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New Versions of Locating Indices and Their Significance in Predicting the Physicochemical Properties of Benzenoid Hydrocarbons

Suha Wazzan [1,*,†] and Anwar Saleh [2,†]

[1] Department of Mathematics, Science Faculty, King Abdulaziz University, Jeddah 21589, Saudi Arabia
[2] Department of Mathematics, Science Faculty, University of Jeddah, Jeddah 21589, Saudi Arabia; asaleh1@uj.edu.sa
* Correspondence: swazzan@kau.edu.sa
† These authors contributed equally to this work.

Abstract: In this paper, we introduce some new versions based on the locating vectors named locating indices. In particular, Hyper locating indices, Randić locating index, and Sambor locating index. The exact formulae for these indices of some well-known families of graphs and for the Helm graph are derived. Moreover, we determine the importance of these locating indices for 11 benzenoid hydrocarbons. Furthermore, we show that these new versions of locating indices have a reasonable correlation using linear regression with physicochemical characteristics such as molar entropy, acentric factor, boiling point, complexity, octanol–water partition coefficient, and Kovats retention index. The cases in which good correlations were obtained suggested the validity of the calculated topological indices to be further used to predict the physicochemical properties of much more complicated chemical compounds.

Keywords: Hyper locating indices; Randić locating index; Sombor locating index; Helm graph; *QSPR* analysis

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1. Introduction

A molecular structure [1] is a graph whose edges correspond to the bonds and vertices of the atoms. Such invariants and indices in graphs have gained increasing interest over time, since they allow scientists to make new classifications for the graphs being studied. One of its many examples is the *QSPR* or quantitative structure–property relationship (see, for example [2–5]) levels of the alkanes (see [6,7]). This index was named after him as the Wiener index. Since the introduction of the Wiener index, around 200 other indices have been defined and studied, such as those presented by Wazzan et al. (see, for example, [8–10]), Gutman (see, for example, [11,12]), and Çevik (see, for example, [13,14]). Some of these indices have been used indirectly or directly in the applications of chemistry, physics, or pharmacology. Since indices have been found to have many applications, many graph theorist still aim to find similar indices and their applications in graph theory. Among the successful attempts are the Sombor $SO(\varsigma)$ and Omega indices $\Omega(\varsigma)$ (see [15,16]) in which the coinvestigator has partaken in these graph invariants studies. Wazzan et al. in [17] introduced two novel topological indices named the first and second locating indices, and in [18] multiplicative locating indices are calculated for families of graphs. In addition, the *QSPR* of hexane and its isomers is investigated by the locating indices. We show that locating indices have positive correlation with at least one property, have structural interpretation, preferably contradistinguish. They can also be generalizable to more advanced analogues, be elementary, not be established based on properties, not be trivially related to other descriptors, be possible to compute effectively, and be based on organizable structure. These reasons motivated us to introduce new versions of these indices, we called them first and second Hyper locating indices, Randić locating index and

Sombor locating index. In 2013, Shirdel et al. [19] introduced a new distance-based group of Zagreb indices named Hyper–Zagreb indices, as $HM_1(\varsigma) = \sum_{v_iv_j \in E(\varsigma)} \left(d_{v_i} + d_{v_j}\right)^2$ and $HM_2(\varsigma) = \sum_{v_iv_j \in E(\varsigma)} \left(d_{v_i} \cdot d_{v_j}\right)^2$. The Randić index of a graph ς introduced by Randić [20] is the most important and widely applied, it is defined as $R(\varsigma) = \sum_{v_iv_j \in E(\varsigma)} \frac{1}{\sqrt{d_{v_i} \cdot d_{v_j}}}$. The Sombor index of a graph ς, which is a novel vertex-degree-based molecular structure descriptor proposed by Gutman [21] is defined as $SO(\varsigma) = \sum_{v_iv_j \in E(\varsigma)} \sqrt{(d_{v_i})^2 + \left(d_{v_j}\right)^2}$. We keep in mind the definition of first and second locating indices given in [17], in order to grasp the importance of this paper. Since this paper is a continuation of our work in [17,22], let us recall the basic facts regarding these indices: let $\varsigma = (V, E)$ be a connected graph with the vertex set $V = \{v_1, v_2, \ldots, v_n\}$ with at least two edges a *locating function* of ς denoted by $\mathcal{F}(\varsigma)$ is a function $\mathcal{F}(\varsigma) : V(\varsigma) \to A^n$ where A is the set of all non-negative integers such that $\mathcal{F}(v_i) = \overrightarrow{v_i} = \langle d(v_1, v_i), d(v_2, v_i), \cdots, d(v_n, v_i)\rangle$, where $d(v_i, v_j)$ is the distance between the vertices v_i and v_j in ς. The vector $\mathcal{F}(v_i)$ is called the *locating vector* corresponding to the vertex v_i, where $\overrightarrow{v_i} \cdot \overrightarrow{v_j}$ is the dot product of the vectors $\overrightarrow{v_i}$ and $\overrightarrow{v_j}$ and $\overrightarrow{v_i} + \overrightarrow{v_j}$ is the sum of vectors $\overrightarrow{v_i}$ and $\overrightarrow{v_j}$ in the integers space A^n such that v_i is adjacent to v_j. For any vector $\overrightarrow{v} = \langle x_1, x_2, \ldots, x_n\rangle$ the magnitude of $\overrightarrow{v}$ is $|\overrightarrow{v}| = \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2}$. In this paper we consider a connected graph $\varsigma = (V, E)$ with an edge set $E(\varsigma)$ [has at least two edges] and vertex set $V = \{v_1, v_2, \cdots, v_r\}$, we introduce the following locating indices:

