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Chemical Applications of Some New Versions of Sombor Index

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Abstract. Topological indices of graphs are numerical descriptors that determine the relationship between the properties of molecules and their structures. In this paper, we introduce three novel vertex-degree-based topological indices that show a good correlation with the Sombor index. We have also derived bounds for them, identified the relationship between them and other topological indices, and finally examined their ability to predict some physico-chemical properties of octane isomers.

Keywords: Sombor index, Graph, Topological indices, Chemical Application.

2000 Mathematics subject classification: 05C09, 92E10; 05C07.

1. Introduction

Suppose $G(V, E)$ be a simple, connected, and undirected graph where $V = V(G)$ is the set of vertices and $E = E(G)$ is the set of edges. For any vertex $x \in V(G)$, $N_x(G)$ represents the set of vertices adjacent to x.

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The degree of x, which is denoted by $d_x(G)$, is defined as the cardinality of $N_x(G)$.

The ordered pair (s,t), where $s = d_x$ and $t = d_y$, is referred to the degree-coordinate (or d-coordinate) of the edge $xy \in E(G)$. In a two-dimensional coordinate system, this pair corresponds to a point known as the degree-point (or d-point) of the edge xy. Using Euclidean metrics, the distance between the (s,t) and the origin of the coordinate system is termed the degree-radius (or d-radius) of the edge xy.

Topological indices are numerical descriptors that are invariant under graph isomorphisms. So far, many types of these indices have been introduced, and numerous papers have been published about them.

Recently, Espinal and Gutman in [3], introduced the elliptic Sombor index of G which is defined as

$$ESO(G) = \sum_{uv \in E(G)} (d_u + d_v)\sqrt{d_u^2 + d_v^2}.$$

Gutman in [4], introduced a vertex-degree-based topological index which is called Sombor index, and defined it by

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2}.$$

Gutman in [5], obtained a new version of Sombor index which is called Euler-Sombor index, and defined it by

$$EU(G) = \sum_{uv \in E(G)} \sqrt{d_u d_v + d_u^2 + d_v^2},$$

he investigated some properties of this index on some special graphs. Tang et al.[14] analyzed the chemical applicability of this version of Sombor index. They established its mathematical properties, determined the extremal values for this Sombor index for all trees, and described the trees that achieve these extremal values. In [6], Gutman and Lepović introduced the generalized Randić index as

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

In [7], Gutman et al. introduced the product of the Sombor index and the modified Sombor index and computed its principal properties. Upper and lower bounds for its product are obtained and the extremal graphs are determined.

Kulli in [9], introduced the modified neighborhood Sombor index and its exponential variant for graphs. He also computed the neighborhood and modified neighborhood Sombor indices, as well as their exponentials, for

several significant dendrimers. Furthermore, he derived various properties of the neighborhood Sombor index.

Liu in [10], introduced multiplicative Sombor index, and some graph transformations which increase or decrease the multiplicative Sombor index. By using these transformations, he determined extremal values of the multiplicative Sombor index of trees and unicyclic graphs.

Ramezani Tousi and Ghods in [11] obtained the molecular graph and the line graph of Glass, and computed their M-polynomial and some topological indices.

Redžepović [13] determined chemical applicability of Sombor indices and studied their predictive and discriminative potentials. He examined that Sombor indices have a strong predictive potential.

Similar studies have been conducted on the Zagreb indices. These indices introduced by Gutman and Trinajstić [8] in 1972 as

$$M_1(G) = \sum_{uv \in E(G)} d_v + d_u, \qquad M_2(G) = \sum_{uv \in E(G)} d_u d_v,$$

and Ranjini et al. [12] redefined them.

In this paper, we introduce three new types of Sombor indices and calculate their exact values for specific graphs. We also examine their relationships with some other topological indices. Additionally, we explore their applications in predicting the physico-chemical properties of materials. It is observed that given their good correlation with material properties, they have the potential to be good predictors.

2. Results and Discussion

The high cost of chemical tests, as well as, the long time and precision required to determine the properties of chemical molecules, have forced scientists to find a way to predict their properties by defining some chemical indices. They examine the compatibility of each of the indices with different molecules, and thereby determine the predictive index of each of them. The general form of these indices are

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

where f is a symmetric positive two-variables function.
In this section we introduce the three novel vertex-degree-based topological indices of graphs. We define the first, second, and third redefined Sombor indices as

(1) $ReSO_1(G) = \sum_{uv \in E(G)} d_u d_v \sqrt{d_u^2 + d_v^2}$.

