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Research Paper

On Relations between Atom-Bond Sum-Connectivity Index and other Degree-Based Indices

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Abstract

The atom-bond sum-connectivity (ABS) index is a novel vertex degree-based topological index defined recently as, $ABS(G) = \sum_{i\sim j}\sqrt{\frac{d_i+d_j-2}{d_i+d_j}} = \sum_{i\sim j}\sqrt{1-\frac{2}{d_i+d_j}}$, where d_i, d_j are degrees of vertices i and j respectively. New findings linking the ABS-index to extensively researched topological indices are presented in this work.

1 Introduction

Throughout the study, G represents a finite simple non-trivial connected graph of order n and size m with the maximum and the minimum degree, Δ and δ respectively.
By considering atoms as vertices and bonds as edges, a graph can be used to depict chemical compounds. Different kinds of topological matrices, such as adjacency or distance matrices, can characterize the connections between the atoms. These matrices can be computationally modified to produce a single number that is commonly referred to as a topological index. Consequently, the topological index may be characterized as two-dimensional descriptors that are simply computed from the molecular graphs and do not need energy reduction of the chemical structure or dependence on how the graph is labelled or shown. Thus, it is a number that correlates with a molecular attribute and describes a chemical structure in graph theoretical terms using the molecular graph [1]. This section defines several topological indices that will be utilized in the next parts. Here $i \sim j$ indicates that vertex i is adjacent to vertex j in graph G.

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Randić index [2]	$R(G) = \sum\limits_{i\sim j} \frac{1}{\sqrt{d_i d_j}}$,
Sum-connectivity index [3]	$\chi(G) = \sum\limits_{i\sim j} \frac{1}{\sqrt{d_i + d_j}}$,
General sum-connectivity index [4]	$\chi_\alpha(G) = \sum\limits_{i\sim j} (d_i + d_j)^\alpha$,
Harmonic index [5]	$H(G) = \sum\limits_{i\sim j} \frac{2}{d_i + d_j}$,
First Zagreb index [6]	$M_1(G) = \sum\limits_{v\in V(G)} d_j^2$,
Hyper Zagreb index [7]	$HM(G) = \sum\limits_{i\sim j} (d_i + d_j)^2$,
Augmented Zagreb-index [8]	$AZI(G) = \sum\limits_{i\sim j} \left(\frac{d_i d_j}{d_i + d_j - 2}\right)^3$,
Sum-connectivity F-index [9]	$SF(G) = \sum\limits_{i\sim j} \frac{1}{\sqrt{d_i^2 + d_j^2}}$,
Atom-bond connectivity index [10]	$ABC(G) = \sum\limits_{i\sim j} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}}$,
General Platt index [11]	$Pl_\alpha(G) = \sum\limits_{i\sim j} (d_i + d_j - 2)^\alpha$.

By combining the fundamental concepts of the sum-connectivity and atom-bond connectivity indices, Akbar Ali et al. [12] introduced the atom-bond sum connectivity index(ABS-index) in 2022 as:

$$ABS(G) = \sum_{i\sim j} \sqrt{\frac{d_i + d_j - 2}{d_i + d_j}} = \sum_{i\sim j} \sqrt{1 - \frac{2}{d_i + d_j}}.$$

It immediately drew the attention of experts working on chemical graph theory. The study of ABS-index of trees and unicyclic graphs was done in [13–16]. In [17], the extremal ABS-index was calculated over all n-vertex chemical trees. The characterisation of the graphs with maximum values of the ABS-index was done in [18], and bounds for the graph ABS-index were provided in [19, 20]. The ABS-index of line graphs was defined and studied in [21].The general ABS-index was defined and explored in [22–24]. So it will be interesting and meaningful to find relationships between the ABS- index with other topological indices. For more details about relationships between different topological indices, one can refer to [25–27].

