ | $3pq- p$ |

**Table-3:** Edge partition of $TUAC_6$ $[p, q]$

**Theorem 5:** *Let G be the graph of an armchair polyhex nanotube $TUAC_6[p, q]$. Then*

$$AC\left(TUAC_6\left[p,\ q\right]\right) = 3pq + \frac{25}{13}p.$$

**Proof:** From definition and by cardinalities of the edge partition of $TUAC_6[p, q]$, we deduce

$$AC\left(TUAC_6\left[p,\ q\right]\right) = \frac{p(2+2)^2}{2(2^2+2^2)} + \frac{2p(2+3)^2}{2(2^2+3^2)} + \frac{(3pq-p)(3+3)^2}{2(3^2+3^2)}$$

$$= 3pq + \frac{25}{13}p.$$

**Theorem 6:** *Let G be the graph of an armchair polyhex nanotube $TUAC_6[p, q]$. Then*

$$CA\left(TUAC_6\left[p,\ q\right]\right) = 3pq + \frac{52}{25}p.$$

**Proof:** From definition and by cardinalities of the edge partition of $TUAC_6[p, q]$, we deduce

$$CA\left(TUAC_6\left[p,\ q\right]\right) = \frac{p2(2^2+2^2)}{(2+2)^2} + \frac{2p2(2^2+3^2)}{(2+3)^2} + \frac{(3pq-p)2(3^2+3^2)}{(3+3)^2}$$

$$= 3pq + \frac{52}{25}p.$$

## 6. RESULTS FOR ZIGZAG POLYHEX NANOTUBES

The zigzag polyhex nanotube is denoted by $TUZC_6$ $[p, q]$, where $p$ is the number of hexagons in a row whereas $q$ is the number of hexagons in a column. A 2-dimensional networks of $TUZC_6$ $[p, q]$ is depicted in FIG. 4.

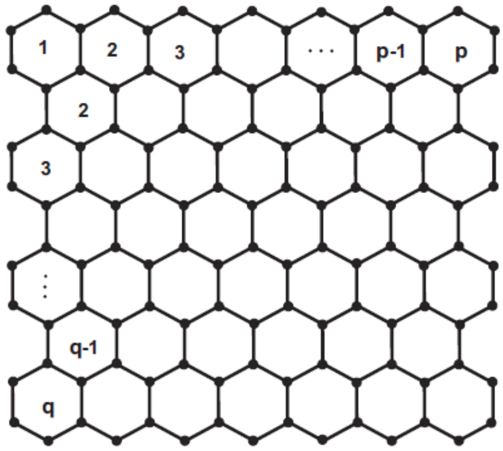


**Figure-4:** A 2-dimensional networks of $TUZC_6[p, q]$

Let $G$ be a graph of a $(p, q)$ dimensional zigzag polyhex nanotube. The graph $G$ has $2p(q+1)$ vertices and $3pq + 2p$ edges. In $G$, there are two types of edges based on degrees of end vertices of each edge. By calculation, the edge partition of $G$ is given in Table 4.

| $d_G(u), d_G(v) \setminus uv \in E(G)$ | (2, 3) | (3, 3) |
|---|---|---|
| Number of edges | $4p$ | $3pq – 2p$ |

**Table-4:** Edge partition of $TUZC_6\,[p, q]$

**Theorem 7:** *Let G be the graph of a zigzag polyhex nanotube* $TUZC_6[p, q]$. *Then*

$$AC\left(TUZC_6\left[p,\ q\right]\right) = 3pq + \frac{24}{13}p.$$

**Proof:** From definition and by cardinalities of the edge partition of $TUZC_6[p, q]$, we deduce

$$AC\left(TUZC_6\left[p,\ q\right]\right) = \frac{4p(2+3)^2}{2(2^2+3^2)} + \frac{(3pq-2p)(3+3)^2}{2(3^2+3^2)}$$

$$= 3pq + \frac{24}{13}p.$$

**Theorem 8:** *Let G be the graph of a zigzag polyhex nanotube* $TUZC_6[p, q]$. *Then*

$$CA\left(TUZC_6\left[p,\ q\right]\right) = 3pq + \frac{54}{25}p.$$

**Proof:** From definition and by cardinalities of the edge partition of $TUZC_6[p, q]$, we deduce

$$CA\left(TUZC_6\left[p,\ q\right]\right) = \frac{p2(2^2+2^2)}{(2+2)^2} + \frac{2p2(2^2+3^2)}{(2+3)^2} + \frac{(3pq-p)2(3^2+3^2)}{(3+3)^2}$$

$$= 3pq + \frac{54}{25}p.$$

## 7. CONCLUSION

In this study, we have introduced the arithmetic-contraharmonic index and contraharmonic-arithmetic index of a graph. Furthermore we have computed these indices for some standard graphs and certain families of nanotubes.

Many questions are suggested by this research, among them are the following:

1. Characterize the AC and CA indices in terms of other degree based topological indices.
2. Obtain the extremal values and extremal graphs of AC and CA indices.
3. Compute the exact values of these two indices for other chemical nanostructures.

 

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