(2) $ReSO_2(G) = \sum_{uv \in E(G)} \sqrt{d_u d_v (d_u^2 + d_v^2)}$.

(3) $ReSO_3(G) = \sum_{uv \in E(G)} \left(\sqrt{d_u d_v} + \sqrt{d_u^2 + d_v^2} \right).$

We will further show that these indices have a good correlation with some other topological indices, making them potentially useful tools for predicting certain physico-chemical properties of materials. Moreover, it may be possible to derive some bounds for these indices according to the certain graph parameters.

Example 2.1. The following statements are true.

(1) Suppose G be a $r-$regular graph with n vertices, then

$$ReSO_1(G) = \frac{nr^4}{2}\sqrt{2}.$$

(2) For the cycle graph C_n, we have $ReSO_2(C_n) = 4n\sqrt{2}$.

(3) If K_n be the complete graph, then

$$ReSO_3(K_n) = \frac{n(n-1)^2}{2}(\sqrt{2}+1).$$

(4) If Q_k be the hypercube graph with $|V(Q_k)| = 2^k$, then

$$ReSO_2(Q_k) = \frac{2^k k^3}{2}\sqrt{2}.$$

Example 2.2. The following statements are true.

(1) Let $K_{p,q}$ be the complete bipartite graph, then

$$ReSO_1(K_{p,q}) = p^2q^2\sqrt{p^2+q^2}.$$

(2) For complete bipartite graph $K_{p,p}$, we have

$$ReSO_2(K_{p,p}) = p^4\sqrt{2}.$$

(3) If S_n be star of order n, then $ReSO_3(S_n) = n\left(\sqrt{1+n^2} + \sqrt{n}\right).$

Trees as an important class of graphs have always been of interest. Here, we have obtained the second redefined Sombor index value for path graphs as the simplest trees.

Theorem 2.3. *If P_n be the path with n vertices, then*

$$ReSO_2(P_n) = \begin{cases} \sqrt{2} & if\ n = 2, \\ 2\sqrt{10} + (n-3)\sqrt{32} & if\ n \geq 3. \end{cases}$$

Similarly, the values of $ReSO_i(P_n)$ for $i = 1, 3$ can be obtained.

Proof. The Theorem is obvious for $n = 2$. Suppose P_n be the path with $n \geq 3$ vertices and $n-1$ edges as $e_1, e_2, \ldots, e_{n-1}$, then e_1 and e_{n-1} have d-coordinate $(1,2)$ and other edges are d-coordinate $(2,2)$, therefore $ReSO_2(P_n) = 2\sqrt{2*5} + (n-3)\sqrt{4*8} = 2\sqrt{10} + (n-3)\sqrt{32}$. □

Obviously, by adding an edge to the graph, the value of the redefined Sombor indices increases. Therefore, the fact that the largest value of these indices occurs for the complete graphs, leads us to the following theorem.

Proposition 2.4. *If K_n represent the complete graph of order n, and $\overline{K_n}$ be its complement, then for any graph G of order n, we have*

$$ReSO_i(\overline{K_n}) \leq ReSO_i(G) \leq ReSO_i(K_n),$$

for $i = 1, 2, 3$, with $ReSO_i(\overline{K_n}) = 0$.

With the same argument, the smallest value of the redefined Sombor indices occurs in trees. Since, the path graph has the minimum Sombor index among trees (see [4]), the following result is obtained.

Theorem 2.5. *If K_n represents the complete graph of order n, and P_n be the path with n vertices, then for any connected graph G of order n, we have*

$$ReSO_i(P_n) \leq ReSO_i(G) \leq ReSO_i(K_n),$$

for $i = 1, 2, 3$.

Similar to the results presented in [1, 2] about the extremal values of some vertex degree-based topological indices, the paths and stars are the bounds of redefined Sombor indices among trees.

Theorem 2.6. *If S_n be the star of order n, and P_n be the path with n vertices, then for any connected tree T of order n, we have*

$$ReSO_i(P_n) \leq ReSO_i(T) \leq ReSO_i(S_n),$$

for $i = 1, 2, 3$. Equality on the left (res. right) holds iff $T \cong P_n$ (res. $T \cong S_n$).