Lemma 1.1. *(Diaz-Metcalf inequality) ([28]). Let x_i and y_i, $i = 1, 2, ..., n$ be real numbers such that $x_i \neq 0$ and $Xx_i \leq y_i \leq Yx_i$ for each $i = 1, 2, ..., n$. Then $(X+Y)\sum\limits_{i=1}^{n} x_i y_i \geq \sum\limits_{i=1}^{n} y_i^2 + XY \sum\limits_{i=1}^{n} x_i^2$ with equality holds if and only if either $y_i = Xx_i$ or $y_i = Yx_i$.*

Lemma 1.2. *([29]). Let $(\varphi_i)_{i=1}^n$ and $(\varpi_i)_{i=1}^n$ be two sequences of real numbers satisfying $0 \leq \varepsilon_1 \leq \varphi \leq \varkappa_1$ and $0 \leq \varepsilon_2 \leq \varpi_i \leq \varkappa_2$ for every i, $i = 1, 2, \ldots, n$. Then,*

$$\sum_{i=1}^{n} \varphi_i^2 \sum_{i=1}^{n} \varpi_i^2 - \left(\sum_{i=1}^{n} \varphi_i \varpi_i\right)^2 \leq \frac{n^2}{4}[\varkappa_1\varkappa_2 - \varepsilon_1\varepsilon_2]^2.$$

Lemma 1.3. *([30]). Let $(a_i)_{i=1}^n$ be a sequence of non-negative and $(b_i)_{i=1}^n$ be a sequence of positive real numbers. Then for any $r \geq 0$, $\sum\limits_{i=1}^{n} \frac{a_i^{r+1}}{b_i^r} \geq \frac{\left(\sum\limits_{i=1}^{n} a_i\right)^{r+1}}{\left(\sum\limits_{i=1}^{n} b_i\right)^r}$, equality attained if and only if $\frac{a_1}{b_1} = \frac{a_2}{b_2} = \cdots = \frac{a_n}{b_n}$.*

Lemma 1.4. *([31]). Let $(\omega_i)_{i=1}^n$ be a sequence of positive real numbers and let $(\alpha_i)_{i=1}^n$ and $(\beta_i)_{i=1}^n$ be two sequences of non-negative real numbers of opposite monotonicity. Then,*

$$\sum_{i=1}^n \omega_i \sum_{i=1}^n \omega_i\alpha_i\beta_i \leq \sum_{i=1}^n \omega_i\alpha_i \sum_{i=1}^n \omega_i\beta_i.$$

Equality is maintained in either scenario if and only if $\beta_1 = \beta_2 = ... = \beta_n$ or $\alpha_1 = \alpha_2 = ... = \alpha_n$.

Lemma 1.5. *([32]). Let $(x_i)_{i=1}^n$ and $(y_i)_{i=1}^n$ be sequences of real numbers and also $z = (z_i)_{i=1}^n$ and $w = (w_i)_{i=1}^n$ be sequences of non-negative real numbers. Then,*

$$\sum_{i=1}^n w_i \sum_{i=1}^n z_i x_i^2 + \sum_{i=1}^n z_i \sum_{i=1}^n w_i y_i^2 \geq 2 \sum_{i=1}^n z_i x_i \sum_{i=1}^n w_i y_i.$$

The equality is only valid if and only if $x = y = k$, where $k = (k, k, \dots, k)$ is a constant sequence, and z_i and w_i are positive.

Remark 1. ([33]). For every edge ij it holds that,

$$\sqrt{\frac{\delta-1}{\Delta}} \leq \sqrt{1-\frac{2}{d_i+d_j}} \leq \sqrt{\frac{\Delta-1}{\delta}}. \tag{1}$$

Lemma 1.6. *([34]). If $\eta_i, \zeta_i \geq 0$ and $\alpha\zeta_i \leq \eta_i \leq \beta\zeta_i$ for $1 \leq i \leq k$, then,*

$$\left(\sum_{i=1}^k \eta_i^2\right)\left(\sum_{i=1}^k \zeta_i^2\right) \leq \frac{1}{4}\left(\sqrt{\frac{\alpha}{\beta}} + \sqrt{\frac{\beta}{\alpha}}\right)\sum_{i=1}^k \eta_i\zeta_i.$$

If $\eta_i > 0$ for some $1 \leq i \leq k$, then equality holds if and only if $\alpha = \beta$ and $\eta = \alpha\beta$ for every $1 \leq i \leq k$.

