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Augmented Zagreb index

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Abstract Inspired by recent work on the atom-bond connectivity (*ABC*) index we propose here a new topological index, *augmented Zagreb index* (*AZI*). The tight upper and lower bounds for chemical trees are obtained. Moreover, it has been shown that among all trees the star has the minimum AZI value. Characterizing trees with maximal augmented Zagreb index remains an open problem for future research.

Keywords Molecular descriptor · Extremal graph · Atom-bond connectivity index · Augmented Zagreb index

1 Introduction

There is a strong and natural parallelism among chemical and graph-theoretical notions. The valency of an atom in graph theory corresponds to the degree of a vertex in molecular graph. The product $d_u d_v$ of the degrees d_u and d_v of the terminal vertices u and v of the edge (chemical bond) uv has attracted a special attention among mathematical chemists and served as a basis for a series of topological indices.

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Let us consider

$$\sum_{uv \in E(G)} (d_u d_v)^{\lambda}$$

where summation goes over all edges of the edge set $E(G)$ of graph G.

For $\lambda = 1$ one obtains well known Zagreb index M_2 [1], and for $\lambda = -1/2$ Randić connectivity index [2], which is together with Wiener [3] and Hosoya index [4] one of mostly used topological index in chemistry. For $\lambda = -1$ one gets modified Zagreb index [5]. The researches on these indices are constantly growing which can be deduced from the number of recent papers on these topics (see for example [6–13] and references cited therein). Most of indices reflect the extent of molecular branching, but there are physico-chemical properties that are dependent on factors rather different than branching which chemical and mathematical properties have been extensively studied [14–19]. In order to take this into account Ernesto Estrada et al. [20] have proposed atom-bond connectivity (ABC) index as

$$ABC\,(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

The ABC has proven to be valuable predictive index in study of heat of formation in alkanes [20] and strain energy of cycloalkanes [21]. We use the same methodology to eliminate the influence of branching from any variable Zagreb index with negative λ by following definition

$$ABC_{\lambda}\,(G) = \sum_{uv \in E(G)} \left(\frac{d_u + d_v - 2}{d_u d_v}\right)^{-\lambda}, \quad \lambda < 0.$$

It can be easily seen that $\lambda = -1/2$ gives ABC index. Another interesting negative value of λ appearing in the study of variable Zagreb indices is $\lambda = -1$ which corresponds to well-known modified Zagreb index. However, it can be shown that exist a direct relation between this quantity and modified Zagreb index as follows:

$$ABC_{-1} = -2M_2^* + n$$

where n is the number of vertices, and M_2^* is the modified Zagreb index of corresponding graph G.

The main goal here is to investigate is there any λ for which ABC_{λ} shows a better prediction power than original ABC index. In order to do this we as resource used a data for heat of formation of octanes. The data are obtained from NIST (National Institute of Stadards and Techology) [23]. Using a computer program we tested predictive power of ABC_{λ} for various values of λ (or more precisely for $\lambda \in [-5, 5]$) in the case of heat of formation of octanes. The best correlation coefficient (R) is obtained when $\lambda = 3.06$ but without any visible loss we can claim that the best correlation coefficient is found when $\lambda = 3$ (see Fig. 1).

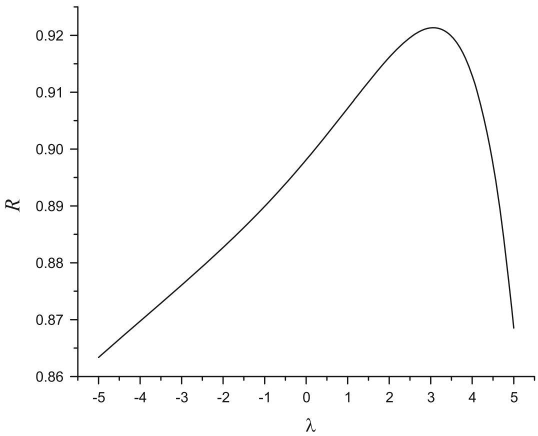


Fig. 1 The absolute value of correlation coefficient versus λ

We also got nearly the same results in the case of heat of formation for heptanes (the best R is obtained for $\lambda = 2.94$).

