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Some results on Arithmetico-Geometrico topological indices

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Abstract

Chemical graph theory plays an indispensable role in QSAR(Quantitative structure activity relationship) and QSPS(Qualitative structure property relationship)research.The molecular physico-chemical properties can be elaborated using the data encoded in their specific chemical (molecular) graphs. Topological indices of molecular descriptions are numerical values associated with a graph that throws light on its topology and are graph invariants.A large number of different invariants have been employed with various degrees of success in quantitative and qualitative structure property research. This paper intends to study AG indices of some standard graphs.

Keywords

Arithmetico-Geometrico index, topological indices, wheel graph, gear graph, sunflower graph, fan graph.

AMS Subject Classification

05C07, 05C76, 92E10.

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Contents

1. Introduction

The numerical values attached with molecular graphs called topological indices play a significant role in chemical studies,analysis and research. A topological index called Weiner index [5] was developed to calculate the boiling point of paraffins, in 1947. A popular index called Zagreb index [3] was defined by Gutman and Trinajstic in 1972 . Thereafter many indices are defined namely [1][2] Randic index, topological index etc. In 2016 [4] V.S. Shigehalli and Rachanna Kanavur introduced arithmetic-geometric indices.In this paper we obtain explicit formula for AG indices of standard class of graphs.

Definition 1.1. *ArithmeticoGeometrico topological index for a non-empty graph G is defined and denoted as*

$$AG(G) = \sum_{xy\varepsilon E(G)} \frac{dx+dy}{2\sqrt{dx.dy}}$$

where dx and dy denote the degrees of the vertices of the edge xy

2. AG indices of some family of graphs

Theorem 2.1. *The AG topological index of path graph*

$$AG(P_n) = \begin{cases} 1 & for n = 2 \\ \frac{3}{\sqrt{2}} + n - 3 & for n \geq 3 \end{cases}$$

Proof. For $n = 2$, there exists a single edge having two pendent vertices.

So, $AG(P_2) = \sum_{xy\varepsilon E(P_2)} \dfrac{dx+dy}{2\sqrt{dx.dy}} = \frac{2}{2} = 1$

For $n = 3$, there are two edges each having ends of degree 1 and 2.

So,

$$\begin{aligned}AG(P_3) &= \sum_{xy\varepsilon E(P_3)} \frac{dx+dy}{2\sqrt{dx.dy}} \\ &= \frac{1+2}{2\sqrt{1.2}} + \frac{2+1}{2\sqrt{2.1}} \\ &= \frac{2.3}{2\sqrt{2}} = \frac{3}{\sqrt{2}} \\ &= \frac{3}{\sqrt{2}} + (3-3)\end{aligned}$$

For $n = 4$, there are two pendent edges each of which have end vertices of degree 1 and 2 and one edge with end vertices of degree 2 each. So,

$$\begin{aligned}AG(P_4) &= \sum_{xy\in E(P_4)} \frac{dx+dy}{2\sqrt{dx.dy}} \\ &= \frac{1+2}{2\sqrt{1.2}} + \frac{2+2}{2\sqrt{2.2}} + \frac{2+1}{2\sqrt{2.1}} \\ &= \frac{2.3}{2\sqrt{2}} + 1 \\ &= \frac{3}{\sqrt{2}} + 1 = \frac{3}{\sqrt{2}} + (4-3)\end{aligned}$$

For P_n, there are two pendent edges each of which have end vertices of degree 1 and 2 and $n-3$ edge with end vertices of degree 2 each.Hence

$$\begin{aligned}AG(P_n) &= \sum_{xy\in E(P_n)} \frac{dx+dy}{2\sqrt{dx.dy}} \\ &= \frac{1+2}{2\sqrt{1.2}} + \frac{2+2}{2\sqrt{2.2}} + \frac{2+2}{2\sqrt{2.2}} + \ldots\ldots + \frac{2+1}{2\sqrt{2.1}} \\ &= \frac{2.3}{2\sqrt{2}} + n - 3 \\ &= \frac{3}{\sqrt{2}} + (n-3)\end{aligned}$$

□

Theorem 2.2. $AG(C_n) = n$

Proof. For $n = 3$, there are 3 vertices each of which has degree 2.

