Comparison Between Three Types of General Indices For Measuring the Heat Capacities and Standard Molecular Entropies of Benzenoid Hydrocarbons

Abdul Wafi Haji Ismail[a], Sakander Hayat[a,*]

[a]Faculty of Science, Universiti Brunei Darussalam, Jalan Tungku Link, Gadong BE1410, Brunei Darussalam

ARTICLE INFO

Keywords:
Benzenoid System
Heat Capacity
Standard Molecular Entropy
General Randić Index
General Sum-Connectivity Index
General Sombor Index

ABSTRACT

This article shows that three examined topological indices, namely the general Randić index R_α, the general sum-connectivity index SCI_α and the general Sombor index SO_α - when the real number α is in some interval - are closely related molecular descriptors. By comparing these three, it is evident that the indices $R_{-1.238343022}$ and $R_{-1.948234553}$ are the best for measuring the standard heat capacity ΔH and the standard molecular entropy E, respectively, of lower benzenoid hydrocabons.

1. Introduction

Suppose G is a simple graph which has an edge set $E(G)$. Let d_a and d_b, respectively, denote degrees of the vertices a and b, in G.

The *Randić index* of G, proposed in [1] (1975), is a very well-known molecular descriptor whose mathematical and chemical properties have been examined extensively in [2, 3, 4, 5, 6], which is defined as such:

$$R(G) = \sum_{(a,b)\in E(G)} \frac{1}{\sqrt{d_a \cdot d_b}} \tag{1}$$

Then, in 1998, Bollobás and Erdös [7] - with the intention of extending the utility of the aforementioned index - generalized it to the *general Randić index*:

$$R_\alpha(G) = \sum_{(a,v)\in E(G)} (d_a \cdot d_b)^\alpha, \tag{2}$$

where $\{\alpha \in \mathbb{R} \mid \alpha \neq 0\}$.

There has been numerous contributions in chemical and mathematical literature in regards to the general Randić index [3, 8, 9, 10, 11].

Additionally, in more recent times, four kinds of new connectivity indices have also been introduced [12, 13, 14, 15].

For a graph G, its *sum-connectivity index* and the generalisation of said index, the *general sum-connectivity index* of G are defined as

$$SCI(G) = \sum_{(a,b)\in E(G)} \frac{1}{\sqrt{d_a + d_b}} \tag{3}$$

and

$$SCI_\alpha(G) = \sum_{(a,b)\in E(G)} (d_a + d_b)^\alpha, \tag{4}$$

respectively, where $\{\alpha \in \mathbb{R} \mid \alpha \neq 0\}$. More applications of these two indices can be found in [12, 13, 16, 17].

Then, the *Sombor index* and its generalisation the *general Sombor index* of G are defined as

$$SO(G) = \sum_{(a,b)\in E(G)} \frac{1}{\sqrt{{d_a}^2 + {d_b}^2}} \tag{5}$$

and

$$SO_\alpha(G) = \sum_{(a,b)\in E(G)} ({d_a}^2 + {d_b}^2)^\alpha, \tag{6}$$

respectively, where $\{\alpha \in \mathbb{R} \mid \alpha \neq 0\}$.

Obviously,

$$\begin{aligned} R(G) &= R_{-0.5}(G) \\ SCI(G) &= SCI_{-0.5}(G) \\ SO(G) &= SO_{-0.5}(G). \end{aligned}$$

2. Materials and Methods

Each benzenoid hydrocarbons can naturally be represented by a benzenoid system, which is a finite, connected plane graph with no cut vertices, and in which each interior face is bounded by a regular hexagon with sides of length 1.

The definitions below are introduced in [18]. Suppose B is a benzenoid system with v vertices and h hexagons. For each path $p_1 - p_2 - \cdots - p_{k+1}$ of length $k (k \geq 1, k \in \mathbb{N})$ in B, we can associate with it the vertex degree sequence $(d_{p_1}, d_{p_2}, \ldots, d_{p_{k+1}})$. Then, a *fjord*, *cove*, *bay*, and *fissure*, are paths of degree sequences (2, 3, 3, 3, 3, 2), (2, 3, 3, 3, 2), (2, 3, 3, 2), and (2, 3, 2), respectively, by going along the perimeter of B, as illustrated in Figure 1.

Fjords, coves, bays, and fissures are all considered different types of *inlets*. The number of inlets, r, then, is defined as the total number of fjords, coves, bays, and fissures summed.

Suppose a benzenoid system B has h hexagons, r inlets and v vertices. Let n_{ij} denote the number of B's edges which

*Corresponding author
Email addresses: wafibismail@gmail.com (A.W.H. Ismail); sakander1566@gmail.com (S. Hayat)

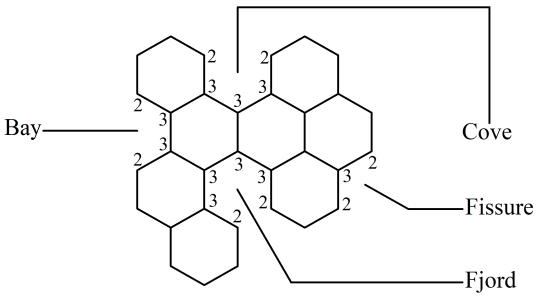

Figure 1: Cove, fissure, fjord and bay in a hexagonal system.

