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A Variant of Atom Bond Sum Connectivity Index

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Abstract

Topological index is a numerical graph invariant derived from molecular graph. The atom bond sum connectivity index drew a lot of interest from chemical graph theorists in a short period of time. Nowadays, the degree sum of a vertex's first neighbors is recognized as a useful parameter in chemical graph theory. Keeping these two facts in mind, the neighborhood degree sum based ABS index ($NABS$) is put forward in this study. It is defined as

$$NABS(G) = \sum_{uv \in E(G)} \sqrt{\frac{\mu_G(u) + \mu_G(v) - 2}{\mu_G(u) + \mu_G(v)}},$$

where $\mu_G(u)$ represents the sum of degrees of all the vertices in a graph G adjacent to the vertex u. The role of this index in structure-property modelling and isomer discrimination is investigated. The extremal graphs for $NABS$ are identified in case of tree, bipartite, unicyclic and general graphs in terms of different graph parameters including graph order and size, maximum and minimum degree, independence number, chromatic number, etc.

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1 Introduction

In the field of chemical graph theory, atoms and bonds are equivalent to vertices and edges, respectively, within a molecule. This approach helps to capture characteristics of structures and investigate how they impact several physico-chemical properties and behaviors [10, 23]. Topological index is a number representing a graph's structure. In the middle of the 1970s, Randić introduced the Randić index [25] to evaluate the saturated hydrocarbon's degree of branching. The Randić index of a graph G has the following formulation:

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)\, d_G(v)}}. \tag{1}$$

where $d_G(u)$ represents the degree of the vertex u in G. By modifying the Randić index, Estrada et al. [11] introduced the atom-bond connectivity (ABC) index of graphs. The works related to ABC index can be found in [3, 7, 12–14, 16], and the probabilistic inference of this index is shown in [12]. The ABC index of a graph G has the following formulation:

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

Another study conducted by Zhou et al. [29] introduces modifications to the Randić index. They replace $d_G(u)\, d_G(v)$ with $d_G(u) + d_G(v)$ in the formulation (1), naming this modified index as the sum-connectivity index. The sum-connectivity index of a graph G has the following definition:

$$SC(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u) + d_G(v)}}. \tag{3}$$

By combining the concept of the SC index and ABC index, the atom-bond sum-connectivity (ABS) index was developed by Ali et al. [2,4]. The

definition of the ABS index for a graph G is as follows:

$$ABS(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u) + d_G(v)}}. \tag{4}$$

Let $N_G(u)$ be the collection of vertices adjacent to u, i.e., $N_G(u) = \{v \in V(G) : uv \in E(G)\}$. The parameter $\mu_G(u)$ is referred in some recent works [19,20] as the neighborhood degree sum of u. The topological indices based on this parameter are found to be very useful in chemical graph theory [6, 8, 18, 21, 22]. For some recent works on the ABS index, readers are referred to [1, 24]. This fact motivated us to present the neighborhood degree sum based ABS index ($NABS$). It is defined as:

$$NABS(G) = \sum_{uv \in E(G)} \sqrt{\frac{\mu_G(u) + \mu_G(v) - 2}{\mu_G(u) + \mu_G(v)}}. \tag{5}$$

Reti et al. [26] generalized the indices based on neighborhood degree sum of vertices. Let $f(x, y)$ be symmetric real valued function. Then the general neighborhood degree sum-based index for a graph G is defined as

$$I(G) = \sum_{uv \in E(G)} f\left(\mu_G(u), \mu_G(v)\right).$$

If we consider $f(x, y) = \sqrt{\frac{x+y-2}{x+y}}$ on the aforesaid formula, then the $NABS$ index is generated.

Quantitative Structure-Property Relationship (QSPR) analysis serves as a computational technique in chemistry, aiming to identify connections between chemical compound's molecular structure and related chemical or physical properties. Topological indices play a crucial role in QSPR studies, as they provide a numerical representation of the connectivity patterns within a molecular graph. The idea is to identify quantitative relationships that can predict a property based on the molecular structure alone, without the need for extensive experimental data. To get more insight on this direction, readers are referred to [5,9,15]. We aim to investigate the significance of the $NABS$ index in QSPR analysis. The isomer discrimination

ability of this index is also explored. Sharp bounds of this index are derived for class of trees, unicyclic, bipartite, and general connected graphs in terms of graph order and size, maximum and minimum degree, independence and chromatic number with identifying extremal graphs. Rest of this work consider following terms and notations. We use n, m, Δ and δ to represent the order, size, maximum degree and minimum degree of graph, respectively. To signify the average degree of a vertex $u \in V(G)$, we use $m_G(u)$.

2 Chemical significance

Various topological indices are available, and their numbers continue to increase. However, most of these indices are treated purely mathematically, without considering their chemical significance. To aid in the selection of a relevant molecular descriptor from a wide array of candidates, a compilation of valuable components has been formulated, among which is the ability to estimate the properties and activities of molecules. QSPR analysis is typically conducted on both theoretical attributes and experimental measurements of certain benchmark chemicals to assess the predictive capacity of topological indices. The objective of this study is to elucidate the chemical relevance of the neighborhood degree sum based ABS index. Octane isomers were initially examined as benchmark datasets, and some hydrocarbons with cyclic substructures were subsequently considered since octanes lack cycles. Table 1 provide specific numerical values for the $NABS$ index and various properties are detailed.

