MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **85** (2021) 211-244

ISSN 0340 - 6253

Augmented Zagreb Index: Extremal Results and Bounds

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(Received May 29, 2020)

Abstract

The augmented Zagreb index (AZI) is a molecular structure descriptor introduced about a decade ago. It is defined as

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

where d_u is the degree of the vertex u, and the summation goes over all pairs of adjacent vertices of the underlying molecular graph. Chemical applicability of AZI was tested in several studies, where it was found that in most cases AZI outperforms other structure descriptors of this type. This survey paper outlines extremal results and bounds on AZI that have been reported until now.

1 Introduction

In recent decades, graph theoretical tools have successfully been applied in chemistry, or more specifically in quantitative structure-property relationship studies to predict the physicochemical properties of molecules [41,64]. The screening of chemical libraries using the traditional methods, like HTS (high-throughput screening), is expensive and time consuming. Several alternative methods for the aforementioned purpose have been developed, and one of such methods involves molecular structure descriptors (or molecular descriptors, for simplicity) [26, 27]. Following Todeschini and Consonni [74], we define a *molecular descriptor* as "*the final result of a logical and mathematical procedure which transforms chemical information encoded within a symbolic representation of a molecule into a useful number or the result of some standardized experiment*".

The (chemical) graph theoretical notation and terminology that are not defined in this paper can be found in standard textbooks, like [12, 14, 46, 51, 75]. Throughout this paper, by a graph we mean a graph containing neither loops nor multiple edges. Also, all graphs discussed in this paper are connected and finite. Most of the definitions used in upcoming sections are presented in Section 2.

A molecular descriptor that is calculated from a molecular graph (a graph of a molecule in which vertices and edges correspond to the considered molecule's atoms and bonds, respectively) is usually known as a *topological index* [75]. From graph theoretical point of view, a topological index TI of a graph G is simply a graph invariant of G, that is the numerical quantity associated with G satisfying $TI(G) = TI(G')$ for every graph G' isomorphic to G.

Throughout this paper, by G is denoted a (molecular) graph with vertex set $\mathbf{V}(G)$ and edge set $\mathbf{E}(G)$, possessing $|\mathbf{V}(G)| = n$ vertices and $|\mathbf{E}(G)| = m$ edges. The parameters n and m are, respectively, the order and size of the graph G. The edge of G, connecting the vertices u and v will be denoted by uv. The degree d_w of a vertex $w \in \mathbf{V}(G)$ is the number of first neighbors of w in G.

Among the topological indices that have found applications in chemistry, a considerable number depend on vertex-degrees or/and edge-degrees of the molecular graph. The atom-bond connectivity (ABC) index is one of such topological indices. The ABC index was proposed in 1998 by Estrada et al. [35]. For a (molecular) graph G it is defined as

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

Note that the factor $\sqrt{2}$, present in the original definition of the ABC index is usually ignored because of an obvious reason. In the remaining part of this paper, we also neglect this factor from the original definition of the ABC index. Note also that $d_u + d_v - 2$ is actually the degree of the edge $uv \in \mathbf{E}(G)$. (The degree of the edge uv is the number of edges incident with uv.) Thus, we may say that the ABC index depends on vertex–degrees as well as edge–degrees of the considered graph [35].

The ABC index was initially devised for predicting the heats of formation of alkanes [35]. Later, Estrada [34] examined whether this index can be used to predict some other physicochemical properties of molecules and found that it provides also a good model for the stability of linear and branched alkanes as well as of the strain energy of cycloalkanes. In [49], because of some doubts about the very good correlating ability of the ABC index with the heats of formation of alkanes, a critical re-examination was conducted and it was concluded that the considered doubts need to be abandoned and that the ABC index may successfully be applied to predict the heats of formation of alkanes.

Inspired by the success of the ABC index, Furtula, Graovac, and Vukičević [37] devised the following modified version of the ABC index and referred it as the "*augmented Zagreb index*" (AZI):

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

In fact, the authors of [37] examined a generalized version of the ABC index, namely

$$ABC(\alpha, G) = \sum_{uv \in \mathbf{E}(G)} \left(\frac{d_u + d_v - 2}{d_u \, d_v} \right)^{-\alpha}$$

and found that it has the best correlating property for $\alpha \approx 3$.

The predictive power of AZI is better than that of the ABC index and this index provides a valuable tool in the study of the heat of formation of heptanes and octanes [37]. Gutman and Tošović [48] tested the correlation abilities of 20 vertex–degree–based topological indices for the case of standard heats of formation and normal boiling points of octane isomers, and found that AZI yields the best results. The same conclusion was obtained in [45], when another set of 7 vertex–degree–based topological indices were tested for the these two properties of octane isomers. Moreover, Furtula, Gutman, and Dehmer [38] undertook a comparative study of 12 vertex–degree–based topological indices by examining the smoothness of the considered indices for trees of orders $6, 7, \ldots, 13$ and concluded that AZI has the greatest structure sensitivity; see also [42]. The latest investigation on the smoothness of topological descriptors, using quite a different methodology, was also favorized the AZI along with a few other degree–based indices [70]. AZI was also considered in [29] for its possible applications.

The present survey is an attempt to collect the bounds and extremal results on AZI that have been reported till now. The remaining part of this paper is organized as follows. In the next section, the definitions and notation are listed that are used in upcoming sections. Section 3 consists of two subsections: the first one is concerned with lower bounds on AZI whereas the second one contains the upper bounds on AZI. Section 4 is also subdivided into two subsections: the first one consists of the extremal results regarding minimal AZI and the second one is devoted to gathering extremal results on maximal AZI.

2 Preliminaries

In this section, we specify the notation and definitions that will be used in the upcoming sections.

By an *n-vertex graph*, we mean a graph of order n, i.e., $|\mathbf{V}(G)| = n$. As usual, the n-vertex path, cycle, star, and complete graphs are denoted by P_n, C_n, S_n, and K_n, respectively. A connected graph without cycles is a *tree*.

A *t-partite graph* is a graph whose vertex set can be partitioned into $t \geq 2$ sets $A_1, A_2, \ldots, A_t$ in such a way that all the vertices in A_i are pairwise non-adjacent for $i = 1, 2, \ldots, t$. The sets $A_1, A_2, \ldots, A_t$ are said to be the partite sets. If, in addition, every vertex of the set A_i is adjacent to all the vertices of the other partite sets for $i = 1, 2, \ldots, t$, then the graph is known as the *complete t-partite graph.* A (complete) 2-partite graph is also called *(complete) bipartite graph* and in that case the pair (A_1, A_2) is called bipartition.

A graph with maximum degree at most 4 is called a *molecular graph.* A *pendent vertex* of a graph is a vertex of degree 1. An edge of a graph incident with a pendent vertex is called a *pendent edge.* A *branching vertex* of a graph is a vertex of degree greater than 2. The *minimum non-pendent vertex degree* of a graph G of maximum degree at least 2 is the least number among all the degrees of non-pendent vertices of G. The number of edges incident with an edge e of a graph is called the *edge degree* of e. The *maximum edge degree* of a graph G of size at least 1 is the largest number among all the edge degrees of G.

A sequence consisting of all the vertex degrees of a graph G is the *degree sequence* of G. The set of all different elements of the degree sequence of a graph is the *degree set.* A graph whose degree set is singleton, say $\{t\}$, is a *regular graph* or *t-regular graph.* A graph whose degree set consists of only two elements is *bidegreed.* A *semiregular bipartite graph* is a bidegreed bipartite graph in which all the vertices of each set of the bipartition have the same degree.