satisfies the conditions $d_a = i$ and $d_b = j$, where d_a and d_b, respectively, are the degrees of the ends a and b of an edge. By Lemma 1 in [18]

$$n_{22} = v - 2h - r + 2, \quad n_{23} = 2r, \quad n_{33} = 3h - r - 3. \quad (7)$$

By (2) and (7), the benzenoid system B has the general Randić index

$$\begin{aligned} R_\alpha(B) &= n_{22}4^\alpha + n_{23}6^\alpha + n_{33}9^\alpha \\ &= (4^\alpha)v + (3\cdot 9^\alpha - 2\cdot 4^\alpha)h \\ &\quad + (2\cdot 6^\alpha - 4^\alpha - 9^\alpha)r + 2\cdot 4^\alpha - 3\cdot 9^\alpha, \end{aligned} \quad (8)$$

by (4) and (7), the general sum-connectivity index

$$\begin{aligned} SCI_\alpha(B) &= n_{22}4^\alpha + n_{23}5^\alpha + n_{33}6^\alpha \\ &= (4^\alpha)v + (3\cdot 6^\alpha - 2\cdot 4^\alpha)h \\ &\quad + (2\cdot 5^\alpha - 4^\alpha - 6^\alpha)r + 2\cdot 4^\alpha - 3\cdot 6^\alpha, \end{aligned} \quad (9)$$

and by (6) and (7), the general Sombor index

$$\begin{aligned} SO_\alpha(B) &= n_{22}8^\alpha + n_{23}13^\alpha + n_{33}18^\alpha \\ &= (8^\alpha)v + (3\cdot 18^\alpha - 2\cdot 8^\alpha)h \\ &\quad + (2\cdot 13^\alpha - 8^\alpha - 18^\alpha)r + 2\cdot 8^\alpha - 3\cdot 18^\alpha. \end{aligned} \quad (10)$$

In (8), (9) and (10), h, r and v, respectively, are the number of hexagons, inlets and vertices in B, and $\{\alpha \in \mathbb{R} \mid \alpha \neq 0\}$.

The molecular structure, heat capacity ΔH, standard molecular entropy E, general Randić index R_α, general sum-connectivity index SCI_α, and general Sombor index SO_α are shown in Table 1 for 30 lower benzenoid hydrocarbons.

3. Results and Discussion

The following results conclude that the general Randić index R_α, the general sum-connectivity index SCI_α and the general Sombor index SO_α - for α in some interval - can quite accurately reproduce the heat capacity and the standard molecular entropy of the lower benzenoid hydrocarbons.

From the data shown in Table 1, we have produced six curves, as illustrated in Figures 2 to 5. For these 30 lower benzenoids, the correlation coefficient curves for their thermodynamic properties (ΔH in Figures 2 and 3, E in Figures 4 and 5) and the indices (R_α, SCI_α or SO_α) are

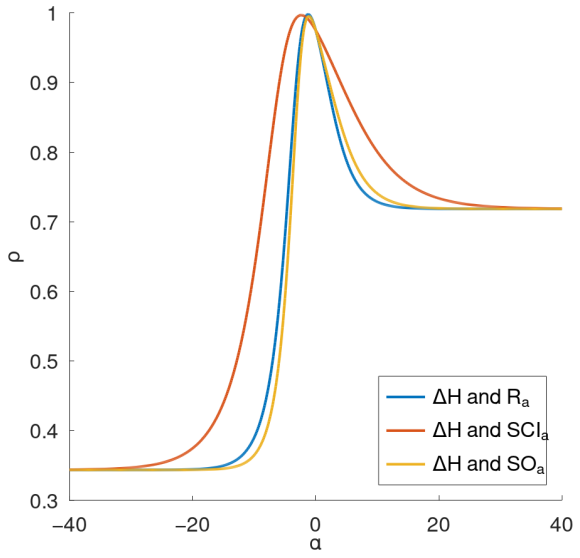

Figure 2: Correlation coefficient curves between general indices and ΔH of lower benzenoids (far-view)

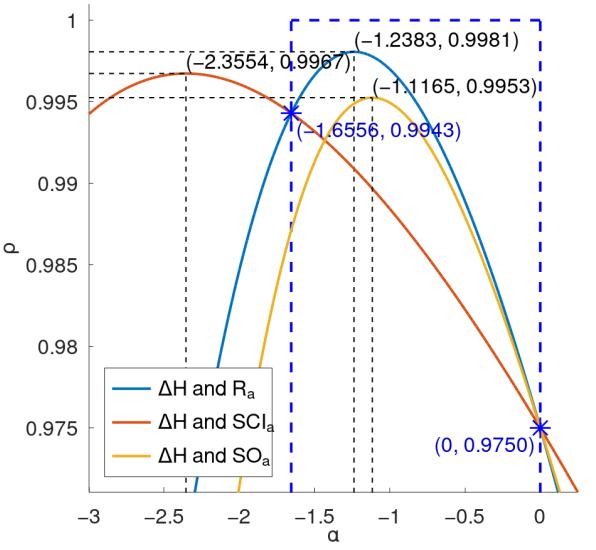

Figure 3: Correlation coefficient curves between general indices and ΔH of lower benzenoids

drawn in the respective figures in solid lines, distinguished by colors.