Proof. The lower bound follows from Theorem 2.5. In order to deduce the upper bound, Suppose s be a vertex of T with neighbors $t_1, t_2, \ldots, t_k, z$, such that $d_T(t_i) = 1, i = 1, 2, \ldots, k$. Let T', be the tree obtained from T, by the transformation shown in Figure 1. If $d_z = 1$, then $T = S_n$ and

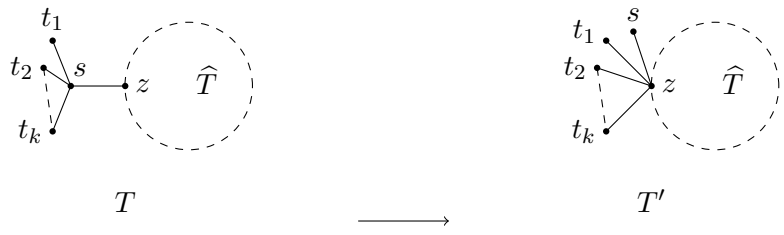

FIGURE 1. Transformation of graph

equality holds. Let $T \neq S_n$, therefore $d_z = l \geq 2$, and

$$\begin{aligned}
ReSO_1(T') &= d_z d_s \sqrt{d_z^2 + d_s^2} + \sum_{i=1}^{k} d_z d_{t_i} \sqrt{d_z^2 + d_{t_i}^2} \\
&\quad + \sum_{\widehat{t} \in V(\widehat{T})} d_z d_{\widehat{t}} \sqrt{d_z^2 + d_{\widehat{t}}^2} + \sum_{\substack{\widehat{t_i}\widehat{t_j} \in E(\widehat{T}) \\ \widehat{t_i}, \widehat{t_j} \neq z}} d_{\widehat{t_i}} d_{\widehat{t_j}} \sqrt{d_{\widehat{t_i}}^2 + d_{\widehat{t_j}}^2} \\
&= (l+k)\sqrt{(l+k)^2 + 1} + \sum_{i=1}^{k} (l+k)\sqrt{(l+k)^2 + 1} \\
&\quad + \sum_{\widehat{t} \in V(\widehat{T})} (l+k) d_{\widehat{t}} \sqrt{(l+k)^2 + d_{\widehat{t}}^2} + \sum_{\substack{\widehat{t_i}\widehat{t_j} \in E(\widehat{T}) \\ \widehat{t_i}, \widehat{t_j} \neq z}} d_{\widehat{t_i}} d_{\widehat{t_j}} \sqrt{d_{\widehat{t_i}}^2 + d_{\widehat{t_j}}^2} \\
&= (k+1)(l+k)\sqrt{(l+k)^2 + 1} + \sum_{\widehat{t} \in V(\widehat{T})} (l+k) d_{\widehat{t}} \sqrt{(l+k)^2 + d_{\widehat{t}}^2} \\
&\quad + \sum_{\substack{\widehat{t_i}\widehat{t_j} \in E(\widehat{T}) \\ \widehat{t_i}, \widehat{t_j} \neq z}} d_{\widehat{t_i}} d_{\widehat{t_j}} \sqrt{d_{\widehat{t_i}}^2 + d_{\widehat{t_j}}^2}.
\end{aligned}$$

Moreover

$$\begin{aligned}
ReSO_1(T) &= d_z d_s \sqrt{d_z^2 + d_s^2} + \sum_{i=1}^{k} d_s d_{t_i} \sqrt{d_s^2 + d_{t_i}^2} \\
&\quad + \sum_{\widehat{t} \in V(\widehat{T})} d_z d_{\widehat{t}} \sqrt{d_z^2 + d_{\widehat{t}}^2} + \sum_{\substack{\widehat{t_i}\widehat{t_j} \in E(\widehat{T}) \\ \widehat{t_i}, \widehat{t_j} \neq z}} d_{\widehat{t_i}} d_{\widehat{t_j}} \sqrt{d_{\widehat{t_i}}^2 + d_{\widehat{t_j}}^2} \\
&= l(k+1)\sqrt{l^2 + (k+1)^2} + \sum_{i=1}^{k} (k+1)\sqrt{(k+1)^2 + 1} \\
&\quad + \sum_{\widehat{t} \in V(\widehat{T})} l d_{\widehat{t}} \sqrt{l^2 + d_{\widehat{t}}^2} + \sum_{\substack{\widehat{t_i}\widehat{t_j} \in E(\widehat{T}) \\ \widehat{t_i}, \widehat{t_j} \neq z}} d_{\widehat{t_i}} d_{\widehat{t_j}} \sqrt{d_{\widehat{t_i}}^2 + d_{\widehat{t_j}}^2} \\
&= l(k+1)\sqrt{l^2 + (k+1)^2} + k(k+1)\sqrt{(k+1)^2 + 1} \\
&\quad + \sum_{\widehat{t} \in V(\widehat{T})} l d_{\widehat{t}} \sqrt{l^2 + d_{\widehat{t}}^2} + \sum_{\substack{\widehat{t_i}\widehat{t_j} \in E(\widehat{T}) \\ \widehat{t_i}, \widehat{t_j} \neq z}} d_{\widehat{t_i}} d_{\widehat{t_j}} \sqrt{d_{\widehat{t_i}}^2 + d_{\widehat{t_j}}^2}.
\end{aligned}$$