So $AG(C_3) = \sum_{xy\in E(C_3)} \frac{dx+dy}{2\sqrt{dx.dy}} = 3.\frac{2+2}{2\sqrt{2.2}} = 3.1 = 3$

Each graph C_n has n edges with each of its vertices with degree 2 and so,$AG(C_n) = \sum_{xy\in E(C_n)} \frac{dx+dy}{2\sqrt{dx.dy}} = n.\frac{2+2}{2\sqrt{2.2}} = n$ □

Theorem 2.3. $AG(K_n) = \binom{n}{2}$

Proof. For the complete graph K_n there are $\frac{n(n-1)}{2}$ edges and each vertex is of degree $n-1$.So,

$$\begin{aligned}AG(K_n) &= \sum_{xy\in E(K_n)} \frac{dx+dy}{2\sqrt{dx.dy}} \\ &= \sum_{uv\in E(K_n)} \frac{n-1+n-1}{2\sqrt{(n-1)(n-1)}} \\ &= \sum_{xy\in E(K_n)} 1 = \frac{n(n-1)}{2} = \binom{n}{2}\end{aligned}$$

□

Theorem 2.4. $AG(K_{1,n}) = \frac{(n+1)\sqrt{n}}{2}$

Proof. For the star graph $K_{1,n}$, all the n edges have one end vertex of degree 1 and other of degree n.So,

$$\begin{aligned}AG(K_{1,n}) &= \sum_{xy\in E(K_{1,n})} \frac{dx+dy}{2\sqrt{dx.dy}} \\ &= \sum_{xy\in E(K_{1,n})} \frac{1+n}{2\sqrt{1.n}} \\ &= \frac{1+n}{2\sqrt{1.n}} \sum_{xy\in E(K_{1,n})} 1 \\ &= \frac{1+n}{2\sqrt{1.n}}.n = \frac{(1+n)\sqrt{n}}{2}\end{aligned}$$

□

Definition 2.5. *The wheel W_n ,$n \geq 3$ is a graph constructed by attaching a mid-vertex v with all the vertices of an $n-$ cycle .The mid-vertex has degree n and all other vertices are of degree 3. Also it has $n+1$ vertices and $2n$ edges.*

Theorem 2.6. *For a wheel with order $n+1$,*

$$AG(W_n) = n(1 + \frac{3+n}{2\sqrt{3n}})$$

Proof. The edges of W_n can be partitioned into two sets E_1 and E_2 as follows.

$$E_1 = E(C_n) \in E(W_n)$$
$$E_2 = E(W_n - E(C_n))$$

$$\begin{aligned}AG(W_n) &= \sum_{xy\in E(W_n)} \frac{dx+dy}{2\sqrt{dx.dy}} \\ &= \sum_{xy\in E(E_1)} \frac{dx+dy}{2\sqrt{dx.dy}} + \sum_{xy\in E(E_2)} \frac{dx+dy}{2\sqrt{dx.dy}} \\ &= \sum_{xy\in E(E_1)} \frac{3+3}{2\sqrt{3.3}} + \sum_{xy\in E(E_2)} \frac{3+n}{2\sqrt{3.n}} \\ &= \sum_{xy\in E(E_1)} 1 + \frac{3+n}{2\sqrt{3.n}} \sum_{xy\in E(E_2)} 1 \\ &= n + \frac{3+n}{2\sqrt{3.n}} n = n(1 + \frac{3+n}{2\sqrt{3.n}})\end{aligned}$$

□

Corollary 2.7. *For a wheel W_{2n} with order $2n+1$*
$AG(W_{2n}) = 2n(1+\frac{3+2n}{2\sqrt{6n}})$

Theorem 2.8. *For an $r-$ regular graph of order n ,*

$$AG(G) = \frac{nr}{2}$$

.

Proof. For an $r-$ regular graph of order n ,there are $\frac{nr}{2}$ edges. So $AG(G) = \sum_{xy\in E(G)} \frac{r+r}{2\sqrt{r.r}} = \sum_{xy\in E(G)} 1 = \frac{nr}{2}$ □

Corollary 2.9. $AG(K_n) = \binom{n}{2}$

Note that K_n is an $(n-1)$regular graph of order n.

