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Extremal Results and Bounds for Atom–Bond Sum–Connectivity Index

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Abstract

The ABS (atom-bond sum-connectivity) index is a topological index, that was introduced in 2022 by amalgamating the main ideas of two well-examined indices. Mathematical aspects (especially, extremal results and bounds) of the ABS index have already been studied considerably. The primary goal of this review paper is to collect known bounds and extremal results regarding the ABS index. Several new extremal results, which follow easily from existing general results, are also given. Moreover, a number of open problems and conjectures, arising from the reported results, are proposed.

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1 Introduction

This paper is a survey of mathematical properties of the recently introduced "atom-bond sum-connectivity index", ABS

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

which, at the first glance, is a minor modification of the much older, and much more detailed studied "atom-bond connectivity index", ABC

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

Indeed, such "modified" graph invariants are often encountered in the present-day chemical graph theory. However, in spite of their algebraic similarity, the mathematical properties of the indices ABS and ABC are profoundly different. This is best seen by comparing the characterization of the trees of a fixed order n, whose ABS- and ABC-values are minimal. In the case of ABS index, this characterization is an easy task (see Theorem 1). On the other hand, the minimum-ABC n-order tree has an extremely complex structure, whose characterization required many years of research (see [51]), and was achieved only recently [36, 37, 57] (see also [45] for the case of molecular trees). Furthermore, whereas the problem of characterizing trees with the minimum ABC index over the class of all trees having a fixed number of pendent vertices was not easy (for example, see [10]), this is not the case with the ABS index (see [20]).

Such great differences between the properties of ABC and ABS indices justify the elaboration of a separate mathematical theory of the ABS index. In the present paper, the main results obtained along these lines are outlined, and directions for further research are indicated.

Most of the terms of graph theory and chemical graph theory that is used in the present paper is taken from [24,26,96] and [87,92], respectively.

In chemical graph theory, numerical graph invariants are commonly referred to as topological indices. Such indices' purpose is to predict physicochemical properties of chemical compounds. The Platt index (for example, see [9]), introduced in [79, 80], is one of the first topological indices used in chemistry. This index is defined as

$$Pl(G) = \sum_{uv \in E(G)} (d_u + d_v - 2)\,,$$

where $E(G)$ is the edge set of G and d_u denotes the degree of the vertex $u \in V(G)$. Note that the "$d_u + d_v - 2$" is the degree of the edge $uv \in E(G)$. Thus, the Platt index of G is simply the sum of all edge degrees of G. It holds that $Pl(G) = M_1(G) - 2|E(G)|$, where M_1 is the first Zagreb index (for example, see [25]), which was introduced in [55] within the study of the π-electron energy of conjugated molecules. Details about the first Zagreb index (and hence the Platt index) can be found in review articles [11,25,53] and the related references cited therein.

In the mid-1970s, Randić [82] introduced a topological index, which he named "branching index", within the study of molecular branching. The original name is now rarely used; this index is nowadays known as the "connectivity index" or the "Randić index" (see for example, [65]). Recent usage of this index in chemistry can be found in [35]. The Randić index of G is defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u\, d_v}}\ .$$

The Randić index is among the most-studied and most-applied topological indices; for example, see the books [63,64,85], review articles [49,65,83,84] and related references listed therein.

Intense research on the Randić index induced its modifications in various ways; for example, see [73]. The atom-bond connectivity (ABC) index [40] (see also [41, 54]) and the sum-connectivity (SC) index [103] are two well-known and well-studied modified versions of the Randić index. These indices for a graph G are defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u\, d_v}} \quad \text{and} \quad SC(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}.$$

One can see that the expression "$d_u + d_v - 2$" (that is, the degree of the edge uv, used in the definition of the Platt index) has been taken into consideration in the Randić index for defining the ABC index. (In the original definition [40] of the ABC index, the factor "$\sqrt{2}$" was present, which was later dropped [41, 54] from its definition). The SC index was defined by replacing the product of degrees "$d_u\, d_v$" with the addition of degrees "$d_u + d_v$" in the definition of the Randić index. We refer the reader to the review articles [10, 37] and [19] for more details on mathematical properties of the ABC and SC indices, respectively.

In [12], by amalgamating the main idea of the ABC and SC indices, a new topological index was put forward, namely the atom-bond sum-connectivity (ABS) index. This index is defined as

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

Here, it should be noted that the ABS index is a special case of a generalization given in [86]. The chemical applicability of the ABS index was examined in [1,6,13,77] on several data sets, and it was concluded that the predictive applicability of this index is comparable to those of the ABC, SC, and Randić indices. Mathematical aspects (especially, extremal results and bounds) of the ABS index have also been studied considerably. The objective of this review article is to collect known bounds and extremal results concerning this index. Several new extremal results, which follow easily from existing general results, are also given. Moreover, a number of open problems and conjectures, arising from the reported results, are proposed.

The rest of this paper is organized as follows. Section 2 provides notions and definitions of those concepts that will be used in the subsequent sections. Section 3 consists of two subsections: the first one is devoted to the extremal results regarding the minimum ABS index, while the second one is about the maximum ABS index. Section 4 is also divided into two subsections: the first one deals with the upper bounds of the ABS index, while the second one is related to its lower bounds.

2 Preliminaries

In this section, needed notions and definitions are presented.

By an *n-order graph*, we mean a graph of order n. The *size* of a graph G is the number of edges of G. The n-order star, path, complete, and cycle graphs are denoted by S_n, P_n, K_n, and C_n, respectively. By a *molecular graph*, we mean a connected graph of the maximum degree at most 4. A vertex of degree 0 (1, respectively) is called an *isolated vertex* (*pendent vertex*, respectively). By an *isolated edge*, we mean an edge both of whose end-vertices have degree 1. An edge of a graph whose end-vertices have degrees i and j is referred to as an *(i,j)-edge*. For a vertex u of a graph G, we denote by $N_G(u)$ (or simply by $N(u)$ when there is no chance of confusion about G) the set of those vertices of G that are adjacent to u. A graph containing no cycle of length 3 is known as a *triangle-free graph*. By following Anderson and Harary [22], we say that a graph is *unicyclic* if it is connected and has exactly one cycle. By a *connected bicyclic* (*tricyclic*, respectively) *graph*, we mean an n-order connected graph of size $n+1$ ($n+2$, respectively).

For an integer ℓ greater than 1, a graph G is said to be an *ℓ-partite graph* if the vertex set of G can be partitioned into ℓ sets $B_1, B_2, \cdots, B_\ell$ so that for every choice $u, v \in B_i$, where $i = 1, 2, \cdots, \ell$, the $uv \notin E(G)$; if G is an ℓ-partite graph, then $(B_1, B_2, \cdots, B_\ell)$ is known as the *ℓ-partition* of G and each set B_i is known as the *partite set* of G. If, in addition, for every $u \in B_i$ and $v \in B_j$, with $i \neq j$, we have $uv \in E(G)$, then G is known as the *complete ℓ-partite graph*. If G is a complete ℓ-partite graph with the ℓ-partition $(B_1, B_2, \cdots, B_\ell)$ such that $|B_i| = r_i$ for $i = 1, 2, \cdots, \ell$ then such graph is denoted by $K_{r_1, r_1, \ldots, r_\ell}$. A 2-partite graph is also known as a *bipartite graph* and a 2-partition of a bipartite graph is also known as a *bipartition*. A bipartite graph G with the bipartition (B_1, B_2) is said to be a *semiregular bipartite graph* if $d_u = s$ for every $u \in B_1$ and $d_v = t$ for every $v \in B_2$, where $s \neq t$.

The *union* of the graphs $H_1, H_2, \cdots, H_r$, with $r \geq 2$, is denoted by $H_1 \cup H_2 \cdots \cup H_r$ and is defined as the graph with the vertex set $V(H_1 \cup H_2 \cdots \cup H_r) = V(H_1) \cup V(H_2) \cdots \cup V(H_r)$ and the edge set $E(H_1 \cup H_2 \cdots \cup$

$H_r) = E(H_1) \cup E(H_2) \cdots \cup E(H_r)$. The union of t copies of a graph G is simply denoted as tG; that is,

$$\underbrace{G \cup G \cdots \cup G}_{t-\text{times}} = tG$$

Two graphs H_1 and H_2 are said to be disjoint if their vertex sets are disjoint. Throughout this paper, wherever we use the concept of the union, we assume there that this operation is applied to disjoint graphs.

The *complement of a graph* G is denoted by $\overline{G}$ and is defined as the graph having the vertex set $V(\overline{G}) = V(G)$, while $uv \in E(\overline{G})$ if and only if $uv \notin E(G)$.

The *join* of two graphs H_1 and H_2 is denoted as $H_1 + H_2$ and is defined as the graph with the vertex set $V(H_1 \cup H_2) = V(H_1) \cup V(H_2)$ and the edge set

$$E(H_1 \cup H_2) = E(H_1) \cup E(H_2) \cup \{uv \ : \ u \in V(H_1), v \in V(H_2)\}.$$

The *line graph* of a graph G is denoted as $L(G)$ and is defined as the graph with the vertex set $V(L(G)) = E(G)$, where two vertices $e_1, e_2 \in V(L(G))$ are adjacent if and only if the edges e_1 and e_2 share a common vertex in G.

Let S be a subset of the vertex set of a graph G. We denote by $G - S$ the graph obtained from G by removing the vertices of S as well as the edges incident to them. We denote the graph $G - (V(G) \setminus S)$ as $G[S]$. Let W be a subset of $E(G)$. We denote by $G - W$ the graph obtained from G by removing the edges of W.

By a *clique* of a graph G, we mean a complete subgraph of G. A *maximum clique* of G is a clique containing the greatest possible number of vertices of G. The *clique number* of G is the order of a maximum clique of G.

The *chromatic number* of a graph G is the smallest number of colors required to color the elements of $V(G)$ such that no two adjacent vertices have the same color.

A *dominating set* of a graph G is a subset D of $V(G)$ such that if

$u \in V(G)$ then either u has a neighbor in D or $u \in D$. A *minimum dominating set* of G is a dominating set of G with the smallest possible number of elements. The *domination number* of G is the cardinality of a minimum dominating set of G.