In the light of the above presented results, we define augmented Zagreb index AZI by:

$$AZI\,(G) = ABC_3\,(G) = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2} \right)^3 .$$

Recently, we have studied extremal properties of ABC index of trees and chemical trees [22]. Although we apply the similar methodology here, we obtain somewhat different results.

2 AZI index of chemical trees

Theorem 1 *Let G_n be a chemical tree with $n \geq 3$ vertices. Then,*

$$\frac{4}{27}\,(35n - 111) \leq AZI\,(G_n) \leq \begin{cases} 8\,(n-1)\,, & 3 \leq n \leq 9; \\ \frac{4825}{64}, & n = 10; \\ \frac{1376}{135} n - \frac{416}{15}, & n \geq 11. \end{cases} \quad . \tag{1}$$

Both bounds are tight, i.e. more precisely, there are infinitely many values of n and chemical trees G'_n such that

$$AZI\,\left(G'_n\right) = \frac{4}{27}\,(35n - 111),$$

and there are infinitely many values of n and chemical trees G''_n such that

$$AZI\,\left(G''_n\right) = \frac{32}{135}\,(43n - 117).$$

Proof First, let us prove that

$$AZI\,(G_n) \geq \frac{4}{27}\,(35n - 111). \tag{2}$$

If G_n has less than 5 vertices, the claim is trivial, hence, let us assume that G_n has at least 5 vertices. Let us observe the function

$$f\,(G_n) = \sum_{uv \in E(G)} \left(\left(\frac{d_u d_v}{d_u + d_v - 2} \right)^3 - 8 \right).$$

The following relation is equivalent to (2)

$$f\,(G_n) \geq -\frac{76}{27}\,(n+3). \tag{3}$$

Denote $\alpha_{ij} = \frac{i+j-2}{i \cdot j} - 8$. Suppose to the contrary that there are some n and some chemical tree H_n^1 with n vertices such that

$$f\left(H_n^1\right) < -\frac{76}{27}\,(n+3).$$

Let H_n^2 be such tree with minimal value of $m_{12} + m_{13}$ and among those with the same such value, let H_n^2 be tree that corresponds to the smallest n. It holds:

Claim A $f\,(P_n) = 0 > -\frac{76}{27}\,(n+3)\,.$

□

Let us show that $m_{11}\left(H_n^2\right) = m_{12}\left(H_n^2\right) = m_{13}\left(H_n^2\right) = 0$. Obviously $m_{11}\left(H_n^2\right) = 0$, hence in the opposite case, we have one of the following two cases:

Case 1 $m_{12}\left(H_n^2\right) > 0.$

Let u_1 be a vertex of degree 2 adjacent to the vertex v of degree 1. Let w be the vertex of degree larger then 2 closest to v (this vertex has to exist, because of the Claim A). Denote the path from v to w by $vu_1u_2\ldots u_xw$ (possibly equal to vu_1w). Let H_{n-x}^3 be a graph obtained by deletion of vertices $v, u_1, \ldots, u_{x-1}$ (possibly just vertex v if $x = 1$). Since,

$$m_{12}\left(H_{n-x}^3\right) + m_{13}\left(H_{n-x}^3\right) \leq m_{12}\left(H_n^2\right) + m_{13}\left(H_n^2\right) \text{ and } n\left(H_{n-x}^3\right) < n\left(H_n^2\right).$$

It follows that

$$f\left(H_{n-x}^3\right) \geq -\frac{76}{27}\,((n-x)+3),$$

but

$$f\left(H_{n-x}^{3}\right)=f\left(H_{n}^{2}\right)-\alpha_{12}-(x-1)\,\alpha_{22}-\alpha_{2d_w}+\alpha_{1d_w}=f\left(H_n\right)+\alpha_{1d_w}$$
$$\leq f\left(H_n\right)<-\frac{76}{27}\left(n+3\right)<-\frac{76}{27}\left(\left(n-x\right)+3\right),$$

which is a contradiction.

Case 2 $m_{13}\left(H_n^2\right)>0$.

