Correlation potential of general product-connectivity and general sum-connectivity graphical indices for evaluating physicochemical properties of benzenoid hydrocarbons

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ABSTRACT

This article shows that two examined topological indices, namely the general Randić index R_α and the general sum-connectivity index SCI_α - when the real number α is in some interval - are closely related molecular descriptors. By comparing these two, it is evident that the indices $R_{-0.33030}$ and $R_{-1.72056}$ are the best for measuring the boiling point bp and the enthalpy of formation ΔH_f^o, 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].

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

Obviously,

$$R(G) = R_{-0.5}(G)$$
$$SCI(G) = SCI_{-0.5}(G)$$

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.

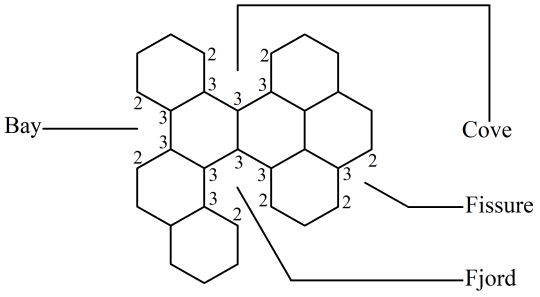

Figure 1: Cove, fissure, fjord and bay in a hexagonal system.

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.

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

$$n_{22} = v-2h-r+2, \quad n_{23} = 2r, \quad n_{33} = 3h-r-3. \quad (5)$$

By (2) and (5), the benzenoid system B has the general Randić index

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

by (4) and (5), the general sum-connectivity index

$$\begin{aligned} SCI_\alpha(B) &= n_{22}4^\alpha + n_{23}5^\alpha + n_{33}6^\alpha \\ &= (4^\alpha)v + (3\cdot 6^\alpha - 2\cdot 4^\alpha)h \\ &\quad + (2\cdot 5^\alpha - 4^\alpha - 6^\alpha)r + 2\cdot 4^\alpha - 3\cdot 6^\alpha, \end{aligned} \quad (7)$$

In (6) and (7), 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, boiling point bp, enthalpy of formation ΔH_f^0, general Randić index R_α, and general sum-connectivity index SCI_α are shown in Table 1 for 30 lower benzenoid hydrocarbons.

Table 1
The molecular structure, boiling point bp, enthalpy of formation ΔH_f^0, general Randić index R_α, and general sum-connectivity index SCI_α of 22 lower benzenoid hydrocarbons