A *k-polygonal system* is a connected geometric figure formed by concatenating congruent regular k-polygons side to side in a plane in such a way that the figure divides the plane into one external (infinite) region and a finite number of internal (finite) regions, provided that all internal regions are congruent regular k-polygons. In a k-polygonal system, two polygons sharing a common side is referred to as *adjacent polygons*. By the *characteristic graph* of a k-polygonal system, we mean a graph CG whose vertices represent k-polygons of the considered system and two vertices u and v of CG are adjacent if and only if the k-polygons corresponding to u and v are adjacent. (Such a graph is sometimes also called the *inner dual* of G.) A *k-polygonal chain* (*catacondensed k-polygonal system*, respectively,) is a k-polygonal system whose characteristic graph is the path graph (tree, respectively). In a k-polygonal chain, a k-polygon adjacent to exactly one (two, respectively) k-polygon(s) is referred to as *external* (*internal*, respectively) *k-polygon*. For $k = 3, 4, 5, 6$, a k-polygonal system is known as a *triangular system*, *polyomino system*, *pentagonal system*, *hexagonal system*, respectively. A graph can be used to represent a k-polygonal system, with the vertices representing the points where two sides of any k-polygon meet and the edges representing the k-polygons' sides. In the rest of this article, by a k-polygonal system we mean the graph corresponding to the considered k-polygonal system.

By a *linear triangular chain*, we mean a triangular chain of maximum degree at most 4. A maximal linear triangular (polyomino, respectively) sub-chain of a triangular (polyomino, respectively) chain T is known as a *segment* of T. By an *external segment* of a triangular (polyomino, respectively) chain, we mean a segment containing at least one external polygon. A segment that is not external is referred to as an *internal segment*. The number of polygons in a segment is known as its *length*. A non-linear triangular chain in which one external segment has length 3 and the other external segment has length either 3 or 4, and every internal segment (if exists) has length 4, is known as a *zigzag triangular chain*.

In a polyomino chain, a *kink* is an internal square containing a vertex of degree 2; in a hexagonal chain, a *kink* is an internal hexagon containing an edge connecting vertices of degree 2. A *linear polyomino chain* (*linear hexagonal chain*, respectively) is the one containing no kink. A non-linear polyomino chain consisting of only kinks and external squares is known as a *zigzag polyomino chain*.

In a catacondensed hexagonal system, a *branched hexagon* is the one adjacent to three other hexagons.

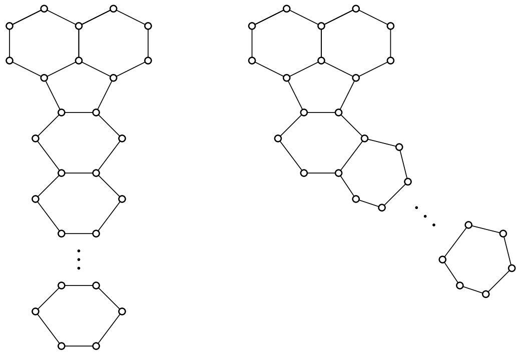
By *isomeric hexagonal systems*, we mean the hexagonal systems that have an equal number of vertices and an equal number of edges.

Consider two hexagonal systems H_1 and H_2. Let $u, v \in V(H_1)$ be vertices of degree 2 having a common neighbor of degree 3. Let $x, y \in V(H_2)$ be two adjacent vertices of degree 2. A *fluoranthene system* F is a molecular graph obtained from the hexagonal systems H_1 and H_2 by inserting the edges ux and vy. If, in addition, F satisfies 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 has only neighbors of degree 2 in H_2; see Figure 1, which depicts a fluoranthene linear chain and a fluoranthene system that is not a fluoranthene linear chain (because in this case, condition (iii) is not satisfied).

The SC index, defined in the previous section, was generalized in [104]. For a graph G, its *general SC index* is defined as

$$SC_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha.$$

For $\alpha = -1, 1/2, 1$, the general SC index SC_α corresponds to the *harmonic index* $H = 2SC_{-1}$ (which was first considered in [42]), the *reciprocal sum-connectivity index* $RSC = SC_{1/2}$ (see [15,52]), the *first Zagreb index* $M_1 = SC_1$, respectively.



(a) (b)

Figure 1. (a)A fluoranthene linear chain (b) A fluoranthene system that is not a fluoranthene linear chain.

The *general Platt index* [9] of a graph G is defined as

$$Pl_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v - 2)^\alpha,$$

provided that G does not contain any component isomorphic to the path P_2 whenever $\alpha < 0$. The index Pl_{-1} is known as the *modified Platt index* [16], denoted as ${}^{m}Pl$.

3 Extremal results

This section is devoted to collecting and presenting results concerning the extremum values of the ABS index. This section is divided into two subsections: the first one provides the extremal results regarding the minimum ABS index, while the second one deals with the maximum ABS index.

3.1 Minimum ABS index

In this section, first we present existing results concerning the minimum ABS index and then we establish such type of results by utilizing existing general results. We start with the following simple but notable result. Although the problem of determining graphs attaining the minimum ABC index among all trees of a fixed order was a hard problem (for example, see [10, 36, 37, 57, 57]), the corresponding problem for the ABS index was quite easy:

Theorem 1. [12] *In the class of all n-order trees, with $n \geq 4$, the path P_n uniquely attains the minimum ABS index.*

In Theorem 1, if the text "n-order trees, with $n \geq 4$," is replaced with "n-order connected graphs, with $n \geq 3$," then the modified statement remains valid [12]. Also, in Theorem 1, if "all n-order trees" and "the path" are replaced with "line graphs of all n-order trees" and "the line graph of the path", respectively, then the resulting statement remains true [47].

By Theorem 1, P_n uniquely achieves the minimum ABS index over the class of all molecular n-order trees for $n \geq 4$; over the same class, for $n \geq 13$, trees attaining second to sixth minimum ABS index were determined in [105].

Since $ABS(P_2) = 0 < ABS(P_n)$ for $n \geq 3$, among all trees with 2 pendent vertices, P_2 uniquely achieves the minimum ABS index. For the case when the number of pendent vertices in a tree is greater than 2, we have the next result, which gives a solution to an open problem posed in [13].

Theorem 2. [20] *The star S_{p+1} uniquely attains the minimum ABS index among all trees with $p \geq 3$ pendent vertices.*

The problem of characterizing trees with the minimum ABC index over the class of all trees having a fixed number of pendent vertices was not easy (for example, see [10]); on the other hand, this problem for the ABS index was rather easy (see Theorem 2). Since the extremal tree in Theorem 2 is not a molecular tree for $p \geq 5$, it seems to be interesting to consider the following problem.

Problem 1. *Characterize graphs that attain the minimum ABS index among all molecular trees with $p \geq 5$ pendent vertices.*

For a fixed integer $p \geq 3$, let $\mathbb{T}(1, 3; p)$ be the class of all trees with p pendent vertices such that every member of $\mathbb{T}(1, 3; p)$ consists of vertices of degrees 1 and 3 only. For $n \geq 3p-2 \geq 7$, denote by $\mathbb{T}^\star(n,p)$ the class of all trees whose arbitrary member $T^\star(n,p)$ is obtained from some $T(1,3;p) \in \mathbb{T}(1,3;p)$ by subdividing every pendent edge of $T(1,3;p)$ at least once, such that the total number of subdivisions performed is $n-2p+2$, which is the number of vertices of degree 2 in $T^\star(n,p)$; for example, see Figure 2.

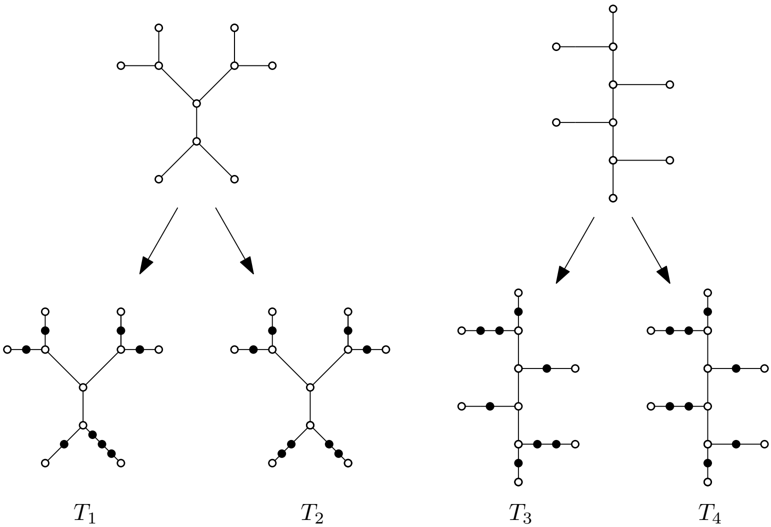


Figure 2. Some trees T_1, T_2, T_3, T_4, belonging to the class $\mathbb{T}^\star(18,6)$.

The next result was proved independently in [20, 74].

Theorem 3. [20, 74] *Among all n-order trees with p pendent vertices, only the member(s) of* $\mathbb{T}^\star(n,p)$ *attain(s) the minimum ABS index for* $n \geq 3p-2 \geq 7$.

Note that every member of the class $\mathbb{T}^\star(n,p)$ is a molecular tree. Thus, if the text "n-order trees" in Theorem 3 is replaced with "n-order molecular trees" then the resulting statement remains true (see also Corollary 3.12 in [39]).

A tree having exactly two non-pendent vertices is known as a double star. By a balanced double star, we mean a double star in which the degrees of non-pendent vertices differ by at most 1.

Theorem 4. [20] *Among all trees of order $p+2$ with $p \geq 4$ pendent vertices, the balanced double star uniquely attains the minimum ABS index.*

The problem concerning the minimum ABS index of n-order trees with $p \geq 4$ pendent vertices, for $p+3 \leq n \leq 3p-3$, was left open in [20].

Problem 2. [20] *Characterize tree(s) attaining the minimum ABS index among all n-order trees with $p \geq 4$ pendent vertices, where $p+3 \leq n \leq 3p-3$.*

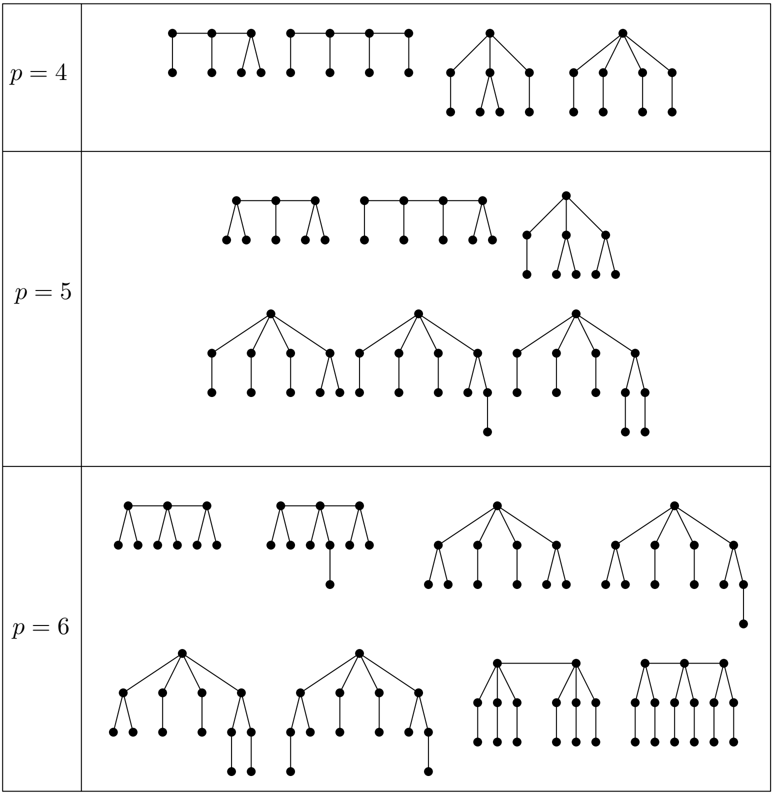


Figure 3. The graphs that provide solution to Problem 2 for $p = 4, 5, 6$.