On the other hand

$$\sum_{\widehat{t}\in V(\widehat{T})}(l+k)d_{\widehat{t}}\sqrt{(l+k)^2+d_{\widehat{t}}^2}\geq\sum_{\widehat{t}\in V(\widehat{T})}ld_{\widehat{t}}\sqrt{l^2+d_{\widehat{t}}^2},$$

and

$$\begin{aligned}(k+1)(l+k)\sqrt{(l+k)^2+1}=&k(k+1)\sqrt{(l+k)^2+1}\\&+(k+1)l\sqrt{(l+k)^2+1}\\&\geq k(k+1)\sqrt{(k+1)^2+1}\\&+(k+1)l\sqrt{(k+1)^2+l^2}.\end{aligned}$$

Therefore, using the above inequlities, and comparing the amounts of $ReSO_1(T')$ and $ReSO_1(T)$ implies that $ReSO_1(T')\geq ReSO_1(T)$. If $T'=S_n$ is proven, then the proof is complete, otherwise, we will repeat the above process a finite number of times until the result is obtained. The proof for $i=2,3$ is similar. □

The maximum and minimum vertex degrees are two important parameters of a graph for establishing new bounds. Here, we derive some bounds for $ReSO_i$ where $i=1,2,3$, based on these values. The proof of the next Theorem is a consequence of the inequality $\delta\leq d_u(G)\leq\Delta$.

Theorem 2.7. *Let G be a simple and connected graph with m edges, and let δ and Δ denote the minimum and maximum degrees of the vertices of G respectively, then*

(1) $\sqrt{2}m\delta^3\leq ReSO_1(G)\leq\sqrt{2}m\Delta^3$.
(2) $\sqrt{2}m\delta^2\leq ReSO_2(G)\leq\sqrt{2}m\Delta^2$.
(3) $(1+\sqrt{2})m\delta\leq ReSO_3(G)\leq(1+\sqrt{2})m\Delta$.

Equality holds iff G be regular.

3. Relationship between redefined Sombor indices and other vertex-degree-based topological indices

In this section, we explore the connections between the redefined Sombor indices and various other topological indices. The redefined Sombor indices showed good correlations with some existing topological indices. Table 1 asserts the possibililty of the establishment of some mathematical relationships among these indices. In the following, we prove some of these relationships.

Proposition 3.1. *For any arbitrary graph G, we have*

$$ReSO_3(G)\leq 2ReSO_2(G).$$

TABLE 1. The correlation coefficients of the redefined Sombor indices with some existing indices.

	M_1	M_2	EU	SO	R	$ReSO_1$	$ReSO_2$	$ReSO_3$
$ReSO_1$	0.96	0.99	0.95	0.94	-0.87	1.00	0.90	0.97
$ReSO_2$	0.91	0.90	0.91	0.90	-0.85	0.90	1.00	0.87
$ReSO_3$	0.97	0.96	0.96	0.96	-0.91	0.97	0.87	1.00

Proposition 3.2. *For any arbitrary graph G, we have*

$$ReSO_2(G) \leq ReSO_1(G).$$

Equality holds if and only if G be a finite union of K_2 graphs.

Proposition 3.3. *If $M_1(G)$ be first Zagreb index and $SO(G)$ be Sombor index of graph G, then*

$$ReSO_2(G) \leq \frac{M_1(G)}{2} SO(G).$$

Equality holds if and only if $G \cong K_2$.