BHs	Structure	bp	ΔH_f^0	R_α	SCI_α
Benzene		80.1	75.2	$6\cdot 4^\alpha$	$6\cdot 4^\alpha$
Naphthalene		218	141	$6\cdot 4^\alpha+4\cdot 6^\alpha+9^\alpha$	$6\cdot 4^\alpha+4\cdot 5^\alpha+6^\alpha$
Phenanthrene		338	202.7	$7\cdot 4^\alpha+6\cdot 6^\alpha+3\cdot 9^\alpha$	$7\cdot 4^\alpha+6\cdot 5^\alpha+3\cdot 6^\alpha$
Anthracene		340	222.6	$6\cdot 4^\alpha+8\cdot 6^\alpha+2\cdot 9^\alpha$	$6\cdot 4^\alpha+8\cdot 5^\alpha+2\cdot 6^\alpha$
Chrysene		431	271.1	$8\cdot 4^\alpha+8\cdot 6^\alpha+5\cdot 9^\alpha$	$8\cdot 4^\alpha+8\cdot 5^\alpha+5\cdot 6^\alpha$
Benzo[a]anthracene		425	277.1	$7\cdot 4^\alpha+10\cdot 6^\alpha+4\cdot 9^\alpha$	$7\cdot 4^\alpha+10\cdot 5^\alpha+4\cdot 6^\alpha$
Triphenylene		429	275.1	$9\cdot 4^\alpha+6\cdot 6^\alpha+6\cdot 9^\alpha$	$9\cdot 4^\alpha+6\cdot 5^\alpha+6\cdot 6^\alpha$
Tetracene		440	310.5	$6\cdot 4^\alpha+12\cdot 6^\alpha+3\cdot 9^\alpha$	$6\cdot 4^\alpha+12\cdot 5^\alpha+3\cdot 6^\alpha$
Benzo[a]pyrene		496	296	$7\cdot 4^\alpha+10\cdot 6^\alpha+7\cdot 9^\alpha$	$7\cdot 4^\alpha+10\cdot 5^\alpha+7\cdot 6^\alpha$
Benzo[e]pyrene		493	289.9	$8\cdot 4^\alpha+8\cdot 6^\alpha+8\cdot 9^\alpha$	$8\cdot 4^\alpha+8\cdot 5^\alpha+8\cdot 6^\alpha$
Perylene		497	319.2	$8\cdot 4^\alpha+8\cdot 6^\alpha+8\cdot 9^\alpha$	$8\cdot 4^\alpha+8\cdot 5^\alpha+8\cdot 6^\alpha$
Anthanthrene		547	323	$6\cdot 4^\alpha+12\cdot 6^\alpha+9\cdot 9^\alpha$	$6\cdot 4^\alpha+12\cdot 5^\alpha+9\cdot 6^\alpha$
Benzo[ghi]perylene		542	301.2	$7\cdot 4^\alpha+10\cdot 6^\alpha+10\cdot 9^\alpha$	$7\cdot 4^\alpha+10\cdot 5^\alpha+10\cdot 6^\alpha$
Dibenzo[a,c]anthracene		535	348	$9\cdot 4^\alpha+10\cdot 6^\alpha+7\cdot 9^\alpha$	$9\cdot 4^\alpha+10\cdot 5^\alpha+7\cdot 6^\alpha$
Dibenzo[a,h]anthracene		535	335	$8\cdot 4^\alpha+12\cdot 6^\alpha+6\cdot 9^\alpha$	$8\cdot 4^\alpha+12\cdot 5^\alpha+6\cdot 6^\alpha$
Dibenzo[a,j]anthracene		531	336.3	$8\cdot 4^\alpha+12\cdot 6^\alpha+6\cdot 9^\alpha$	$8\cdot 4^\alpha+12\cdot 5^\alpha+6\cdot 6^\alpha$
Picene		519	336.9	$9\cdot 4^\alpha+10\cdot 6^\alpha+7\cdot 9^\alpha$	$9\cdot 4^\alpha+10\cdot 5^\alpha+7\cdot 6^\alpha$
Coronene		590	296.7	$6\cdot 4^\alpha+12\cdot 6^\alpha+12\cdot 9^\alpha$	$6\cdot 4^\alpha+12\cdot 5^\alpha+12\cdot 6^\alpha$
Dibenzo(a,h)pyrene		596	375.6	$8\cdot 4^\alpha+12\cdot 6^\alpha+9\cdot 9^\alpha$	$8\cdot 4^\alpha+12\cdot 5^\alpha+9\cdot 6^\alpha$
Dibenzo(a,i)pyrene		594	366	$8\cdot 4^\alpha+12\cdot 6^\alpha+9\cdot 9^\alpha$	$8\cdot 4^\alpha+12\cdot 5^\alpha+9\cdot 6^\alpha$
Dibenzo(a,l)pyrene		595	393.3	$9\cdot 4^\alpha+10\cdot 6^\alpha+10\cdot 9^\alpha$	$9\cdot 4^\alpha+10\cdot 5^\alpha+10\cdot 6^\alpha$
Pyrene		393	221.3	$6\cdot 4^\alpha+8\cdot 6^\alpha+5\cdot 9^\alpha$	$6\cdot 4^\alpha+8\cdot 5^\alpha+5\cdot 6^\alpha$

3. Results and Discussion

The following results conclude that the general Randić index R_α, and the general sum-connectivity index SCI_α - for α in some interval - can quite accurately reproduce the boiling point and enthalpy of formation of the lower benzenoid hydrocarbons.

From the data shown in Table 1, we have produced four curves, as illustrated in Figures 2 to 4. For these 22 lower benzenoids, the correlation coefficient curves for their thermodynamic properties (bp in Figures 2 and 3, ΔH_f^0 in Figures 4 and 5) and the indices (R_α or SCI_α) are drawn in the respective figures in solid lines, distinguished by colors.