Comparing the three general indices, the general Randić index R_α is the best measure of *standard heat capacity* ΔH for benzenoid hydrocarbons for $\alpha \in (-1.6556, 0)$, as shown in Figure 3, while for other α, the sum-connectivity index SCI_α is the best.

On the other hand, as measures of *standard molecular entropy* E of benzenoid hydrocarbons, the general Randić index R_α is the best for $\alpha \in (-2.5788, 0)$, as can be seen in Figure 5, while for other α, the sum-connectivity index SCI_α is the best.

Table 1
The molecular structure, heat capacity ΔH, standard molecular entropy E, general Randić index R_α, general sum-connectivity index SCI_α, and general Sombor index SO_α of 30 lower benzenoid hydrocarbons

Molecule	Structure	ΔH	E	R_α	SCI_α	SO_α
Benzene		83.019	269.722	$6\cdot 4^\alpha$	$6\cdot 4^\alpha$	$6\cdot 8^\alpha$
Naphthalene		133.325	334.155	$6\cdot 4^\alpha+4\cdot 6^\alpha+9^\alpha$	$6\cdot 4^\alpha+4\cdot 5^\alpha+6^\alpha$	$6\cdot 8^\alpha+4\cdot 13^\alpha+18^\alpha$
Anthracene		184.194	389.475	$6\cdot 4^\alpha+8\cdot 6^\alpha+2\cdot 9^\alpha$	$6\cdot 4^\alpha+8\cdot 5^\alpha+2\cdot 6^\alpha$	$6\cdot 8^\alpha+8\cdot 13^\alpha+2\cdot 18^\alpha$
Phenanthrene		183.654	395.882	$7\cdot 4^\alpha+6\cdot 6^\alpha+3\cdot 9^\alpha$	$7\cdot 4^\alpha+6\cdot 5^\alpha+3\cdot 6^\alpha$	$7\cdot 8^\alpha+6\cdot 13^\alpha+3\cdot 18^\alpha$
Tetracene		235.165	444.724	$6\cdot 4^\alpha+12\cdot 6^\alpha+3\cdot 9^\alpha$	$6\cdot 4^\alpha+12\cdot 5^\alpha+3\cdot 6^\alpha$	$6\cdot 8^\alpha+12\cdot 13^\alpha+3\cdot 18^\alpha$
Benzo[c]phenanthrene		233.497	447.437	$8\cdot 4^\alpha+8\cdot 6^\alpha+5\cdot 9^\alpha$	$8\cdot 4^\alpha+8\cdot 5^\alpha+5\cdot 6^\alpha$	$8\cdot 8^\alpha+8\cdot 13^\alpha+5\cdot 18^\alpha$
Benzo[a]phenanthrene		234.568	457.958	$7\cdot 4^\alpha+10\cdot 6^\alpha+4\cdot 9^\alpha$	$7\cdot 4^\alpha+10\cdot 5^\alpha+4\cdot 6^\alpha$	$7\cdot 8^\alpha+10\cdot 13^\alpha+4\cdot 18^\alpha$
Chrysene		234.638	455.839	$8\cdot 4^\alpha+8\cdot 6^\alpha+5\cdot 9^\alpha$	$8\cdot 4^\alpha+8\cdot 5^\alpha+5\cdot 6^\alpha$	$8\cdot 8^\alpha+8\cdot 13^\alpha+5\cdot 18^\alpha$
Triphenylene		233.558	450.418	$9\cdot 4^\alpha+6\cdot 6^\alpha+6\cdot 9^\alpha$	$9\cdot 4^\alpha+6\cdot 5^\alpha+6\cdot 6^\alpha$	$9\cdot 8^\alpha+6\cdot 13^\alpha+6\cdot 18^\alpha$
Pyrene		200.815	399.491	$6\cdot 4^\alpha+8\cdot 6^\alpha+5\cdot 9^\alpha$	$6\cdot 4^\alpha+8\cdot 5^\alpha+5\cdot 6^\alpha$	$6\cdot 8^\alpha+8\cdot 13^\alpha+5\cdot 18^\alpha$
Pentacene		286.182	499.831	$6\cdot 4^\alpha+16\cdot 6^\alpha+4\cdot 9^\alpha$	$6\cdot 4^\alpha+16\cdot 5^\alpha+4\cdot 6^\alpha$	$6\cdot 8^\alpha+16\cdot 13^\alpha+4\cdot 18^\alpha$
Benzo[a]tetracene		285.056	513.857	$7\cdot 4^\alpha+14\cdot 6^\alpha+5\cdot 9^\alpha$	$7\cdot 4^\alpha+14\cdot 5^\alpha+5\cdot 6^\alpha$	$7\cdot 8^\alpha+14\cdot 13^\alpha+5\cdot 18^\alpha$
Dibenzo[a,h]anthracene		284.037	508.537	$8\cdot 4^\alpha+12\cdot 6^\alpha+6\cdot 9^\alpha$	$8\cdot 4^\alpha+12\cdot 5^\alpha+6\cdot 6^\alpha$	$8\cdot 8^\alpha+12\cdot 13^\alpha+6\cdot 18^\alpha$