Figure 3 provides solution to Problem 2 for $p = 4, 5, 6$, see [20]. However, for $p \geq 7$, Problem 2 remains open. To obtain better insight into some structural properties of the extremal trees of Problem 2, we performed a computer search for $p = 7, 8, 9$; for these values of p, the obtained extremal trees are depicted in Figures 4, 5, 6, respectively.

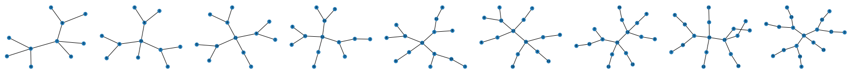


Figure 4. Trees attaining the minimum ABS index among all n-order trees with 7 pendent vertices, where $10 \le n \le 18$.

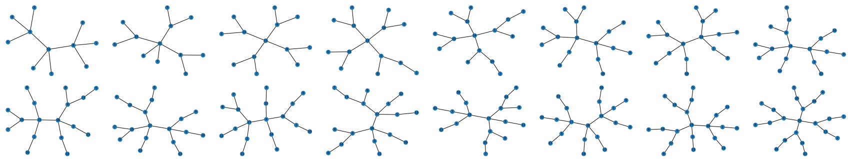


Figure 5. Trees attaining the minimum ABS index among all n-order trees with 8 pendent vertices, where $11 \le n \le 21$.

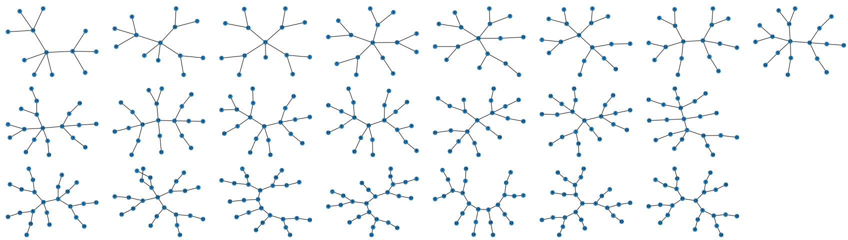


Figure 6. Trees attaining the minimum ABS index among all n-order trees with 9 pendent vertices, where $12 \le n \le 24$.

Next, we present a result, obtained in a recent preprint [60], concerning the minimum ABS index of n-order trees with a fixed maximum degree.

Theorem 5. [60] *In the class of all n-order trees of maximum degree Δ,*

(i) *only a tree(s) having exactly one branching vertex, adjacent to Δ vertices of degree 2 attain(s) the minimum ABS index, when $3 \le \Delta \le \lfloor (n-1)/2 \rfloor$;*

(ii) *only a tree(s) possessing exactly one branching vertex, having $n-\Delta-1$ neighbors of degree 2 and $2\Delta+1-n$ pendent neighbor(s), attain(s) the minimum ABS index, when $\lceil (n-1)/2 \rceil \le \Delta \le n-3$.*

Now, we shift the focus of our attention toward results on the minimum ABS index of graphs containing cycles.

Theorem 6. [13] *In the class of all n-order unicyclic graphs, with $n \geq 4$, the cycle C_n uniquely attains the minimum ABS index.*

In Theorem 6, if the text "all n-order unicyclic graphs" and "the cycle" are replaced with "line graphs of all n-order unicyclic graphs" and "the line graph of the cycle", respectively, then the modified statement remains valid [47].

Let $\mathbb{U}_n$ be the class of those n-order unicyclic graphs that are obtained by adding an edge between a vertex of the cycle C_{n-k} and a pendent vertex of the path P_k, where $k \geq 2$.

Theorem 7. [13] *The member(s) of the class $\mathbb{U}_n$ uniquely attain(s) the second-minimum ABS index among all n-order unicyclic graphs for every $n \geq 5$.*

Since the extremal graphs mentioned in Theorems 6 and 7 are molecular ones, if the text "unicyclic graphs" in the statements of these theorems is replaced with "molecular unicyclic graphs", then the modified statements remains valid.

The graphs that attain the third-minimum ABS index among all n-order molecular unicyclic graphs, for $n \geq 7$, were determined in [105].

Theorem 8. [77] *The graph formed by adding an edge between a pendent vertex of the path P_{n-k} and a vertex of the cycle C_k, uniquely attains the minimum ABS index among all n-order unicyclic graphs of girth k, where $3 \leq k \leq n-2$.*

The graphs attaining the second-minimum value of the ABS index over the class of all n-order unicyclic graphs of girth k, with $3 \leq k \leq n-2$, were also determined in [77].

Let $U_{n,g}^{\ell_1,\ell_2,\ldots,\ell_r}$ be the n-order unicyclic graph obtained by attaching r paths to a single vertex of the cycle C_g such that the attached paths have lengths $\ell_1, \ell_2, \ldots, \ell_r$ provided that $\sum_{i=1}^{r} \ell_i = n - g$, where $3 \leq g \leq n-2$.

Theorem 9. [75] *Among all n-order unicyclic graphs with maximum degree Δ,*

(i) *the member(s) of* $\left\{U_{n,3}^{\ell_1,\ell_2,\ldots,\ell_{\Delta-2}} : 1 \le \ell_i \le 2, \textit{for } i = 1, 2 \ldots, \Delta - 2\right\}$ *attain(s) the minimum ABS index, when* $\frac{n+2}{2} \le \Delta \le n-2$*;*

(ii) *the member(s) of* $\left\{U_{n,g}^{\ell_1,\ell_2,\ldots,\ell_{\Delta-2}} : g \ge 3, \ell_i \ge 2, \textit{for } i = 1, 2 \ldots, \Delta - 2\right\}$ *attain(s) the minimum ABS index, when* $3 \le \Delta < \frac{n+2}{2}$.

Theorem 10. [105] *Only the graphs depicted in Figure 7 attain the minimum ABS index over the class of all n-order bicyclic molecular graphs for* $n \ge 6$.

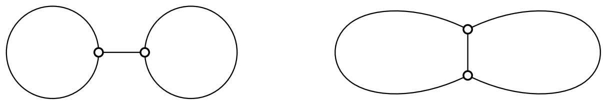


Figure 7. The bicyclic graphs referred in Theorem 10.

The graphs attaining the second-minimum *ABS* index over the class of all n-order bicyclic molecular graphs, for $n \ge 6$, were also determined in [105].

Theorem 10 suggests the following conjecture.

Conjecture 1. *Only the graphs depicted in Figure 7 attain the minimum ABS index over the class of all n-order connected bicyclic graphs for every* $n \ge 6$.

Theorem 11. [105] *The graph formed by inserting* $n-4$ *vertices of degree 2 on one of the edges of the complete graph* K_4 *(see Figure 8) uniquely attains the minimum ABS index among all n-order tricyclic molecular graphs for* $n \ge 6$.

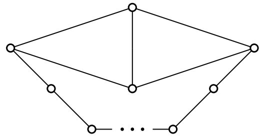


Figure 8. The tricyclic graph referred in Theorem 11 and Conjecture 2.

The graphs attaining the second-minimum *ABS* index among all n-order tricyclic molecular graphs, for $n \ge 6$, were also determined in [105].

Theorem 11 suggests the following conjecture.

Conjecture 2. *The graph depicted in Figure 8 uniquely attains the minimum ABS index among all n-order connected tricyclic graphs for every $n \geq 6$.*

Theorem 12. [12] *In the class of all non-trivial n-order graphs, only the graphs having the maximum degree at most 1 attain the minimum ABS index.*

In the rest of this subsection, we collect those extremal results concerning the minimum ABS index that can be derived from existing extremal results about general BID indices.

A cut vertex of a connected graph G is a vertex whose removal makes G a disconnected graph. By a 2-connected graph G, we mean a non-complete and connected graph containing no cut vertex.

From Theorem 4.2 of [90], the next result follows.

Theorem 13. *Among all 2-connected graphs of order n, the cycle C_n uniquely attains the minimum ABS index for every $n \geq 4$.*

By Theorem 8 of [95], the value of a BID index, defined via a function $b(x, y)$, is decreasing if and only if

$$b(x+1, y+1) - b(x+1, y) < b(x, y+1) - b(x, y),$$

for all positive integers x and y. Note that if $b(x_1, x_2) = \sqrt{\frac{x_1+x_2-2}{x_1+x_2}}$ then the function f defined by

$$f(x_1, x_2) = b(x_1, x_2+1) - b(x_1, x_2)$$

is strictly decreasing in x_1 for all real numbers x_1 and x_2 greater than or equal to 1. Thus, $f(x+1, y) < f(x, y)$ for all positive integers x and y. Thus, the ABS index is deescalating. Results concerning the minimum ABS index over the class of all

- trees,
- unicyclic graphs of minimum degree 1,

- connected bicyclic graphs of minimum degree 1,
- connected graphs of minimum degree 1,

with a given degree sequence, follow from [72], see also [93, 100, 102].

For a connected r-cyclic graph H of order $n-k$, the graph $K_k + H$ is known as a k-cone r-cyclic graph, where $k \geq 1$; a 0-cone graph is simply a connected graph, see [71]. Since the ABS index is deescalating, from Corollary 2.1 and Theorem 2.3 of [71], one obtains the graphs attaining the minimum ABS index over the class of all k-cone

- trees,
- unicyclic graphs,
- bicyclic graphs,

with a given degree sequence for $k \geq 0$.

A subgraph H of a graph G is said to be a spanning subgraph if $V(H) = V(G)$; in addition, if H is a tree then H is called a spanning tree of G. The following problem is a special case of a general problem attacked in [38]:

Problem 3. *INSTANCE: A graph G and a real number k.*
QUESTION: Does G has a spanning tree T with $ABS(T) \leq k$?

Theorem 1 of [38] implies that Problem 1 is NP-complete.

Next, we obtain results concerning the minimum ABS index of k-polygonal systems; for definitions of polygonal chains and related concepts, see Section 2.

The following result is a consequence of the second part of Corollary 3.2 of [7].

Theorem 14. [7] *Over the family of all those triangular chains with $t \geq 4$ triangles in which every vertex has degree less than or equal to 5, the linear triangular chain uniquely attains the minimum ABS index.*

From the first part of Theorem 2.10 of [17], the next result follows.

