MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **98** (2027) 419–429
ISSN: 0340–6253
doi: 10.46793/match.98-1.24426

Counterexamples to a Conjecture on the Maximum ABC Index of Graphs with Fixed Cyclomatic Number

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(Received June 26, 2026)

Abstract

The atom–bond connectivity (ABC) index is a classical degree-based topological index in chemical graph theory. Ali, Das, Dimitrov, and Furtula conjectured that a specific star-based graph $H_{n,\nu}$ uniquely maximizes the ABC index among all connected graphs on n vertices with cyclomatic number ν, where $5 \leq \nu \leq n-3$. We disprove this conjecture in two regimes. First, for $\nu = n-3$, we show that the complete bipartite graph $K_{2,n-2}$ has a larger ABC index than $H_{n,n-3}$ for all $n \geq 10$, implying failure at the minimum admissible order $n = \nu + 3$ for all $\nu \geq 7$. Second, for every fixed $\nu \geq 5$, we construct an infinite family of graphs based on $K_{2,\nu+1}$ with pendant attachments that exceed the ABC index of $H_{n,\nu}$ for all sufficiently large n.

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These counterexamples show that dense bipartite structures can outperform the conjectured star-based graphs and therefore must be taken into account in any future characterization of ABC-extremal graphs under fixed cyclomatic number constraints.

1 Introduction

Chemical graph theory studies graph-theoretic models of chemical compounds, where vertices represent atoms and edges represent chemical bonds. Numerical quantities derived from molecular structures are called molecular descriptors, among which topological indices play an important role. For a graph G, a topological index **TI** is a numerical graph invariant satisfying $\mathbf{TI}(G) = \mathbf{TI}(H)$ whenever $G \cong H$ [2]. The first topological index, introduced by Wiener in 1947 [16], was originally proposed for the study of structural properties of organic compounds, including paraffin boiling points.

Among various topological indices, degree-based indices have attracted considerable attention due to their simple definitions and wide chemical applications. Among them, the Zagreb index and the Randić index are two of the most important and extensively studied molecular descriptors introduced in the 1970s [8, 9, 13]. These indices have found numerous applications in quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) [10–12, 15].

The atom-bond connectivity (ABC) index was introduced by Estrada et al. [6] as a degree-based molecular descriptor motivated by chemical applications. Later, Estrada [5] demonstrated its applicability to the study of alkanes and cycloalkanes. Since then, the ABC index has attracted considerable attention, and numerous mathematical results concerning this index have been obtained; see, for instance, [3, 4, 7] and the comprehensive survey [1].

We use the normalized ABC index defined in [1], which omits the global factor $\sqrt{2}$ from the original definition. Thus, the standard ABC index satisfies $ABC_{\mathrm{std}}(G) = \sqrt{2}ABC(G)$ under our notation. This normalization does not affect the extremal graphs. Among the known maximum results, the star is extremal among trees, and star-based constructions are

extremal for several small cyclomatic numbers. Motivated by the tree, unicyclic, bicyclic, tricyclic and tetracyclic cases, Ali, Das, Dimitrov and Furtula proposed a general conjecture for fixed cyclomatic number at least five. We show here that the conjectured pattern breaks down as soon as larger cyclomatic numbers are considered.

Our counterexamples are elementary. In the dense boundary case, complete bipartite graphs $K_{2,n-2}$ already beat the conjectured graph. Moreover, for every fixed $\nu \geq 5$, a graph obtained from $K_{2,\nu+1}$ by attaching pendant vertices gives infinitely many further counterexamples. The proofs require only degree counts and explicit inequalities.

2 Definitions, notation and the conjecture

All graphs in this note are finite, simple and connected. For a graph G, its vertex set and edge set are denoted by $V(G)$ and $E(G)$. The *order* and *size* of G are $|V(G)|$ and $|E(G)|$, respectively. The degree of $v \in V(G)$ is denoted by $d_G(v)$, or simply by $d(v)$ when the graph is clear. A vertex of degree one is called a *pendant vertex*. The star on n vertices is denoted by S_n, and the complete bipartite graph with partite sets of sizes p and q is denoted by $K_{p,q}$.