A graph G containing no cycles is an *acyclic graph.* (If, in addition, G is connected, then it is a *tree.*) The minimum number of edges of a connected graph G whose removal makes G acyclic is its *cyclomatic number.* By a *unicyclic graph*, we mean a graph with cyclomatic number 1. Similarly, a *bicyclic graph* is the one that has cyclomatic number 2. It is easy to observe that every (connected) unicyclic graph has same order and size, while every (connected) bicyclic graph of order n has size $n + 1$.

The *girth* of a graph G containing at least one cycle is the minimum length of a cycle of G. A graph in which every edge lies on at most one cycle is known as a *cactus graph.*

The *diameter* of a graph G is the largest distance between any two vertices of G.

A *matching* in a graph is a set of pairwise non-adjacent edges. A *maximum matching* is the one that covers as many edges as possible. The *matching number* of a graph is the number of edges in a maximum matching. A matching M, in a graph G, such that every vertex of G is incident with an edge of M is called a *perfect matching.*

A tree containing exactly one branching vertex (= vertex of degree greater than 2) is known as a *starlike tree.* The n-vertex starlike tree with no vertex of degree 2, i.e., with $n - 1$ pendent vertices, is the *star*, S_n. The tree obtained from two stars S_a and S_b, by joining their branching vertices is called a *double star.* If $|a - b| \leq 1$, then this double star is said to be *balanced.*

For $r \geq 2$, a path $P : v_1v_2 \cdots v_r$ in a graph G is said to be an internal path if both the vertices v_1, v_r are branching and every other vertex (if exists) of P has degree 2.

The *complement of a graph G*, denoted by $\overline{G}$, is the graph whose vertex set is $\mathbf{V}(\overline{G}) = \mathbf{V}(G)$ whereas $uv \in \mathbf{E}(\overline{G})$ if and only if $uv \notin \mathbf{E}(G)$. The *union* $H \cup K$ of two graphs H and K is the graph with the vertex set $\mathbf{V}(H) \cup \mathbf{V}(K)$ and the edge set $\mathbf{E}(H) \cup \mathbf{E}(K)$. The *join* $H + K$ of two graphs H and K is the graph with the vertex set $\mathbf{V}(H) \cup \mathbf{V}(K)$ and the edge set $\mathbf{E}(H) \cup \mathbf{E}(K) \cup \{uv \mid u \in \mathbf{V}(H), v \in \mathbf{V}(K)\}$.

The *vertex connectivity* of a nontrivial connected graph is the minimum number of vertices whose removal gives rise to a disconnected or trivial graph. The *edge connectivity* of a nontrivial connected graph is the minimum number of edges whose removal gives rise to a disconnected graph.

A *k-polygonal system* is a connected geometric figure obtained by concatenating congruent regular k-polygons side to side in a plane in such a way that the figure divides the plane into one infinite (external) region and a number of finite (internal) regions, and all internal regions must be congruent regular k-polygons. In a k-polygonal system, two polygons are said to be adjacent if they share a side. The *characteristic graph* (or *dualist* or *inner dual*) of a given k-polygonal system consists of vertices corresponding to k-polygons of the system; two vertices are adjacent if and only if the corresponding k-polygons are adjacent. A k-polygonal system whose characteristic graph is the path graph (respectively, tree) is called *k-polygonal chain* (respectively, *catacondensed k-polygonal system*).

Among k-polygonal systems, those with $k = 6$ are of outstanding importance in chemical graph theory. These are referred to as *hexagonal systems* or *benzenoid systems*; for details see [31, 43]. A hexagonal system H consists of h hexagons (i.e., h internal regions of size 6). It possesses n vertices, some of which belonging to its boundary and some being internal. If the number of internal vertices is n_i, then the hexagonal system H possesses $n = 4h + 2 - n_i$ vertices and $m = 5h + 1 - n_i$ edges. If $n_i = 0$, then the hexagonal system is said to be *catacondensed*. The vertices of a hexagonal system are of degree 2 and 3. The number of degree 3 vertices is $2h - 2$.

A *fluoranthene system* F is a molecular graph constructed from two hexagonal systems, H_1 and H_2. Let u, v be two degree 2 vertices of H_1, separated by a degree 3 vertex. Let x, y be two adjacent degree 2 vertices of H_2. Then F is obtained by joining u, v and x, y by means of two new edges. If, in addition, F satisfying the following three conditions then F is called a *fluoranthene linear chain*: (i) H_1 has only two hexagons (ii) H_2 is the hexagonal linear chain (iii) each of the vertices x, y is adjacent to only vertices of degree 2 in H_2. Note that F consists of $h(H_1) + h(H_2)$ hexagons and has one pentagon. Fluoranthene systems have also been extensively studied in chemical graph theory; for details see [44].

In a k-polygonal chain, a k-polygon adjacent to exactly one (respectively, two) k-polygon(s) is called *external* (respectively, *internal*) *k-polygon*. Any k-polygonal system can be represented by a graph, in which the edges represent the sides of a k-polygon while the vertices correspond to the points where two sides of a k-polygon meet. In the remaining part of this paper, by a k-polygonal system we always mean the graph corresponding to the k-polygonal system.

A 3-polygonal (triangular) chain in which every vertex has degree at most 4 is called a *linear triangular chain*. (Note that for every triangular chain T_n, there exist a 6-polygonal (hexagonal) system whose characteristic graph is isomorphic to T_n.)

A subgraph H of a graph G satisfying the following property is called an *induced subgraph*: $uv \in \mathbf{E}(H)$ whenever $u, v \in \mathbf{V}(H)$ and $uv \in \mathbf{E}(G)$. An induced subgraph of a triangular chain T_n is said to be a *segment* if it is a maximal linear triangular sub-chain of T_n. A segment containing external triangle(s) is called *external segment*. Suppose that a triangular chain T_n has s segments $S_1, S_2, S_3, ..., S_s$. The number of triangles in a segment S_i (where $1 \leq i \leq s$) is its *length*. The s-tuple $(a_1, a_2, \ldots, a_s)$ is said to be the *length vector* of T_n if and only if a_i is the length of S_i for $i = 1, 2, \ldots, s$. If $(a_1, a_2, \ldots, a_s)$ is a length vector of T_n and $s \geq 3$, then we assume that a_1, a_s are the lengths of the external segments.

In a 4-polygonal (polyomino) chain, an internal square having a vertex of degree 2 is known as a kink. In a 5-polygonal (pentagonal)/6-polygonal (hexagonal) chain, a kink is an internal pentagon/hexagon that contains an edge connecting vertices of degree 2. A *linear polyomino/pentagonal/hexagonal chain* is the one, without kinks. A *zigzag polyomino/pentagonal/hexagonal chain* is the one, consisting of only kinks and external polygons. A *segment* in a polyomino/pentagonal/hexagonal chain is a maximal linear sub-chain, including the kinks and/or external polygons at its ends. The number of polygons in a segment is called its *length*. A segment is said to be *external* (*internal*, respectively) if it contains (does not contain, respectively) external polygons. Two segments that have a polygon in common are called *adjacent segments*.

The hexagonal systems with equal number of hexagons and equal number of internal vertices are *isomeric*. Also, isomeric hexagonal systems have equal number of vertices and equal number of edges. Paths along the perimeter of a hexagonal system having degree sequences (2, 3, 2), (2, 3, 3, 2), (2, 3, 3, 3, 2), (2, 3, 3, 3, 3, 2) are known as *fissure, bay, cove, fjord,* respectively. The sum of the number of fissures, bays, coves, and fjords of a hexagonal system S is its *number of inlets*.

In a catacondensed hexagonal system, a hexagon adjacent to three other hexagons is referred to as a *branched hexagon*, while a hexagon that is adjacent to two other hexagons and that contains an edge connecting the vertices of degree 2 is called a *kink*.