Theorem 15. [17] *The linear polyomino chain uniquely attains the minimum ABS index among all polyomino chains with $s \geq 3$ squares.*

Since no extremal result from [18] concerning pentagonal chains is applicable for the ABS index, it would be nice to establish such results for this index.

The second part of Theorem 9 of [34], or Corollary 2.12 of [81], gives the following result.

Theorem 16. [34, 81] *Only those catacondensed hexagonal systems that contain* $\lfloor h/2 \rfloor - 1$ *branched hexagons and* $\lceil h/2 - \lfloor h/2 \rfloor \rceil$ *kinks attain the minimum* ABS *index among all catacondensed hexagonal systems with* $h \geq 3$ *hexagons.*

The following result follows from Theorem 2 of [91].

Theorem 17. [91] *Among all catacondensed fluoranthene systems with* h *hexagons, the system shown in Figure 9 has the minimum* ABS *index for every* $h \geq 5$.

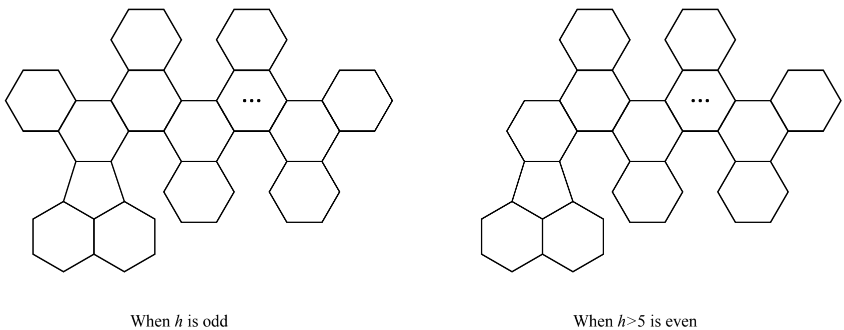


Figure 9. The fluoranthene system referred in Theorem 17.

Corresponding to Theorem 17, we refer the reader to the second part of Theorem 8 in [56].

Theorem 5(a) of [32] provides the systems attaining the minimum ABS index in the class of all isomeric hexagonal systems.

Additional extremal results regarding the minimum ABS index of different types of hexagonal systems can be easily obtained from general results reported in [8, 31, 33].

3.2 Maximum ABS index

In this section, first we present existing results concerning the maximum ABS index and then we establish such type of results by utilizing existing general results. Although the trees attaining the minimum ABS index and the ones attaining the minimum ABC index over the class of all n-order trees, for $n \geq 10$, are not the same; in the case of maximization, such trees are the same, as stated in the following theorem:

Theorem 18. [12] *In the class of all n-order trees, with $n \geq 4$, the star S_n uniquely attains the maximum ABS index.*

In Theorem 18, if the texts "all n-order trees" and "the star" are replaced with "line graphs of all n-order trees" and "the line graph of the star", respectively, then the modified statement remains valid [47].

Theorem 19. [78] *Among all n-order trees having p pendent vertices, the tree $S_{n,p}$ uniquely attains the maximum ABS index, where $3 \leq p \leq n-2$ and $S_{n,p}$ is the tree formed by attaching $p-1$ pendent vertices to exactly one pendent vertex of the path graph P_{n-p+1} of order $n-p+1$.*

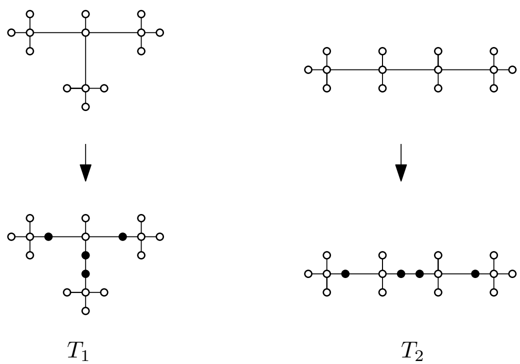


Figure 10. Two examples, T_1 and T_2, of trees belonging to the class $\mathbb{T}_e^{\dagger}(18,10)$.

For a fixed even integer $p \geq 6$, let $\mathbb{T}_e(1,4;p)$ be the class of all trees with p pendent vertices such that every member of $\mathbb{T}_e(1,4;p)$ consists of vertices of degrees 1 and 4 only. For $n \geq 2p-3 \geq 9$, p being even, denote by $\mathbb{T}_e^{\dagger}(n,p)$ the class of all trees whose arbitrary member $T_e^{\dagger}(n,p)$ is obtained from some $T_e(1,4;p) \in \mathbb{T}_e(1,4;p)$ by replacing every $(4,4)$-edge of $T_e(1,4;p)$ with a path of length at least 2, such that the total number of vertices of degree 2 in $T_e^{\dagger}(n,p)$ is $n - \frac{3p}{2} + 1$; for example, see Figure 10.

Theorem 20. [39] *Among all n-order molecular trees with p pendent vertices, only the member(s) of $\mathbb{T}_e^{\dagger}(n,p)$ attain(s) the maximum ABS index, where p is even and $n \geq 2p - 3 \geq 9$.*

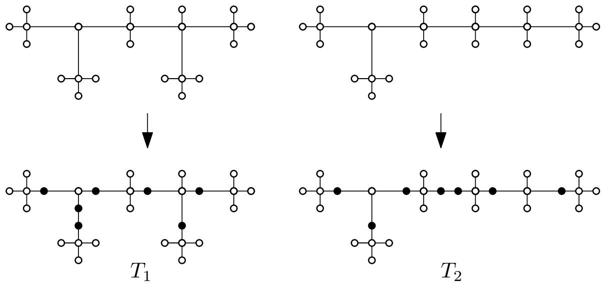


Figure 11. Two examples, T_1 and T_2, of trees belonging to the class $\mathbb{T}_o^{\dagger}(29,15)$.

For a fixed odd integer $p \geq 9$, let $\mathbb{T}_o(1,3,4;p)$ be the class of all trees with p pendent vertices such that every member of $\mathbb{T}_o(1,3,4;p)$ does not contain any vertex of degree 2 and it contains exactly one vertex of degree 3, which is adjacent to three vertices of degree 4. For $n \geq 2p - 2 \geq 16$, p being odd, denote by $\mathbb{T}_o^{\dagger}(n,p)$ the class of all trees whose arbitrary member $T_o^{\dagger}(n,p)$ is obtained from some $T_o(1,3,4;p) \in \mathbb{T}_o(1,3,4;p)$ by replacing every $(i,4)$-edge of $T_o(1,3,4;p)$ with a path of length at least 2, such that the total number of vertices of degree 2 in $T_o^{\dagger}(n,p)$ is $n - \frac{3p-1}{2}$, where $i = 3,4$; for example, see Figure 11.

Theorem 21. [39] *Only the member(s) of $\mathbb{T}_o^{\dagger}(n,p)$ attain(s) the maximum ABS index over the class of all n-order molecular trees with p pendent vertices, where p is odd and $n \geq 2p - 2 \geq 16$.*

Theorems 20 and 21 suggest the following problem.

Problem 4. *Characterize trees attaining the maximum ABS index in the* *class of all n-order molecular trees with p pendent vertices for sufficiently large p and $n \leq 2p-4$.*

By a *matching* in a graph G, we mean a subset S of $E(G)$ such that the members of S are pairwise non-adjacent. A *maximum matching* of G is the one possessing the maximum possible number of edges of G. The *matching number* of G is the cardinality of a maximum matching of G. By subdividing an edge uv of a graph G, we mean obtaining a new graph G' from G by inserting a new vertex w and replacing the edge uv with two new edges uw, wv. The next result was proved independently in [59, 101].

Theorem 22. [59,101] *The tree formed by subdividing $\beta-1$ edge(s) of the star $S_{n-\beta+1}$ uniquely attains the maximum ABS index in the class of all n-order trees with matching number β, where $n \geq 4$ and $1 \leq \beta \leq \lfloor n/2 \rfloor$.*

By replacing the phrase "matching number" with "domination number" in Theorem 22, the resulting statement remains true (see [101]).

A perfect matching S of a graph G is a matching such that every vertex of G is incident to exactly one edge of S.

Theorem 23. [94] *Among all molecular n-order trees with perfect matching, the tree depicted in Figure 12 uniquely attains the maximum ABS index, where $n = 2k + 12 \geq 14$.*

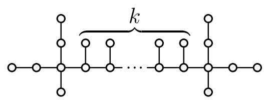


Figure 12. The tree referred in Theorem 23.

Theorem 24. [59] *In the class of all n-order trees with diameter d, the tree formed by attaching $n-d$ pendent edge(s) to exactly one of the pendent vertices of the path P_d uniquely attains the maximum ABS index, where $n \geq d+1 \geq 3$.*

Next, we turn our attention to extremal results involving cyclic graphs.

Theorem 25. [13] *The graph formed by connecting two pendent vertices with an edge in the star S_n, uniquely attains the maximum ABS index among all n-order unicyclic graphs, for every $n \geq 4$.*

The unique graph with the second-maximum ABS index, among all n-order unicyclic graphs for every $n \geq 5$, was also reported in [13].

Theorem 26. [76] *The graph formed by attaching $n-g$ pendent vertices to a single vertex of the cycle C_g, uniquely attains the maximum ABS index over the class of all n-order unicyclic graphs with girth g, where $3 \leq g \leq n-2$.*

The graphs with the second-maximum ABS index, among all n-order unicyclic graphs with a given girth, were also reported in [76].

Theorem 27. [1] *The graph formed by adding two new adjacent edges in the star S_n, uniquely attains the maximum ABS index among all n-order connected bicyclic graphs, for every $n \geq 5$.*

Theorem 28. [3] *Among all molecular n-order graphs of size m, with $n-1 \leq m \leq 2n$ and $n \geq 13$,*

(i) *only the graph(s) containing no vertices of degrees 2 and 3 attain the maximum ABS index, when $n+m \equiv 0 \pmod 3$, and this maximum value is*

$$\frac{(25-4\sqrt{5}\,)m + 4(2\sqrt{5}-5)n}{10\sqrt{3}},$$

(ii) *only the graph(s) containing no vertex of degree 2 and containing exactly one vertex of degree 3, adjacent to three vertices of degree 4, attain the maximum ABS index, when $n+m \equiv 1 \pmod 3$, and this maximum value is*

$$\frac{(25-4\sqrt{5}\,)m + 4(2\sqrt{5}-5)n}{10\sqrt{3}} + \frac{45\sqrt{35} - 140\sqrt{3} - 7\sqrt{15}}{105},$$

(iii) *only the graph(s) containing no vertex of degree 3 and containing exactly one vertex of degree 2, adjacent to two vertices of degree 4, attain the maximum ABS index, when $n+m \equiv 2 \pmod 3$, and this maximum value is*

$$\frac{(25-4\sqrt{5}\,)m + 4(2\sqrt{5}-5)n}{10\sqrt{3}} - \frac{2(5-5\sqrt{2}+\sqrt{5}\,)}{5\sqrt{3}}.$$

The case $m = n - 1$ of Theorem 28 was first proved in [12].