A noteworthy correlation is observed between the $NABS$ index and the standard enthalpy of vaporization ($DHVAP$), entropy (S), and acentric factor (AF) of octanes. To evaluate the $NABS$ index's performance, we investigate the following relationship.

$$\mathsf{P} = \mathsf{S}\ (\pm 2 \times \mathsf{E}_1)\ \mathsf{D} + \mathsf{I}\ (\pm 2 \times \mathsf{E}_2), \tag{6}$$

In Equation (6), P represents the property, S denotes the slope, D corre-

Table 1. $NABS$ index and various properties for octane isomers.

Octanes	$NABS$	$DHVAP$	S	AF
$C8:1$	5.837578059	111.67	9.915	0.397898
$C8:2$	5.939919045	109.84	9.484	0.377916
$C8:3$	5.960534307	111.26	9.521	0.371002
$C8:4$	5.936123932	109.32	9.483	0.371504
$C8:5$	5.967003651	109.43	9.476	0.362472
$C8:6$	6.064463460	103.42	8.915	0.339426
$C8:7$	6.063658052	108.02	9.272	0.348247
$C8:8$	6.053708823	106.98	9.029	0.344223
$C8:9$	6.038878417	105.72	9.051	0.35683
$C8:10$	6.107927373	104.74	8.973	0.322596
$C8:11$	6.098552680	106.59	9.316	0.340345
$C8:12$	6.086982966	106.06	9.209	0.332433
$C8:13$	6.178609585	101.48	9.081	0.306899
$C8:14$	6.21860559	101.31	8.826	0.300816
$C8:15$	6.153464783	104.09	8.402	0.30537
$C8:16$	6.25079367	102.06	8.897	0.293177
$C8:17$	6.184270664	102.39	9.014	0.317422
$C8:18$	6.353024302	93.06	8.41	0.255294

sponds to descriptors, and I stands for the intercept, respectively. We use E_1, E_2 to denote errors. We conduct regression analysis that includes significance F (SF), the F-test (F), and the standard error (SE), apart from R for more precise evaluation. In the context of S, $DHVAP$ and AF, the structure-property relationships generated by $NABS$ are as follows.

$$S = -33.066(\pm 6.13)NABS + 306.553(\pm 37.306)), \tag{7}$$

$$SE = 1.619, \quad F = 116.316, \quad SF = 9.5 \times 10^{-9}, \quad R^2 = 0.879$$

$$DHVAP = -2.576(\pm 0.761)NABS + 24.798(\pm 4.620)), \tag{8}$$
$$SE = 0.201, \quad F = 45.839, \quad SF = 4.5 \times 10^{-6}, \quad R^2 = 0.741$$

$$AF = -0.273(\pm 0.023)NABS + 1.995(\pm 0.142)), \tag{9}$$
$$SE = 0.006, \quad F = 537.218, \quad SF = 9.74 \times 10^{-14}, \quad R^2 = 0.971$$

In Figure 1, the linear relations (7), (8) are fitted. The linear fitting of the relation (9) as seen in Figure 2.

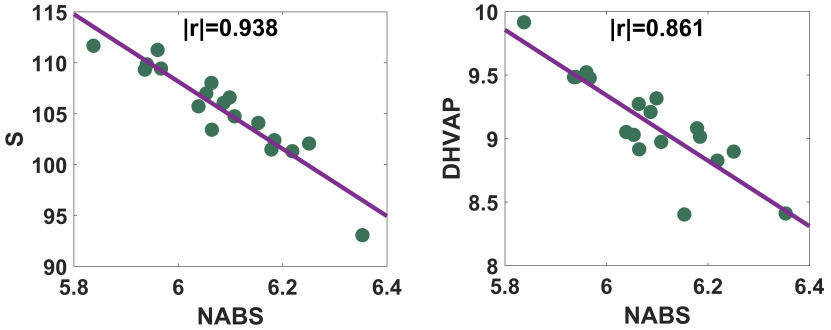

Figure 1. Linear fittings of $NABS$ with S and $DHVAP$ for octanes.

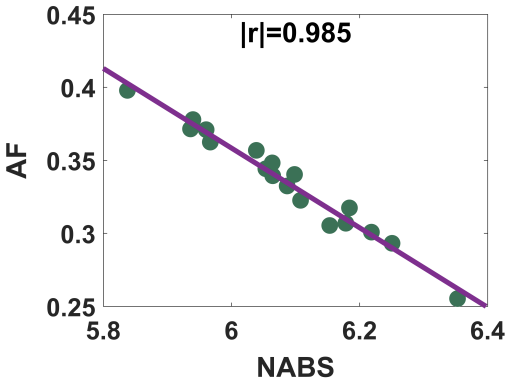

Figure 2. Linear fitting between $NABS$ and AF for octanes.