Proof. Since $\sqrt{xy} \leq \frac{x+y}{2}$, we have $\sqrt{d_u d_v (d_u^2 + d_v^2)} \leq \frac{d_u + d_v}{2}\sqrt{d_u^2 + d_v^2}$, therefore,

$$\begin{aligned} ReSO_2(G) &= \sum_{uv \in E(G)} \sqrt{d_u d_v (d_u^2 + d_v^2)} \\ &\leq \sum_{uv \in E(G)} (\frac{d_u + d_v}{2}) \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2} \\ &= \frac{M_1(G)}{2} SO(G). \end{aligned}$$

□

Proposition 3.4. *For any arbitrary graph G, we have*

$$ReSO_2(G) \leq \frac{1}{2} ESO(G).$$

Equality holds if and only if G be a regular graph.

Proposition 3.5. *If $M_1(G)$ be first Zagreb index of graph G, then*

$$EU(G) \leq M_1(G), \qquad EU(G) \leq ReSO_3(G).$$

Proof. Since $\sqrt{d_u d_v + d_u^2 + d_v^2} \leq \sqrt{2d_u d_v + d_u^2 + d_v^2} = d_u + d_v$, then $EU \leq M_1(G)$. The rest of the proof comes from the inequality

$$\sqrt{d_u d_v + d_u^2 + d_v^2} \leq \sqrt{d_u d_v} + \sqrt{d_u^2 + d_v^2}.$$

□

Proposition 3.6. *If $M_1(G)$ be first Zagreb index and $SO(G)$ be Sombor index of connected graph G, then*

$$ReSO_3(G) \leq \frac{M_1(G)}{2} + SO(G).$$

Equality holds if and only if G be a regular graph.

Proof. Since $\sqrt{d_u d_v} + \sqrt{d_u^2 + d_v^2} \leq \frac{d_u+d_v}{2} + \sqrt{d_u^2 + d_v^2}$, then

$$ReSO_3(G) \leq \frac{M_1(G)}{2} + SO(G).$$

□

Proposition 3.7. *If $M_1(G)$ be first Zagreb index and $SO(G)$ be Sombor index of connected graph G, then*

$$ReSO_1(G) \leq \frac{M_1^2}{4} SO(G).$$

Equality holds if and only if $G \cong K_2$.

Proof. Since $xy \leq (\frac{x+y}{2})^2$, we have $ReSO_1(G) \leq \frac{M_1^2}{4} SO(G)$. □

Proposition 3.8. *Let G be a simple and connected graph, $R_\alpha(G)$ and $SO(G)$ are the generalized Randić and Sombor indices of G, respectively, then*

$$\sqrt{2} R^3_{\frac{1}{2}}(G) \leq ReSO_1(G),$$

with equality iff G be regular.

Proof. Since $xy \leq \frac{x^2+y^2}{2}$ for $x, y \in \mathcal{R}$ with equality iff $x = y$, therefore

$$\sqrt{2}(d_u d_v)^{\frac{3}{2}} \leq d_u d_v \sqrt{d_u^2 + d_v^2}.$$

□

The following proposition is proven in [5]. Here, we present a shorter proof of it.

Proposition 3.9. *Let G be a simple and connected graph, then*

$$SO(G) < EU(G) \leq \sqrt{\frac{3}{2}} SO(G).$$

Proof. It suffices to show that

$$x^2 + y^2 < x^2 + y^2 + xy \leq \frac{3}{2}(x^2 + y^2),$$

for $x, y > 0$. The left inequality is obvious. For the right inequality, let $y = mx$, then

$$x^2 + y^2 + xy = x^2(1 + m^2 + m)$$
$$\leq x^2(1 + m^2 + \frac{1 + m^2}{2}) = \frac{3}{2}x^2(1 + m^2) = \frac{3}{2}(x^2 + y^2).$$

□

The proof of the following proposition is strightforward.

Proposition 3.10. *Let G be a simple and connected graph, then*

(1) $SO(G) \leq ReSO_3(G) \leq (1 + \frac{1}{\sqrt{2}})SO(G)$.

(2) $SO(G) \leq ReSO_2(G) \leq \Delta SO(G)$.

(3) $SO(G) \leq ReSO_1(G) \leq \Delta^2 SO(G)$.

4. Applications

In this section, we concentrate on the predictive capacity of redefined Sombor indices for framing linear regression models, to predict some physico-chemical properties (Entropy(S), standard enthalpy of vaporisation (ΔH_{vap}), acentric factor(AcentFac), Narumi simple topological index(SNar), and Narumi harmonic topological index(HNar)) of isomers of octane. By using isomers, the influence of molecular size on the predictive model is eliminated. The experimental data were collected from the molecular descriptors database, available at moleculardescriptors.eu and are shown in Table 2.