2 Relation between ABS-index with other degree-based topological indices

In [12], an upper bound for the ABS- index is presented using the harmonic index, we now present some lower bounds using the harmonic index.

Theorem 2.1. *For any graph G with $\Delta \geq 2$,*

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

(ii) $ABS(G) \geq 2\frac{\sqrt{m(m-H(G))\sqrt{\delta\Delta(\delta-1)(\Delta-1)}}}{\sqrt{\delta(\delta-1)}+\sqrt{\Delta(\Delta-1)}}$.

Further, the equality holds if and only if G is a regular graph.

Proof. (i) By taking $y_{ij} = \sqrt{1-\frac{2}{d_i+d_j}}$, $x_{ij} = 1$, for each edge $i \sim j$, and using Equation (1), by substituting $X = \sqrt{\frac{\delta-1}{\Delta}}$ and $Y = \sqrt{\frac{\Delta-1}{\delta}}$ in Lemma 1.1, we get:

$$\left(\sqrt{\frac{\delta-1}{\Delta}} + \sqrt{\frac{\Delta-1}{\delta}}\right)\sum_{i\sim j}\sqrt{1-\frac{2}{d_i+d_j}} \geq \sum_{i\sim j}\left(1-\frac{2}{d_i+d_j}\right) + \sqrt{\frac{\delta-1}{\Delta}}\sqrt{\frac{\Delta-1}{\delta}}\sum_{i\sim j}1.$$

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

yields the desired result.
(ii) By taking $\eta_{ij} = \sqrt{1 - \frac{2}{d_i+d_j}}$, $\zeta_{ij} = 1$, for each edge $i \sim j$, and using Equation (1), by substituting $\alpha = \sqrt{\frac{\delta-1}{\Delta}}$ and $\beta = \sqrt{\frac{\Delta-1}{\delta}}$ in Lemma 1.6, we get:

$$\sum_{i\sim j}\left(1 - \frac{2}{d_i + d_j}\right)\sum_{i\sim j} 1 \leq \left(\sum_{i\sim j}\sqrt{1 - \frac{2}{d_i + d_j}}\right)^2 \frac{\left(\sqrt{\frac{\delta-1}{\Delta}} + \sqrt{\frac{\Delta-1}{\delta}}\right)^2}{4\sqrt{\frac{\delta-1}{\Delta}}\sqrt{\frac{\Delta-1}{\delta}}}.$$

This implies that,

$$m(m - H(G)) \leq (ABS(G))^2 \frac{\left(\sqrt{\delta(\delta-1)} + \sqrt{\Delta(\Delta-1)}\right)^2}{4\sqrt{\delta\Delta(\delta-1)(\Delta-1)}}.$$

Furthermore, by Lemma 1.6 and Equation (1), equality holds if and only if $\sqrt{\frac{\delta-1}{\Delta}} = \sqrt{\frac{\Delta-1}{\delta}}$ and
$\sqrt{1 - \frac{2}{d_i+d_j}} = \sqrt{\frac{\delta-1}{\Delta}}$, which is possible if and only if G is a regular graph. ■

In [20], it is proved that for any connected graph G with the minimum degree δ and the maximum degree Δ,

$$ABS(G) \geq \sqrt{\delta(\delta-1)}. \qquad (2)$$

If G is a graph with $\delta = 1$ and $\Delta \geq 2$, then the lower bound in Equation (2) is zero but bounds obtained in Theorem 2.1 are nonzero. Thus, the lower bounds obtained in Theorem 2.1 are better than the lower bound in Equation (2) for $\delta = 1$ and $\Delta \geq 2$.

We present a bound for atom-bond sum connectivity index using the harmonic index and sum-connectivity F-index.