Let u be a vertex of degree 3 adjacent to vertex of u' of degree 1 and vertices v and w. Without loss of generality, we may assume that $d_v \leq d_w$. Let us distinguish three subcases:

Subcase 2.1 $(d_v, d_w) \in \{(1,1),(1,2),(1,3),(2,2),(2,3)\}$
Let H_{n+1}^4 be a tree obtained by adding one pendant vertex to u. Note that

$$m_{12}\left(H_{n+1}^{4}\right)+m_{13}\left(H_{n+1}^{4}\right)<m_{12}\left(H_{n}^{2}\right)+m_{13}\left(H_{n}^{2}\right),$$

but

$$\begin{aligned}
&f\left(H_{n+1}^{4}\right)\\
&=f\left(H_n\right)+\alpha_{14}+\left(\alpha_{14}-\alpha_{13}\right)+\left(a_{4d_v}-\alpha_{3d_v}\right)+\left(a_{4d_w}-\alpha_{3d_w}\right)\\
&<-\frac{76}{27}\left(\left(n+1\right)+3\right)+\left[\frac{76}{27}+\alpha_{14}+\left(\alpha_{14}-\alpha_{13}\right)+\left(a_{4d_v}-\alpha_{3d_v}\right)+\left(a_{4d_w}-\alpha_{3d_w}\right)\right]\\
&<\left\{\begin{array}{l}\text{simple calculation shows that in each of the observed cases it holds}\\ \frac{76}{27}+\alpha_{14}+\left(\alpha_{14}-\alpha_{13}\right)+\left(a_{4d_v}-\alpha_{3d_v}\right)+\left(a_{4d_w}-\alpha_{3d_w}\right)<0\end{array}\right\}\\
&<-\frac{76}{27}\left(\left(n+1\right)+3\right),
\end{aligned}$$

which is a contradiction.

Subcase 2.2 $(d_v, d_w) \in \{(2,4),(3,3),(3,4),(4,4)\}$
Let H_{n-1}^5 be a tree obtained by deletion of vertex u'. Note that

$$m_{12}\left(H_{n-1}^{5}\right)+m_{13}\left(H_{n-1}^{5}\right)<m_{12}\left(H_{n}^{2}\right)+m_{13}\left(H_{n}^{2}\right),$$

but

$$f\left(H_{n-1}^{5}\right)=f\left(H_{n}^{2}\right)-a_{13}+\left(a_{2d_v}-\alpha_{3d_v}\right)+\left(a_{2d_w}-\alpha_{3d_w}\right)$$
$$<-\frac{76}{27}\left(\left(n-1\right)+3\right)-\frac{76}{27}-a_{13}+\left(a_{2d_v}-\alpha_{3d_v}\right)+\left(a_{2d_w}-\alpha_{3d_w}\right)$$

$$< \left\{ \begin{array}{l} \text{simple calculation shows that in each of the observed cases it holds} \\ -\frac{76}{27} - a_{13} + \left(a_{2d_v} - \alpha_{3d_v}\right) + \left(a_{2d_w} - \alpha_{3d_w}\right) < 0 \end{array} \right\}$$

$$< -\frac{76}{27}\left((n-1)+3\right),$$

which is a contradiction.

Subcase 2.3 $(d_v, d_w) = (1, 4)$
Let H_{n-2}^6 be a tree obtained by deletion of vertices u' and v. Note that

$$m_{12}\left(H_{n-2}^6\right) + m_{13}\left(H_{n-2}^6\right) < m_{12}\left(H_n^2\right) + m_{13}\left(H_n^2\right),$$

but

$$\begin{aligned} f\left(H_{n-2}^6\right) &= f\left(H_n^2\right) - 2a_{13} + (a_{14} - \alpha_{34}) \\ &< -\frac{76}{27}\left((n-2)+3\right) + \left[-2\cdot\frac{76}{27} - 2a_{13} + (a_{14} - \alpha_{34})\right] \\ &< -\frac{76}{27}\left((n-2)+3\right), \end{aligned}$$

which is a contradiction. Contradiction is obtained in both cases, hence indeed: $m_{11}\left(H_n^2\right) = m_{12}\left(H_n^2\right) = m_{13}\left(H_n^2\right) = 0$, i.e. $n_1\left(H_n^2\right) = m_{14}\left(H_n^2\right)$. Therefore,