Most of the well-known degree-based topological indices can be obtained from the following general setting [54, 78]:

$$BID(G) = \sum_{uv \in E(G)} f(d_u, d_v), \tag{1}$$

where f is a non-negative real valued symmetric function of d_u and d_v. The topological indices of the form (1) will be referred to as *bond incident degree indices* [76], BID indices in short [6]. In Table 1, we list some choices of the function f for which Eq. (1) corresponds to the topological indices considered in the upcoming sections.

Table 1. Some topological indices considered in the present survey. It needs to be mentioned that the modified second Zagreb index M_2^* coincides with the so-called first-order overall index [11, 65].

Function $f(d_u, d_v)$	Eq. (1) corresponds to	Symbol
$d_u + d_v$	first Zagreb index [50]	M_1
$2(d_u + d_v)^{-1}$	harmonic index [36]	H
$(d_u + d_v)^{-1/2}$	sum–connectivity index [84]	X
$d_u\, d_v$	second Zagreb index [47]	M_2
$(d_u\, d_v)^{-1/2}$	Randić index [71]	R
$(d_u\, d_v)^{-1}$	modified second Zagreb index [65]	M_2^*
$\sqrt{\frac{d_u+d_v-2}{d_u\, d_v}}$	atom–bond connectivity index [35]	ABC
$2\sqrt{d_u\, d_v}(d_u + d_v)^{-1}$	geometric–arithmetic index [77]	GA
$\left(\frac{d_u\, d_v}{d_u+d_v-2}\right)^3$	augmented Zagreb index [37]	AZI

3 Bounds

Let G be a graph with a given set $\mathcal{A}$ of graph invariants (for example, order, size, maximum degree, etc.) and let Θ be a bound on the $AZI(G)$ in terms of the elements of $\mathcal{A}$. We say that the bound Θ is the best possible if and only if for every choice of the values of the parameters of $\mathcal{A}$ there exists at least one graph attaining this bound. In this section, we list only those bounds on AZI that are not best possible over the given graph family, or better to say, we shall present bounds on AZI for some quite general graph classes. However, if one restricts his/her observation to more special class of graphs, then sharper results may hold in a such specific case. These kinds of results will be presented in Section 4.

3.1 Lower bounds on augmented Zagreb index

Recall that a tree with maximum degree at most 4 is called a *molecular tree*. In the seminal paper [37], a simple lower bound on AZI for an arbitrary molecular tree in terms of its order was obtained.

Theorem 1. [37] *If T is a molecular tree of order $n \geq 3$, then*

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

If $n \equiv 1 \pmod 4$ and if T is isomorphic to the tree depicted in Figure 1, then equality in (2) *holds.*

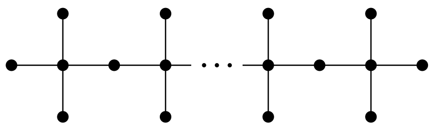

Figure 1. Tree of order $n \equiv 1 \pmod 4$, for which equality in (2) holds.

Note that if $n \equiv 1 \pmod 4$, then equality in (2) holds not only for the tree shown in Figure 1, but also for every tree satisfying $m_{2,4} = (n-5)/2$ and $m_{1,4} = (n+3)/2$, where $m_{i,j}$ is the number of edges whose one end-vertex has degree i and the other end-vertex has degree j.

Let us count the number of extremal graphs for $n \equiv 1 \pmod 4$. Let us denote their set by E_n and let us denote by χ_n the set of all chemical trees with n vertices. Considering that only $m_{i,j}$ that are greater than 0 are $m_{1,4}$ and $m_{2,4}$, it follows that operation that contracts all vertices of degree 2 (i.e. removes vertex of degree 2 with adjacent edges and connects its neighbors by an edge) and removing of all pendent vertices (together with adjacent edge) is bijection from set E_n to set $\chi_{(n-1)/4}$. The numbers χ_n are calculated in [13, 69].

A lower bound for AZI of n-vertex molecular trees with fixed numbers of pendent vertices was given in [32] where also the corresponding extremal trees were characterized. The next two results may be considered as extensions of Theorem 1 for unicyclic and bicyclic molecular graphs.

Theorem 2. [8] *If G is a unicyclic molecular graph of order n, then*

$$AZI(G) \geq \frac{140}{27}\, n\,,$$

with equality if and only if $n \equiv 0 \pmod 4$, the maximum degree of G is 4, and each edge of G has one end-vertex of degree 4 and the other end-vertex is of degree 1 or 2.

Theorem 3. [8] *If G is a bicyclic molecular graph of order n, then*

$$AZI(G) \geq \frac{4}{27}(35n + 111)\,,$$

with equality if and only if $n \equiv 3 \pmod 4$, the maximum degree of G is 4, and each edge of G has one end-vertex of degree 4 and the other end-vertex is of degree 1 or 2.

In [57], several lower bounds on AZI are obtained in terms of various graph parameters.

Theorem 4. [57] *If G is a graph of size m and minimum degree $\delta \geq 2$, then*

$$AZI(G) \geq \frac{m\,\delta^6}{8(\delta-1)^3}\,,$$

with equality if and only if G is either a δ-regular graph, $\delta > 2$, or every edge of G has at least one end-vertex of degree 2 when $\delta = 2$.

Corollary 5. [57] *If G is a graph of order n and minimum degree $\delta \geq 2$ then*

$$AZI(G) \geq \frac{n\,\delta^7}{16(\delta-1)^3}\,,$$

with equality if and only if G is a δ-regular graph.

Theorem 6. [57] *Let G be a graph of size $m \geq 2$ and maximum degree Δ. Let p be the number of pendent vertices of G. If q is the number of non-pendent edges of G having at least one end-vertex of degree 2 then*

$$AZI(G) \geq \frac{729(m-p-q)}{64} + 8q + p\left(\frac{\Delta}{\Delta-1}\right)^3\,,$$

with equality if and only if at least one end-vertex of uv has degree 2, or both the end-vertices of uv have degree 3 for every non-pendent edge $uv \in \mathbf{E}(G)$, and every pendent edge of G is incident with a vertex of degree Δ.

Theorem 7. [57] *Let G be a graph of size $m \geq 2$ and maximum degree Δ. If p is the number of pendent vertices of G then*

$$AZI(G) \geq 8(m-p) + p\left(\frac{\Delta}{\Delta-1}\right)^3 ,$$

with equality if and only if at least one end-vertex of uv has degree 2 for every non-pendent edge $uv \in \mathbf{E}(G)$, and every pendent edge of G is incident with a vertex of degree Δ.

Since every molecular graph has maximum degree at most 4, the next result is a direct consequence of Theorem 7.

Corollary 8. [57] *If G is a molecular graph of size $m \geq 2$ and if p is the number of pendent vertices of G, then*

$$AZI(G) \geq 8(m-p) + \frac{64}{27}p ,$$

with equality if and only if at least one end-vertex of uv has degree 2 for every non-pendent edge $uv \in \mathbf{E}(G)$ and every pendent edge of G is incident with a vertex of degree 4.

Theorem 9. [57] *If G is a graph of size $m \geq 2$ and maximum degree Δ, then*

$$AZI(G) \geq m\left(\frac{\Delta}{\Delta-1}\right)^3 ,$$

with equality if and only if G is the star graph.

The bound on AZI given in the next theorem is stronger than that in Theorem 9.

Theorem 10. [79] *Let $\Psi_{n,m,\Delta}$ be the class of graphs of order n, size m, and maximum degree Δ, whose each edge has one end-vertex of degree Δ and the other end-vertex of degree 1 or 2. If G is a graph of order n, size m, and maximum degree Δ, $2 \leq \Delta \leq n-1$, then*

$$AZI(G) \geq \left(2n - m - \frac{2m}{\Delta}\right)\left(\frac{\Delta}{\Delta-1}\right)^3 + 16\left(m - n + \frac{m}{\Delta}\right) ,$$

with equality if and only if G is the path graph for $\Delta = 2$, and $G \in \Psi_{n,m,\Delta}$ with $m \equiv 0 \pmod{\Delta}$ for $\Delta \geq 3$.