The R^2 values indicate that the variability in data for S, $DHVAP$,

and AF accounts for 88%, 74%, and 97% of the variance, respectively. Notably, the blue circles corresponding to AF in Figure 2 are positioned closer to the regression line than other data points. A decrease in the SE (standard error) value indicates a stronger regression relationship. All the equations mentioned result in a small SE, with AF exhibiting particularly low values. The model's consistency improves with a higher F-value, and in Model (9), the F-value is relatively high. The model is considered statistically reliable when the SF (significance F) value is less than 0.05, and in each case, the SF value is significantly less than 0.05. Therefore, it can be concluded that the $NABS$ index outperforms S and $DHVAP$ in explaining the acentric factor. Moving forward, external validation of the established model for AF is carried out using the nonane isomer as an external dataset. The dataset is partitioned into training and test sets in an 80 : 20 ratio using the Python scikit-learn machine learning module. The training set is used to generate the model, which is subsequently validated using the test set.

$$AF = -0.314(\pm 0.043)NABS + 2.55(\pm 0.306), \qquad (10)$$
$$SE = 0.015, \quad F = 203.669, \quad SF = 8.22 \times 10^{-14}, \quad R^2 = 0.89.$$

Equation (10) represents the structure-property relationship within the training set, with the data variance amounting to 89%. The test set demonstrates a data variance of 84%, confirming the meaningfulness of external validation. Now, we compare the performance of $NABS$ with other known indices. The concept of $NABS$ originates from the atom-bond sum-connectivity (ABS) index. Ali et al. [4] explored that the ABS index somewhat outperforms the connectivity index (R), sum-connectivity index (SCI), and atom-bond connectivity index (ABC). The correlation coefficients of these indices with S, $DHVAP$, and AF are listed in Table 2.

Table 2 illustrates that concerning $DHVAP$, the efficacy of $NABS$ is comparatively lower than the other four indices. However, for S and AF, it exhibits superior performance compared to the existing indices.

Next, we investigate certain benzenoid hydrocarbons (BHC) for analysis.

Table 2. The correlation coefficients between ABS, R, SCI, ABC, and $NABS$ with respect to S, $DHVAP$, and AF for octanes.

	ABS	R	SCI	ABC	$NABS$
S	0.885	0.906	0.923	0.815	**0.938**
$DHVAP$	0.954	0.958	0.961	0.917	0.861
AF	0.880	0.904	0.929	0.808	**0.985**

The molecular structures for BHC are seen in Figure 3. The $NABS$ index demonstrates a notable correlation between benzenoid hydrocarbons and the boiling point (BP). The linear regression equation including stastical parameters are reported as follows:

$$BP = 21.559(\pm 1.063)NABS + 20.527(\pm 23.641), \quad (11)$$
$$SE = 10.963, \quad F = 1642.76, \quad SF = 6.48 \times 10^{-20}, \quad R^2 = 0.989.$$

According to relation (11), 99% of observations fit the model related to BP, and the F-value is also significantly large. The linear fitting of this relation is depicted in Figure 4.

The correlation coefficients of ABS, R, SCI, ABC, and $NABS$ with BP for benzenoid hydrocarbons are reported in Table 3.

Table 3. The correlation coefficients of ABS, R, SCI, ABC, and $NABS$ with BP for benzenoid hydrocarbons.

	ABS	R	SCI	ABC	$NABS$
BP	0.993	0.996	0.997	0.996	**0.994**

The fundamental aim of a molecular descriptor is to establish correlations between structure and property. However, a good description should distinguish each structure clearly and include as many structural details as possible. Generating a single descriptor for distinct isomers is a problem that many indices encounter; this issue is known as degeneracy. This degeneracy is quantified by sensitivity [17], expressed as $S_{\mathrm{D}} = 1 - \frac{N_{\mathrm{D}}}{N}$, where N and N_{D} represent the total number of isomers and the total quantity