As seen in Table 3, the correlation coefficients of the redefined Sombor indices with certain physico-chemical properties, is better compared to other topological indices in some cases. Therefore, these indices may contain useful information for prediction these properties. The motivation for selecting these specific physico-chemical properties, is that the redefined Sombor indices provide relatively strong linear correlations, with their respective correlation coefficients, which are greater than 0.8. The results are presented in Table 3.

The scatter plot depicted in Figures 2, 3, 4, 5, 6, demonstrates a linear dependence between physico-chemical properties and redefined Sombor indices. All analyzed correlations reveal linear relationships between the redefined Sombor indices and these physico-chemical properties.
Therefore, we use a regression model for modeling to obtain a linear relationship between physico-chemical properties and Sombor indices. The

TABLE 2. Physico-chemical properties of isomers of octane with $ReSO_i$, $i = 1, 2, 3$.

Molecule	$ReSO_1$	$ReSO_2$	$ReSO_3$	S	ΔH_{vap}	$AcentFac$	$SNar$	$HNar$
octane	65.51	34.6	31.44	111.67	9.92	0.40	4.16	1.60
2-methylheptane	79.02	39.91	33.97	109.84	9.48	0.38	3.87	1.50
3-methylheptane	84.32	40.77	33.96	111.26	9.52	0.37	3.87	1.50
4-methylheptane	84.32	40.77	33.96	109.32	9.48	0.37	3.87	1.50
3-ethylhexane	89.63	41.63	33.94	109.43	9.48	0.36	3.87	1.50
2,2-dimethylhexane	112.3	51.86	38.97	103.42	8.92	0.34	3.47	1.39
2,3-dimethylhexane	104.06	46.81	36.45	108.02	9.27	0.35	3.58	1.41
2,4-dimethylhexane	97.83	46.08	36.49	106.98	9.03	0.34	3.58	1.41
2,5-dimethylhexane	92.52	45.22	36.51	105.72	9.05	0.36	3.58	1.41
3,3-dimethylhexane	124.79	53.77	38.97	104.74	8.973	0.32	3.47	1.39
3,4-dimethylhexane	109.36	47.67	36.44	106.59	9.32	0.34	3.58	1.41
2-methyl-3-ethylpentane	109.36	47.67	36.44	106.06	9.21	0.33	3.58	1.41
3-methyl-3-ethylpentane	146.18	55.68	38.97	101.48	9.09	0.31	3.47	1.39
2,2,3-trimethylpentane	145.06	59.53	41.43	101.31	8.83	0.30	3.18	1.32
2,2,4-trimethylpentane	125.86	57.17	37.4	104.09	8.40	0.31	3.18	1.32
2,3,3-trimethylpentane	152.2	60.57	41.44	102.06	8.90	0.29	3.18	1.32
2,3,4-trimethylpentane	123.8	52.84	38.95	102.39	9.01	0.32	3.30	1.33
2„2,3,3-tetramethylbutane	189.46	56.4	46.39	93.06	8.41	0.26	2.78	1.23

TABLE 3. The correlation coefficient of different topological indices with S, ΔH_{vap}, AcenFac, HNar and SNar.

	$ReSO_1$	$ReSO_2$	$ReSO_3$	EU	SO	M_1	M_2	R
S	-0.96	-0.84	-0.97	-0.95	-0.95	-0.95	-0.94	0.91
ΔH_{vap}	-0.82	-0.87	-0.84	-0.94	-0.95	-0.94	-0.81	0.96
$AcentFac$	-0.98	-0.93	-0.95	-0.97	-0.96	-0.97	-0.99	0.90
$HNar$	-0.91	-0.92	-0.93	-0.97	-0.96	-0.97	-0.93	0.96
$SNar$	-0.94	-0.91	-0.95	-0.99	-0.98	-0.99	-0.95	0.97

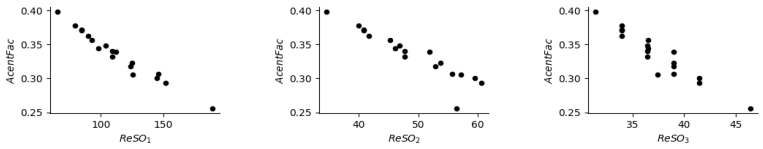

FIGURE 2. The correlation between $AcentFac$ and $ReSO_i$ for 18 isomers of octane.

scatter plots are shown in Figures 7, 8, 9, 10, 11, and the coefficients of these linear equations are presented in Table 4. The coefficients in the regression models are determined through a Python script, utilizing the scikit-learn machine learning framework.