The first Hyper locating index:

$$HM_1^{\mathcal{L}}(\varsigma) = \sum_{v_iv_j \in E(\varsigma)} |\overrightarrow{v_i} + \overrightarrow{v_j}|^2 . \tag{1}$$

Second Hyper locating index:

$$HM_2^{\mathcal{L}}(\varsigma) = \sum_{v_iv_j \in E(\varsigma)} (\overrightarrow{v_i} \cdot \overrightarrow{v_j})^2 . \tag{2}$$

The Randić locating index:

$$R^{\mathcal{L}}(\varsigma) = \sum_{v_iv_j \in E(\varsigma)} \frac{1}{\sqrt{\overrightarrow{v_i} \cdot \overrightarrow{v_j}}} . \tag{3}$$

The Sombor locating index:

$$SO^{\mathcal{L}}(\varsigma) = \sum_{v_iv_j \in E(\varsigma)} \sqrt{|\overrightarrow{v_i}|^2 + |\overrightarrow{v_j}|^2}. \tag{4}$$

The topological indices with a high positive correlation factor play a crucial role in quantitative structure–property relationships $(QSPR)$ and quantitative structure–activity relationships $(QSAR)$ analysis. In order to predict the validity of these new versions of locating indices we consider one branch of Benzene which is the polycyclic aromatic hydrocarbons. For the two other kinds the linear and branched hydrocarbons, whose properties can also be described by these kind of indices, according to the result obtained in this report, we can predict the validities of the new version of locating indices in the other two kind of hydrocarbons. Hence, we leave this investigation for future work. Benzene (C_6H_6) is an organic chemical compound composed of six carbon atoms joined in a planar ring with one hydrogen atom attached to each ring. Benzene is classified as a hydrocarbon because it contains only hydrogen and carbon atoms. Benzene is a natural ingredient of crude oil and is one of the basic petrochemicals. It is described as an aromatic hydrocarbon due to the cyclic connected pi bonds between the carbon atoms. The abbreviation of it is PhH. Benzene is a colorless and highly flammable liquid. It is used as a precursor to the synthesis of more complex chemical structure, such as cumene and ethylbenzene. The toxicity of benzene limits its use in consumer items despite its popularity as a major industrial chemical [23].

To test the predictive ability of these new indices, we discuss the linear regression analysis of 11 benzenoid hydrocarbons, which are used many times to approach the efficiency of any topological descriptor in quantitative structure property relationships. We inspect the following physicochemical properties: boiling point (BP), molar entropy (S), acentric factor (ϖ), octanol–water partition coefficient $(logP)$, complexity (C), and Kovats retention index (RI).

2. New Versions of Locating Indices for Some Known Graphs

In this section, by considering new versions of locating indices, we will determine their values for some special graphs such as complete graph, complete bipartite graph, and cycle, wheel and path graph.