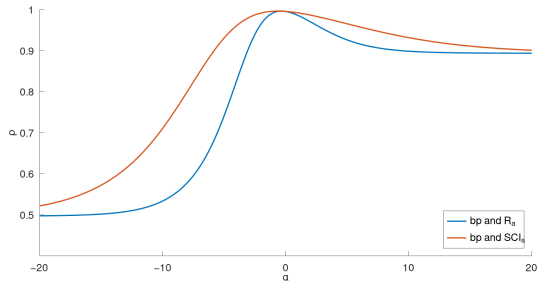

Figure 2: Correlation coefficient curves between general indices and bp of lower benzenoids (far-view)

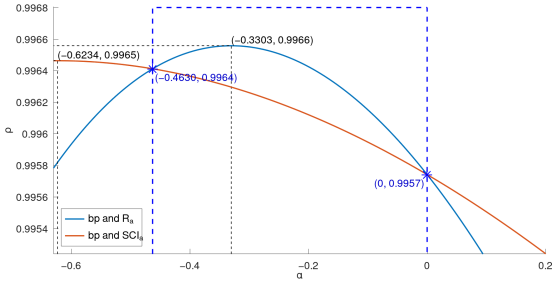

Figure 3: Correlation coefficient curves between general indices and bp of lower benzenoids

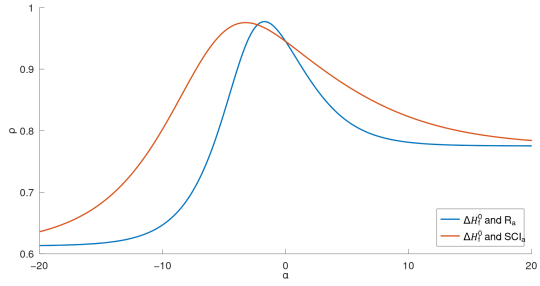

Figure 4: Correlation coefficient curves between general indices and ΔH_f^0 of lower benzenoids (far-view)

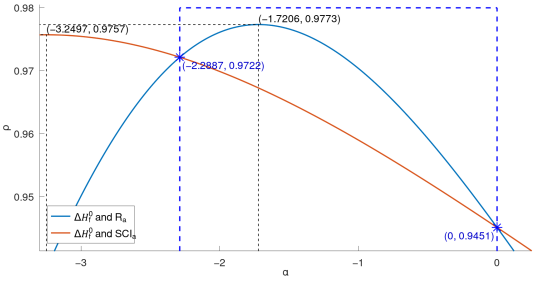

Figure 5: Correlation coefficient curves between general indices and ΔH_f^0 of lower benzenoids

Comparing the two general indices, the general Randić index R_α is the best measure of *boiling point bp* for benzenoid hydrocarbons for $\alpha \in (-0.4630, 0)$, 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 *enthalpy of formation* ΔH_f^o of benzenoid hydrocarbons, the general Randić index R_α is the best for $\alpha \in (-2.2887, 0)$, as can be seen in Figure 5, while for other α, the sum-connectivity index SCI_α is the best.

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

$$\rho(Y, X) = \frac{\sum_{n=1}^{k}(x_n - \bar{x})(y_n - \bar{y})}{\sqrt{\sum_{n=1}^{k}(x_n - \bar{x})^2}\sqrt{\sum_{n=1}^{k}(y_n - \bar{y})^2}} \tag{8}$$

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 $(n = 1, 2, \ldots, k)$, 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

$$s(Y, X) = \sqrt{\frac{1}{k-2}\sum_{n=1}^{k}(y_n - y'_n)^2} \tag{9}$$

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 bp and R_α when α is in some interval. For example, for $\alpha \in [-1.154217, 0.681350]$, bp and R_α has correlation coefficient greater than 0.996558. Similarly, there also exists - for α in different intervals - good correlation between bp and SCI_α, between ΔH_f^0 and R_α, between ΔH_f^0 and SCI_α as in Figure 6.