We note here that Theorem 10 follows also from a more general result, obtained recently in [83]. The next two results are special cases of Theorem 10.

Corollary 11. [79] *If T is a tree of order n and maximum degree Δ, $2 \leq \Delta \leq n-1$, then*

$$AZI(T) \geq \left(n+1-\frac{2(n-1)}{\Delta}\right)\left(\frac{\Delta}{\Delta-1}\right)^3 + 16\left(\frac{n-1}{\Delta}-1\right),$$

with equality if and only if T is the path graph for $\Delta = 2$, and $G \in \Psi_{n,n-1,\Delta}$ with $n \equiv 1 \pmod{\Delta}$ for $\Delta \geq 3$, where $\Psi_{n,n-1,\Delta}$ is same as in Theorem 10.

Corollary 12. [79] *If T is a molecular tree of order $n \geq 3$ then*

$$AZI(T) \geq \frac{4}{27}(35n-111),$$

with equality if and only if $G \in \Psi_{n,n-1,4}$ with $n \equiv 1 \pmod 4$.

Note that the bound given in Corollary 12 is same as that in Theorem 1. However, in Theorem 1 the graphs attaining the bound are not characterized while in Corollary 12 these graphs are characterized.

Theorem 13. [79] *Let G be a graph with $n \geq 3$ vertices, m edges and p pendent vertices. If Δ is the maximum degree of G and δ_1 is the minimum non-pendent vertex degree of G, then*

$$AZI(G) \geq p\left(\frac{\Delta}{\Delta-1}\right)^3 + (m-p)\left(\frac{\delta_1^2}{2(\delta_1-1)}\right)^3,$$

with equality if and only if G is regular or G has the degree set $\{1,\Delta\}$ or G is the graph in which every pendent edge is incident with a vertex of degree Δ and every non-pendent edge has at least one end-vertex of degree 2, or G is the graph of minimum degree 2 and every edge has at least one end-vertex of degree 2.

Theorem 14. [66] *If G is a graph of order $n \geq 3$, size m and maximum degree Δ, then*

$$AZI(G) \geq \frac{m^4}{(n-1)^3}\left(\frac{\Delta^2}{\Delta^2-1}\right)^3.$$

If G is the complete graph then equality sign in the above inequality holds.

The bound given in the next theorem is stronger than the one mentioned in Theorem 14.

Theorem 15. [39] *If G is a graph of order $n \geq 3$, size m, and maximum degree Δ, then*

$$AZI(G) \geq m^4\left(\frac{\Delta}{n(\Delta-1)}\right)^3,$$

with equality if and only if G is a regular graph.

If $m \geq n$ then the bound mentioned in Theorem 15 is stronger than that given in Theorem 9, see [39] for details.

Theorem 16. [3] *If G is a graph of order $n \geq 3$, then*

$$AZI(G) \geq \frac{1536}{343} X(G) \tag{3}$$

$$AZI(G) \geq \frac{343\sqrt{7}}{216} R(G) \tag{4}$$

$$AZI(G) \geq \frac{375}{64} H(G) \tag{5}$$

$$AZI(G) \geq \left(\frac{n-1}{n-2}\right)^{7/2} ABC(G) \tag{6}$$

$$AZI(G) \geq 4M_2^*(G)\,. \tag{7}$$

Equality in (3), *(4), (5), (6), and (7) holds if and only if $G \cong S_9$, $G \cong S_8$, $G \cong S_6$, $G \cong S_n$, and $G \cong P_3$, respectively.*

The next result is an improved variant of Theorem 16 when G has the minimum degree at least 2.

Corollary 17. [3] *If G is a graph with minimum degree $\delta \geq 2$, then*

$$AZI(G) \geq \frac{\delta^{13/2}}{\sqrt{32}(\delta-1)^3} X(G) \tag{8}$$

$$AZI(G) \geq \frac{\delta^7}{8(\delta-1)^3} R(G) \tag{9}$$

$$AZI(G) \geq \frac{\delta^7}{8(\delta-1)^3} H(G) \tag{10}$$

$$AZI(G) \geq \left(\frac{\delta^2}{2(\delta-1)}\right)^{7/2} ABC(G) \tag{11}$$

$$AZI(G) \geq \frac{\delta^6}{8(\delta-1)^3} GA(G) \tag{12}$$

$$AZI(G) \geq \frac{\delta^4}{2(\delta-1)} M_2^*(G)\,. \tag{13}$$

Equality in any of the inequalities (8)–(13) holds if and only if G is a δ-regular graph.

Theorem 18. [39] *(a) If G is a graph of size $m \geq 1$, then*

$$AZI(G) \geq \frac{m^7}{ABC(G)^6} \, .$$

(b) If G is a graph of order $n \geq 3$ and size m, then

$$AZI(G) \geq \frac{m^4}{\left[n - 2M_2^*(G)\right]^3} \, .$$

Equality in any of the above two inequalities holds if and only if G is a regular graph or a semiregular bipartite graph, or G is a graph in which each edge is incident with at least one vertex of degree 2.

Each of the two bounds given in Theorem 18 is stronger than the bound in Theorem 14. Also, if either $m \geq n$ or $m \geq 2$, then each of the two bounds in Theorem 18 is stronger than the one given in Theorem 9, see [39] for details.

Theorem 19. [39] *(a) If G is a graph of size $m \geq 2$, then*

$$AZI(G) \geq \frac{m^7}{\left[(M_1(G) - 2m)M_2^*(G)\right]^3} \, ,$$

with equality if and only if G is either a regular graph or a semiregular bipartite graph.
(b) If G is a graph of order $n \geq 3$ and size m, then

$$AZI(G) \geq \frac{m^7}{\left[(n-1)(m - M_2^*(G))\right]^3} \, ,$$

with equality if and only if G is either a star graph or a complete graph.
(c) If G is a graph of order $n \geq 3$ and size m, then

$$AZI(G) \geq m^4 \left(\frac{M_2(G)}{n\, M_2(G) - 2m^2} \right)^3 \, ,$$

with equality if and only if G is either a regular graph or a semiregular bipartite graph.
(d) If G is a graph of size $m \geq 2$ and maximum edge-degree Δ', then

$$AZI(G) \geq \frac{M_2(G)^3}{\Delta' \left[M_1(G) - 2m\right]^2} \, ,$$

with equality if and only if G is either a regular graph or a semiregular bipartite graph.

Theorem 20. [8] *Let G be a graph of order $n \geq 3$, such that its complement $\overline{G}$ is connected. Let Δ, δ_1, p, $\overline{\Delta}$, $\overline{\delta_1}$, and $\overline{p}$ denote the maximum degree, minimal non-pendent* *vertex degree, the number of pendent vertices in* G *and* $\overline{G}$*, respectively. If* $\alpha = \min\{\delta_1, \overline{\delta_1}\}$ *and* $\beta = \max\{\Delta, \overline{\Delta}\}$*, then*

$$AZI(G) \geq (p+\overline{p})\left(\frac{n-2}{n-3}\right)^3\left[1-\left(\frac{n-2}{2}\right)^3\right]+\binom{n}{2}\left(\frac{\alpha^2}{2\alpha-2}\right)^3 - AZI(\overline{G}),$$

with equality if and only if $G \cong P_4$ *or* G *is isomorphic to an* r*-regular graph with* $2r+1$ *vertices.*

Lower bounds on AZI of graphs under various operations can be found in [28, 33, 40, 58, 72].

3.2 Upper bounds on augmented Zagreb index

In this section, we list only those upper bounds on AZI that are not best possible over the given graph family.