Corollary 2.10. *For the Peterson graph PG, $AG(PG) = 15$.*

Definition 2.11. *A gear graph G_n of order $2n+1$ is a wheel graph where a vertex is appended between each pair of adjacent vertices of the outer cycle . Note that it has 3n edges .*

Theorem 2.12. $AG(G_n) = \frac{n}{2\sqrt{3}}(\frac{3+n}{\sqrt{n}}+5\sqrt{2})$ *where G_n is the gear graph of order $2n+1$.*

Proof. The edges of G_n can be partitioned as follows,
$E_1 = \{xy|deg(x) = n \text{ and } deg(y) = 3\}$
$E_2 = \{xy|deg(x) = 2 \text{ and } deg(y) = 3\}$

$$\begin{aligned}AG(G_n) &= \sum_{xy\in E(E_1)} \frac{dx+dy}{2\sqrt{dx.dy}} + \sum_{xy\in E(E_2)} \frac{dx+dy}{2\sqrt{dx.dy}}\\ &= \sum_{xy\in E(E_1)} \frac{n+3}{2\sqrt{n.3}} + \sum_{xy\in E(E_2)} \frac{2+3}{2\sqrt{2.3}}\\ &= \frac{n+3}{2\sqrt{3n}} \sum_{xy\in E(E_1)} 1 + \frac{5}{2\sqrt{6}} \sum_{xy\in E(E_2)} 1\\ &= \frac{n+3}{2\sqrt{3n}}.n + \frac{5}{2\sqrt{6}}.2n = \frac{n}{2\sqrt{3}}(\frac{n+3}{\sqrt{n}}+5\sqrt{2})\end{aligned}$$

□

Definition 2.13. *The sunflower graph SF_n is a modified wheel with an additional n vertices $w_0, w_1, w_2, \ldots, w_{n-1}$ where w_i is joined to vertices of the edge e_ie_{i+2} for $i = 0,1,2,\ldots,n-1$ where $i+1$ is taken modulo n.The mid-vertex has degree n , the cycle vertices with degree 5 and each w_i with degree 2.*

Theorem 2.14. *For the sunflower graph SF_n of order $2n+1$,* $AG(SF_n) = n(\frac{5+n}{2\sqrt{5n}}+1+\frac{7}{\sqrt{10}})$

Proof. The edges of SF_n can be partitioned into E_1, E_2, E_3 as follows.
$E_1 = \{xy|deg(x) = n \text{ and } deg(y) = 5\}$
$E_2 = \{xy|deg(x) = 5 \text{ and } deg(y) = 5\}$
$E_3 = \{xy|deg(x) = 5 \text{ and } deg(y) = 2\}$

$$\begin{aligned}AG(SF_n) &= \sum_{xy\in E(E_1)} \frac{dx+dy}{2\sqrt{dx.dy}} + \sum_{xy\in E(E_2)} \frac{dx+dy}{2\sqrt{dx.dy}}\\ &\quad + \sum_{xy\in E(E_3)} \frac{dx+dy}{2\sqrt{dx.dy}}\\ &= \sum_{xy\in E(E_1)} \frac{n+5}{2\sqrt{5n}} + \sum_{xy\in E(E_2)} \frac{5+5}{2\sqrt{5.5}} + \sum_{xy\in E(E_3)} \frac{5+2}{2\sqrt{5.2}}\\ &= \frac{n+5}{2\sqrt{5n}} \sum_{xy\in E_1} 1 + \sum_{xy\in E_2} 1 + \frac{7}{2\sqrt{10}} \sum_{xy\in E_3}\\ &= \frac{n+5}{2\sqrt{5n}}.n + n + \frac{7}{2\sqrt{10}}.2n\\ &= n(\frac{n+5}{2\sqrt{5n}}+1+\frac{7}{\sqrt{10}})\end{aligned}$$

□

Definition 2.15. *A helm graph H_n is a $2n+1$ ordered graph generated from a wheel W_n with degree 4 and degree 1 vertices.*

Theorem 2.16. *For the helm graph H_n of order $2n+1$,* $AG(H_n) = n(\frac{n+4}{4\sqrt{n}}+\frac{9}{4})$

Proof. The edges of H_n can be partitioned into three :E_1, E_2, E_3 as follows.
$E_1 = \{xy|deg(x) = n \text{ and } deg(y) = 4\}$
$E_2 = \{xy|deg(x) = 4 \text{ and } deg(y) = 4\}$
$E_3 = \{xy|deg(x) = 4 \text{ and } deg(y) = 1\}$