Definition 2.1. [5] The *atom–bond connectivity index* of a graph G is

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

For a single edge uv, the corresponding summand is called its ABC contribution.

Definition 2.2. [1] The *cyclomatic number* of a connected graph G with n vertices and m edges is defined as $\nu(G) = m - n + 1$. A connected graph with cyclomatic number ν is sometimes called a *ν-cyclic graph*.

Formally, if S_n has vertex set $V(S_n) = \{c, v_1, v_2, \ldots, v_{n-1}\}$ where c is the central vertex and $v_1, \ldots, v_{n-1}$ are pendant vertices, and we choose

$p = v_1$, then $E(H_{n,\nu}) = E(S_n) \cup \{\, pv_i \mid i = 2, 3, \ldots, \nu + 1 \,\}$. Hence, $H_{n,\nu}$ has n vertices and cyclomatic number $\nu(H_{n,\nu}) = \nu$.

Ali, Das, Dimitrov and Furtula stated the following conjecture (conjecture 4.1 of [1]).

Conjecture 1. *[1] If ν and n are integers satisfying $5 \leq \nu \leq n - 3$, then among all connected n-vertex graphs with cyclomatic number ν, only the graph $H_{n,\nu}$ has maximum ABC index, which is equal to*

$$(n - \nu - 2)\sqrt{\frac{n-2}{n-1}} + \sqrt{\frac{n + \nu - 2}{(\nu + 1)(n-1)}} + \nu\sqrt{2}. \tag{1}$$

The original survey also records extremal results for dense graphs without pendant vertices. In particular, $K_{2,n-2}$ maximizes the ABC index among connected graphs of order n, size $2n - 4$, and minimum degree at least two [14]. This naturally motivates a comparison between $K_{2,n-2}$ and the conjectured graph in the class of all connected graphs. It turns out that the conjectured graph has a smaller ABC index than $K_{2,n-2}$ when $\nu = n - 3$.

Our main contributions are as follows:

(i) We show that the conjecture fails in the boundary case $\nu = n - 3$ by establishing that $K_{2,n-2}$ has a larger ABC index than $H_{n,n-3}$ for all $n \geq 10$.

(ii) For every fixed $\nu \geq 5$, we construct an infinite family of counterexamples based on $K_{2,\nu+1}$ with pendant attachments.

(iii) These counterexamples show that dense bipartite structures can outperform the conjectured star-based graphs and therefore must be taken into account in any future characterization of ABC-extremal graphs under fixed cyclomatic number constraints.

3 Counterexamples at the minimum admissible order

Theorem 1. *For every integer $n \geq 10$,*

$$\mathrm{ABC}(K_{2,n-2}) > \mathrm{ABC}(H_{n,n-3}).$$

Proof. First consider the complete bipartite graph $K_{2,n-2}$. It has order n and size $|E(K_{2,n-2})| = 2(n-2)$. Since $K_{2,n-2}$ is connected, its cyclomatic number is $\nu(K_{2,n-2}) = |E(K_{2,n-2})| - |V(K_{2,n-2})| + 1 = n-3$. Moreover, in $K_{2,n-2}$, every vertex in the part of size 2 has degree $n-2$, while every vertex in the part of size $n-2$ has degree 2. Hence every edge has degree type $(n-2, 2)$ and contributes $\sqrt{\frac{(n-2)+2-2}{2(n-2)}} = \frac{1}{\sqrt{2}}$ to the ABC index. Since there are $2(n-2)$ edges, we obtain

$$\mathrm{ABC}(K_{2,n-2}) = 2(n-2) \cdot \frac{1}{\sqrt{2}} = (n-2)\sqrt{2}. \tag{2}$$