Theorem 21. [37] *If* T *is a molecular tree of order* $n \geq 3$ *then*

$$AZI(T) \leq \begin{cases} 8(n-1) & \text{if } 3 \leq n \leq 9, \\ \dfrac{4825}{64} & \text{if } n = 10, \\ \dfrac{1376}{135}n - \dfrac{416}{15} & \text{if } n \geq 11. \end{cases} \tag{14}$$

If n *is at least 12 and satisfies* $n \equiv 2 \pmod 5$*, and if* T *is isomorphic to the tree depicted in Figure 2, then equality in* (14) *holds.*

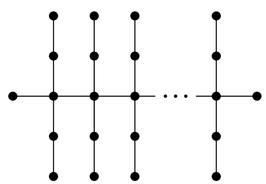

Figure 2. The tree of order $n \geq 12$ satisfying $n \equiv 2 \pmod 5$, that attains the equality in (14).

Note that if $n \equiv 2 \pmod 5$, then equality in (14) holds not only for the tree shown in Figure 2, but also for every tree satisfying $m_{1,2} = m_{2,4} = 2\cdot(n-2)/5$, $m_{4,4} = (n-2)/5 - 1$ and $m_{1,4} = 2$. (Recall that $m_{i,j}$ denotes the number of edges whose one end-vertex has degree i and the other end–vertex has degree j.)

The next two results can be considered as extensions of Theorem 21 for the unicyclic and bicyclic molecular graphs.

Theorem 22. [8] *If G is a unicyclic molecular graph of order n, then*

$$AZI(G) \leq \frac{1376}{135}\, n\,. \tag{15}$$

If $G \cong U_n'$, then equality in (15) *holds, where U_n' is depicted in Figure 3.*

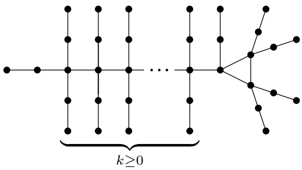

Figure 3. The unicyclic graph U_n' of order n satisfying $n = 5k + 15 \geq 15$, that attains equality in (15).

Theorem 23. [8] *If G is a molecular bicyclic graph of order n, then*

$$AZI(G) \leq \frac{1376}{135}\, n + \frac{416}{15}\,. \tag{16}$$

If $G \cong B_n'$, then equality in (16) *holds, where B_n' is depicted in Figure 4.*

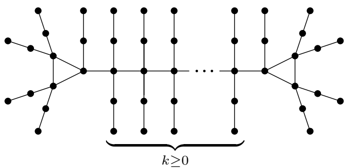

Figure 4. The bicyclic graph B_n' of order n satisfying $n = 5k + 26 \geq 26$, that attains equality in (16).

Theorem 24. [57] *If G is a molecular graph of size $m \geq 2$, then*

$$AZI(G) \leq \frac{512}{27}\, m\,,$$

with equality if and only if G is a 4-regular graph.

Corollary 25. [57] *If G is a molecular graph of order $n \geq 3$, then*

$$AZI(G) \leq \frac{1024}{27}\, n\,,$$

with equality if and only if G is a 4-regular graph.

Theorem 26. [57] *Let G be a graph of size $m \geq 2$ and has maximum degree Δ. Let p be the number of pendent vertices. If q is the number of non-pendent edges having at least one end-vertex of degree 2, then*

$$AZI(G) \leq 8(p+q) + (m-p-q)\left(\frac{\Delta^2}{2(\Delta-1)}\right)^3 ,$$

with equality if and only if at least one end-vertex of the edge uv has degree 2 or both the end-vertices of uv have degree Δ for every $uv \in \mathbf{E}(G)$.

Theorem 27. [57] *If G is a graph of size $m \geq 2$ and has maximum degree Δ, then*

$$AZI(G) \leq m\left(\frac{\Delta^2}{2(\Delta-1)}\right)^3 ,$$

with equality if and only if G is a path or a Δ-regular graph.

Corollary 28. [57] *If G is a graph of order $n \geq 3$ and has maximum degree Δ, then*

$$AZI(G) \leq \frac{n\,\Delta^7}{16(\Delta-1)^3} ,$$

with equality if and only if G is a Δ-regular graph.

Theorem 29. [79] *Let G be a graph with $n \geq 3$ vertices, m edges and p pendent vertices. If Δ is the maximum degree of G and δ_1 is the minimum non-pendent vertex degree of G, then*

$$AZI(G) \leq p\left(\frac{\delta_1}{\delta_1-1}\right)^3 + (m-p)\left(\frac{\Delta^2}{2(\Delta-1)}\right)^3 ,$$

with equality if and only if either G is regular or G has the degree set $\{1, \Delta\}$.

Theorem 30. [3] *If G is a graph of order $n \geq 3$ then*

$$AZI(G) \leq \frac{\sqrt{(n-1)^{13}}}{\sqrt{32}(n-2)^3}\,X(G) \tag{17}$$

$$AZI(G) \leq \frac{(n-1)^7}{8(n-2)^3}\,R(G) \tag{18}$$

$$AZI(G) \leq \frac{(n-1)^7}{8(n-2)^3}\,H(G) \tag{19}$$

$$AZI(G) \leq \left(\frac{(n-1)^2}{2(n-2)}\right)^{7/2} ABC(G) \tag{20}$$

$$AZI(G) \leq \frac{(n-1)^4}{2(n-2)} M_2^*(G) , \tag{21}$$

where equality in any of the inequalities (17)–(21) holds if and only if $G \cong K_n$.

Theorem 31. [3] *If G is a graph of order $n \geq 3$ and minimum degree at least 2, then*

$$AZI(G) \leq \frac{(n-1)^6}{8(n-2)^3}\, GA(G)\,,$$

with equality if and only if $G \cong K_n$.

In [3], it was asked to find a sharp upper bound on AZI of a graph G of order $n \geq 3$ and minimum degree 1 in terms of n and $GA(G)$. This problem seems to be still open.

Theorem 32. [8] *Let G be a graph of order $n \geq 3$, such that its complement $\overline{G}$ is connected. Let Δ, δ_1, p, $\overline{\Delta}$, $\overline{\delta_1}$, and $\overline{p}$ denote the maximum degree, minimal non-pendent vertex degree, number of pendent vertices in G and $\overline{G}$, respectively. If $\alpha = \min\{\delta_1, \overline{\delta_1}\}$ and $\beta = \max\{\Delta, \overline{\Delta}\}$, then*

$$AZI(G) \leq \binom{n}{2}\left(\frac{\beta^2}{2\beta-2}\right)^3 - AZI(\overline{G})\,,$$

with equality if and only if $G \cong P_4$ or G is isomorphic to an r-regular graph with $2r+1$ vertices.

Upper bounds on AZI of graphs under several graph operations can be found in [28, 33, 40, 58, 72].

4 Extremal results

In this section, we list the extremal results concerning AZI, reported till date. We remark here that the best possible bounds on AZI over certain classes of graphs follow directly from the results listed in this section.

4.1 Extremal results concerning minimal AZI

Studies of extremal problems concerning minimal AZI were initiated by the paper [37], where the problem of characterizing the graph(s) having minimal AZI in the class of all trees of a given order was solved.

Theorem 33. [37] *Among trees of order $n \geq 4$, only the star S_n has minimal AZI, equal to*

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

Theorem 33 was proven also in [25, 57] by an alternative method. From Theorem 33, it follows directly that S_n is the unique graph having minimal AZI in the class of all starlike trees of order $n \geq 7$. This fact was proven in [10].