$$\begin{aligned} f\left(H_n^2\right) &= \sum_{2\le i\le j\le 4} m_{ij}\left(H_n^2\right)\cdot\alpha_{ij} + n_1\left(H_n^2\right)\cdot a_{14} \\ &= \{\text{analogously as in the paper[22]}\} \\ &= \sum_{2\le i\le j\le 4} \frac{\alpha_{ij} + 2\cdot\left(\frac{i-2}{i} + \frac{j-2}{j}\right)\cdot\alpha_{14}}{\frac{\frac{5}{2}i-4}{i} + \frac{\frac{5}{2}j-4}{j}} \\ &\quad \cdot\left(\left(\frac{\frac{5}{2}i-4}{i} + \frac{\frac{5}{2}j-4}{j}\right)\cdot m_{ij}\left(H_n\right)\right) + 4\alpha_{14}. \end{aligned} \tag{4}$$

It can be shown that

$$\max_{2\le i\le j\le 4} \frac{\alpha_{ij} + 2\cdot\left(\frac{i-2}{i} + \frac{j-2}{j}\right)\cdot\alpha_{14}}{\frac{\frac{5}{2}i-4}{i} + \frac{\frac{5}{2}j-4}{j}} \ge -\frac{76}{27}.$$

Putting this in (4), we get:

$$\begin{aligned} f\left(H_n^2\right) &\ge -\frac{76}{27}\sum_{2\le i\le j\le 4}\left(\left(\frac{\frac{5}{2}i-4}{i} + \frac{\frac{5}{2}j-4}{j}\right)\cdot m_{ij}\left(H_n^2\right)\right) + 4\alpha_{14} \\ &= \{\text{analogously as in the paper [22]}\} \end{aligned}$$

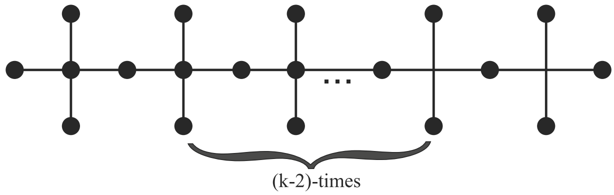


Fig. 2 Graphs G'_{4k+1}

$$= -\frac{76}{27}\left(n_1\left(H_n^2\right) + n_2\left(H_n^2\right) + n_3\left(H_n^2\right) + n_4\left(H_n^2\right) - 5\right) + 4\alpha_{14}$$
$$= -\frac{76}{27}(n-5) + 4\left(\frac{64}{27} - 8\right) = -\frac{76}{27}(n+3).$$

This proves the inequality. In order to prove that this bound is attainable, let us define graphs G'_n, where $n = 4k+1$ for $k \geq 2$ as it is shown in Fig. 2.

Simple calculation shows that $AZI\left(G'_n\right) = \frac{4}{27}(35n - 111)$. Let us prove the upper bound. If $n \leq 16$, the claim can be easily checked by computer. Hence, suppose that $n \geq 17$. We need to prove that:

$$AZI(G_n) \leq \frac{1376}{135}n - \frac{416}{15} \tag{5}$$

Let us observe the function

$$g(G_n) = \sum_{uv \in E(G)} \left(8 - \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3\right). \tag{6}$$

Denote $\beta_{ij} = 8 - \left(\frac{i \cdot j}{i+j-2}\right)^3$. Note that:

$$g(G_n) = (n-1)\cdot 8 - AZI(G_n)$$
$$AZI(G_n) = (n-1)\cdot 8 - g(G_n).$$

Hence, (5) can be rewritten as

$$(n-1)\cdot 8 - g(G_n) \leq \frac{1376}{135}n - \frac{416}{15}$$
$$g(G_n) \geq -\frac{296}{135}n + \frac{296}{15}$$