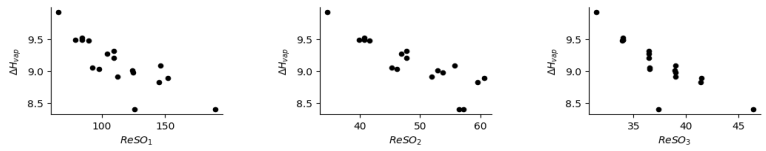

FIGURE 3. The correlation between the ΔH_{vap} and $ReSO_i$ for 18 isomers of octane.

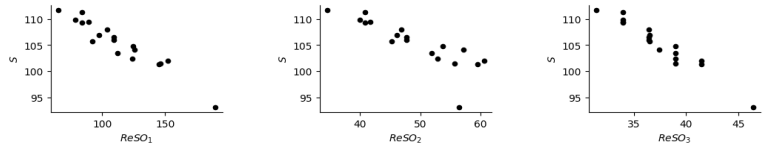

FIGURE 4. The correlation between the S and $ReSO_i$ for 18 isomers of octane.

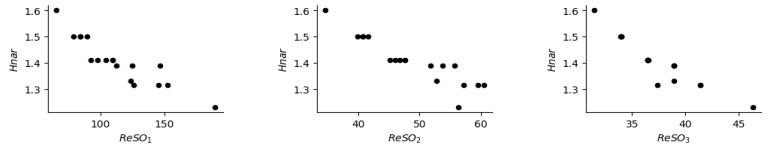

FIGURE 5. The correlation between the $HNar$ and $ReSO_i$ for 18 isomers of octane.

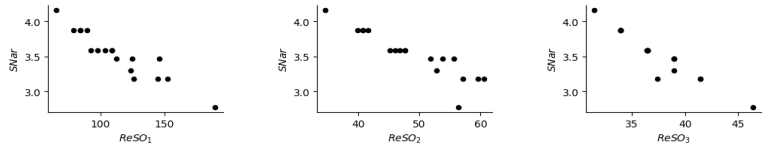

FIGURE 6. The correlation between the $SNar$ and $ReSO_i$ for 18 isomers of octane.

In the model described by equation 4.1, one of the physico-chemical properties is forecasted by using only one of the redefined Sombor indices. The tested regression models are outlined as follows:

$$S, \Delta H_{vap}, AcentFac, HNar, SNar \approx A * ReSO_i + B \ ; \ i = 1, 2, 3, \quad (4.1)$$

Here, A, represents the regression coefficient and B, denotes the regression constant. The values for A and B are presented in Table 4.

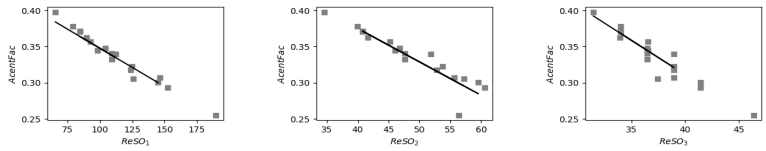

FIGURE 7. The regression model with $AcentFac$ and $ReSO_i$ for 18 isomers of octane.

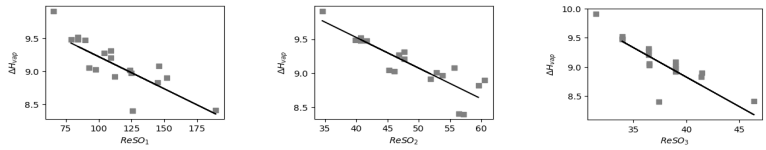

FIGURE 8. The regression model with ΔH_{vap} and $ReSO_i$ for 18 isomers of octane.

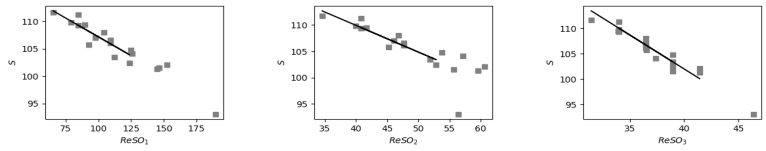

FIGURE 9. The regression model with S and $ReSO_i$ for 18 isomers of octane.