Dibenzo[a,j]anthracene		284.088	507.395	$8\cdot 4^\alpha+12\cdot 6^\alpha+6\cdot 9^\alpha$	$8\cdot 4^\alpha+12\cdot 5^\alpha+6\cdot 6^\alpha$	$8\cdot 8^\alpha+12\cdot 13^\alpha+6\cdot 18^\alpha$
Pentaphene		285.148	506.076	$7\cdot 4^\alpha+14\cdot 6^\alpha+5\cdot 9^\alpha$	$7\cdot 4^\alpha+14\cdot 5^\alpha+5\cdot 6^\alpha$	$7\cdot 8^\alpha+14\cdot 13^\alpha+5\cdot 18^\alpha$
Benzo[g]chrysene		284.595	512.523	$10\cdot 4^\alpha+8\cdot 6^\alpha+8\cdot 9^\alpha$	$10\cdot 4^\alpha+8\cdot 5^\alpha+8\cdot 6^\alpha$	$10\cdot 8^\alpha+8\cdot 13^\alpha+8\cdot 18^\alpha$
Pentahelicene		284.870	500.734	$9\cdot 4^\alpha+10\cdot 6^\alpha+7\cdot 9^\alpha$	$9\cdot 4^\alpha+10\cdot 5^\alpha+7\cdot 6^\alpha$	$9\cdot 8^\alpha+10\cdot 13^\alpha+7\cdot 18^\alpha$
Benzo[c]chrysene		284.503	510.307	$9\cdot 4^\alpha+10\cdot 6^\alpha+7\cdot 9^\alpha$	$9\cdot 4^\alpha+10\cdot 5^\alpha+7\cdot 6^\alpha$	$9\cdot 8^\alpha+10\cdot 13^\alpha+7\cdot 18^\alpha$
Picene		284.785	509.210	$9\cdot 4^\alpha+10\cdot 6^\alpha+7\cdot 9^\alpha$	$9\cdot 4^\alpha+10\cdot 5^\alpha+7\cdot 6^\alpha$	$9\cdot 8^\alpha+10\cdot 13^\alpha+7\cdot 18^\alpha$
Benzo[b]chrysene		284.740	513.879	$8\cdot 4^\alpha+12\cdot 6^\alpha+6\cdot 9^\alpha$	$8\cdot 4^\alpha+12\cdot 5^\alpha+6\cdot 6^\alpha$	$8\cdot 8^\alpha+12\cdot 13^\alpha+6\cdot 18^\alpha$
Dibenzo[a,c]anthracene		284.233	511.770	$9\cdot 4^\alpha+10\cdot 6^\alpha+7\cdot 9^\alpha$	$9\cdot 4^\alpha+10\cdot 5^\alpha+7\cdot 6^\alpha$	$9\cdot 8^\alpha+10\cdot 13^\alpha+7\cdot 18^\alpha$
Dibenzo[b,g]phenanthrene		284.552	509.611	$8\cdot 4^\alpha+12\cdot 6^\alpha+6\cdot 9^\alpha$	$8\cdot 4^\alpha+12\cdot 5^\alpha+6\cdot 6^\alpha$	$8\cdot 8^\alpha+12\cdot 13^\alpha+6\cdot 18^\alpha$
Perylene		251.175	461.545	$8\cdot 4^\alpha+8\cdot 6^\alpha+8\cdot 9^\alpha$	$8\cdot 4^\alpha+8\cdot 5^\alpha+8\cdot 6^\alpha$	$8\cdot 8^\alpha+8\cdot 13^\alpha+8\cdot 18^\alpha$
Benzo[e]pyrene		250.568	463.738	$8\cdot 4^\alpha+8\cdot 6^\alpha+8\cdot 9^\alpha$	$8\cdot 4^\alpha+8\cdot 5^\alpha+8\cdot 6^\alpha$	$8\cdot 8^\alpha+8\cdot 13^\alpha+8\cdot 18^\alpha$
Benzo[a]pyrene		251.973	468.712	$7\cdot 4^\alpha+10\cdot 6^\alpha+7\cdot 9^\alpha$	$7\cdot 4^\alpha+10\cdot 5^\alpha+7\cdot 6^\alpha$	$7\cdot 8^\alpha+10\cdot 13^\alpha+7\cdot 18^\alpha$
Hexahelicene		336.098	555.409	$10\cdot 4^\alpha+12\cdot 6^\alpha+9\cdot 9^\alpha$	$10\cdot 4^\alpha+12\cdot 5^\alpha+9\cdot 6^\alpha$	$10\cdot 8^\alpha+12\cdot 13^\alpha+9\cdot 18^\alpha$
Benzo[ghi]perylene		267.543	472.295	$7\cdot 4^\alpha+10\cdot 6^\alpha+10\cdot 9^\alpha$	$7\cdot 4^\alpha+10\cdot 5^\alpha+10\cdot 6^\alpha$	$7\cdot 8^\alpha+10\cdot 13^\alpha+10\cdot 18^\alpha$
Hexacene		337.204	554.784	$6\cdot 4^\alpha+20\cdot 6^\alpha+5\cdot 9^\alpha$	$6\cdot 4^\alpha+20\cdot 5^\alpha+5\cdot 6^\alpha$	$6\cdot 8^\alpha+20\cdot 13^\alpha+5\cdot 18^\alpha$
Coronene		285.041	468.796	$6\cdot 4^\alpha+12\cdot 6^\alpha+12\cdot 9^\alpha$	$6\cdot 4^\alpha+12\cdot 5^\alpha+12\cdot 6^\alpha$	$6\cdot 8^\alpha+12\cdot 13^\alpha+12\cdot 18^\alpha$
Ovalene		368.518	551.708	$6\cdot 4^\alpha+16\cdot 6^\alpha+19\cdot 9^\alpha$	$6\cdot 4^\alpha+16\cdot 5^\alpha+19\cdot 6^\alpha$	$6\cdot 8^\alpha+16\cdot 13^\alpha+19\cdot 18^\alpha$