Theorem 2.2. *For any graph G, $ABS(G) \leq \sqrt{(m - H(G))SF(G)\sqrt{2}\Delta}$. Equality holds if and only if G is regular.*

Proof. By taking $r = 1$, $a_{ij} = \sqrt{\frac{d_i+d_j-2}{d_i+d_j}}$ and $b_{ij} = \frac{1}{\sqrt{d_i^2+d_j^2}}$, for each edge $i \sim j$, in Lemma 1.3, we get:

$$\frac{\left(\sum_{i\sim j}\sqrt{\frac{d_i+d_j-2}{d_i+d_j}}\right)^2}{\sum_{i\sim j}\frac{1}{\sqrt{d_i^2+d_j^2}}} \leq \sum_{i\sim j}\left(1 - \frac{2}{d_i + d_j}\right)\sqrt{d_i^2 + d_j^2}.$$

This implies that,

$$\frac{(ABS(G))^2}{SF(G)} \leq [m - H(G)]\,\sqrt{2}\Delta.$$

Furthermore, by Lemma 1.3, equality holds if and only if G is regular. ■

Next, by employing the first Zagreb index, sum-connectivity/general sum-connectivity index and Randić index some bounds are presented.

Theorem 2.3. *For any graph G,*

$$\sqrt{(M_1(G)-2m)\chi_{-1}(G)-\frac{m^2}{4}\left(\sqrt{\frac{\Delta-1}{\delta}}-\sqrt{\frac{\delta-1}{\Delta}}\right)^2}\leq ABS(G)\leq\sqrt{\chi_{-1}(G)(M_1(G)-2m)}.$$

Furthermore, equality holds if and only if G is a regular graph and R.H.S equality is also holds for semiregular bipartite graph,

Proof. By taking $\varphi_{ij}=\sqrt{d_i+d_j-2}$, $\varpi_{ij}=\frac{1}{\sqrt{d_i+d_j}}$, for each edge $i\sim j$, $\varepsilon_1=\sqrt{2\delta-2}$, $\varkappa_1=\sqrt{2\Delta-2}$, $\varepsilon_2=\frac{1}{\sqrt{2\Delta}}$ and $\varkappa_2=\frac{1}{\sqrt{2\delta}}$ in Lemma 1.2, we have:

$$\begin{aligned}&\frac{m^2}{4}\left(\sqrt{\frac{\Delta-1}{\delta}}-\sqrt{\frac{\delta-1}{\Delta}}\right)^2\\&\geq\sum_{i\sim j}(d_i+d_j-2)\sum_{i\sim j}\frac{1}{d_i+d_j}-\left(\sum_{i\sim j}\sqrt{\frac{d_i+d_j-2}{d_i+d_j}}\right)^2\\&=(M_1(G)-2m)\chi_{-1}(G)-(ABS(G))^2,\end{aligned}$$

and by taking $a_{ij}=\sqrt{\frac{d_i+d_j-2}{d_i+d_j}}$, $b_{ij}=\frac{1}{d_i+d_j}$, for each edge $i\sim j$, and $r=1$ in Lemma 1.3, we get:

$$\frac{\left(\sum\limits_{i\sim j}\sqrt{\frac{d_i+d_j-2}{d_i+d_j}}\right)^2}{\sum\limits_{i\sim j}\frac{1}{d_i+d_j}}\leq\sum_{i\sim j}(d_i+d_j-2).$$

This implies that:

$$\frac{(ABS(G))^2}{\chi_{-1}(G)}\leq M_1(G)-2m.$$

If graph G is regular, then on both sides equality holds and if G is a complete bipartite graph, then equality holds on the R.H.S. ■

Theorem 2.4. *([19]). For any graph G of size m without isolated vertices, $ABS(G)\leq\sqrt{\frac{(M_1(G)-2m)H(G)}{2}}$. Equality holds if and only if G is a regular or semiregular bipartite graph.*

By using the fact that, $\frac{H(G)}{2}=\chi_{-1}(G)$, the result coincides with the upper bound of Theorem 2.3.

The following corollary follows from the fact that $M_1(G)-2m=pl(G)$, where $pl(G)$ is the Platt index of graph G.