$$\begin{aligned}AG(H_n) &= \sum_{xy\in E(H_n)} \frac{dx+dy}{2\sqrt{dx.dy}}\\ &= \sum_{xy\in E(E_1)} \frac{dx+dy}{2\sqrt{dx.dy}} + \sum_{xy\in E(E_2)} \frac{dx+dy}{2\sqrt{dx.dy}}\\ &\quad + \sum_{xy\in E(E_3)} \frac{dx+dy}{2\sqrt{dx.dy}}\\ &= \sum_{xy\in E(E_1)} \frac{n+4}{2\sqrt{4n}} + \sum_{xy\in E(E_2)} \frac{4+4}{2\sqrt{4.4}} + \sum_{xy\in E(E_3)} \frac{4+1}{2\sqrt{4.1}}\\ &= \frac{n+4}{2\sqrt{4n}} \sum_{xy\in E_1} 1 + \sum_{xy\in E_2} 1 + \frac{5}{2\sqrt{4}} \sum_{xy\in E_3} 1\\ &= \frac{n+4}{2\sqrt{4n}}.n + n + \frac{5}{4}.n\\ &= n(\frac{n+4}{2\sqrt{4n}}+\frac{9}{4})\end{aligned}$$

□

3. AG index of Graph operations.

Definition 3.1. *The sum G_1+G_2 of graphs G_1 and G_2 of order n_1 and n_2 and disjoint vertex set $V(G_1)$ and $V(G_2)$ respectively consists of $G_1 \cup G_2$ and edges joining a vertex* *of G_1 and a vertex of G_2 so that $|V(G_1+G_2)| = |V(G_1)| + |V(G_2)| = n_1+n_2$ and degree of each vertex v belonging to G_1 in G_1+G_2 is $deg(v)+n_2$ and degree of each vertex v belonging to G_2 in G_1+G_2 is $deg(v)+n_1$.Also $E(G_1+G_2) = E(G_1)\cup E(G_2)\cup\{uv|u\in V(G_1), v\in V(G_2)\}$*

Definition 3.2. *Fan graph $F_{m,n}$ is a join of P_n and the compliment of the graph K_m. That is, $\bar{K_m}+P_n$ is called a fan graph and it has $m+n$ vertices and $mn+n-1$ edges.*

Theorem 3.3.

$$AG(\bar{K_m}+P_n) = \frac{m(m+n+1)}{\sqrt{n(m+1)}} + \frac{(n-2)(m+n+2)}{\sqrt{n(m+2)}} + \frac{2m+3}{\sqrt{(m+1)(m+2)}} + |n-3| \text{ for } n\geq 2$$

Proof. The edge set of $\bar{K_m}+P_n$ can be partitioned into four sets as follows.
$E_1 = \{E(\bar{K_m}+P_n)|$ each edge with terminal vertices of degree n and $m+1\}$
$E_2 = \{E(\bar{K_m}+P_n)|$ each edge with terminal vertices of degree n and $m+2\}$
$E_3 = \{E(\bar{K_m}+P_n)|$ each edge with terminal vertices of degree $m+1$ and $m+2\}$
$E_4 = \{E(\bar{K_m}+P_n)|$ each edge with terminal vertices of degree $m+2\}$
Now E_1 contains $2m$ edges, E_2 contains $2(n-2)$ edges, E_3 contains $(n-2)m$ edges and E_4 contains $(n-3)$ edges.

$$\begin{aligned}AG(\bar{K_m}+P_n) &= \sum_{xy\in E(\bar{K_m}+P_n)} \frac{dx+dy}{2\sqrt{dx.dy}}\\ &= \sum_{xy\in E_1}\frac{dx+dy}{2\sqrt{dx.dy}} + \sum_{xy\in E_2}\frac{dx+dy}{2\sqrt{dx.dy}}\\ &+ \sum_{xy\in E_3}\frac{dx+dy}{2\sqrt{dx.dy}} + \sum_{xy\in E_4}\frac{dx+dy}{2\sqrt{dx.dy}}\\ &= \sum_{xy\in E_1}\frac{n+m+1}{2\sqrt{n(m+1)}} + \sum_{xy\in E_2}\frac{n+m+2}{2\sqrt{n(m+2)}}\\ &+ \sum_{xy\in E_3}\frac{m+1+m+2}{2\sqrt{(m+1)(m+2)}}\\ &+ \sum_{xy\in E_4}\frac{2(m+2)}{2\sqrt{(m+2)(m+2)}}\\ &= m\frac{n+m+1}{2\sqrt{n(m+1)}} + (n-2)\frac{n+m+2}{\sqrt{n(m+2)}}\\ &+ \frac{2m+3}{\sqrt{(m+1)(m+2)}} + n-3\end{aligned}$$

□

Corollary 3.4.

$$AG(\bar{K_m}+P_3) = \frac{m(m+4)}{\sqrt{3(m+1)}} + \frac{(m+5)}{\sqrt{3(m+2)}} + \frac{2m+3}{\sqrt{(m+1)(m+2)}}$$