In the field of statistics, for a series of k measurements of X and Y, denoted by x_n and y_n $(n = 1, 2, \dots, k)$, the *correlation coefficient (ρ) of X and Y* is defined by

$$\rho(Y,X) = \frac{\sum_{n=1}^{k}(x_n-\bar{x})(y_n-\bar{y})}{\sqrt{\sum_{n=1}^{k}(x_n-\bar{x})^2}\sqrt{\sum_{n=1}^{k}(y_n-\bar{y})^2}} \quad (11)$$

where $\bar{x} = \frac{1}{k}\sum_{n=1}^{k} x_n$ and $\bar{y} = \frac{1}{k}\sum_{n=1}^{k} y_n$.

Then with the series x_n and y_n $(n = 1, 2, \dots, k)$, a *regression line* $y' = ax + b$ where $\{a, b \in \mathbb{R}\}$ can be calculated. This is known as the *least square line* or a *line of best fit*. The *standard error of fit* is defined as

$$s(Y,X) = \sqrt{\frac{1}{k-2}\sum_{n=1}^{k}(y_n-y_n')^2} \quad (12)$$

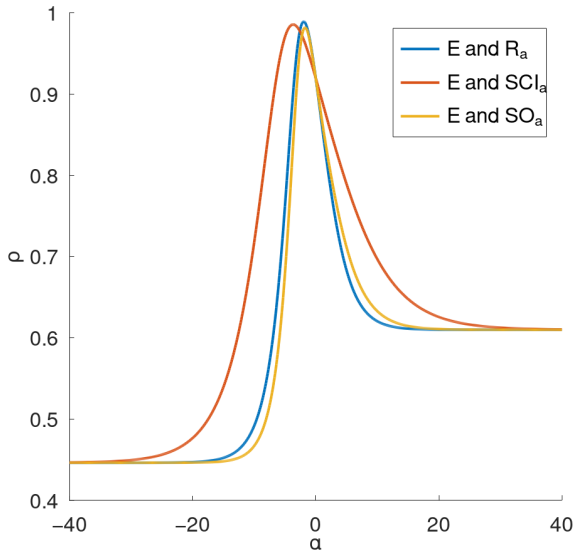

Figure 4: Correlation coefficient curves between general indices and E of lower benzenoids (far-view)

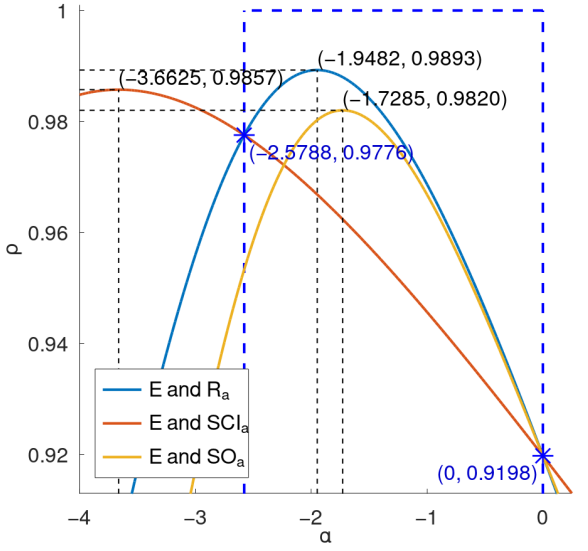

Figure 5: Correlation coefficient curves between general indices and E of lower benzenoids

where $y'_n = ax_n + b$ (the regression line's resulting predicted value).

The standard error of fit and correlation coefficient are both key goodness-of-fit measures in regression analysis. Using various mathematical or statistical software, they can be easily obtained.

There exists good correlation between ΔH and R_α when α is in some interval. For example, for $\alpha \in [-1.8384, -0.5499]$, ΔH and R_α has correlation coefficient greater than 0.99000. Similarly, there also exists - for α in different intervals - good correlation between ΔH and SCI_α, between ΔH and SO_α, between E and R_α, between E and SCI_α, and between E and SO_α as in Figure 6.