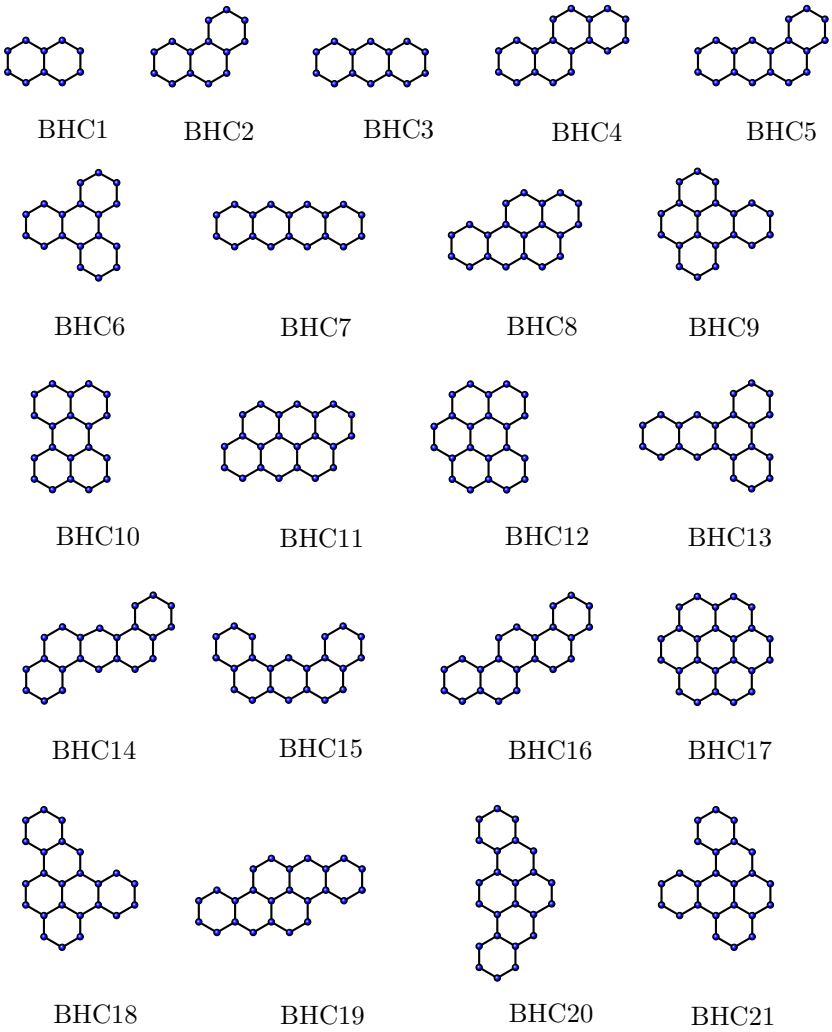

Figure 3. Molecular graphs of benzenoid hydrocarbons.

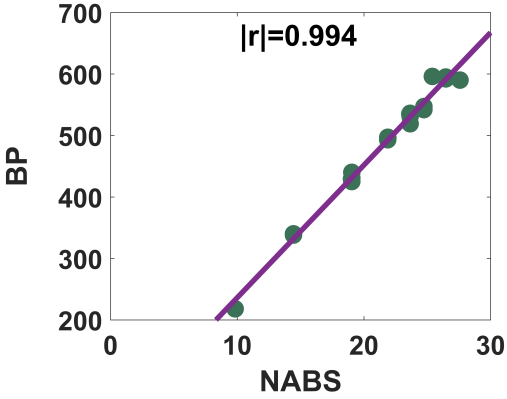

Figure 4. Linear fitting of $NABS$ with BP for benzenoid hydrocarbons.

not identifiable by the index D, respectively. The isomer discrimination ability of D is directly proportional to S_{D}. Figure 5 and Table 4 compares the sensitivity of $NABS$ with that of some well-established descriptors. It is clear that $NABS$ exerts better isomer discrimination ability than other well-known indices for octane, nonane and decane isomers.

Table 4. The sensitivity values of various indices for isomers of octane, nonane, and decane.

	M_1	F	M_2	R	ISI	SDD	SCI	ABC	ABS	$NABS$
Octane	0.333	0.389	0.722	0.889	0.722	0.889	0.889	0.889	0.889	1
Nonane	0.200	0.229	0.457	0.800	0.686	0.686	0.800	0.800	0.800	1
Decane	0.107	0.133	0.28	0.667	0.547	0.547	0.627	0.627	0.627	1

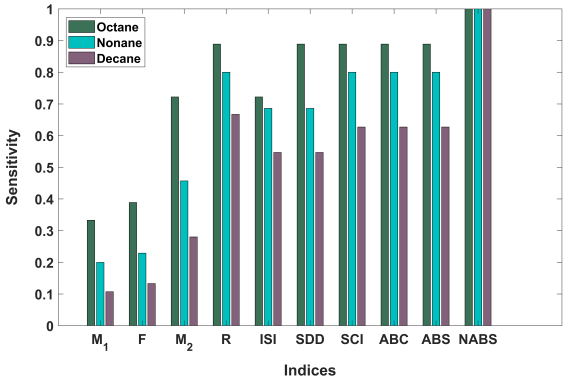

Figure 5. Comparison of isomer discrimination ability of different indices.

3 Bounds of NABS index

In this section we derive some crucial bounds of the $NABS$ index and characterize the extremal graphs. A Turan graph is a complete multipartite graph where the sizes of the partite sets differ by at most one. First, we report some inequalities that will be used later.

Lemma 1. *([27]) For a connected graph G of m edges and order n, such that it is K_{q+1}-free graph, we have*

$$m \leq \left(1 - \frac{1}{q}\right) \frac{n^2}{2}.$$

Equality in the above inequality occurs iff G is Turan graph.