Theorem 34. [56] *(a) In the class of trees of order $n \geq 6$, only the tree obtained from the star of order $n-1$ by attaching a new pendent vertex to any pendent vertex, has the second minimal AZI, equal to*

$$\frac{(n-2)^3}{(n-3)^2} + 16\,.$$

(b) In the class of trees of order $n \geq 6$, only the tree obtained from the path graph of order 3, by attaching $\lfloor (n-3)/2 \rfloor$ pendent vertices to the one end-vertex and $\lceil (n-3)/2 \rceil$ pendent vertices to the other end-vertex, has the third minimal AZI, equal to

$$\frac{(\lfloor (n-3)/2 \rfloor + 1)^3}{(\lfloor (n-3)/2 \rfloor)^2} + \frac{(\lceil (n-3)/2 \rceil + 1)^3}{(\lceil (n-3)/2 \rceil)^2} + 16\,.$$

In [56], the problem of characterizing the graph(s) having minimal AZI in the class of all n-vertex trees with a given number of pendent vertices was solved for $n \geq 5$.

Theorem 35. [56] *(a) For $2 \leq p \leq n-3$, among trees with n vertices and p pendent vertices, only the tree obtained from the path graph of order $n - \lfloor p/2 \rfloor - \lceil p/2 \rceil$ by attaching $\lfloor p/2 \rfloor$ pendent vertices to the one end-vertex and $\lceil p/2 \rceil$ pendent vertices to the other end-vertex, has the minimal AZI, equal to*

$$\frac{(\lfloor p/2 \rfloor + 1)^3}{(\lfloor p/2 \rfloor)^2} + \frac{(\lceil p/2 \rceil + 1)^3}{(\lceil p/2 \rceil)^2} + 8(n-p-1)\,.$$

(b) Among trees with $n \geq 5$ vertices and $n-2$ pendent vertices, only the tree specified in Theorem 34(a) has minimal AZI.

In the class of n-vertex trees with a given diameter, the unique graph having minimal AZI was characterized in [55] for $n \geq 6$.

Theorem 36. [55] *Among all the trees of order $n \geq 6$ and diameter 3, only the tree specified in Theorem 34(a) has the minimal AZI.*

Note that Theorems 35(b) and 36 are equivalent because a tree T of order $n \geq 6$ has $n-2$ pendent vertices if and only if T has diameter 3.

Theorem 37. [55] *For $4 \leq d \leq n-2$, among trees of order n and diameter d, only the tree obtained from the path graph of order $n - \lfloor (n-d+1)/2 \rfloor - \lceil (n-d+1)/2 \rceil$*

by attaching $\lfloor (n-d+1)/2 \rfloor$ *pendent vertices to the one end-vertex and* $\lceil (n-d+1)/2 \rceil$ *pendent vertices to the other end-vertex, has minimal* AZI*, equal to*

$$\frac{(\lfloor (n-d+1)/2 \rfloor + 1)^3}{(\lfloor (n-d+1)/2 \rfloor)^2} + \frac{(\lceil (n-d+1)/2 \rceil + 1)^3}{(\lceil (n-d+1)/2 \rceil)^2} + 8(d-2)\,.$$

The next theorem is a special case of a more general result proven in [20].

Theorem 38. [20] *Among trees with* $n \geq 8$ *vertices and with exactly two branching vertices, the extremal graph specified in Theorem 34(b) is the unique tree with minimal* AZI*.*

In [73], the problem of characterizing the graph(s) having minimal AZI in the class of all n-vertex trees/unicyclic graphs with a perfect matching was addressed for even values of n.

Theorem 39. [73] *For every* $k \geq 3$*, among all trees of order* $2k$ *with a perfect matching, only the tree* T_k^* *depicted in Figure 5 has minimal* AZI*, equal to*

$$\begin{cases} \dfrac{219}{16}k - \dfrac{91}{16} & \textit{if } k \textit{ is odd,} \\[2ex] \dfrac{219}{16}k - \dfrac{295}{64} & \textit{otherwise.} \end{cases}$$

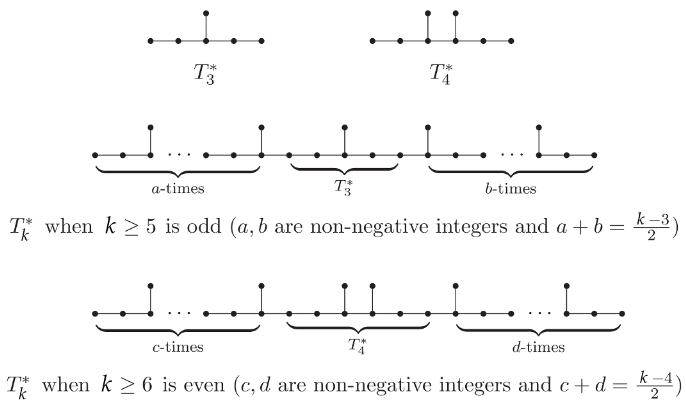

Figure 5. The tree T_k^* mentioned in Theorem 39.

Theorem 40. [73] *For every $k \geq 2$, among all unicyclic graphs of order $2k$ with a perfect matching, only the graph U_k^* depicted in Figure 6 has minimal AZI, equal to*

$$\begin{cases} \dfrac{219}{16}\,k + \dfrac{69}{64} & \text{if } k \text{ is odd,} \\[2ex] \dfrac{219}{16}\,k & \text{otherwise.} \end{cases}$$

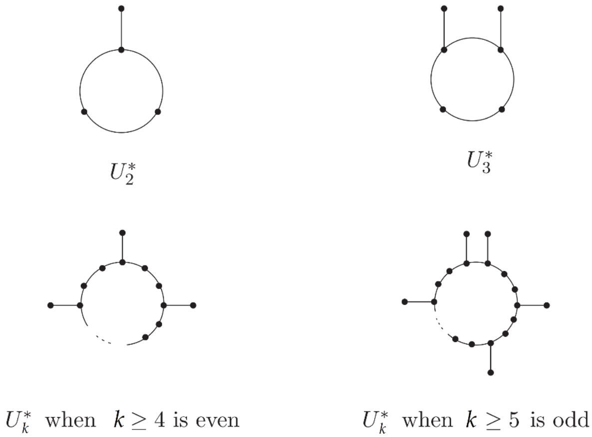

Figure 6. The graph U_k^* mentioned in Theorem 40.

The next theorem is a special case of a more general result proven in [80].

Theorem 41. [80] *In the class of trees of order at least 4, with a given degree sequence, the tree(s) having maximal ABC index have minimal AZI.*

Theorem 42. [57] *Among unicyclic graphs of order n and girth g, the unique graph $C_{n,n-g}$ has minimal AZI, equal to*

$$\frac{(n-g)(n-g+2)^3}{(n-g+1)^3} + 8g\,,$$

where $C_{n,n-g}$ is the graph obtained from the cycle C_g by attaching $n-g$ pendent vertices to one vertex of C_g.

Theorem 43. [57] *Among unicyclic graphs with n vertices and p pendent vertices, the unique graph $C_{n,p}$ has minimal AZI, equal to*

$$\frac{p(p+2)^3}{(p+1)^3} + 8(n-p)\,,$$

where $C_{n,p}$ is same as in Theorem 42.

The next result follows directly from Theorem 42 as well as from Theorem 43.

Corollary 44. [57] *In the class of unicyclic graphs with* $n \geq 4$ *vertices,* $C_{n,n-3}$ *is the unique graph with minimal* AZI*, equal to*

$$\frac{(n-3)(n-1)^3}{(n-2)^3} + 24\,.$$

The next result was proven both in [56] and [81], independently.

Theorem 45. [56, 81] *Among unicyclic graphs with* $n \geq 6$ *vertices, the unique graph* $C_{n,n-4}$ *has the second minimal* AZI*, equal to*

$$\frac{(n-4)(n-2)^3}{(n-3)^3} + 32\,,$$

where $C_{n,n-4}$ *is same as in Theorem 42.*

Theorem 44 for $n \geq 4$ and Theorem 45 for $n \geq 9$ are special cases of a more general result proven recently in [63].