After simple calculation, this inequality can be transformed to

$$g(G_n) \geq \frac{n-9}{5}\cdot\beta_{44}$$

Suppose to the contrary that there is some n and some chemical tree H_n^7 with $n \geq 11$ vertices such that

$$g\left(H_n^7\right) < \frac{n-9}{5} \cdot \beta_{44}.$$

Let H_n^8 be such graph with minimal value of $m_{13}+m_{14}$. Let us show that $m_{11}\left(H_n^8\right) = m_{13}\left(H_n^8\right) = m_{14}\left(H_n^8\right) = 0$. Obviously $m_{11}\left(H_n^8\right) = 0$, hence in the opposite case, there is a vertex u of degree 1 that is adjacent to vertex v of degree either 3 or 4. Let H_{n+1}^9 be a graph obtained from graph H_n^2 by splitting edge uv in the path of length 2. It holds:

$$m_{13}\left(H_{n+1}^9\right) + m_{14}\left(H_{n+1}^9\right) < m_{13}\left(H_n^8\right) + m_{14}\left(H_n^8\right),$$

but

$$\begin{aligned} g\left(H_{n+1}^9\right) &= g\left(H_n^8\right) + \beta_{12} + \beta_{2d_v} - \beta_{1d_v} = g\left(H_n^8\right) - \beta_{1d_v} < g\left(H_n^8\right) - \min_{i=3,4} \beta_{1i} \\ &< \frac{n-9}{5} \cdot \beta_{44} - \min_{i=3,4} \beta_{1i} = \frac{(n+1)-9}{5} \cdot \beta_{44} + \left(-\min_{i=3,4} \beta_{1i} - \frac{1}{5}\beta_{44}\right) \\ &< \frac{(n+1)-9}{5} \cdot \beta_{44}, \end{aligned}$$

which is a contradiction. Hence, indeed $m_{11}\left(H_n^8\right) = m_{13}\left(H_n^8\right) = m_{14}\left(H_n^8\right) = 0$. Now, let us observe the class Γ_1 of chemical trees H_n^{10} with $n \geq 11$ vertices such that:

1) $g\left(H_n^{10}\right) < \frac{n-9}{5} \cdot \beta_{44}$;
2) $m_{11}\left(H_n^{10}\right) = m_{13}\left(H_n^{10}\right) = m_{14}\left(H_n^{10}\right) = 0$.

Note that Γ_1 is non-empty, because at least H_n^8 is in this class. Let H_n^{11} be the graph in this class with the smallest value of $n_2\left(H_n^{11}\right) - n_1\left(H_n^{11}\right) > 0$. Let us prove that $n_1\left(H_n^{11}\right) = n_2\left(H_n^{11}\right)$.

Suppose to the contrary. Condition 1) implies that H_n^{11} has at least 17 vertices, because the claim is verified for all graphs with at most 16 vertices. Let u be vertex of degree 2 adjacent to vertices v and w of degrees greater than 1. Let H_{n-1}^{12} be a graph obtained from H_n^{11} by deleting vertex v (and its incident edges) and adding edge vw. Note that:

$$\begin{aligned} g\left(H_{n-1}^{12}\right) &= g\left(H_n^{11}\right) - \beta_{2d_v} - \beta_{2d_w} + \beta_{d_v d_w} = g\left(H_n^{11}\right) + \beta_{d_v d_w} \\ &\leq \frac{n-9}{5} \cdot \beta_{44} < \frac{(n-1)-9}{5} \cdot \beta_{44}, \end{aligned}$$

which is contradiction with minimality of $n_2\left(H_n^{11}\right) - n_1\left(H_n^{11}\right) > 0$.

Now, let us observe the class Γ_2 of graphs H_n^{13} in Γ_1 such that $n_1\left(H_n^{13}\right) = n_2\left(H_n^{13}\right)$. We have just proved that this class is non-empty. Let graph H_n^{14} be the graph with the smallest value q_3, where q_3 is the number of vertices of degree 3 that are adjacent to at least two vertices of degree greater than 2. Let us prove that $q_3\left(H_n^{14}\right)=0$. Suppose to the contrary that there is a vertex u of degree 3 adjacent to at least two vertices v and w of degree greater than 2 and to vertex z of degree 2, 3 or 4. Let us observe graph H_{n+2}^{15} obtained by adding vertices v' and v'' and edges uv' and $v'v''$ to graph H_n^{14}. Note that:

$$\begin{aligned}
g\left(H_{n+2}^{15}\right) &= g\left(H_n^{14}\right)+\beta_{24}+\beta_{12}+\left(\beta_{4d_v}-\beta_{3d_v}\right)+\left(\beta_{4d_w}-\beta_{3d_w}\right)+\left(\beta_{4d_z}-\beta_{3d_z}\right)\\
&< g\left(H_n^{14}\right)+2\cdot\max_{i=3,4}\left(\beta_{4d_v}-\beta_{3d_v}\right)+\max_{i=2,3,4}\left(\beta_{4d_v}-\beta_{3d_v}\right)\\
&= g\left(H_n^{14}\right)+2\cdot\max_{i=3,4}\left(\beta_{4d_v}-\beta_{3d_v}\right)<\frac{n-9}{5}\cdot\beta_{44}+2\cdot\max_{i=3,4}\left(\beta_{4d_v}-\beta_{3d_v}\right)\\
&= \frac{(n+2)-9}{5}\cdot\beta_{44}+\left[-\frac{2}{5}\beta_{44}+2\cdot\max_{i=3,4}\left(\beta_{4d_v}-\beta_{3d_v}\right)\right]\\
&< \frac{(n+2)-9}{5}\cdot\beta_{44}
\end{aligned}$$

Therefore, H_{n+2}^{15} is in Γ_2, but this is in contradiction with minimality of $q_3\left(H_n^{14}\right)$. Hence, indeed $q_3\left(H_n^{14}\right)=0$.

Since, every vertex of degree 3 is adjacent to two vertices of degree 2 that are adjacent to vertices of degree 1, and H_n^{14} is connected and $n\geq 17$, it follows that $m_{33}\left(H_n^{14}\right)=0$. Also, it follows that $n_4\left(H_n^{14}\right)>0$. Further, vertices of degree 4 create subtree of H_n^{14}, hence $m_{44}\left(H_n^{14}\right)=n_4\left(H_n^{14}\right)-1$. Also, $m_{33}\left(H_n^{14}\right)=0$ and $n_1\left(H_n^{14}\right)=n_2\left(H_n^{14}\right)=m_{12}\left(H_n^{14}\right)$ implies that $m_{34}\left(H_n^{14}\right)=n_3\left(H_n^{14}\right)$. Summarizing this, we get:

$$\begin{aligned}
&n_1\left(H_n^{14}\right)=n_2\left(H_n^{14}\right)\\
&m_{11}\left(H_n^{14}\right)=m_{13}\left(H_n^{14}\right)=m_{14}\left(H_n^{14}\right)=m_{22}\left(H_n^{14}\right)=m_{33}\left(H_n^{14}\right)=0\\
&m_{12}\left(H_n^{14}\right)=n_1\left(H_n^{14}\right)\\
&m_{44}\left(H_n^{14}\right)=n_4\left(H_n^{14}\right)-1\\
&m_{23}\left(H_n^{14}\right)+m_{24}\left(H_n^{14}\right)=n_2\left(H_n^{14}\right)\\
&m_{24}\left(H_n^{14}\right)+m_{34}\left(H_n^{14}\right)+2m_{44}\left(H_n^{14}\right)=4n_4\left(H_n^{14}\right)\\
&m_{23}\left(H_n^{14}\right)+m_{34}\left(H_n^{14}\right)=3n_3\left(H_n^{14}\right)
\end{aligned}$$

Solving the last three equations (and taking into the account that $m_{44}\left(H_n^{14}\right)=n_4\left(H_n^{14}\right)-1$) we get:

$$m_{23}\left(H_n^{14}\right)=-\frac{1}{2}\left(2-n_2\left(H_n^{14}\right)-3n_3\left(H_n^{14}\right)+2n_4\left(H_n^{14}\right)\right)$$

$$m_{24}\left(H_n^{14}\right) = -\frac{1}{2}\left(-2 - n_2\left(H_n^{14}\right) + 3n_3\left(H_n^{14}\right) - 2n_4\left(H_n^{14}\right)\right)$$
$$m_{34}\left(H_n^{14}\right) = -\frac{1}{2}\left(-2 + n_2\left(H_n^{14}\right) - 3n_3\left(H_n^{14}\right) - 2n_4\left(H_n^{14}\right)\right)$$