By Figures 3 and 4, we have that, for 30 lower benzenoids, $R_{-1.2383}$ and $R_{-1.9482}$, respectively, are the most linearly correlated with ΔH and E among all Randić indices, $SCI_{-2.3554}$ and $SCI_{-3.6625}$, respectively, are the most linearly correlated with ΔH and E among all sum-connectivity indices, while $SO_{-1.1165}$ and $SO_{-1.7285}$, respectively, are the most linearly correlated with ΔH and E among all Sombor indices. The linear correlations (with 95% confidence intervals) between the thermodynamic properties (ΔH and E) and all the aforementioned indices, respectively, are given below:

$$\begin{aligned} \Delta H &= -19.567(\pm 6.822) \\ &\quad + 96.678(\pm 2.333)\, R_{-1.23834}, \\ \rho(\Delta H, R_{-1.23834}) &= 0.998063, \\ s(\Delta H, R_{-1.23834}) &= 3.66806, \end{aligned} \tag{13}$$

$$\begin{aligned} \Delta H &= -18.259(\pm 8.829) \\ &\quad + 453.527(\pm 14.229)\, SCI_{-2.35541}, \\ \rho(\Delta H, SCI_{-2.35541}) &= 0.996732, \\ s(\Delta H, SCI_{-2.35541}) &= 4.76278, \end{aligned} \tag{14}$$

$$\begin{aligned} \Delta H &= -16.364(\pm 10.584) \\ &\quad + 175.079(\pm 6.629)\, SO_{-1.116549}, \\ \rho(\Delta H, SO_{-1.116549}) &= 0.995251, \\ s(\Delta H, SO_{-1.116549}) &= 5.73935, \end{aligned} \tag{15}$$

$$\begin{aligned} E &= 129.723(\pm 19.850) \\ &\quad + 379.673(\pm 21.698)\, R_{-1.94823}, \\ \rho(E, R_{-1.94823}) &= 0.989277, \\ s(E, R_{-1.94823}) &= 9.43091, \end{aligned} \tag{16}$$

$$\begin{aligned} E &= 132.844(\pm 22.745) \\ &\quad + 4049.697(\pm 267.589)\, SCI_{-3.66247}, \\ \rho(E, SCI_{-3.66247}) &= 0.985743, \\ s(E, SCI_{-3.66247}) &= 10.86489, \end{aligned} \tag{17}$$

$$\begin{aligned} E &= 136.413(\pm 25.344) \\ &\quad + 907.902(\pm 67.543)\, SO_{-1.72854}, \\ \rho(E, SO_{-1.72854}) &= 0.9820298, \\ s(E, SO_{-1.72854}) &= 12.18666, \end{aligned} \tag{18}$$

where s and ρ are the standard error of fit and correlation coefficient respectively.

Figure 7 shows scatter plots between the standard heat capacity ΔH and the indices $R_{-1.23834}$, $SCI_{-2.35541}$, and $SO_{-1.116549}$, as well as scatter plots between the standard molecular entropy E and the indices $R_{-1.94823}$, $SCI_{-3.66247}$, and $SO_{-1.72854}$ for the 30 lower benzenoids.

It is obvious from Equations (13) to (18), that the Randić indices $R_{-1.23834}$ and $R_{-1.94823}$, respectively, are the best for measuring the heat capacities and standard molecular entropies among all the examined indices.