Corollary 2.5. *For any graph G,*

$$\sqrt{pl(G)\chi_{-1}(G)-\frac{m^2}{4}\left(\sqrt{\frac{\Delta-1}{\delta}}-\sqrt{\frac{\delta-1}{\Delta}}\right)^2}\leq ABS(G)\leq\sqrt{\chi_{-1}(G)Pl(G)}.$$

Furthermore, equality holds on the left-hand side if and only if for regular graphs and on the right-hand side if and only if for complete bipartite graphs and R.H.S equality is also holds for complete bipartite graph.

The following inequality proved in [35],

$$M_1(G) \leq 2m(\delta+\Delta) - n\delta\Delta.$$

Equality holds if and only if G is a regular graph. Now the upper bound of Theorem 2.3, can be written as $ABS(G) \leq \sqrt{2m(\delta+\Delta-1) - n\delta\Delta\chi_{-1}(G)}$.

Theorem 2.6. *For any graph G, $ABS(G) \leq \frac{(M_1(G)-2m)\chi(G)}{m}$ with equality holds if and only if G is K_2.*

Proof. By taking $\alpha_{ij} = \sqrt{d_i+d_j-2}$, $\beta_{ij} = \frac{1}{\sqrt{d_i+d_j}}$, for each edge $i \sim j$, and $\omega_{ij} = 1$, in Lemma 1.4 as α_{ij} and β_{ij} are of opposite monotonicity we have:

$$\sum_{i\sim j} 1 \sum_{i\sim j} \sqrt{\frac{d_i+d_j-2}{d_i+d_j}} \leq \sum_{i\sim j} \sqrt{d_i+d_j-2} \sum_{i\sim j} \frac{1}{\sqrt{d_i+d_j}}. \tag{3}$$

This implies that:

$$mABS(G) \leq \sum_{i\sim j}(d_i+d_j-2) \sum_{i\sim j} \frac{1}{\sqrt{d_i+d_j}}.$$

Thus,

$$mABS(G) \leq (M_1(G)-2m)\chi(G).$$

Furthermore, by Lemma 1.4, equality holds if and only if $\alpha_1 = \alpha_2 = \cdots = \alpha_n$ or $\beta_1 = \beta_2 = \cdots = \beta_n$ and using the fact that $\sqrt{d_i+d_j-2} = (d_i+d_j-2)$ if and only if $d_i = d_j = 1$. ■

The following corollary is an immediate result of Equation (3).

Corollary 2.7. *For any graph G, $ABS(G) \leq \frac{Pl_{\frac{1}{2}}(G)\chi(G)}{m}$ with equality holds if and only if G is a regular graph.*

In [36], it is proved that for any graph G with m edges,

$$ABS(G) \leq \sqrt{\frac{m}{2\delta}(M_1(G)-m) + \chi(G)}. \tag{4}$$

If G is a r-regular graph of order n and size m, then the upper bound in Equation (4) reduces to $\frac{n\sqrt{r}}{2}\left[\sqrt{\left(r-\frac{1}{2}\right)+\frac{1}{\sqrt{2}}}\right]$ and the upper bound in Corollary 2.7 reduces to $\frac{n\sqrt{r}}{2}\sqrt{r-1} = ABS(G)$. Thus the upper bound in the Corollary 2.7 is sharper than the upper bound in Equation (4) for a regular graph G.

Theorem 2.8. *For any graph G, $ABS(G) \leq \frac{m\sqrt{2\Delta-2}}{R(G)}\left[\frac{n}{8\delta} + \chi_{-1}(G)\right]$.*

Proof. By taking $x_{ij} = \frac{1}{\sqrt{d_i+d_j}}$, $y_{ij} = 2\frac{\sqrt{d_id_j}}{d_i+d_j}$, $z_{ij} = \sqrt{d_i+d_j-2}$ and $w_i = \frac{d_i+d_j}{d_id_j}$, for each edge $i \sim j$ in Lemma 1.5, we get:

$$\begin{aligned} &2\sum_{i\sim j}\sqrt{\frac{d_i+d_j-2}{d_i+d_j}} \sum_{i\sim j}\frac{2}{\sqrt{d_id_j}} \\ &\leq \sum_{i\sim j}\frac{d_i+d_j}{d_id_j}\sum_{i\sim j}\frac{\sqrt{d_i+d_j-2}}{d_i+d_j} + \sum_{i\sim j}\sqrt{d_i+d_j-2}\sum_{i\sim j}\frac{4}{d_i+d_j}. \end{aligned}$$