On the other hand, applying $\nu = n-3$ gives

$$\mathrm{ABC}(H_{n,n-3}) = (n-3)\sqrt{2} + \sqrt{\frac{n-2}{n-1}} + \sqrt{\frac{2n-5}{(n-1)(n-2)}}. \tag{3}$$

Therefore, by (2) and (3), it is enough to prove that

$$\sqrt{2} > \sqrt{\frac{n-2}{n-1}} + \sqrt{\frac{2n-5}{(n-1)(n-2)}}. \tag{4}$$

Set $A = \sqrt{\frac{n-2}{n-1}}, B = \sqrt{\frac{2n-5}{(n-1)(n-2)}}$. Then $A > 0$ and $B > 0$ for $n \geq 10$, and (4) is equivalent to $\sqrt{2} > A + B$. Since both sides are positive, this is equivalent to

$$2 - A^2 - B^2 > 2AB. \tag{5}$$

A direct calculation gives

$$2 - A^2 - B^2 = 2 - \frac{n-2}{n-1} - \frac{2n-5}{(n-1)(n-2)} = \frac{n^2-4n+5}{(n-1)(n-2)} > 0.$$

Hence each side of (5) takes a positive value, which permits us to square the inequality (5). After simplification,

$$(2 - A^2 - B^2)^2 - 4A^2B^2 = \frac{(n-3)(n^3 - 13n^2 + 39n - 35)}{(n-1)^2(n-2)^2}. \qquad (6)$$

It remains to show that the right-hand side of (6) is positive. Since $n \geq 10$, we have $n - 3 > 0$ and $(n-1)^2(n-2)^2 > 0$. Hence it suffices to prove $n^3 - 13n^2 + 39n - 35 > 0$. Let $p(x) = x^3 - 13x^2 + 39x - 35$. Then $p(10) = 55 > 0$. Furthermore, $p'(x) = 3x^2 - 26x + 39$ and $p''(x) = 6x - 26$. For $x \geq 10$, we have $p''(x) > 0$. Therefore $p'(x)$ is increasing on $[10, \infty)$. Since $p'(10) = 300 - 260 + 39 = 79 > 0$, it follows that $p'(x) > 0$ for all $x \geq 10$. Consequently, $p(x)$ is increasing on $[10, \infty)$, and so $p(n) \geq p(10) > 0$ for every integer $n \geq 10$.

Thus the right-hand side of (6) is positive, which proves (5), and hence (4). Combining this with (2) and (3), we get $\mathrm{ABC}(K_{2,n-2}) > \mathrm{ABC}(H_{n,n-3})$ for all $n \geq 10$.

Finally, both graphs have order n and cyclomatic number $n - 3$, but $K_{2,n-2}$ has a larger ABC index than the conjectured graph $H_{n,n-3}$. Therefore, we provide counterexamples to Conjecture 1. ■

Equivalently, Theorem 1 gives a counterexample at the smallest admissible order $n = \nu + 3$ whenever $\nu \geq 7$.

Corollary 2. *For every integer $\nu \geq 7$, $\mathrm{ABC}(K_{2,\nu+1}) > \mathrm{ABC}(H_{\nu+3,\nu})$. Consequently, the conjecture of [1] fails at the minimal graph order $n = \nu + 3$ allowed by the condition $\nu \leq n - 3$.*

Proof. This follows immediately from Theorem 1 by setting $n = \nu + 3$, since $\nu \geq 7$ implies $n \geq 10$. ■

4 Fixed cyclomatic number

The preceding section disproves the conjecture in the extremal case $\nu = n - 3$. We now show that the failure persists beyond this boundary case.

Let n and ν be integers such that $n \geq \nu + 3$. Let $A = \{a_1, \ldots, a_{\nu+1}\}$ and $B = \{b_1, \ldots, b_{n-\nu-3}\}$, where A, B, and $\{x, y\}$ are pairwise disjoint.