Lemma 2. *[8] For any vertex $u \in V(G)$, we have*

$$\mu_G(u) = d_G(u)\, m_G(u) \leq 2m - d_G(u) - (n - d_G(u) - 1)\, \delta.$$

Theorem 1. *Let $f(x, y)$ be a non-negative symmetric real valued function, which is strictly increasing in x, y for $x \geq 1$, $y \geq 1$. Let $uv \notin E(G)$ for a graph G with max $\{\mu_G(u), \mu_G(v)\} \geq 1$. Then show that*

$$I(G + uv) = \sum_{uv \in E(G+uv)} f\big(\mu_G(u), \mu_G(v)\big) > \sum_{uv \in E(G)} f\big(\mu_G(u), \mu_G(v)\big) = I(G).$$

Proof. Let us consider $\mu_G(u) \geq \mu_G(v) \geq 0$. We assume $\mu_G(v) = 0$, which implies $\mu_G(u) \geq 1$. Therefore

$$\begin{aligned} & I(G+uv) - I(G) \\ &= \sum_{w \in N_G(u)} \Big[f\big(\mu_G(u)+1,\, \mu_G(w)+1\big) - f\big(\mu_G(u),\, \mu_G(w)\big) \Big] \\ &\quad + f\left(\mu_G(u)+1,\, d_G(u)+1\right) > 0. \end{aligned}$$

Now we consider $\mu_G(v) \geq 1$. Thus, we obtain

$$\begin{aligned} & I(G+uv) - I(G) \\ &= \sum_{w \in N_G(u)} \Big[f\big(\mu_G(u)+d_G(v)+1,\, \mu_G(w)+1\big) - f\big(\mu_G(u),\, \mu_G(w)\big) \Big] \\ &\quad \sum_{w' \in N_G(v)} \Big[f\big(\mu_G(v)+d_G(u)+1,\, \mu_G(w')+1\big) - f\big(\mu_G(v),\, \mu_G(w')\big) \Big] \\ &\quad + f\big(\mu_G(u)+d_G(v)+1,\, \mu_G(v)+d_G(u)+1\big) > 0. \end{aligned}$$

Hence the proof is completed. ■

Employing Theorem 1, we get the following corollary.

Corollary 2. *For two non-adjacent and non-isolated vertices u, v in G, we have*

$$NABS(G+uv) > NABS(G).$$

Using Corollary 2, we obtain following results.

Corollary 3. *Let G be a graph of order n, then we obtain*

$$NABS(G) \leq \frac{n\sqrt{n^2-2n}}{2},$$

where equality appears iff $G \cong K_n$.

Corollary 4. *For a bipartite graph G of order n, we obtain*

$$NABS(G) \leq \sqrt{\left\lceil \frac{n}{2} \right\rceil \left\lfloor \frac{n}{2} \right\rfloor \left(\left\lceil \frac{n}{2} \right\rceil \left\lfloor \frac{n}{2} \right\rfloor - 1 \right)},$$

where equality occurs iff $G \cong K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$.

Proof. For a bipartite graph G (of order n) having partite sets U, V such that $|U| = x \geq y = |V|$, (say). Then $x + y = n$ and $x \geq y \geq 1$. Using Corollary 2, one can write

$$NABS(G) \leq NABS(K_{x,y}) = \sqrt{xy(xy-1)} \leq \sqrt{\left\lceil \frac{n}{2} \right\rceil \left\lfloor \frac{n}{2} \right\rfloor \left(\left\lceil \frac{n}{2} \right\rceil \left\lfloor \frac{n}{2} \right\rfloor - 1 \right)}.$$

Moreover, the equality appears iff $G \cong K_{\lceil \frac{n}{2} \rceil, \lfloor \frac{n}{2} \rfloor}$. ■

In the context of a graph G, an independent set S (where $S \subseteq V(G)$) is characterized by the absence of edges between its vertices. The independence number, denoted by α, represents the size of the largest such independent set in the graph. A graph labeled as a complete split graph $CS(n, \alpha)$ (where $1 \leq \alpha \leq n$) consists of a clique containing $n - \alpha$ nodes and a stable set containing α nodes. Notably, each node in the clique is connected to every node in the stable set.

Corollary 5. *For a graph G having n nodes with independence number α, we have*

$$NABS(G) \leq (n-\alpha)\,\alpha \sqrt{1 - \frac{2}{(n-1)\,(n-\alpha) + (n-1)^2 - (\alpha-1)\,\alpha}} + \frac{(n-\alpha)\,(n-\alpha-1)}{2} \sqrt{1 - \frac{1}{(n-1)^2 - (\alpha-1)\,\alpha}},$$

where equality holds iff $G \cong CS(n, \alpha)$.