Note that, $\frac{\sqrt{d_i+d_j-2}}{d_i+d_j} \leq \frac{\sqrt{2\Delta-2}}{2\delta}$ and $\sqrt{d_i+d_j-2} \leq \sqrt{2\Delta-2}$.
Thus,

$$4ABS(G)R(G) \leq m\sqrt{2\Delta-2}\left[\frac{n}{2\delta}+4\chi_{-1}(G)\right].$$

■

Lemma 2.9. *([37]). For a non-trivial graph G, $R(G) \geq \sqrt{2}SF(G)$.*

The following corollary is a direct consequence of Theorem 2.8 and Lemma 2.9.

Corollary 2.10. *For any graph G, $ABS(G) \leq \frac{m\sqrt{\Delta-1}}{SF(G)}\left[\frac{n}{8\delta}+\chi_{-1}(G)\right]$.*

Now, we provide some bounds by considering the hyper Zagreb index and the first Zagreb index.

Theorem 2.11. *For any graph G, $ABS(G) \leq \frac{1}{\sqrt{2\delta}}\left[HM(G)+4m-4M_1(G)\right]$, with equality holds if and only if G is K_2.*

Proof. By definition,

$$\begin{aligned} ABS(G) &\leq \sum_{i\sim j}\frac{(d_i+d_j-2)^2}{\sqrt{d_i+d_j}} \\ &\leq \frac{1}{\sqrt{2\delta}}\left[\sum_{i\sim j}(d_i+d_j)^2+4m-4\sum_{i\sim j}(d_i+d_j)\right] \\ &= \frac{1}{\sqrt{2\delta}}\left[HM(G)+4m-4M_1(G)\right]. \end{aligned}$$

■

Now we relate ABS-index with the augmented Zagreb index.

Theorem 2.12. *For any graph G with $\delta \geq 2$, $ABS(G) \geq \sqrt{\frac{m^3\delta^6(\delta-1)}{8\Delta(\Delta-1)^3AZI(G)}}$. Furthermore, equality holds if and only if G is a regular graph.*

Proof. By taking $r=2$, $a_{ij}=\frac{d_id_j}{d_i+d_j-2}$ and $b_{ij}=\sqrt{\frac{d_i+d_j-2}{d_i+d_j}}$, for each edge $i\sim j$ in Lemma 1.3, we get:

$$\sum_{i\sim j}\left(\frac{d_id_j}{d_i+d_j-2}\right)^3\frac{d_i+d_j}{d_i+d_j-2} \geq \frac{\left(\sum_{i\sim j}\frac{d_id_j}{d_i+d_j-2}\right)^3}{\left(\sum_{i\sim j}\sqrt{\frac{d_i+d_j-2}{d_i+d_j}}\right)^2}.$$

This implies that,

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

Therefore,

$$ABS(G) \geq \sqrt{\frac{m^3\delta^6(\delta-1)}{8\Delta(\Delta-1)^3 AZI(G)}}.$$

Furthermore, by Lemma 1.3 equality holds if and only if G is a regular graph. ■

Theorem 2.13. *([38]). (i) For any connected graph with $m \geq 2$, $AZI(G) \leq \frac{m\Delta^6}{8(\Delta-1)^3}$. (ii) For a connected graph G with $n \geq 3$, $AZI(G) \leq \frac{n\Delta^7}{16(\Delta-1)^3}$ with equality holds in (i) if and only if G is a path or Δ-regular graph and in (ii) if and only if G is a Δ-regular graph.*

By using Theorems 2.12 and 2.13 we get the following result.

Corollary 2.14. *For any graph G with $\delta \geq 2$,*

(i) $ABS(G) \geq m\delta^3\sqrt{\frac{\delta-1}{\Delta^7}}$.