Theorem 29. [6] *The complete bipartite graph $K_{\lceil n/2\rceil,\lfloor n/2\rfloor}$ uniquely attains the maximum ABS index over the class of all triangle-free graphs of order $n \geq 4$.*

In Theorem 29, if the text "triangle-free graphs" is replaced with "bipartite graphs" then the resulting statement remains true [6].

Theorem 30. [6] *Among all graphs of size $m \geq 2$, the star S_{m+1} uniquely attains the maximum ABS index.*

Theorem 31. [12] *In the class of all non-trivial n-order graphs, the complete graph K_n uniquely possesses the maximum ABS index.*

The *vertex connectivity* of a non-trivial connected graph G is the least number of vertices whose removal makes G either a disconnected graph or a trivial graph. Similarly, the *edge connectivity* of G is the least number of edges whose removal makes G a disconnected graph. The next result, concerning the vertex connectivity, was proved independently in [5, 67].

Theorem 32. [5, 67] *Among all n-order connected graphs with the vertex connectivity at most r, such that $1 \leq r \leq n-2$ and $n \geq 5$, the graph $K_n^{(r)}$ uniquely attains the maximum ABS index, where $K_n^{(r)}$ is the graph obtained from the complete graph K_{n-1} by joining a new vertex (through edges) to exactly r vertices of K_{n-1}.*

Recall that the vertex connectivity of a connected graph G is at most the edge connectivity of G. Hence, in Theorem 32, if the text "vertex connectivity" is replaced with "edge connectivity" then the resulting statement remains valid [67].

It is a well-known fact that the vertex connectivity of a graph G is less than or equal to the minimum degree of G. Thus, Theorem 32 implies the next result.

Theorem 33. [21] *The graph $K_n^{(r)}$, defined in Theorem 32, uniquely attains the maximum ABS index among all n-order connected graphs of minimum degree δ, where $1 \leq \delta \leq n-2$.*

Theorem 34. [5] *Over the class of all n-order connected graphs with matching number β, such that $1 \leq \beta \leq \lfloor n/2 \rfloor - 1$ and $n \geq 5$, the graph $K_\beta + \overline{K}_{n-\beta}$ uniquely attains the maximum ABS index. If $\beta = \lfloor n/2 \rfloor$, then K_n uniquely attains the maximum ABS index over the aforementioned class of graphs.*

In Theorem 34, if the text "matching number β" is replaced with "matching number at most β" then the resulting statement remains true [67].

By a *nearly k-regular graph* of order $n \geq 3$, with $k \geq 1$, we mean a graph having $n - 1$ vertices of degree k and one vertex of degree $k - 1$.

Theorem 35. [21] *Among all n-order connected graphs of maximum degree $\Delta \geq 1$,*

(i) *only Δ-regular graph(s) achieve(s) the maximum ABS index, when $n\Delta$ is even;*

(ii) *only nearly Δ-regular graph(s) achieve(s) the maximum ABS index, when $n\Delta$ is odd.*

Denote by $B(n, r)$ the complete r-partite graph with n vertices such that the number of vertices in any two partite sets of $B(n, r)$ differs by at most 1, where $r \geq 2$.

Theorem 36. [21] *In the class of all n-order connected graphs with chromatic number χ, the graph $B(n, \chi)$ uniquely attains the maximum ABS index, where $\chi \geq 3$ and $n \geq 5$.*

It is a well-known fact that the chromatic number of a connected graph G is 2 if and only if G is bipartite. Also, every bipartite graph is triangle-free. Thus, by Theorem 29, if the condition "$\chi \geq 3$" in Theorem 36 is replaced with "$\chi \geq 2$" then the resulting statement remains valid (see also [67]); this resulting statement follows also from Theorem 3.2 of [89]. Furthermore, if the text "chromatic number" and the constraint "$\chi \geq 3$" in Theorem 36 are replaced with "clique number" and "$\chi \geq 2$", respectively, then again the resulting statement remains true [67].

A subset S of the vertex set of a graph G is said to be an *independent set* if the members S are pairwise non-adjacent. By a *maximum independent vertex set* of a graph G, we mean an independent set possessing the maximum possible number of vertices of G. The *independence number* of a graph G is the cardinality of a maximum independent set of G.

Theorem 37. [21] *Among all non-trivial n-order connected graphs with independence number α, the graph $K_{n-\alpha}+\overline{K}_\alpha$ uniquely achieves the maximum ABS index.*

Since the sum of the independence number and vertex cover number of an n-order graph G is always n (for example, see [96]), Theorem 37 gives the graph attaining the maximum ABS index among all connected graphs of a given order and fixed vertex cover number.

Theorem 38. [21] *The graph formed by attaching p pendent vertices to exactly one vertex of the complete graph K_{n-p}, uniquely achieves the maximum ABS index over the class of all n-order connected graphs with p pendent vertices, where $0 \leq p \leq n-3$.*

In the rest of this subsection, we collect those extremal results concerning the maximum ABS index that can be derived from existing extremal results about general BID indices.

A graph in which the degrees of any two adjacent vertices differ by 1 is known as a *stepwise irregular graph* [50]. By Theorem 4.4 of [2], we have the next result.

Theorem 39. [2] *In the class of all stepwise irregular graphs of order $n \geq 5$,*

(i) *only the complete bipartite graph $K_{(n-1)/2,(n+1)/2}$ attains the maximum ABS index, when n is odd;*

(ii) *only the graph G_n attains the maximum ABS index, when $n \equiv 0 \pmod{n}$ and n is even, where G_n is the graph with degree set $\left\{\frac{n-4}{2}, \frac{n-2}{2}, \frac{n}{2}\right\}$ such that the number of vertices with degrees $\frac{n-4}{2}$, $\frac{n-2}{2}$, $\frac{n}{2}$ are $\frac{n}{4}, \frac{n}{2}, \frac{n}{4}$, respectively;*

(iii) *only the graph(s) of the class $\mathbb{G}_n$ attain(s) the maximum ABS index, when n is even and $n \equiv 2 \pmod{n}$, where $\mathbb{G}_n$ is the class of graphs with degree set $\{\frac{n-2}{4}, \frac{n+2}{4}\}$ such that the number of vertices with degrees $\frac{n-2}{4}, \frac{n+2}{4}$ are $\frac{n+2}{2}, \frac{n-2}{2}$, respectively.*

The next result provides a useful tool for establishing several extremal results concerning the maximum ABS index.

Theorem 40. [12] *If u and v are non-adjacent non-isolated vertices of a graph G, then $ABS(G) < ABS(G + uv)$, where $G + uv$ is the graph obtained from G by adding the edge uv.*

A *cut edge* (or a *bridge*) of a graph G is an edge whose removal increases the number of components of G. Proposition 2 of [97] and Theorem 40 yield the next result.

Theorem 41. [97] *If G is a graph attaining the maximum ABS index among all connected n-order graphs with r cut edges, namely $e_1, e_2, \ldots, e_r$, then every component of the graph $G - \{e_1, e_2, \ldots, e_r\}$ is complete.*

From Proposition 1.1 of [28] and Theorem 40, the following result is deduced.

Theorem 42. [28] *If G is a graph attaining the maximum ABS index among all bipartite n-order graphs with r cut edges, namely $e_1, e_2, \ldots, e_r$, then every component of the graph $G - \{e_1, e_2, \ldots, e_r\}$ is either a complete bipartite graph or K_1.*

Recall that a cut vertex of a connected graph G is a vertex whose removal makes G a disconnected graph. By a block B of G, we mean a maximal connected subgraph of G such that B does not contain any cut vertex.

Proposition 1 of [97] and Theorem 40 yield the next result.

Theorem 43. [97] *If G is a graph attaining the maximum ABS index among all connected n-order graphs with r cut vertices, then every block of G is complete and every cut vertex of G is contained in exactly two blocks.*

The minimum number of vertices of a graph G whose removal makes G a bipartite graph is known as the *vertex bipartiteness* (or *bipartite vertex frustration*) of G, see [43,98]. By using Theorem 40 in Proposition 1 of [30], we obtain the following result.

Theorem 44. [30] *If G is a graph possessing the maximum ABS index over the class of all connected n-order graphs with the vertex bipartiteness at most r, where $1 \le r \le n-2$, then there exist positive integers s and t such that $s+t=n-r$ and G is of the form $K_r + K_{s,t}$.*

In [46], the concept of vertex bipartiteness was generalized to vertex k-partiteness for $k \ge 2$. The minimum number of vertices of a graph G whose removal makes G a k-partite graph is known as the *vertex k-partiteness* of G. From Theorem 3.2 of [46] and Theorem 40, the next result (a general form of Theorem 44) follows.

Theorem 45. [46] *If G is a graph possessing the maximum ABS index over the class of all connected n-order graphs with the vertex k-partiteness at most r, where $1 \le r \le n-2$, then there exist k positive integers $t_1, t_2, \ldots, t_k$ such that $\sum_{i=1}^{k} t_i = n-r$ and G is of the form $K_r + K_{t_1,t_2,\ldots,t_k}$.*

A *vertex cut U* of a connected graph G is a subset of $V(G)$ such that the graph $G-U$ is disconnected. A vertex cut of G with the least possible number of elements is known as a minimum vertex cut of G.

By using Proposition 1.1 of [27] and keeping in mind Theorem 40, we arrive at the following result.

Theorem 46. [27] *Let G be a graph possessing the maximum ABS index over the class of all connected bipartite graphs of order n with the vertex connectivity κ. Let S be a minimum vertex cut of G. If the graph $G-S$ has a nontrivial component, then $G-S$ has exactly two components, namely H_1 and H_2, such that the graphs $G[S \cup V(H_1)]$ and $G[S \cup V(H_2)]$ are complete bipartite.*

Here, we remark that some extra work is required to completely characterize the extremal graphs in Theorems 41, 42, 43, 44, 45 and 46. Thus, the following problem arises.

Problem 5. *Characterize graphs attaining the maximum ABS index over the graph classes considered in Theorems 41, 42, 43, 44, 45 and 46.*

From Theorem 2.1 of [89] (see also Proposition 1 in [29]), the next result follows.