Define $G_{n,\nu}$ by $V(G_{n,\nu}) = \{x, y\} \cup A \cup B$ and $E(G_{n,\nu}) = \{xa_i, ya_i : 1 \leq i \leq \nu+1\} \cup \{xb_j : 1 \leq j \leq n-\nu-3\}$. Equivalently, $G_{n,\nu}$ is obtained from $K_{2,\nu+1}$ by attaching $n-\nu-3$ pendant vertices to one of the two vertices in the part of size 2.

Lemma 4.1. *Let n and ν be integers with $n \geq \nu+3$. Then $G_{n,\nu}$ has cyclomatic number ν and*

$$\mathrm{ABC}(G_{n,\nu}) = (\nu+1)\sqrt{2} + (n-\nu-3)\sqrt{\frac{n-3}{n-2}}. \tag{7}$$

Proof. By construction, $G_{n,\nu}$ has order n and $|E(G_{n,\nu})| = 2(\nu+1) + (n-\nu-3) = n+\nu-1$. Since $G_{n,\nu}$ is connected, its cyclomatic number is $\nu(G_{n,\nu}) = |E(G_{n,\nu})| - |V(G_{n,\nu})| + 1 = \nu$.

The vertex degrees in $G_{n,\nu}$ are $d(x) = n-2, d(y) = \nu+1$ and $d(a) = 2 (a \in A)$ and every vertex in B is pendant. For each $a \in A$, the edges xa and ya have degree types $(n-2, 2)$ and $(\nu+1, 2)$, respectively. Hence each of them contributes $\frac{1}{\sqrt{2}}$ to the ABC index. Since there are $2(\nu+1)$ such edges, their total contribution is $(\nu+1)\sqrt{2}$.

Finally, each of the $n-\nu-3$ pendant edges incident with x has degree type $(n-2, 1)$ and contributes $\sqrt{\frac{(n-2)+1-2}{(n-2)\cdot 1}} = \sqrt{\frac{n-3}{n-2}}$. Summing these contributions gives (7). ∎

Theorem 3. *Let $\nu \geq 5$ be fixed and let $M_\nu = \sqrt{2} - 1 - \frac{1}{\sqrt{\nu+1}}$. If*

$$n \geq \left\lceil \max\left\{ \nu+3,\ 2 + \frac{4}{M_\nu},\ 1 + \frac{2(\nu-1)}{M_\nu\sqrt{\nu+1}} \right\} \right\rceil, \tag{8}$$

then $\mathrm{ABC}(G_{n,\nu}) > \mathrm{ABC}(H_{n,\nu})$. Consequently, for every fixed cyclomatic number $\nu \geq 5$, Conjecture 1 admits infinitely many counterexamples.

Proof. Since $\nu \geq 5$, we have $\frac{1}{\sqrt{\nu+1}} \leq \frac{1}{\sqrt{6}} < \sqrt{2} - 1$, and hence $M_\nu > 0$. By

(1) and Lemma 4.1, we have

$$\mathrm{ABC}(G_{n,\nu}) - \mathrm{ABC}(H_{n,\nu}) = \sqrt{2} + (n-\nu-3)\sqrt{\frac{n-3}{n-2}} - (n-\nu-2)\sqrt{\frac{n-2}{n-1}} - \sqrt{\frac{n+\nu-2}{(\nu+1)(n-1)}}. \tag{9}$$

Set

$$A_n = \sqrt{\frac{n-2}{n-1}}, \qquad C_n = \sqrt{\frac{n-3}{n-2}}, \qquad R_n = \sqrt{\frac{n+\nu-2}{(\nu+1)(n-1)}}.$$

Then (9) can be written as

$$\mathrm{ABC}(G_{n,\nu}) - \mathrm{ABC}(H_{n,\nu}) = \sqrt{2} - A_n - R_n - (n-\nu-3)(A_n - C_n). \tag{10}$$