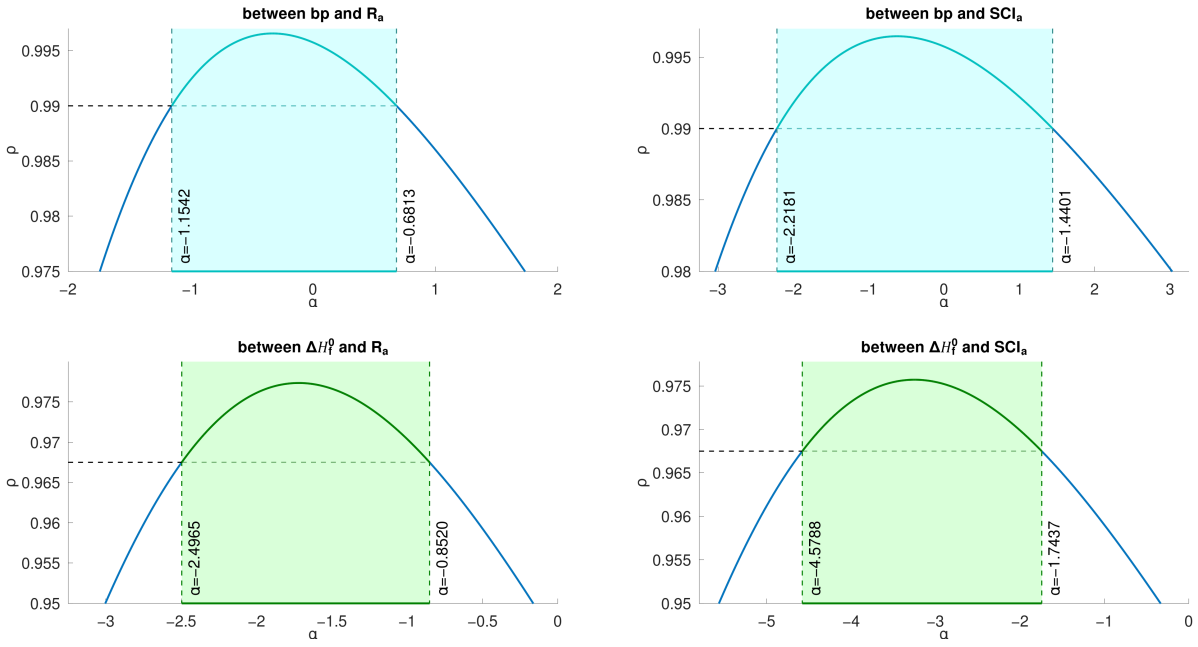

Figure 6: Intervals for good ρ for bp-R_α, bp-SCI_α, ΔH_f^0-R_α, ΔH_f^0-SCI_α for lower benzenoids.

By Figures 3 and 5, we have that, for 22 lower benzenoids, $R_{-0.33030}$ and $R_{-1.72056}$, respectively, are the most linearly correlated with bp and ΔH_f^0 among all Randić indices, $SCI_{-0.62336}$ and $SCI_{-3.24966}$, respectively, are the most linearly correlated with bp and ΔH_f^0 among all sum-connectivity indices. The linear correlations (with 95% confidence intervals) between the thermodynamic properties (bp and ΔH_f^0) and all the aforementioned indices, respectively, are given below:

$$\begin{aligned} bp &= 39.693(\pm 1.540) \\ &\quad - 42.183(\pm 20.161)\ R_{-0.33030}, \\ \rho(bp, R_{-0.33030}) &= 0.996558, \\ s(bp, R_{-0.33030}) &= 10.9571, \end{aligned} \tag{10}$$

$$\begin{aligned} bp &= 59.430(\pm 2.334) \\ &\quad - 40.884(\pm 20.388)\ SCI_{-0.62336}, \\ \rho(bp, SCI_{-0.62336}) &= 0.996463, \\ s(bp, SCI_{-0.62336}) &= 11.1067, \end{aligned} \tag{11}$$

$$\begin{aligned} \Delta H_f^0 &= 300.943(\pm 30.399) \\ &\quad - 85.181(\pm 38.305)\ R_{-1.72056}, \\ \rho(\Delta H_f^0, R_{-1.72056}) &= 0.977344, \\ s(\Delta H_f^0, R_{-1.72056}) &= 16.5206, \end{aligned} \tag{12}$$

$$\begin{aligned} \Delta H_f^0 &= 2486.468(\pm 260.362) \\ &\quad - 82.232(\pm 39.402)\ SCI_{-3.24966}, \\ \rho(E, SCI_{-3.24966}) &= 0.975715, \\ s(E, SCI_{-3.24966}) &= 17.0968, \end{aligned} \tag{13}$$

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

Figure 7 shows scatter plots between the boiling point bp and the indices $R_{-0.33030}$, and $SCI_{-0.62336}$, as well as scatter plots between the enthalpy of formation ΔH_f^0 and the indices $R_{-1.72056}$, and $SCI_{-3.24966}$ for the 30 lower benzenoids.