Theorem 46. [57] *From the class of bicyclic graphs with* n *vertices and* p *pendent vertices,* $0 \leq p \leq n-5$*, only member(s) of the class* $\mathcal{B}_{n,p}$ *attain(s) the minimal* AZI*-value, equal to*

$$\frac{p(p+4)^3}{(p+3)^3} + 8(n-p+1)\,,$$

where $\mathcal{B}_{n,p}$ *is the class of bicyclic graphs obtained by identifying one vertex of two cycles* C_r *and* C_s*, and then attaching* $p = n - r - s + 1$ *pendent vertices to the common vertex.*

Theorem 46 does not give any information about finding graphs with minimal AZI among bicyclic graphs with $n \geq 5$ vertices and $n-4$ pendent vertices. The next two theorems, independently proven in [56] and [81], provide the respective solution.

Theorem 47. [56, 81] *Among bicyclic graphs with* $n \geq 5$ *vertices and* $n-4$ *pendent vertices, the unique graph obtained from the star* S_n *by adding two new adjacent edges, has minimal* AZI*, equal to*

$$\frac{(n-4)(n-1)^3}{(n-2)^3} + \frac{27(n-1)^3}{n^3} + 32\,.$$

Theorem 48. [56, 81] *In the class of bicyclic graphs with* $n \geq 5$ *vertices, the unique graph obtained from the star* S_n *by adding two non-adjacent edges, has minimal* AZI*, equal to*

$$\frac{(n-5)(n-1)^3}{(n-2)^3} + 48\,.$$

Theorem 49. [1] *Among cactus graphs with $n \geq 4$ vertices and k cycles, the unique graph obtained from the star S_n by adding k pairwise non-adjacent edges, has minimal AZI, equal to*

$$(n-2k-1)\left(\frac{n-1}{n-2}\right)^3 + 24k\,.$$

Theorem 50. [52] *(a) For $2 \leq p \leq n-3$, among cactus graphs with n vertices and p pendent vertices, only the extremal tree specified in Theorem 35(a) has minimal AZI.*
(b) Among cactus graphs with $n \geq 5$ vertices and $n-2$ pendent vertices, only the extremal tree specified in Theorem 34(a) has minimal AZI.

Because of the fact that AZI of a graph $G \ncong K_n$ is less than AZI of the graph obtained from G by adding an edge [57], Theorem 50 follows also from Theorem 35.

Theorem 51. [57] *Among graphs of order $n \geq 3$, only the star S_n has minimal AZI, and this minimal value is given in Theorem 33.*

Theorem 51 follows directly from Theorem 9. Theorem 51 was proven also in [22] by using an alternative method.

Theorem 52. [56] *In the class of graphs of order $n \geq 5$, only the extremal tree mentioned in Theorem 34(a) has the second minimal AZI.*

Denote by $\mathfrak{T}_n$ the class of triangular chains with $n \geq 4$ triangles in which every vertex has degree at most five. Note that $\mathfrak{T}_n$ is actually a subclass of the class of all characteristic graphs of hexagonal systems. For $n \geq 6$, let T_n^- be the triangular chain with the length vector $(3, x, 3)$, where $x \geq 4$.

Theorem 53. [2] *For $n \geq 9$, T_n^- is the unique triangular chain with minimal AZI among the members of $\mathfrak{T}_n$.*

Theorem 54. [6] *Among all polyomino chains with $n \geq 3$ squares, only the linear polyomino chain has minimal AZI.*

Let Ω_n be the class of pentagonal chains with $n \geq 3$ pentagons in which every internal segment of length 3 (if it exists) contains no edge connecting vertices of degree 3.

Theorem 55. [7] *For $n \geq 3$, only the linear pentagonal chain has minimal AZI among the members of Ω_n.*

Theorem 56. [18] *Among isomeric hexagonal systems, only those having maximal number of inlets have minimal AZI.*

The next result is a special case of Theorem 9 of [30].

Theorem 57. [30] *Among catacondensed hexagonal systems with h hexagons, only the linear hexagonal chain has minimal AZI.*

Theorem 57 was proven independently also in [62, 67, 82]. Additional results on minimal AZI of certain hexagonal systems can be found by using the results obtained in [5, 9, 16, 17, 30, 68].

Theorem 58. [53] *Among catacondensed fluoranthene systems with h hexagons, only the fluoranthene linear chain has minimal AZI.*

Theorem 58 was independently proven also in [59]. More results concerning the minimal AZI of fluoranthene systems can be found in [53, 59].

4.2 Extremal results concerning maximal AZI

In this section, we list the extremal results regarding maximal AZI. The following theorem is a special case of a more general result, proved in [80].

Theorem 59. [80] *Among trees of order at least 4 and with a given degree sequence, the tree(s) having minimal ABC have maximal AZI.*

Recall that a tree containing exactly one branching vertex is called a starlike tree.

Theorem 60. [10] *In the class of starlike trees of order $n \geq 7$, only the tree(s) in which every edge is incident with at least one vertex of degree 2, has/have maximal AZI and this maximal value is $8(n-1)$.*

Note that if G is a tree having exactly one branching vertex in Theorem 26, then $p+q=m=n-1$ and hence we have Theorem 60.

In [21], the problem of finding graph(s) with maximal AZI in the class of trees with given order and with given number of branching vertices was addressed – however, its complete solution has been left as an open problem.

Theorem 61. [21] *Among trees with $n \geq 19$ vertices and exactly two branching vertices, the balanced double star is the unique tree with maximal AZI.*

Theorem 62. [21] *Among trees with* $n \geq 35$ *vertices and exactly three branching vertices, the unique graph obtained from the star* S_5 *by attaching* $\lfloor (n-5)/2 \rfloor$ *pendent vertices to one pendent vertex of* S_5 *and* $\lceil (n-5)/2 \rceil$ *pendent vertices to another pendent vertex, has maximal* AZI.

Note that the next two theorems are equivalent because a tree T of order $n \geq 6$ has $n-2$ pendent vertices if and only if T has diameter 3.

Theorem 63. [56] *Among trees with* $n \geq 6$ *vertices and exactly* $n-2$ *pendent vertices, the balanced double star is the unique tree with maximal* AZI, *equal to*

$$\frac{(\lfloor (n-2)/2 \rfloor + 1)^3}{(\lfloor (n-2)/2 \rfloor)^2} + \frac{(\lceil (n-2)/2 \rceil + 1)^3}{(\lceil (n-2)/2 \rceil)^2} + 8\,.$$

Theorem 64. [55] *Among trees of order* $n \geq 6$ *and diameter* 3, *the balanced double star is the unique tree with maximal* AZI.

The following problem was considered in [1].

Problem 65. [1] *Among cactus graphs with* $n \geq 4$ *vertices and* k *cycles, characterize the graph(s) having maximal* AZI.

For $k = 0$, Problem 65 is equivalent to characterizing the tree(s) with maximal AZI. (In what follows, we call such a tree as the "n-vertex tree with maximal AZI".) In [1], the n-vertex trees with maximal AZI were characterized for $n \leq 9$ and some structural properties of such trees were established for $n \geq 10$. One of such property is that an n-vertex tree with maximal AZI contains no internal path of length greater than 1. In [60], it was found that the balanced double star is the unique n-vertex tree with maximal AZI for every $n \in \{10, 11, 12, \ldots, 200\}$ and hence the following conjecture was posed.

Conjecture 66. [60] *The balanced double star is the unique* n*-vertex tree with maximal* AZI *for* $n \geq 19$.