We now estimate the three terms on the right-hand side. First, $A_n \le 1$. Moreover, $R_n = \frac{1}{\sqrt{\nu+1}}\sqrt{1+\frac{\nu-1}{n-1}}$. Using $\sqrt{1+t} \le 1 + t/2$ for $t \ge 0$, we obtain

$$R_n \le \frac{1}{\sqrt{\nu+1}} + \frac{\nu-1}{2(n-1)\sqrt{\nu+1}}. \tag{11}$$

Since $A_n^2 - C_n^2 = \frac{n-2}{n-1} - \frac{n-3}{n-2} = \frac{1}{(n-1)(n-2)}$, we get $A_n - C_n = \frac{A_n^2 - C_n^2}{A_n + C_n} = \frac{1}{(n-1)(n-2)(A_n+C_n)}$. For $n \ge 4$, both A_n and C_n are at least $1/\sqrt{2}$, and therefore $A_n + C_n \ge \sqrt{2}$. Hence

$$(n-\nu-3)(A_n - C_n) \le \frac{n-\nu-3}{\sqrt{2}\,(n-1)(n-2)} \le \frac{n}{\sqrt{2}\,(n-1)(n-2)} \le \frac{1}{n-2}. \tag{12}$$

Combining (10), (11), and (12), and using $A_n \le 1$, gives

$$\mathrm{ABC}(G_{n,\nu}) - \mathrm{ABC}(H_{n,\nu}) \ge \sqrt{2} - 1 - \frac{1}{\sqrt{\nu+1}} - \frac{\nu-1}{2(n-1)\sqrt{\nu+1}} - \frac{1}{n-2} = M_\nu - \frac{\nu-1}{2(n-1)\sqrt{\nu+1}} - \frac{1}{n-2}. \tag{13}$$

By the choice of n in (8), we have $n-2 \ge \frac{4}{M_\nu}, n-1 \ge \frac{2(\nu-1)}{M_\nu\sqrt{\nu+1}}$.

Therefore, $\frac{1}{n-2} \leq \frac{M_\nu}{4}$ and $\frac{\nu-1}{2(n-1)\sqrt{\nu+1}} \leq \frac{M_\nu}{4}$. It follows from (13) that

$$\mathrm{ABC}(G_{n,\nu}) - \mathrm{ABC}(H_{n,\nu}) \geq M_\nu - \frac{M_\nu}{4} - \frac{M_\nu}{4} = \frac{M_\nu}{2} > 0.$$

Thus $\mathrm{ABC}(G_{n,\nu}) > \mathrm{ABC}(H_{n,\nu})$.

Since the threshold (8) is finite for every fixed $\nu \geq 5$, the above inequality holds for all sufficiently large n. Hence, for every fixed cyclomatic number $\nu \geq 5$, there are infinitely many orders n for which the conjectured graph $H_{n,\nu}$ is not extremal. This proves the theorem. ■

Therefore, for every fixed cyclomatic number $\nu \geq 5$, the family $G_{n,\nu}$ yields infinitely many counterexamples to Conjecture 1. The explicit threshold in (8) is only a sufficient bound obtained from the estimates above and is not intended to be optimal.

5 Concluding remarks

In this paper, we disprove a conjecture on the maximum ABC index for graphs with fixed cyclomatic number. We show that the conjectured star-based structure is not extremal when $\nu = n-3$ and $n \geq 10$, and, for every fixed $\nu \geq 5$, at all sufficiently large orders. Our counterexamples show that dense bipartite structures can outperform the conjectured star-based graphs. They do not characterize the true maximizers or imply that all extremal graphs are bipartite.

Accordingly, any future characterization of ABC-extremal graphs under fixed cyclomatic number constraints should take such non-tree-like dense structures into account. Determining the true extremal graphs remains a problem for future research.

***Acknowledgment*:** The authors would like to thank the editor and the kind anonymous referees for their insightful comments that helped to improve the paper's final edition. This research was supported by the Tianjin Technology Innovation Guidance Special Project (Fund)– enterprise science and technology commissioner project (No. 25YDTPJC00870).

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