Corollary 3.5.

$$AG(\bar{K_2}+P_3) = \frac{m(m+4)}{\sqrt{3(m+1)}} + \frac{(m+5)}{\sqrt{3(m+2)}} + \frac{2m+3}{\sqrt{(m+1)(m+2)}}$$

$\bar{K_2}+P_3$ is the join of complement of K_2 and P_3.It has 5 vertices and 8 edges. The vertex set are of 2 types E_1 and E_2 and E_1 has 4 edges with end vertices of degree 3 and 3 and E_2 also has 4 edges with end vertices of degree 3 and 4.

$$\begin{aligned}AG(\bar{K_2}+P_3) &= \frac{2(2+4)}{\sqrt{3(2+1)}} + \frac{(2+5)}{\sqrt{3(2+2)}}\\ &+ \frac{2.2+3}{\sqrt{(2+1)(2+2)}}\\ &= 4+\frac{7}{2\sqrt{3}} + \frac{7}{2\sqrt{3}} = 4+\frac{7}{\sqrt{3}}\end{aligned}$$

Definition 3.6. *A unicyclic graph which has a unique subgraph isomorphc to a cycle. A vertex on the cycle is called cyclic vertex. Here we consider unicyclic graph with cycle C_n associated with a star $K_{1,m}$ to each cyclic vertex.A pendent on a unicyclic graph is a path of length one with exactly one vertex on the cycle.The non-cyclic vertex of a pendent is called pendent vertex.For every $m,n\in N$ with $n\geq 3$, there is a graph obtained by appending m pendents to each cycle vertex of C_n.That is ,attaching a copy of $K_{1,m}$ at its vertex of degree m to each cycle vertex.We denote it by the symbol $C_n\odot K_{1,m}$.*

Theorem 3.7. $AG(C_n\odot K_{1,m}) = n[1+\frac{m(m+3)}{2\sqrt{m+2}}]$

Proof. We have
$|E(C_n\odot K_{1,m})| = n+mn = n(m+1) = |V(C_n)||V(K_{1,m})|$

$$\begin{aligned}AG(C_n\odot K_{1,m}) &= \sum_{xy\in E(C_n\odot K_{1,m})}\frac{dx+dy}{2\sqrt{dx.dy}}\\ &= \sum_{xy\in C_n\in C_n\odot K_{1,m}}\frac{dx+dy}{2\sqrt{dx.dy}}\\ &+ \sum_{xy\in K_{1,m}\in C_n\odot K_{1,m}}\frac{dx+dy}{2\sqrt{dx.dy}}\\ &= \sum_{xy\in C_n\in C_n\odot K_{1,m}}\frac{m+2+m+2}{2\sqrt{(m+2)(m+2)}}\\ &+ \sum_{xy\in K_{1,m}\in C_n\odot K_{1,m}}\frac{m+2+1}{2\sqrt{(m+2)1}}\\ &= n+\frac{m+3}{2\sqrt{(m+2)}}mn = n(1+\frac{m+3}{2\sqrt{(m+2)}})\end{aligned}$$

□

Definition 3.8. *A friendship graph f_n is a collection of n triangles with a common vertex ,ie, $f_n = K_1 + nK_2$. It can be obtained from a wheel W_{2n} with a single cycle C_{2n} by eliminating alternate edges of the cycle.Let v_c denotes the central vertex, then $d(v_c) = 2n$.Note that f_n has $2n+1$ vertices and $3n$ edges.*

Theorem 3.9. *For a friendship graph f_n of order $2n+1$,*
$AG(f_n) = n(1 + \frac{2(n+1)}{\sqrt{n}})$

Proof. The edges of f_n can be partitioned into two types as follows.
$E_1 = \{xy|deg(x) = deg(y) = 2\}$
$E_2 = \{xy|deg(x) = 2 \text{ and } deg(y) = 2n\}$

$$\begin{aligned} AG(f_n) &= \sum_{xy \in E_1} \frac{dx+dy}{2\sqrt{dx.dy}} + \sum_{xy \in E_2} \frac{dx+dy}{2\sqrt{dx.dy}} \\ &= \sum_{xy \in E_1} \frac{2+2}{2\sqrt{2.2}} + \sum_{xy \in E_2} \frac{2n+2}{2\sqrt{2n.2)}} \\ &= \sum_{xy \in E_1} 1 + \sum_{xy \in E_2} 1 \\ &= n(1 + \frac{2(n+1)}{\sqrt{n}}) \end{aligned}$$

□

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