In [60], it was also proven that every pendent vertex of an n-vertex tree, $n \geq 19$, with maximal AZI is adjacent to a branching vertex, which together with a property proven in [1] implies that such a tree contains no vertex of degree 2. Conjecture 66 was proven for all trees of order $n \geq 19$ that have at most 3 branching vertices [21]. Recently, Conjecture 66 has been proven completely in [61]. The problems of finding graph(s) with maximal AZI from the following classes of graphs were posed in [61]: (i) n-vertex trees with a given diameter, (ii) n-vertex trees with a given number of pendent vertices, (iii) n-vertex graphs with a fixed size greater than $n-1$.

Theorem 67. [57] *Among graphs of order $n \geq 3$, only the complete graph has maximal AZI, equal to*

$$\frac{n(n-1)^7}{16(n-2)^3}\,.$$

Note that Theorem 67 follows directly from Corollary 28. However, in [57], Theorem 67 was proven in some other way. Theorem 67 was proven also in [22] by using another method.

Theorem 68. [57] *Among graphs of order $n \geq 3$, only the graph $K_n - e$ has the second maximal AZI, equal to*

$$2(n-2)^4\left(\frac{n-1}{2n-5}\right)^3 + \frac{(n-3)(n-1)^6}{16(n-2)^2}\,,$$

where $K_n - e$ is the graph obtained from the complete graph K_n by removing an edge.

From the class of graphs of order $n \geq 5$, the graphs having third, fourth, and fifth maximal AZI are characterized in [56].

Theorem 69. [57] *If $\sum_{i=1}^{t} r_i = n \geq 3$, then among all t-partite graphs with $r_1, r_2, \ldots, r_t$ vertices in their t-partite sets, only the complete t-partite graph $K_{r_1,r_2,\ldots,r_t}$ has maximal AZI, equal to*

$$\sum_{1\leq i\leq j\leq t} \frac{r_i\, r_j\, (n-r_i)^3\, (n-r_i)^3}{(2n-r_i-r_j-2)^3}\,.$$

Theorem 70. [57] *Among bipartite graphs of order $n \geq 4$, only the complete bipartite graph $K_{\lfloor n/2\rfloor,\lceil n/2\rceil}$ has maximal AZI, equal to*

$$\frac{\left(\lfloor n/2\rfloor\,\lceil n/2\rceil\right)^4}{(n-2)^3}\,.$$

Theorem 71. [4] *In the class graphs of order $n \geq 5$ and vertex connectivity at most $\kappa \geq 2$, $K_\kappa + (K_1 \cup K_{n-\kappa-1})$ is the unique graph having maximal AZI and this maximal value is*

$$\frac{\kappa(\kappa-1)}{16}\left(\frac{(n-1)^2}{n-2}\right)^3 + \kappa^4\left(\frac{n-1}{n+\kappa-3}\right)^3 + \frac{(n-\kappa-1)(n-\kappa-2)}{16}\left(\frac{(n-2)^2}{n-3}\right)^3$$
$$+\ \kappa(n-\kappa-1)\left(\frac{(n-2)(n-1)}{2n-5}\right)^3.$$

Theorem 72. [4] *(a) For $2 \leq \beta < \lfloor \frac{n}{2} \rfloor$, among graphs of order n and matching number at most β, $K_\beta + \overline{K}_{n-\beta}$ is the unique graph having maximal AZI, equal to*

$$\frac{\beta(\beta-1)(n-1)^6}{16(n-2)^3} + \beta^4 (n-\beta) \left(\frac{n-1}{n+\beta-3} \right)^3 .$$

(b) In the class graphs of order $n \geq 4$ and matching number at most $\lfloor \frac{n}{2} \rfloor$, K_n is the unique graph having maximal AZI, equal to

$$\frac{n(n-1)^7}{16(n-2)^3} .$$

If we replace the condition "$\kappa \geq 2$" with "$\kappa \geq 1$" in Theorem 71, and the condition "$2 \leq \beta < \lfloor \frac{n}{2} \rfloor$" with "$1 \leq \beta < \lfloor \frac{n}{2} \rfloor$" in Theorem 72(a), then the resulting statements remain true [15]. Since the vertex connectivity of a graph G cannot be greater than the edge connectivity, we have the following result.

Theorem 73. [15] *For $1 \leq \kappa' \leq n-2$, in the class of graphs of order $n \geq 5$ and edge connectivity at most κ', $K_{\kappa'} + (K_1 \cup K_{n-\kappa'-1})$ is the unique graph having maximal AZI, equal to the expression obtained by replacing κ by κ' in Theorem 71.*

Theorem 74. [6] *Among polyomino chains with $n \geq 6$ squares, let B_n^+ be a polyomino chain with maximal AZI. The following structural properties of B_n^+ hold:*
(i) Every segment of B_n^+ has length less than 4 (and consequently B_n^+ has at least 3 segments).
(ii) No two segments of B_n^+ with lengths 2 are adjacent.
(iii) If at least one external segment of B_n^+ has length 2. Then no two internal segments of lengths 3 are adjacent.
(iv) If an external segment of B_n^+ has length 3, then its adjacent segment has also length 3.

Note that the problem of finding maximal-AZI polyomino chain(s) with a fixed number of polygons was left open in [6], and has not been settled until now.

Recall that Ω_n is the class of pentagonal chains with $n \geq 3$ pentagons in which every external segment of length 3 (if it exists) contains no edge connecting the vertices of degree 3.

Theorem 75. [7] *For $n \geq 3$, among members of Ω_n, only the zigzag pentagonal chain has maximal AZI .*

Theorem 76. [18] *Among isomeric hexagonal systems, those having minimal number of inlets have maximal* AZI.

The next result is a special case of Theorem 9 of [30].

Theorem 77. [30] *Among catacondensed hexagonal systems with* h *hexagons, only the system having* $\lfloor h/2 \rfloor - 1$ *branched hexagons and* $\lceil h/2 - \lfloor h/2 \rfloor \rceil$ *kinks has maximal* AZI.

Theorem 77 was proven independently also in [62,67,82]. Additional results concerning maximal AZI of certain hexagonal systems can be found by using the results from [5,16, 17].

Theorem 78. [53] *Among catacondensed fluoranthene systems with* h *hexagons, only* E_h*, shown in Figure 7, has maximal* AZI.

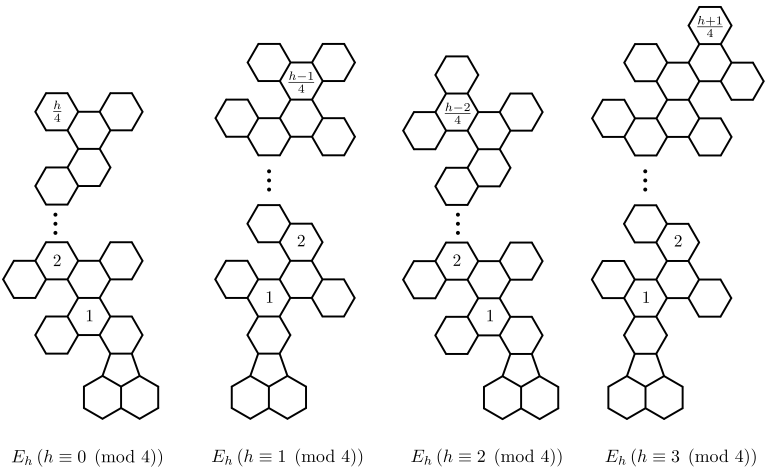

Figure 7. The fluoranthene system E_h, mentioned in Theorem 78.

Theorem 78 was independently proven also in [59]. More results on maximal AZI of fluoranthene systems can be found in [53, 59].

Acknowledgments: B.F. is supported by the Serbian Ministry of Education, Science and Technological Development (Agreement No. 451-03-68/2020-14/200122).

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