Theorem 47. *The complete bipartite graph $K_{\beta,n-\beta}$ uniquely achieves the maximum ABS index among all connected bipartite graphs of order n with the matching number β, where $2 \le \beta \le \lfloor n/2 \rfloor$.*

A subset S of the vertex set (edge set, respectively) of a graph G is said to be a *vertex cover* (edge cover, respectively) if every edge (vertex, respectively) of G is incident to at least one vertex (edge, respectively) of S. A *minimum vertex cover* (edge cover, respectively) of G is the one with the minimum cardinality among all vertex covers (edge covers, respectively) of G. The *vertex cover number* (edge cover number, respectively) of G is the cardinality of a minimum vertex cover (edge cover, respectively) of G.

Remark. Since the vertex cover number and the matching number of every connected bipartite graph are the same (by König-Egeváry theorem), if the text "matching number" in Theorem 47 is replaced with "vertex cover number" then the resulting statement of Theorem 47 remains true.

Since the sum of the matching number and edge cover number of an n-order graph G without isolated vertices is always n (see [44, 88]). Thus, by Theorem 47, we have the next result.

Theorem 48. *The complete bipartite graph $K_{r,n-r}$ uniquely achieves the maximum ABS index among all connected bipartite graphs of order n with the edge cover number r, where $\lceil n/2 \rceil \le r \le n-2$.*

Since the sum of the independence number and vertex cover number of an n-order graph G is always n (for example, see [89, 96]), and because of Remark 3.2, if the text "edge cover number" in Theorem 48 is replaced with "independence number" then the resulting statement remains true.

Next, we obtain results concerning the maximum ABS index of k-polygonal systems; for definitions of polygonal chains and related concepts, see Section 2.

The following result is a consequence of the second part of Corollary 3.3 of [7].

Theorem 49. [7] *Over the family of all those triangular chains with* $t \geq 4$ *triangles in which every vertex has degree less than or equal to* 5*, the zigzag triangular chain uniquely attains the maximum* ABS *index.*

The next result follows from the first part of Theorem 2.12 of [17].

Theorem 50. [17] *Among all those polyomino chains with* $s \geq 3$ *squares in which no internal segment of length* 3 *possesses any* $(3,3)$*-edge, the zigzag polyomino chain uniquely attains the maximum* ABS *index.*

Since no extremal result from [18] concerning pentagonal chains is applicable for the ABS index, it would be nice to establish such results for this index.

The second part of Theorem 9 of [34], or Corollary 2.11 of [81], gives the next result.

Theorem 51. [34, 81] *The linear hexagonal chain uniquely attains the maximum* ABS *index among all catacondensed hexagonal systems with* $h \geq 3$ *hexagons.*

The following result follows from either Theorem 1 of [91] or Theorem 8 of [56].

Theorem 52. [56,91] *Among all catacondensed fluoranthene systems with* h *hexagons, the fluoranthene linear chain has the maximum* ABS *index for every* $h \geq 5$*.*

From several general results reported in [56], one may obtain some additional results about the maximum ABS index of fluoranthene systems.

Theorem 5(a) of [32] provides the systems attaining the maximum ABS index in the class of all isomeric hexagonal systems.

Additional extremal results regarding the maximum ABS index of different types of hexagonal systems can be easily obtained from general results reported in [8, 23, 31, 33, 66].

4 Bounds

This section consists of two subsections: the first one deals with the ABS index's upper bounds, while the second one is related to the ABS index's lower bounds.

4.1 Upper bounds

Theorem 53. [6] *For a triangle-free graph G of order n and size $m \geq 2$, it holds that*

$$ABS(G) \leq m\sqrt{\frac{n-2}{n}}$$

with equality if and only if G is complete bipartite.

Theorem 54. [4] *If G is a connected graph of order n, size m and maximum degree $\Delta \geq 2$, then*

$$ABS(G) \leq \frac{n\Delta - 2m}{\sqrt{\Delta^2 - 1}} + \frac{m(\Delta + 1) - n\Delta}{\sqrt{\Delta(\Delta - 1)}}, \tag{1}$$

where the equality in (1) holds if and only if the degree set of G is either $\{\Delta\}$ or $\{1, \Delta\}$.

Theorem 55. [12] *If G has m edges, then*

$$ABS(G) \leq \sqrt{m(m - H(G))}$$

with equality if and only if either $m = 0$ or there exists a fixed positive integer k such that $d_u + d_v = k$ for every edge $uv \in E(G)$.

Theorem 56. [60] *If G is a connected non-trivial graph of size m, maximum degree Δ and minimum degree δ, then*

$$ABS(G) \leq m\sqrt{\frac{\Delta - 1}{\delta}},$$

with equality if and only if G is regular.

Theorem 57. [60] *If G is a connected non-trivial graph with order n, maximum degree Δ, clique number α and minimum degree δ, then*

$$ABS(G) \leq \frac{n^2(\alpha-1)}{2\alpha}\sqrt{\frac{\Delta-1}{\delta}},$$

with equality if and only if G is a complete α-partite graph whose all partite sets have the same number of elements.

Theorem 58. [60] *If G is a graph with size $m \geq 1$ and chromatic number χ, then*

$$ABS(G) \leq m\sqrt{\frac{2m-\chi}{2m}},$$

with equality if and only if G is either a complete graph or the union of a complete graph and some isolated vertices.

Theorem 59. [68] *If G is a connected graph of maximum degree Δ, then*

$$ABS(G) \leq \sqrt{\Delta(\Delta-1)}\,R(G) \quad \textit{and} \quad ABS(G) \leq \sqrt{\Delta(\Delta-1)}\,H(G),$$

where the equality in either of the inequalities holds if and only if G is regular.

Upper bounds on the ABS index of n-order molecular trees in terms of the Randić index and n can be found in [62].

Theorem 60. [61] *Let G be a connected graph of size m and maximum degree Δ. Then*

$$ABS(G) \leq m\sqrt{1-\frac{1}{\Delta}}$$

where the equality holds if G is regular.

Theorem 61. [61] *If G is a graph having t isolated edges then*

$$ABS(G) \leq Pl_{1/2}(G)\sqrt{\frac{H(G)}{2}-t}\,.$$

If G has m edges (from which t are isolated edges) then

$$ABS(G) \leq (SC(G)-t)\,\sqrt{m-t-1}\,,$$

where the equality holds if and only if G is the union of a star graph and t isolated edges.

Theorem 62. [16] *If G is a graph of minimum degree at least 1, then*

$$ABS(G) \leq \sqrt{SC(G)(RSC(G) - 2 \cdot SC(G))};$$

in addition, if G has size m then

$$ABS(G) \leq \sqrt{\frac{(M_1(G) - 2m)\, H(G)}{2}},$$

where in these inequalities the equality holds if and only if G is either a regular graph or a semiregular bipartite graph.

Since $Pl(G) = M_1(G) - 2m$, the second inequality in Theorem 62 can be written as

$$ABS(G) \leq \sqrt{\frac{Pl(G)H(G)}{2}}.$$

Theorem 63. [16] *If G is an n-order graph of size m, minimum degree $\delta \geq 1$ and maximum degree Δ, then*

$$ABS(G) \leq \sqrt{\frac{(2m(\Delta + 2\delta - 1) + \Delta\delta^2 ID(G) - n\delta(2\Delta + \delta))\, H(G)}{2}} \tag{2}$$

and

$$ABS(G) \leq \sqrt{\frac{(2m(\Delta + \delta - 1) - n\Delta\delta)H(G)}{2}}, \tag{3}$$

where $ID(G)$ is the inverse degree index of G (for example, see [11])

$$ID(G) = \sum_{u \in V(G)} \frac{1}{d_u}.$$

On the other hand, if G is an n-order tree of maximum degree Δ, with $n \geq 3$, then

$$ABS(G) \leq \sqrt{\frac{\Delta(n-2)H(G)}{2}}. \tag{4}$$

The equality in the inequalities (2) and (4) holds if and only if $\Delta = d_1 = \cdots = d_t \geqslant d_{t+1} = \cdots = d_n = \delta$, for some $t \in \{1, 2, \ldots, n-1\}$, where

$(d_1, d_2, \ldots, d_n)$ is the degree sequence of G in non-increasing form and δ is the minimum degree of G. The equality in (3) holds if and only if G is either a regular graph or a semiregular bipartite graph.

We remark here that inequality (2) is stronger than (3), see [16]. Some additional upper bounds on the ABS index can be found in [16, 48, 61].

4.2 Lower bounds

Following [101], we define the class $\mathbb{T}$ of trees recursively as follows.

- The path graph P_{3k} of order $3k$ is a member of $\mathbb{T}$, where $k \geq 1$.
- For $T \in \mathbb{T}$, let v be a pendent vertex of T. If T' is a tree generated from T and P_{3t} by adding an edge between v and a pendent vertex of P_{3t}, then $T' \in \mathbb{T}$.
- For $T \in \mathbb{T}$, let $v \in V(T)$ be a vertex of degree 2 such that every member of $N_T(v)$ has degree 2 and v belongs to a minimum dominating set of T. If T' is a tree generated from T and P_{3t+1} by adding an edge between v and a pendent vertex of P_{3t+1}, then $T' \in \mathbb{T}$.

Theorem 64. [101] *Let T be an n-order tree with domination number γ, where $n \geq 3$ and $1 \leq \gamma \leq \lfloor n/2 \rfloor$. Then*

$$ABS(T) \geq \left(\frac{\sqrt{3}}{3} + \frac{3\sqrt{15}}{5} - \frac{3\sqrt{2}}{2} \right)(n - 3\gamma) + \frac{3\sqrt{2}}{2}\gamma + \left(\frac{2\sqrt{3}}{3} - \frac{3\sqrt{2}}{2} \right),$$

with equality if and only if $T \in \mathbb{T}$.

Theorem 65. [60] *If G is a connected non-trivial graph of size m, maximum degree Δ and minimum degree δ, then*

$$ABS(G) \geq m\sqrt{\frac{\delta - 1}{\Delta}},$$

with equality if and only if G is regular.

Theorem 66. [60] *If G is a connected graph of size m, maximum degree Δ and minimum degree $\delta \geq 2$, then*

$$ABS(G) \geq \frac{2\,H(G)\sqrt{\Delta\delta(\Delta-1)(\delta-1)} + M_1(G) - 2m}{2\left(\sqrt{\delta(\delta-1)} + \sqrt{\Delta(\Delta-1)}\,\right)},$$

with equality if and only if G is regular, where $M_1(G)$ and $H(G)$ are the first Zagreb and harmonic indices of G, respectively.

Theorem 67. [60] *If G is an n-order graph of size m, then*

$$ABS(G) \geq m - \sqrt{2}\,SC(G),$$

with equality if and only if G is a 1-regular graph, where $SC(G)$ is the sum-connectivity index of G.

Theorem 68. [68] *If G is a connected graph of minimum degree δ, then*

$$ABS(G) \geq \sqrt{\delta(\delta-1)}\,R(G) \quad \text{and} \quad ABS(G) \geq \sqrt{\delta(\delta-1)}\,H(G),$$

where the equality in either of the inequalities holds if and only if G is regular.