(ii) $ABS(G) \geq \frac{\delta^3}{\Delta^4}\sqrt{\frac{2(\delta-1)m^3}{n}}$.

Furthermore, in either case, equality holds if and only if G is regular.

In the next section, we examine the correlation between the ABS- index with other degree-based topological indices considered in the study.

3 Correlation between the ABS index and other degree-based topological indices

The correlation between the ABS index and other degree-based topological indices listed above was examined on a collection of twenty-one cycloalkanes, see Figure 1. Table 1 lists the values of the indices used in the study. A correlation graph (Figure 2) was used to depict the results. The vertices are designed to represent degree-based topological indices. If the absolute value of the Pearson correlation coefficient between two vertices exceeds 0.95, then they are connected by an edge. Figure 2 shows that the ABS-vertex has a degree 7, indicating a strong correlation with other degree-based topological indices in this study. Theorem 2.8 shows the correlation matrix among these indices.

The results indicate that most of the physicochemical information of cycloalkanes, carried by the other degree-based indices considered in this study can be harvested with the ABS index.

4 Concluding remarks

In the theory of topological indices, determining the upper and lower bounds as well as the connection between topological indices are essential and extensively researched problems. We derive several constraints in this study that relate the atom-bond sum connectivity index to the harmonic index, the first, hyper and augmented Zagreb indices, the general sum-connectivity index, the Randić index, and the sum-connectivity F-index. The computational investigation on the correlations of the atom-bond sum connectivity index with other degree-based topological indices value of cycloalkanes considered in this study shows that it is well-correlated with most of the degree-based topological indices.

Table 1: Different degree-based topological indices of cycloalkanes.

	ABS	R	M_1	H	χ_{-1}	χ	SF	HM	AZI
CA1	4.9497	3.5	28	3.5	1.75	3.5	2.4749	112	14
CA2	5.0847	3.3938	30	3.3	1.65	3.3944	2.2851	130	13.3333
CA3	5.1941	3.3045	32	3.1333	1.5667	3.3027	2.13	150	12.8333
CA4	5.3035	3.2071	34	2.9667	1.4833	3.2109	1.9929	170	12.3333
CA5	5.0225	3.4319	30	3.3667	1.6833	3.419	2.3399	132	14
CA6	5.2197	3.2877	32	3.1	1.55	3.2889	2.09541	148	12.6667
CA7	5.3035	3.2152	34	2.9667	1.4833	3.2109	1.9748	170	12.3333
CA8	5.2157	3.2701	34	3.0667	1.5333	3.2493	2.06413	174	13.1667
CA9	5.4702	3.0654	38	2.7048	1.3524	3.0586	1.7532	216	11.6333
CA10	5.4385	3.101	36	2.7667	1.3833	3.1054	1.8032	188	11.6667
CA11	5.3997	3.1278	36	2.819	2.819	3.1279	1.8558	192	11.9
CA12	5.2157	3.2678	34	3.0667	1.5333	3.2493	2.0677	174	13.6667
CA13	5.5974	2.9571	40	2.5167	1.2583	2.9589	1.5941	236	11
CA14	5.1319	3.3425	32	3.2	1.6	3.3272	2.1847	152	13.5
CA15	5.1574	3.3257	32	3.1667	1.5833	3.3134	2.1502	150	13.3333
CA16	5.3118	3.1885	36	2.919	1.4595	3.1662	1.9305	196	12.7333
CA17	5.3374	3.1658	36	2.8857	1.4429	3.1524	1.9106	194	12.5667
CA18	5.0225	3.4319	30	3.3667	1.6833	3.419	2.3399	132	14
CA19	5.0225	3.4319	30	3.3667	1.6833	3.419	2.3399	132	14
CA20	5.1319	3.3425	32	3.2	1.6	3.3272	2.1847	152	13.5
CA21	5.2157	3.2678	34	3.0667	1.5333	3.2493	2.0677	174	13.1667

Table 2: Correlation coefficient matrix.