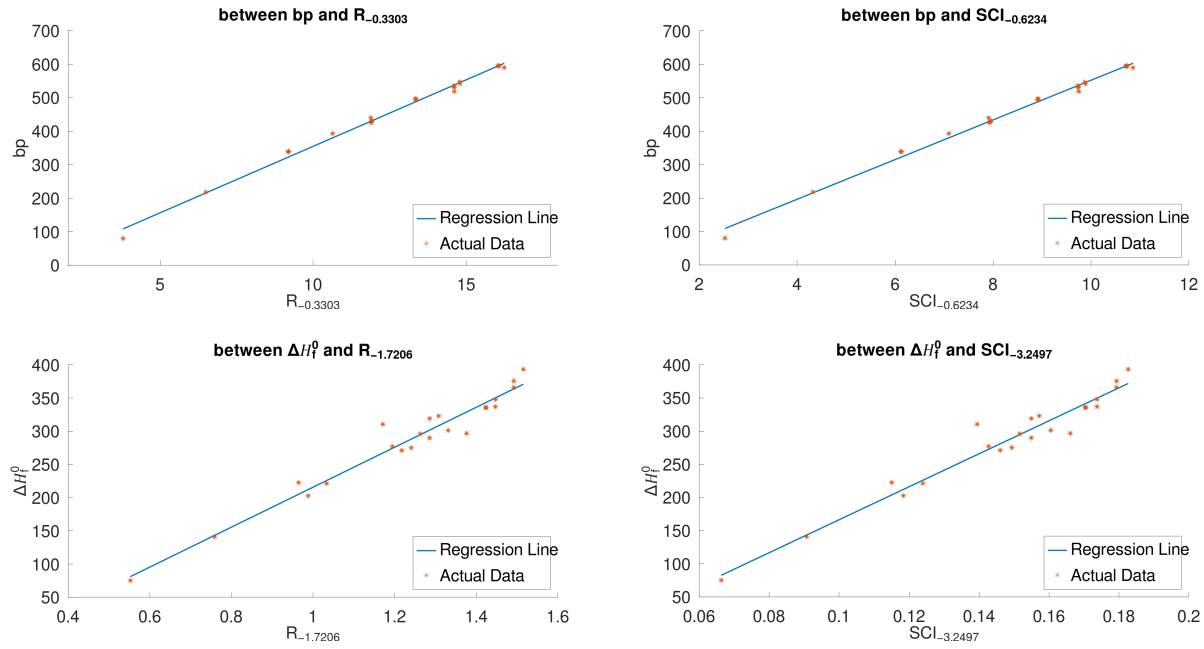

Figure 7: Scatter plots of bp-$R_{-0.33030}$, bp-$SCI_{-0.62336}$, ΔH_f^0-$R_{-1.72056}$, ΔH_f^0-$SCI_{-3.24966}$ for lower benzenoids.

It is obvious from Equation (10), Equation (11), Equation (12) and Equation (13), that the Randić indices $R_{-0.33030}$ and $R_{-1.72056}$, respectively, are the best for measuring the boiling point and enthalpy of formation among all the examined indices.

4. Conclusion

We showed in this paper that there is good correlation between boiling point (bp) and general Randić index (R_α), between bp and general sum-connectivity index (SCI_α), as well as between enthalpy of formation (ΔH_f^0) and R_α, between ΔH_f^0 and SCI_α when α in some intervals (as in Figure 6) for benzenoid hydrocarbons. Moreover, for $\alpha \in (-0.4630, 0)$ and $\alpha \in (-2.2887, 0)$ (marked with blue dashed lines in Figures 3 and 5), R_α - compared to SCI_α - is the best measure of boiling point and enthalpy of formation, respectively, of G. For α outside those intervals, SCI_α is the best measure of both boiling point and enthalpy of formation of G.

5. Future Work

This paper examined the correlation power of the general Randić Index and general sum-connectivity index to determine the boiling point (bp) of benzenoid hydrocarbons, as well as their correlation power to determine the enthalpy of formation (ΔH_f^0) of benzenoid hydrocarbons. We propose further study to be conducted to similarly examine other generalized valency-based indices in determining bp and ΔH_f^0 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/AzriArfan/Correl_of_RandSCI_between_bpandH

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.

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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.