A vertex adjacent to a pendent vertex is known as a quasi-pendent vertex.

Theorem 69. [68] *If G is a connected graph in which the degree of every quasi-pendent vertex is at least 3, then $ABS(G) > R(G)$ and hence $ABS(G) > H(G)$.*

Theorem 70. [14] *Let G be a connected n-order graph of minimum degree at least 2. Then*

$$ABS(G) \geq ABC(G),$$

with equality if and only if G is the cycle graph C_n.

$$ABS(G) > ABC(G) \tag{5}$$

Theorem 71. [14] *If G is any of the following graphs then inequality (5) holds:*

(i) *Line graph of a connected n-order graph K such that $n \geq 5$ and that $K \notin \{P_n, C_n\}$.*

(ii) *A connected graph of size m such that the number of pendent vertices of G is at most $\lfloor m/2 \rfloor$ and the number of vertices of degree 2 in G is zero.*

(iii) *A connected graph of size m such that the number of pendent vertices of G is at most $\lfloor m/2 \rfloor$ and if $v \in V(G)$ is a vertex of degree 2 then v has no neighbor of any of degrees 2, 3 and 4.*

It was found in [14] that inequality (5) in reverse order holds for every n-order tree satisfying $3 \leq n \leq 10$. However, if $n \geq 11$ then there exists at least one n-order tree satisfying inequality (5). These observations lead to the following problem.

Problem 6. [14] *Characterize the trees that satisfy inequality* (5).

Take $\Theta = ABC - ABS$. Employing computer search, it was found in [14] that $\Theta \neq 0$ for all n-order trees satisfying $3 \leq n \leq 15$. It would be of some interest to extend this finding to higher values of n or to discover a tree (or a graph with minimum degree 1) for which $\Theta = 0$ [14].

Let T_n be the number of n-order trees and t_n the number of n-order trees for which $\Theta < 0$. Since $t_n/T_n > 0$ for $n \geq 11$, the following problem is natural to ask.

Problem 7. [14] *Does the* $\lim_{n\to\infty} t_n/T_n$ *exist, and if yes, what is its value?*

Theorem 72. [61] *Let G be a connected graph of size m and minimum degree δ. Then*

$$ABS(G) \geq m\sqrt{1 - \frac{1}{\delta}}$$

where the equality holds if G is regular.

Theorem 73. [61] *For any connected graph G of order at least 3, size m and maximum degree Δ, it holds that*

$$ABS(G) \geq \frac{(M_1(G) - 2m)^{3/2}}{2(\Delta - 1)\sqrt{M_1(G)}},$$

with equality if and only if G is regular.

Theorem 74. [61] *If G is a connected non-trivial graph of size m, then*

$$ABS(G) \geq \sqrt{m(2m - H(G))}.$$

with equality if and only if G is regular.

Theorem 75. [16] *If G is a connected graph of size $r \geq 2$, then*

$$ABS(G) \geq \frac{r^{3/2}}{\sqrt{r + 2\ {}^{m}Pl(G)}}\,,$$

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

Some additional lower bounds on the ABS index can be found in the papers [48, 61].

5 Concluding notes

In the present survey, we presented the main, hitherto established, mathematical results on the atom-bond sum-connected index. By this, we hope to have contributed to the emerging mathematical theory of this recently introduced vertex-degree-based graph invariant. More results along these lines are anticipated, and the open problems and conjectures stated in this survey may help to motivate such future research.

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References

[1] K. Aarthi, S. Elumalai, S. Balachandran, S. Mondal, Extremal values of the atom-bond sum-connectivity index in bicyclic graphs, *J. Appl. Math. Comput.* **69** (2023) 4269–4285.

[2] D. Adiyanyam, E. Azjargal, L. Buyantogtokh, Bond incident degree indices of stepwise irregular graphs, *AIMS Math.* **7** (2022) 8685–8700.

[3] A. M. Albalahi, A. Ali, Z. Du, A. A. Bhatti, T. Alraqad, N. Iqbal, A. E. Hamza, On bond incident degree indices of chemical graphs, *Mathematics* **11** (2023) #27.

[4] A. M. Albalahi, D. Dimitrov, T. Réti, A. Ali, S. Hussain, Bond incident degree indices of connected (n, m)-graphs with fixed maximum degree, *MATCH Commun. Math. Comput. Chem.*, in press.

[5] A. M. Albalahi, Z. Du, A. Ali, On the general atom-bond sum-connectivity index, *AIMS Math.* **8** (2023) 23771–23785.

[6] A. M. Albalahi, E. Milovanović, A. Ali, General atom-bond sum-connectivity index of graphs, *Mathematics* **11** (2023) #2494.

[7] A. Ali, A. A. Bhatti, Extremal triangular chain graphs for bond incident degree (BID) indices, *Ars Comb.* **141** (2018) 213–227.

[8] A. Ali, A. A. Bhatti, Z. Raza, Topological study of tree-like polyphenylene systems, spiro hexagonal systems and polyphenylene dendrimer nanostars, *Quant. Mat.* **5** (2016) 534–538.

[9] A. Ali, D. Dimitrov, On the extremal graphs with respect to bond incident degree indices, *Discr. Appl. Math.* **238** (2018) 32–40.

[10] A. Ali, K. C. Das, D. Dimitrov, B. Furtula, Atom-bond connectivity index of graphs: a review over extremal results and bounds, *Discr. Math. Lett.* **5** (2021) 68–93.

[11] A. Ali, I. Gutman, E. Milovanović, I. Milovanović, Sum of powers of the degrees of graphs: Extremal results and bounds, *MATCH Commun. Math. Comput. Chem.* **80** (2018) 5–84.

[12] A. Ali, B. Furtula, I. Redžepović, I. Gutman, Atom-bond sum-connectivity index, *J. Math. Chem.* **60** (2022) 2081–2093.

[13] A. Ali, I. Gutman, I. Redžepović, Atom-bond sum-connectivity index of unicyclic graphs and some applications, *El. J. Math.* **5** (2023) 1–7.

[14] A. Ali, I. Gutman, I. Redžepović, J. P. Mazorodze, A. M. Albalahi, A. E. Hamza, On the difference of atom-bond sum-connectivity and atom-bond-connectivity indices, *MATCH Commun. Math. Comput. Chem.* **91** (2024) 725–740.

[15] A. Ali, M. Javaid, M. Matejić, I. Milovanović, E. Milovanović, Some new bounds on the general sum-connectivity index, *Commun. Comb. Optim.* **5** (2020) 97–109.

[16] A. Ali, I. Milovanović, E. Milovanović, M. Matejić, Sharp inequalities for the atom-bond (sum) connectivity index, *J. Math. Ineq.* **17** (2023) 1411–1426.

[17] A. Ali, Z. Raza, A. A. Bhatti, Bond incident degree (BID) indices of polyomino chains: a unified approach, *Appl. Math. Comput.* **287-288** (2016) 28–37.

[18] A. Ali, Z. Raza, A. A. Bhatti, Extremal pentagonal chains with respect to bond incident degree indices, *Canad. J. Chem.* **94** (2016) 870–876.

[19] A. Ali, L. Zhong, I. Gutman, Harmonic index and its generalization: extremal results and bounds, *MATCH Commun. Math. Comput. Chem.* **81** (2019) 249–311.

[20] T. A. Alraqad, I. Ž. Milovanović, H. Saber, A. Ali, J. P. Mazorodze, A. A. Attiya, Minimum atom-bond sum-connectivity index of trees with a fixed order and/or number of pendent vertices, *AIMS Math.* **9** (2024) 3707–3721.

[21] T. Alraqad, H. Saber, A. Ali, A. M. Albalahi, On the maximum atom-bond sum-connectivity index of graphs, *Open Math.* **22** (2024) #20230179.

[22] S. S. Anderson, F. Harary, Trees and unicyclic graphs, *Math. Teach.* **60** (1967) 345–348.

[23] L. Berrocal, A. Olivieri, J. Rada, Extremal values of VDB topological indices over hexagonal systems with fixed number of vertices, *Appl. Math. Comput.* **243** (2014) 176–183.

[24] J. A. Bondy, U. S. R. Murty, *Graph Theory*, Springer, London, 2008.

[25] B. Borovićanin, K. C. Das, B. Furtula, I. Gutman, Bounds for Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 17–100.

[26] G. Chartrand, L. Lesniak, P. Zhang, *Graphs & Digraphs*, CRC Press, Boca Raton, 2016.

[27] H. Chen, H. Deng, R. Wu, On extremal bipartite graphs with a given connectivity, *Filomat* **33** (2019) 1531–1540.

[28] H. Chen, R. Wu, On extremal bipartite graphs with given number of cut edges, *Discr. Math. Alg. Appl.* **12** (2020) #2050015.

[29] H. Chen, R. Wu, H. Deng, The extremal values of some topological indices in bipartite graphs with a given matching number, *Appl. Math. Comput.* **280** (2016) 103–109.

[30] H. Chen, R. Wu, H. Deng, The extremal values of some monotonic topological indices in graphs with a given vertex bipartiteness, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 103–120.

[31] R. Cruz, H. Giraldo, J. Rada, Extremal values of vertex-degree topological indices over hexagonal systems, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 501–512.

[32] R. Cruz, I. Gutman, J. Rada, Convex hexagonal systems and their topological indices, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 97–108.

[33] R. Cruz, A. D. Santamaría-Galvis, J. Rada, Extremal values of vertex-degree-based topological indices of coronoid systems, *Int. J. Quantum Chem.* **121** (2021) #e26536.

[34] H. Deng, J. Yang, F. Xia, A general modeling of some vertex-degree based topological indices in benzenoid systems and phenylenes, *Comput. Math. Appl.* **61** (2011) 3017–3023.

[35] D. Desmecht, V. Dubois, Correlation of the molecular cross-sectional area of organic monofunctional compounds with topological descriptors, *J. Chem. Inf. Model.* (2024), https://doi.org/10.1021/acs.jcim.3c01787.

[36] D. Dimitrov, Z. Du, Complete characterization of the minimal-ABC trees, *Discr. Appl. Math.* **336** (2023) 148–194.

[37] D. Dimitrov, Z. Du, The ABC index conundrum's complete solution, *MATCH Commun. Math. Comput. Chem.* **91** (2023) 5–38.

[38] Y. Dong, H. Broersma, Y. Bai, S. Zhang, The complexity of spanning tree problems involving graphical indices, *Discr. Appl. Math.* **347** (2024) 143–154.

[39] J. Du, X. Sun, On bond incident degree index of chemical trees with a fixed order and a fixed number of leaves, *Appl. Math. Comput.* **464** (2024) #128390.

[40] E. Estrada, L. Torres, L. Rodríguez, I. Gutman, An atom-bond connectivity index: modelling the enthalpy of formation of alkanes, *Indian J. Chem. Sec.* **37A** (1998) 849–855.