Proof. First we derive $NABS(CS(n, \alpha))$. For this, we have $\mu_G(u) = (n-1)\,(n-\alpha)$ for $u \in S$ and $\mu_G(u) = (n-1)^2 - (\alpha-1)$ for $u \in V(CS(n, \alpha)) \backslash S$.

$$NABS(CS(n, \alpha)) = \sum_{\substack{uv \in E(CS(n,\,\alpha)),\\ u \in S, v \in V(CS(n,\,\alpha)) \backslash S}} \sqrt{1 - \frac{2}{\mu_G(u) + \mu_G(v)}} + \sum_{\substack{uv \in E(CS(n,\,\alpha)),\\ u \in V(CS(n,\,\alpha)) \backslash S, v \in V(CS(n,\,\alpha)) \backslash S}} \sqrt{1 - \frac{2}{\mu_G(u) + \mu_G(v)}}$$

$$= (n-\alpha)\,\alpha\sqrt{1-\frac{2}{(n-1)\,(n-\alpha)+(n-1)^2-(\alpha-1)\,\alpha}}$$

$$+\frac{(n-\alpha)\,(n-\alpha-1)}{2}\sqrt{1-\frac{1}{(n-1)^2-(\alpha-1)\,\alpha}}.$$

Consequently, equality occurs when $G \cong CS(n,\,\alpha)$. Otherwise, $G \ncong CS(n,\,\alpha)$. Now using Corollary 2 (several times if needed), we obtain

$$NABS(G) < \cdots < NABS(CS(n,\,\alpha)).$$

This completes the proof of the theorem. ■

Theorem 6. *Let T be a tree of order n, then we obtain $NABS(T) \leq \sqrt{(n-1)\,(n-2)}$, where equality occurs iff $T \cong S_n$.*

Proof. Note that $m = n-1$, $\delta = 1$ for a tree T. Employing Lemma 2, we have

$$\mu_G(u) \leq 2m - (n - d_G(u) - 1) - d_G(u) = n-1,$$

for any vertex $u \in V(G)$. For any edge $uv \in E(T)$, we obtain

$$\mu_G(u) + \mu_G(v) \leq 2(n-1),$$

where equality occurs iff $\mu_G(u) = \mu_G(v) = n-1$. Consequently

$$\begin{aligned} NABS(T) &= \sum_{uv\in E(T)}\sqrt{1-\frac{2}{\mu_G(u)+\mu_G(v)}} \\ &\leq \sum_{uv\in E(T)}\sqrt{1-\frac{1}{n-1}} = \sqrt{(n-1)\,(n-2)} \end{aligned}$$

where equality appears iff $\mu_G(u) = \mu_G(v) = n-1$ for all $uv \in E(T)$, that is, iff $T \cong S_n$. ■

Let S_n' be a unicyclic graph generated from star graph by connecting two pendent vertices. We now determine an upper bound of $NABS$ for any unicyclic graph G, and identify the extremal graph.

Theorem 7. *For a unicyclic graph G containing n nodes, we have*

$$NABS(G) \leq (n-3)\sqrt{\frac{n-1}{n}} + 3\sqrt{\frac{n}{n+1}}.$$

The equality holds iff $G \cong S'_n$.

Proof. If ℓ is the length of the cycle in G, then $3 \leq \ell \leq n$. We construct the following cases:

Case 1. $\ell = 3$. Let x, y and z be three vertices on the cycle in G such that $d_G(\mathrm{x}) \geq d_G(\mathrm{y}) \geq d_G(\mathrm{z})$. Let E'' be the collection of edges on the cycle in G.

Case 1.1 $d_G(\mathrm{y}) > 2$. In this case $\mu_G(u) \leq n+1$ for $u \in \{x, y, z\}$ and $\mu_G(u) \leq n-2$ for $u \in V(G)\backslash\{x, y, z\}$. We have

$$\sqrt{1 - \frac{2}{\mu_G(u) + \mu_G(v)}} \leq \sqrt{\frac{n}{n+1}} \quad \text{for} \quad uv \in E''$$

and

$$\sqrt{1 - \frac{2}{\mu_G(u) + \mu_G(v)}} \leq \sqrt{1 - \frac{2}{2n-1}} \quad \text{for} \quad uv \in E(G\backslash E'').$$

One can easily check that

$$\begin{aligned} NABS(G) &= \sum_{uv \in E(G)} \sqrt{1 - \frac{2}{\mu_G(u) + \mu_G(v)}} \\ &\leq 3\sqrt{\frac{n}{n+1}} + (n-3)\sqrt{1 - \frac{2}{2n-1}} \\ &< (n-3)\sqrt{\frac{n-1}{n}} + 3\sqrt{\frac{n}{n+1}}. \end{aligned}$$

Case 1.2 $d_G(\mathrm{y}) = 2$. Then $d_G(\mathrm{z}) = 2$. If all the vertices in $V(G)\backslash\{x, y, z\}$ are adjacent to vertex x, then $G \cong S'_n$. Thus the equality occurs. Otherwise, $x \leq n-2$. Note that $\mu_G(\mathrm{x}) \leq n+1$, $\mu_G(\mathrm{y}) \leq n$, $\mu_G(\mathrm{z}) \leq n$ and

$\mu_G(u) \leq n-1$ for $u \in V(G)\backslash\{x, y, z\}$. Hence

$$\begin{aligned} NABS(G) &= \sum_{uv\in E(G)} \sqrt{1-\frac{2}{\mu_G(u)+\mu_G(v)}} \\ &\leq 2\sqrt{1-\frac{2}{2n+1}}+\sqrt{\frac{n-1}{n}}+(n-3)\sqrt{\frac{n-1}{n}} \\ &< (n-3)\sqrt{\frac{n-1}{n}}+3\sqrt{\frac{n}{n+1}}. \end{aligned}$$