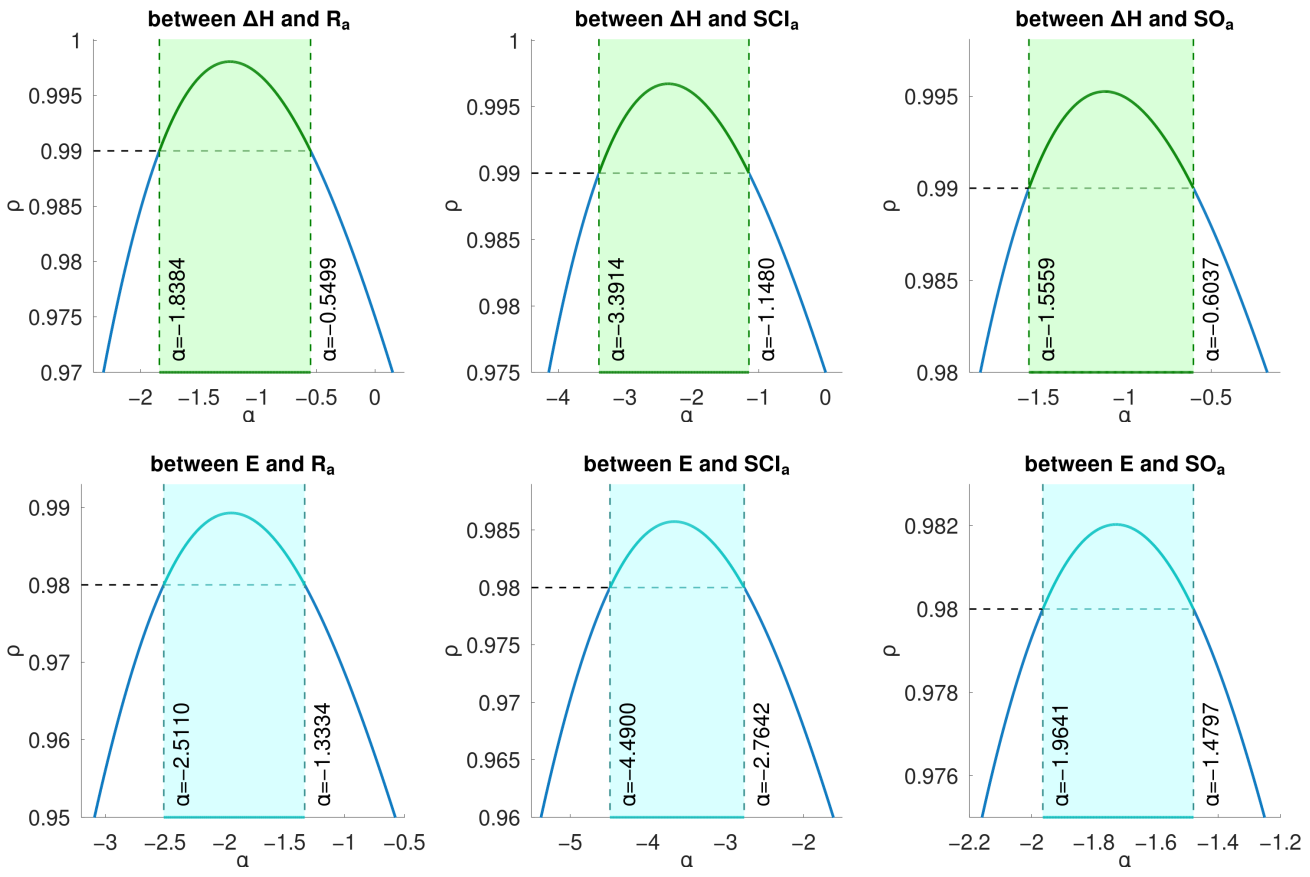

Figure 6: Intervals for good ρ for ΔH-R_α, ΔH-SCI_α, ΔH-SO_α, E-R_α, E-SCI_α and E-SO_α for lower benzenoids.

4. Conclusion

We showed in this paper that there is good correlation between Standard Heat Capacity (ΔH) and general Randić index (R_α), between ΔH and general sum-connectivity index (SCI_α), between ΔH and general Sombor index (SO_α), as well as between Standard Molecular Entropy (E) and R_α, between E and SCI_α, and between E and SO_α when α in some intervals (as in Figure 6) for benzenoid hydrocarbons. Moreover, for $\alpha \in (-1.65556, 0)$ and $\alpha \in (-2.57876, 0)$ (marked with blue dashed lines in Figures 3 and 5), R_α - compared to both SCI_α and SO_α - is the best measure of heat capacity and standard molecular entropy, respectively, of G. For α outside those intevals, SCI_α is the best measure of both heat capacity and standard molecular entropy of G.

5. Future Work

This paper examined the correlation power of the general Randić Index, general sum-connectivity index, and general Sombor index to determine the standard heat capacity (ΔH) of benzenoid hydrocarbons, as well as their correlation power to determine the standard molecular entropy (E) of benzenoid hydrocarbons. We propose further study to be conducted to similarly examine other generalized valency-based indices in determining ΔH and E of benzenoid hydrocarbons.

6. Supporting Information

Octave 7.2 scripts used to generate results and draw Figures 2 to 7 are also provided on GitHub:
https://github.com/wafibismail/Correl_GenInd_HeatCap_Entropy_BenzHCarb

Declarations

Availability of Data and Materials

No datasets were generated or analyzed during the current study; Data sharing not applicable to this article.

Conflict of Interests

The authors declared that they have no conflict of interest in regards to this manuscript.

Authors' contributions

The authors declare that the study was realized in collaboration with equal responsibility. All authors read and approved the final manuscript.

Acknowledgments

We extend our sincerest gratitude to all involved, from lecturers for the relevant knowledge that they have passed down, project supervisor for his expert guidance, friends whose company made the journey meaningful, and authors themselves for the monumental effort and enthusiasm put into the work. It was only with everyone's part that the conducting of this research was able to be as smooth-sailing as it was.