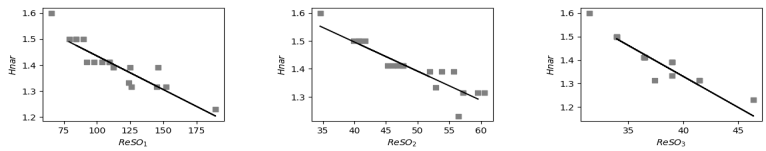

FIGURE 10. The regression model with $HNar$ and $ReSO_i$ for 18 isomers of octane.

The terms R^2, $RMSE$ and R^2_{adj} refer to the coefficients of determination, root mean square error and adjusted coefficient of determination, respectively. The evaluation results shown in Tables 5 indicate that the physico-chemical properties of octane isomers are effectively predicted using straightforward models based on equation 4.1. Specifically, over 90% of the variance in the physico-chemical properties can be accounted for a linear model, in which a single redefined Sombor index is the sole predictor.

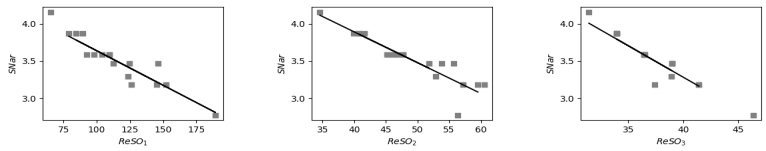

FIGURE 11. The regression model with $SNar$ and $ReSO_i$ for 18 isomers of octane.

TABLE 4. The values for the parameters used in the models.

Parameter	$ReSO_i$	A	B
S	$ReSO_1$	-0.14	120.92
	$ReSO_2$	-0.51	130.21
	$ReSO_3$	-1.34	155.54
ΔH_{vap}	$ReSO_1$	-0.01	10.20
	$ReSO_2$	-0.05	11.33
	$ReSO_3$	-0.10	12.88
$AcentFac$	$ReSO_1$	-0.001	0.45
	$ReSO_2$	-0.005	0.56
	$ReSO_3$	-0.009	0.69
$HNar$	$ReSO_1$	-0.003	1.69
	$ReSO_2$	-0.01	1.91
	$ReSO_3$	-0.02	2.38
$SNar$	$ReSO_1$	-0.01	4.56
	$ReSO_2$	-0.04	5.54
	$ReSO_3$	-0.08	6.67

The results in Tables 5 demonstrate that the physico-chemical properties of octane isomers can be adequately predicted using basic models derived from equation 4.1. Specifically, a linear model using a single redefined Sombor index as the sole predictor explains over 90% of the variance in the physico-chemical properties. Moreover, the errors generated by these models are minimal, particularly for $SNar$. Among all the models, the model using the third redefined Sombor index to predict $SNar$ demonstrated the best performance. Precisely, its R^2 value reaches 96.60%.

To compare the experimental and theoretical results, it is essential to evaluate the model's predictive power using the Root Mean Square Error ($RMSE$) metric. The optimal predictive model will be the one that exhibits the minimum error, i.e., the lowest RMSE, which is defined as

$$RMSE = \sqrt{\frac{1}{n}\sum_{j=1}^{n}(y_j - \widehat{y_j})^2}.$$

TABLE 5. The results of evaluation of the linear regression models.

$ReSO_i$	$R^2(\%)$	$R^2_{adj}(\%)$	$RMSE$
	S		
$ReSO_1$	90.37	87.96	0.92
$ReSO_2$	91.22	89.03	0.87
$ReSO_3$	92.45	90.56	1.02
	ΔH_{vap}		
$ReSO_1$	94.15	92.69	0.10
$ReSO_2$	86.40	83.01	0.14
$ReSO_3$	91.74	89.68	0.12
	$AcentFac$		
$ReSO_1$	94.10	92.63	0.08
$ReSO_2$	92.11	90.14	0.08
$ReSO_3$	93.75	92.19	0.01
	$HNar$		
$ReSO_1$	95.09	93.8	0.02
$ReSO_2$	91.74	89.68	0.03
$ReSO_3$	92.17	90.21	0.03
	$SNar$		
$ReSO_1$	96.60	95.75	0.08
$ReSO_2$	0.96	95.01	0.06
$ReSO_3$	92.63	90.79	0.09

Here y_j represents the observed values of the independent variable, $\widehat{y_j}$ signifies the predicted values of the independent variable, and n denotes the number of samples under consideration.

5. Conclusions

In this paper, we have studied three newly redefined Sombor indices of the first, second, and third types. We have also identified their relationships with some topological indices, as well as their predictive abilities regarding the properties of molecules. In the future, we can explore some bounds to these indices for certain molecular graphs, according to graph parameters.

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