Case 2. $\ell = 4$. Let V' and E' be the collection of nodes and edges on the cycle in G, respectively. For each $u \in V(G)$, there is at least one non-pendant node v for which $uv \notin E(G)$. In this case

$$\sum_{v:\, uv\notin E(G)} d_G(v) \geq (n-d_G(u)-1)+1 = n-d_G(u)$$

and by Lemma 2, we obtain

$$\mu_G(u) \leq 2n-d_G(u)-(n-d_G(u)), \quad \text{that is,} \quad \mu_G(u) \leq n$$

for each $u \in V(G)$. Moreover, in view of Lemma 2, we obtain $\mu_G(u) \leq n-2$ for any $u \in V(G)\backslash V'$, as

$$\sum_{v:\, uv\notin E(G)} d_G(v) \geq (n-d_G(u)-1)+3 = n-d_G(u)+2.$$

It is evident that

$$\sqrt{1-\frac{2}{\mu_G(u)+\mu_G(v)}} \leq \sqrt{\frac{n-1}{n}} \quad \text{for} \quad uv \in E',$$

and

$$\sqrt{1-\frac{2}{\mu_G(u)+\mu_G(v)}} \leq \sqrt{\frac{n-2}{n-1}} \quad \text{for} \quad uv \in E(G\backslash E').$$

Hence

$$NABS(G) = \sum_{uv \in E'} \sqrt{1 - \frac{2}{\mu_G(u) + \mu_G(v)}} + \sum_{uv \in E(G \setminus E')} \sqrt{1 - \frac{2}{\mu_G(u) + \mu_G(v)}}$$

$$\leq 4\sqrt{\frac{n-1}{n}} \times +(n-4)\sqrt{\frac{n-2}{n-1}}$$

$$< (n-3)\sqrt{\frac{n-1}{n}} + 3\sqrt{\frac{n}{n+1}}.$$

Case 3. $\ell \geq 5$. At least two non-pendant nodes are non-adjacent to the vertex u, where u is any vertex in G. In this case we have

$$\sum_{v:\, uv \notin E(G)} d_G(v) \geq (n - d_G(u) - 1) + 2 = n - d_G(u) + 1.$$

By Lemma 2, we obtain

$$\mu_G(u) \leq 2n - d_G(u) - (n - d_G(u) + 1), \quad \text{that is,} \quad \mu_G(u) \leq n - 1$$

for any vertex $u \in V(G)$ as $m = n$. Note that, for each $uv \in E(G)$,

$$\sqrt{1 - \frac{2}{\mu_G(u) + \mu_G(v)}} \leq \sqrt{\frac{n-2}{n-1}}.$$

Hence

$$NABS(G) = \sum_{uv \in E(G)} \sqrt{1 - \frac{2}{\mu_G(u) + \mu_G(v)}}$$

$$\leq n\sqrt{\frac{n-2}{n-1}} < (n-3)\sqrt{\frac{n-1}{n}} + 3\sqrt{\frac{n}{n+1}}.$$

■

Lemma 3. [28] *For a connected graph G, $\mu_G(u) = \mu_G(v)$ for all $u, v \in V(G)$ iff G is a regular graph or a bipartite semi-regular graph.*

Let $\delta_N = min\{\mu_G(u) : u \in V(G)\}$ and $\Delta_N = max\{\mu_G(u) : u \in V(G)\}$.

Theorem 8. *Let G be a connected graph with m edges. Then we obtain*

$$m\sqrt{\frac{\delta_N - 1}{\Delta_N}} \leq NABS(G) \leq m\sqrt{\frac{\Delta_N - 1}{\delta_N}},$$

where both the equalities occur iff G is regular or bipartite semi-regular.

Proof. For $uv \in E(G)$, we obtain

$$\sqrt{\frac{\mu_G(u) + \mu_G(v) - 2}{\mu_G(u) + \mu_G(v)}} = \sqrt{\frac{1}{\mu_G(u) + \mu_G(v)}}.\sqrt{\mu_G(u) + \mu_G(v) - 2}.$$

It follows from

$$\sqrt{(2\delta_N - 2)} \leq \sqrt{\mu_G(u) + \mu_G(v) - 2} \leq \sqrt{(2\Delta_N - 2)}$$

and

$$\sqrt{\frac{1}{2\Delta_N}} \leq \sqrt{\frac{1}{\mu_G(u) + \mu_G(v)}} \leq \sqrt{\frac{1}{2\delta_N}}$$

that

$$m\sqrt{\frac{\delta_N - 1}{\Delta_N}} \leq NABS(G) \leq m\sqrt{\frac{\Delta_N - 1}{\delta_N}}.$$

Both the equalities are satisfied iff $\mu_G(u) = \mu_G(v)$ for all $u, v \in V(G)$. Hence by Lemma 3, the equalities occur iff G is regular or bipartite semi-regular. ■

It is evident that for a graph G, we have $\Delta_N \leq \Delta^2$ and $\delta_N \geq \delta^2$, where the equality occurs iff G is regular. Combining this fact with Theorem 8, we obtain the following result.