Since, $\beta_{12} = \beta_{22} = \beta_{23} = \beta_{24} = 0$, it follows that:

$$\begin{aligned}
& g\left(H_n^{12}\right) \\
&= \frac{1}{2}\left(2 - n_2\left(H_n^{14}\right) + 3n_3\left(H_n^{14}\right) + 2n_4\left(H_n^{14}\right)\right)\cdot\beta_{34} + \left(n_4\left(H_n^{14}\right) - 1\right)\cdot\beta_{44} \\
&= \left\{n_2\left(H_n^{14}\right) = n_1\left(H_n^{14}\right) = n_3\left(H_n^{14}\right) + 2n_4\left(H_n^{14}\right) + 2\right\} \\
&= n_3\left(H_n^{14}\right)\cdot\beta_{34} + n_4\left(H_n^{14}\right)\cdot\beta_{44} - \beta_{44} \\
&= \left(3\cdot n_3\left(H_n^{14}\right) + 5\cdot n_4\left(H_n^{14}\right) + 4\right)\frac{\beta_{44}}{5} + \left(\beta_{34} - \frac{3}{5}\beta_{44}\right)n_3\left(\left(H_n^{14}\right)\right) \\
&\quad -\frac{4}{5}\beta_{44} - \beta_{44} \\
&= \left\{2n_3\left(H_n^{14}\right) + 4n_4\left(H_n^{14}\right) + 4 = 2n_1\left(H_n^{14}\right) = n_1\left(H_n^{14}\right) + n_2\left(H_n^{14}\right)\right\} \\
&= n\left(H_n^{14}\right)\cdot\frac{\beta_{44}}{5} + \left(\beta_{34} - \frac{3}{5}\beta_{44}\right)n_3\left(H_n^{14}\right) - \frac{9}{5}\beta_{44} \\
&= \frac{n\left(H_n^{12}\right) - 9}{5}\beta_{44} + \left(\beta_{34} - \frac{3}{5}\beta_{44}\right)n_3\left(H_n^{12}\right) \geq \frac{n\left(H_n^{12}\right) - 9}{5}\beta_{44}.
\end{aligned}$$

In order to prove that this bound is attainable, let us define graphs G''_n, where $n = 5k + 2$ by the following drawing (Fig. 3):

Simple calculation shows that $AZI\left(G''_n\right) = \frac{1376}{135}n - \frac{416}{15}$. □

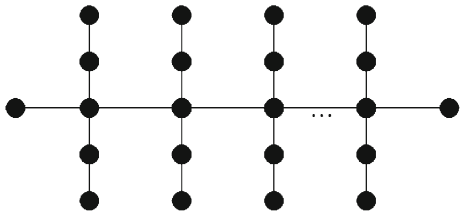
Theorem 2 *Let G_n be a tree with $n \geq 3$ vertices. Then,*

$$AZI\left(G_n\right) \geq (n-1)\cdot\left(\frac{n-1}{n-2}\right)^3.$$

Moreover, the equality holds if and only if G_n is a star.

Proof The results of the paper [22] imply that function $g : \{1, \ldots, n-1\} \times \{1, \ldots, n-1\} \to \mathbb{R}$ defined by $g(x, y) = \frac{x+y-2}{xy}$ is maximized for $(x, y) =$

Fig. 3 Graphs G''_{5k+2}



$(1, n-1)$ or $(x, y) = (n-1, 1)$. Hence,

$$AZI\,(G_n) = \sum_{uv \in E(G_n)} \left(\frac{d_u d_v}{d_u + d_v - 2} \right)$$
$$\geq \sum_{uv \in E(G_n)} \left(\frac{1 \cdot (n-1)}{1 + (n-1) - 2} \right) = (n-1) \cdot \left(\frac{n-1}{n-2} \right)^3 .$$

Moreover equality holds if and only if $\{d_u, d_v\} = \{1, n-1\}$ for each edge uv. The only such graph is a star. □

3 Conclusions

The problem of finding the extremal values of the *AZI* index is completely solved here for chemical trees. Besides chemical trees, general trees are also treated and it has been shown that star tree, S_n, has the maximal *AZI* value. Finding of the minimal *AZI*-value trees, in the case of general trees, remains an open problem.

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