[41] E. Estrada, Atom-bond connectivity and the energetic of branched alkanes, *Chem. Phys. Lett.* **463** (2008) 422–425.

[42] S. Fajtlowicz, On conjectures of Graffiti–II, *Congr. Num.* **60** (1987) 187–197.

[43] S. Fallat, Y. Fan, Bipartiteness and the least eigenvalue of signless Laplacian of graphs, *Lin. Algebra Appl.* **436** (2012) 3254–3267.

[44] T. Gallai, Über extreme Punkt- und Kantenmengen, *Ann. Univ. Sci. Budapest Eötvös Sect. Math.* **2** (1959) 133–138.

[45] W. Gao, The minimum *ABC* index of chemical trees, *Discr. Appl. Math.* **348** (2024) 132–143.

[46] F. Gao, D.-D. Zhao, X.-X. Li, J.-B. Liu, Graphs having extremal monotonic topological indices with bounded vertex k-partiteness, *J. Appl. Math. Comput.* **58** (2018) 413–432.

[47] Y. Ge, Z. Lin, J. Wang, Atom-bond sum-connectivity index of line graphs, *Discr. Math. Lett.* **12** (2023) 196–200.

[48] K. J. Gowtham, I. Gutman, On the difference between atom-bond sum-connectivity and sum-connectivity indices, *Bull. Cl. Sci. Math. Nat. Sci. Math.* **47** (2022) 55–65.

[49] I. Gutman, Degree-based topological indices, *Croat. Chem. Acta* **86** (2013) 351–361.

[50] I. Gutman, Stepwise irregular graphs, *Appl. Math. Comput.* **325** (2018) 234–238.

[51] I. Gutman, B. Furtula, M. B. Ahmadi, S. A. Hosseini, P. S. Nowbandegani, M. Zarrinderakht, The ABC index conundrum, *Filomat* **27** (2013) 1075–1083.

[52] I. Gutman, B. Furtula, I. Redžepović, On topological indices and their reciprocals, *MATCH Commun. Math. Comput. Chem.* **91** (2024) 287–297.

[53] I. Gutman, E. Milovanović, I. Milovanović, Beyond the Zagreb indices, *AKCE Int. J. Graph. Comb.* **17** (2020) 74–85.

[54] I. Gutman, J. Tošović, S. Radenković, S. Marković, On atom-bond connectivity index and its chemical applicability, *Indian J. Chem.* **51A** (2012) 690–694.

[55] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[56] S. He, H. Chen, H. Deng, The vertex–degree–based topological indices of fluoranthene–type benzenoid systems, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 431–458.

[57] S. A. Hosseini, B. Mohar, M. B. Ahmadi, The evolution of the structure of ABC-minimal trees, *J. Comb. Theory Ser. B* **152** (2022) 415–452.

[58] Z. Hu, L. Li, X. Li, D. Peng, Extremal graphs for topological index defined by a degree-based edge-weight function, *MATCH Commun. Math. Comput. Chem.* **88** (2022) 505–520.

[59] Y. Hu, F. Wang, On the maximum atom-bond sum-connectivity index of trees, *MATCH Commun. Math. Comput. Chem.* **91** (2024) 709–723.

[60] Z. Hussain, H. Liu, S. Zhang, H. Hua, Bounds for the atom-bond sum-connectivity index of graphs, *MATCH Commun. Math. Comput. Chem.*, in press.

[61] A. Jahanbani, I. Redžepović, On the generalized ABS index of graphs, *Filomat* **37** (2023) 10161–10169.

[62] A. Kannan, S. Elumalai, S. Mondal, S. Balachandran, On the difference between atom-bond sum-connectivity index and Randić index of binary trees and chemical trees, *Research Square*, `https://doi.org/10.21203/rs.3.rs-3970562/v1`.

[63] L. B. Kier, L. H. Hall, *Molecular Connectivity in Chemistry and Drug Research*, Academic Press, New York, 1976.

[64] L. B. Kier, L. H. Hall, *Molecular Connectivity in Structure–Activity Analysis*, Wiley, New York, 1986.

[65] X. Li, Y. Shi, A survey on the Randić index, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 127–156.

[66] F. Li, Q. Ye, H. Broersma, R. Ye, X. Zhang, Extremality of VDB topological indices over f-benzenoids with given order, *Appl. Math. Comput.* **393** (2021) #125757.

[67] F. Li, Q. Ye, H. Lu, The greatest values for atom-bond sum-connectivity index of graphs with given parameters, *Discr. Appl. Math.* **344** (2024) 188–196.

[68] Z. Lin, On relations between atom-bond sum-connectivity index and other connectivity indices, *Bull. Int. Math. Virtual Inst.* **13** (2023) 249–252.

[69] H. Liu, Z. Du, Y. Huang, H. Chen, S. Elumalai, Note on the minimum bond incident degree indices of k-cyclic graphs, *MATCH Commun. Math. Comput. Chem.* **91** (2024) 255–266.

[70] H. Liu, L. You, H. Chen, Y. Huang, Unified extremal results for (exponential) bond incident degree indices of trees, *MATCH Commun. Math. Comput. Chem.* **92** (2024) 151–164.

[71] M. Liu, I. Tomescu, J. Liu, Unified extremal results for k-apex unicyclic graphs (trees), *Discr. Appl. Math.* **288** (2021) 35–49.

[72] M. Liu, K. Xu, X.-D. Zhang, Extremal graphs for vertex-degree-based invariants with given degree sequences, *Discr. Appl. Math.* **255** (2019) 267–277.

[73] Y. Ma, S. Cao, Y. Shi, I. Gutman, M. Dehmer, B. Furtula, From the connectivity index to various Randić-type descriptors, *MATCH Commun. Math. Comput. Chem.* **80** (2018) 85–106.

[74] V. Maitreyi, S. Elumalai, S. Balachandran, The minimum ABS index of trees with given number of pendent vertices, arXiv:2211.05177.

[75] P. Nithya, S. Elumalai, S. Balachandran, Minimum atom-bond sum-connectivity index of unicyclic graphs with maximum degree, *Discr. Math. Lett.* **13** (2024) 82–88.

[76] P. Nithya, S. Elumalai, S. Balachandran, H. Liu, Maximum atom-bond sum-connectivity index in unicyclic graphs of fixed girth, *MATCH Commun. Math. Comput. Chem.*, in press.

[77] P. Nithya, S. Elumalai, S. Balachandran, S. Mondal, Smallest ABS index of unicyclic graphs with given girth, *J. Appl. Math. Comput.* **69** (2023) 3675–3692.

[78] S. Noureen, A. Ali, Maximum atom-bond sum-connectivity index of n-order trees with fixed number of leaves, *Discr. Math. Lett.* **12** (2023) 26–28.

[79] J. R. Platt, Inuence of neighbor bonds on additive bond properties in paraffins, *Chem. Phys.* **15** (1947) 419–420.

[80] J. R. Platt, Prediction of isomeric differences in paraffin properties, *J. Phys. Chem.* **56** (1952) 328–336.

[81] J. Rada, R. Cruz, I. Gutman, Vertex-degree-based topological indices of catacondensed hexagonal systems, *Chem. Phys. Lett.* **572** (2013) 154–157.

[82] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.

[83] M. Randić, On history of the Randić index and emerging hostility toward chemical graph theory, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 5–124.

[84] M. Randić, The connectivity index 25 years after, *J. Mol. Graph. Model.* **20** (2001) 19–35.

[85] M. Randić, M. Novič, D. Plavšić, *Solved and Unsolved Problems in Structural Chemistry*, CRC Press, Boca Raton, 2016.

[86] Y. Tang, D. B. West, B. Zhou, Extremal problems for degree-based topological indices, *Discr. Appl. Math.* **203** (2016) 134–143.

[87] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1992.

[88] Z. Tuza, Extensions of Gallai's graph covering theorems for uniform hypergraphs, *J. Comb. Theory Ser. B* **52** (1991) 92–96.

[89] T. Vetrík, General approach for obtaining extremal results on degree-based indices illustrated on the general sum-connectivity index, *El. J. Graph Theory Appl.* **11** (2023) 125–133.

[90] T. Vetrík, Degree-based function index of graphs with given connectivity, *Iranian J. Math. Chem.* **14** (2023) 183–194.

[91] D. Vukičević, J. Đurđević, Bond additive modeling 10. Upper and lower bounds of bond incident degree indices of catacondensed fluoranthenes, *Chem. Phys. Lett.* **515** (2011) 186–189.

[92] S. Wagner, H. Wang, *Introduction to Chemical Graph Theory*, CRC Press, Boca Raton, 2018.

[93] H. Wang, Functions on adjacent vertex degrees of trees with given degree sequence, *Central Eur. J. Math.* **12** (2014) 1656–1663.

[94] F. Wang, Y. Zhang, X. Ren, B. Zhang, Maximum atom bond sum connectivity index of molecular trees with a perfect matching, *MATCH Commun. Math. Comput. Chem.*, in press.

[95] P. Wei, M. Liu, I. Gutman, On (exponential) bond incident degree indices of graphs, *Discr. Appl. Math.* **336** (2023) 141–147.

[96] D. B. West, *Introduction to Graph Theory*, Prentice Hall, 2001.

[97] R. Wu, H. Chen, H. Deng, On the monotonicity of topological indices and the connectivity of a graph, *Appl. Math. Comput.* **298** (2017) 188–200.

[98] Z. Yarahmadi, A. R. Ashrafi, Extremal properties of the bipartite vertex frustration of graphs, *Appl. Math. Lett.* **24** (2011) 1774–1777.

[99] J. Ye, M. Liu, Y. Yao, K. C. Das, Extremal polygonal cacti for bond incident degree indices, *Discr. Appl. Math.* **257** (2019) 289–298.

[100] G. Zhang, Y. Chen, Functions on adjacent vertex degrees of graphs with prescribed degree sequence, *MATCH Commun. Math. Comput. Chem.* **80** (2018) 129–139.

[101] Y. Zhang, H. Wang, G. Su, K. C. Das, Extremal problems on the atom-bond sum-connectivity indices of trees with given matching number or domination number, *Discr. Appl. Math.* **345** (2024) 190–206.

[102] X. M. Zhang, X. D. Zhang, R. Bass, H. Wang, Extremal trees with respect to functions on adjacent vertex degrees, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 307–322.

[103] B. Zhou, N. Trinajstić, On a novel connectivity index, *J. Math. Chem.* **46** (2009) 1252–1270.

[104] B. Zhou, N. Trinajstić, On general sum-connectivity index, *J. Math. Chem.* **47** (2010) 210–218.

[105] X. Zuo, A. Jahanbani, H. Shooshtari, On the atom-bond sum-connectivity index of chemical graphs, *J. Mol. Struct.* **1296** (2024) #136849.