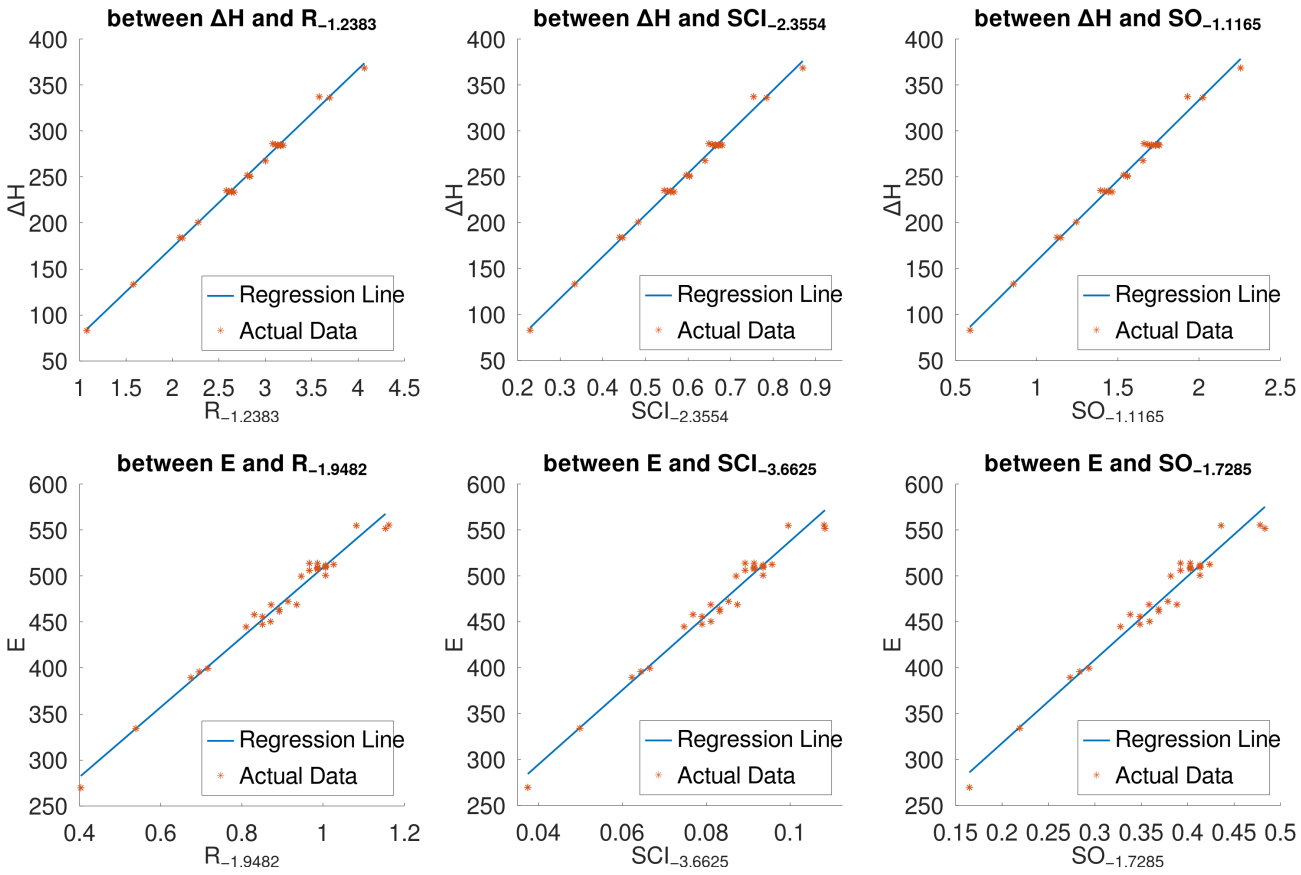

Figure 7: Scatter plots of ΔH-$R_{-1.23834}$, ΔH-$SCI_{-2.35541}$, ΔH-$SO_{-1.116549}$, E-$R_{-1.94823}$, E-$SCI_{-3.66247}$, E-$SO_{-1.72854}$ for lower benzenoids.

References

[1] M. Randic, Characterization of molecular branching, Journal of the American Chemical Society 97 (1975) 6609–6615.

[2] B. Furtula, I. Gutman, Comparing energy and randic energy, Macedonian Journal of Chemistry and Chemical Engineering 32 (2013) 117–123.

[3] N. Trinajstić, Xueliang li, ivan gutman: Mathematical aspects of randić-type molecular structure descriptors, Croatica Chemica Acta 79 (2006) A31–A32.

[4] R. Cruz, I. Gutman, J. Rada, On benzenoid systems with minimal number of inlets, Journal of the Serbian Chemical Society 78 (2013) 1351–1357.

[5] M. Randić, The connectivity index 25 years after, Journal of Molecular Graphics and Modelling 20 (2001) 19–35.

[6] R. Todeschini, V. Consonni, Handbook of molecular descriptors, John Wiley & Sons, 2008.

[7] B. Bollobás, P. Erdös, Graphs of extremal weights, Ars combinatoria 50 (1998) 225.

[8] P. Balister, B. Bollobás, S. Gerke, The generalized randić index of trees, Journal of Graph Theory 56 (2007) 270–286.

[9] J. Li, Y. Li, The asymptotic value of the zeroth-order randić index and sum-connectivity index for trees, Applied Mathematics and Computation 266 (2015) 1027–1030.

[10] F. Li, Q. Ye, Second order randić index of fluoranthene-type benzenoid systems, Applied Mathematics and Computation 268 (2015) 534–546.

[11] X. Li, J. Zheng, Extremal chemical trees with minimum or maximum general randic index, MATCH Commun. Math. Comput. Chem 55 (2006) 381–390.

[12] B. Zhou, N. Trinajstić, On a novel connectivity index, Journal of mathematical chemistry 46 (2009) 1252–1270.

[13] B. Zhou, N. Trinajstić, On general sum-connectivity index, Journal of mathematical chemistry 47 (2010) 210–218.

[14] I. Gutman, Geometric approach to degree-based topological indices: Sombor indices, MATCH Commun. Math. Comput. Chem 86 (2021) 11–16.

[15] C. Phanjoubam, S. M. Mawiong, On general sombor index, arXiv preprint arXiv:2110.03225 (2021).

[16] Z. Du, B. Zhou, N. Trinajstić, On the general sum-connectivity index of trees, Applied Mathematics Letters 24 (2011) 402–405.

[17] J. Liu, et al., On harmonic index and diameter of graphs, J. Appl. Math. Phys 1 (2013) 5–6.

[18] J. Rada, O. Araujo, I. Gutman, Randić index of benzenoid systems and phenylenes, Croatica Chemica Acta 74 (2001) 225–235.