	ABS	R	M_1	H	χ_{-1}	χ	SF	HM	AZI
ABS	1	-0.9985	0.972	-0.9983	-0.163	-0.9938	-0.9968	0.956	-0.961
R	-0.9985	1	-0.9827	0.9998	0.1694	0.998	0.9985	-0.9696	0.9472
M_1	0.972	-0.9827	1	-0.9836	-0.1933	-0.9917	-0.9844	0.9977	-0.8788
H	-0.9983	0.9998	-0.9836	1	0.1725	0.9986	0.9994	-0.9702	0.9448
χ_{-1}	-0.163	0.1694	-0.1933	0.1725	1	0.1801	0.1775	-0.1967	0.1132
χ	-0.9968	0.998	-0.9917	0.9986	0.1801	1	0.9986	-0.9814	0.9275
SF	-0.9968	0.9985	-0.9844	0.9994	0.1775	0.9986	1	-0.9708	0.9393
HM	0.956	-0.9696	0.9977	-0.9702	-0.1967	-0.9814	-0.9708	1	-0.853
AZI	-0.961	0.9472	-0.8788	0.9448	0.1132	0.9275	0.9393	-0.853	1

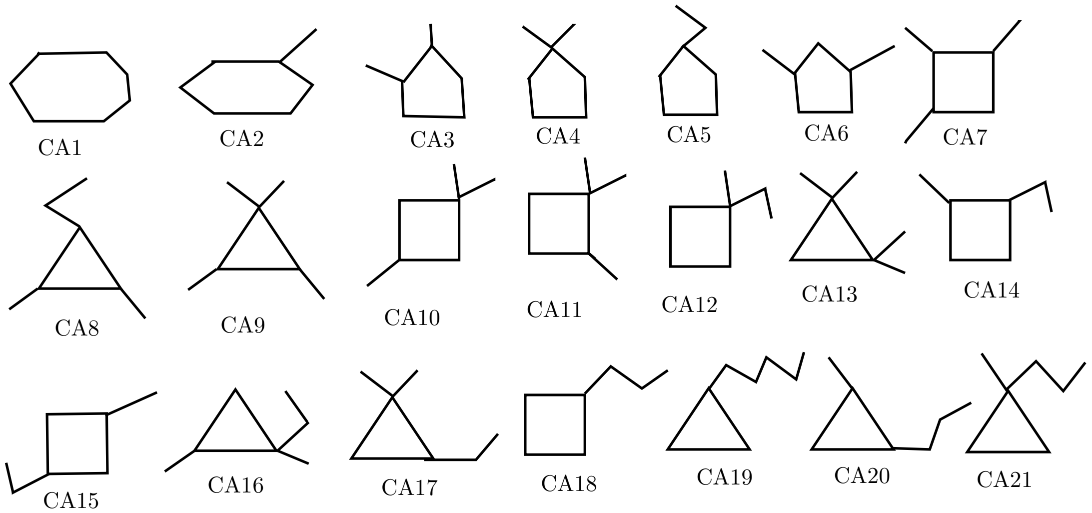

Figure 1: Molecular graphs of cycloalkanes.

Conflicts of Interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

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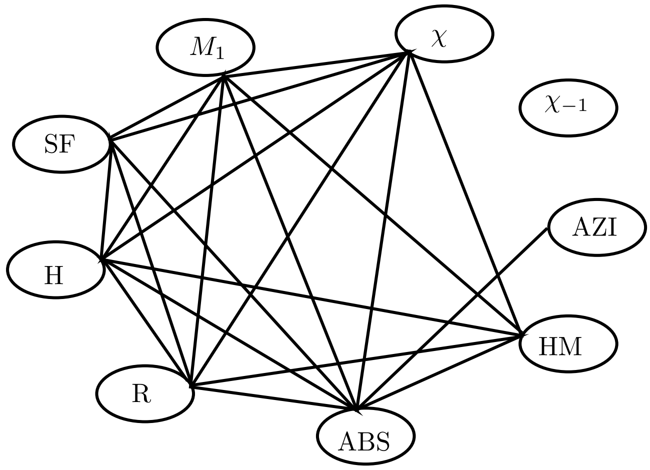

Figure 2: The correlation graph for the investigated degree-based topological indices.

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