Corollary 9. *Let G be a connected graph with m edges. Then we obtain*

$$m\sqrt{\frac{\delta^2 - 1}{\Delta^2}} \leq NABS(G) \leq m\sqrt{\frac{\Delta^2 - 1}{\delta^2}},$$

where both the equalities occur iff G is regular.

Employing Lemma 1 on the above corollary we obtain the following result.

Corollary 10. *For a connected graph G of order n with chromatic number χ (provided χ divides n), we have*

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

where the equality occurs iff G is a complete χ-partite graph, with all partite sets of vertices possess same cardinality.

4 Concluding remarks

The neighborhood degree sum based atom bond sum connectivity index has been introduced in this work parallel to the well-established ABS index. The chemical significance of this index has been extensively investigated. The $NABS$ has been found to adequately explain entropy, standard enthalpy of vaporization, and the acentric factor of octanes. Its performance is notable for AF. Its correlation has been observed to be better for S and AF compared to ABS, R, SCI and ABC. External validation considering nonane isomers has been noticed to be meaningful. This novel index has also remarkable linear relation with the boiling point of benzenoid hydrocarbons. The isomer discrimination ability of $NABS$ outperforms some well-established indices including ABS. Consequently, it can be concluded that the incorporation of $NABS$ into chemical graph theory is not arbitrary but rather essential. The extremal graphs have been characterized for different family of graphs including tree, unicyclic, bipartite, and general connected graph, in terms numerous graph parameters. Future research may delve deeper into the specific advantages of the NABS index in characterizing complex structures and networks, fostering innovation in both mathematical theory and applied sciences.

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

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

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

[5] S. C. Basak, A. K. Bhattacharjee, Computational approaches for the design of mosquito repellent chemicals, *Curr. Med. Chem.* **27** (2020) 32–41.

[6] M. Chamua, R. Moran, A. Pegu, A. Bharali, M-polynomial and neighborhood M-polynomial of some concise drug structures: Azacitidine, Decitabine and Guadecitabine, *J. Mol. Struct.* **1263** (2022) 133197.

[7] K. C. Das, I. Gutman, B. Furtula, On atom-bond connectivity index, *Chem. Phys. Lett.* **511** (2011) 452–454.

[8] K. C. Das, S. Mondal, On neighborhood inverse sum indeg index of molecular graphs with chemical significance, *Inf. Sci.* **623** (2023) 112–131.

[9] K. C. Das, S. Mondal, R. Zahid, On Zagreb connection indices, *Eur. Phys. J. Plus*, **137** (2022) 1242.

[10] M. V. Diudea, I. Gutman, L. Jantschi, *Molecular Topology*, Nova, Huntington, 2001.

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

[12] E. Estrada, The ABC matrix, *J. Math. Chem.* **55** (2017) 1021–1033.

[13] B. Furtula, I. Gutman, M. Ivanović, D. Vukičević, Computer search for trees with minimal ABC index, *Appl. Math. Comput.* **219** (2012) 767–772.

[14] Y. Gao, Y. Shao, The smallest ABC index of trees with n pendent vertices, *MATCH Commun. Math. Comput. Chem.* **76** (2016) 141–158.

[15] D. M. Hawkins, S. C. Basak, X. Shi, QSAR with few compounds and many features, *J. Chem. Inf. Comput.* **41** (2001) 663–670.

[16] 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.

[17] E. V. Konstantinova, The discrimination ability of some topological and information distance indices for graphs of unbranched hexagonal systems, *J. Chem. Inf. Comput. Sci.* **36** (1996) 54–57.

[18] S. Mondal, K. C. Das, On the Sanskruti index of graphs, *J. Appl. Math. Comput.* **69** (2023) 1205–1219.

[19] S. Mondal, N. De, A. Pal, On neighborhood Zagreb index of product graphs, *J. Mol. Struct.* **1223** (2021) 129210.

[20] S. Mondal, N. De, A. Pal, Neighborhood degree sum-based molecular descriptors of fractal and Cayley tree dendrimers, *Eur. Phys. J. Plus* **136** (2021) 1–37.

[21] S. Mondal, S. Barik, N. De, A. Pal, A note on neighborhood first Zagreb energy and its significance as a molecular descriptor, *Chemometr. Intell. Lab. Syst.* **222** (2022) 104494.

[22] S. Mondal, N. De, A. Pal, A note on some novel graph energies, *MATCH Commun. Math. Comput. Chem.* **86** (2021) 663–684.

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

[24] 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.

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

[26] T. Reti, A. Ali, P. Varga, E. Bitay, Some properties of the neighborhood first Zagreb index, *Discrete Math. Lett.* **2** (2019) 10–17.

[27] P. Turan, On an external problem in graph theory, *Mat. Fiz. Lapok* **48** (1941) 436–452.

[28] L. You, Y. Shu, X. D. Zhang, A sharp upper bound for the spectral radius of a nonnegative matrix and applications, *Czech. Math. J.* **66** (2016) 701–715.

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