Lemma 1. *Let ς be the complete graph with three or more vertices r. Then*

1. $HM_1^{\mathcal{L}}(\varsigma) = 2r(r-1)^3$.
2. $HM_2^{\mathcal{L}}(\varsigma) = \dfrac{r(r-1)(r-2)^2}{2}$.
3. $R^{\mathcal{L}}(\varsigma) = \dfrac{r(r-1)}{2\sqrt{r-2}}$.
4. $SO^{\mathcal{L}}(\varsigma) = \dfrac{r\sqrt{(r-1)^3}}{\sqrt{2}}$.

Proof.

1. Let ς be the complete graph with number of vertices $r \geq 3$ for each vertex $v_i \in V(\varsigma)$ let $\overrightarrow{v_i}$ is the locating vector associated with it. Then $\overrightarrow{v_i} = \langle a_1, a_2, \cdots, a_r \rangle$ such that $a_i = 0$ and all the other components equal to 1. Hence $|\overrightarrow{v_i} + \overrightarrow{v_j}|^2 = [2 + 2(r-2)]^2 = 4(r-1)^2$. However, the total number of edges in ς is $\dfrac{r(r-1)}{2}$ and so $HM_1^{\mathcal{L}}(\varsigma) = 2r(r-1)^3$.
2. For any arbitrary locating vectors $\overrightarrow{v_i}$ and $\overrightarrow{v_j}$, where $i \neq j$, we gain $\overrightarrow{v_i} \cdot \overrightarrow{v_j} = r-2$. Therefore $HM_2^{\mathcal{L}}(\varsigma) = \dfrac{r(r-1)(r-2)^2}{2}$.
3. For any arbitrary locating vectors $\overrightarrow{v_i}$ and $\overrightarrow{v_j}$, where $i \neq j$, we gain $\overrightarrow{v_i} \cdot \overrightarrow{v_j} = r-2$. Therefore $\dfrac{1}{\sqrt{\overrightarrow{v_i} \cdot \overrightarrow{v_j}}} = \dfrac{1}{\sqrt{r-2}}$ hence $R^{\mathcal{L}}(\varsigma) = \dfrac{r(r-1)}{2\sqrt{r-2}}$ of the summation over all edges.
4. For each $\overrightarrow{v_i} = \langle a_1, a_2, \cdots, a_r \rangle$ we have $|\overrightarrow{v_i}|^2 = r-1$ and hence $\sqrt{|\overrightarrow{v_i}|^2 + |\overrightarrow{v_j}|^2} = \sqrt{2(r-1)}$. Therefore $SO^{\mathcal{L}}(\varsigma) = \dfrac{r\sqrt{(r-1)^3}}{\sqrt{2}}$.

□

Theorem 1. *Let ς be the complete bipartite graph $K_{r,s}$, where $1 < r \leq s$. Then*

1. $HM_1^{\mathcal{L}}(\varsigma) = rs(9(r+s-2)+2)$.
2. $HM_2^{\mathcal{L}}(\varsigma) = 4rs(r+s-2)^2$.
3. $R^{\mathcal{L}}(\varsigma) = \dfrac{rs}{\sqrt{2(r+s-2)}}$.

4. $SO^{\mathcal{L}}(\varsigma) = rs\sqrt{5(r+s)-8}$.

Proof. Let ς be the complete bipartite graph $K_{r,s}$, where $1 < r \leq s$, with two bipartite sets R and S such that $|R| = r$ and $|S| = s$, by labelling the vertices of ς as $V(\varsigma) = \{v_1, \ldots, v_r, u_1, \ldots, u_s\}$. It is clear that the corresponding locating $\overrightarrow{v_i}$ of the vertex v_i has one zero value in the ith position, $(r-1)$ components of value 2, and s components of value 1 for all $i = 1, 2, \ldots, r$ and the locating vector $\overrightarrow{u_j}$ correspond to the vertex u_j for all $j = 1, 2, \ldots, s$ has one zero value in the jth position, $(s-1)$ components of value 2, and r components of value 1. Therefore

1. For any two adjacent vertices v_i and u_j where $i = 1, 2, \ldots, r$ and $j = 1, 2, \ldots, s$ the locating vector $\overrightarrow{v_i} + \overrightarrow{u_j}$ has $(r-1)$ components of value three, $(s-1)$ components of value three, and two components of value one. Hence, $|\overrightarrow{v_i} + \overrightarrow{u_j}|^2 = 9(r-1) + 9(s-1) + 2 = 9(r+s-2) + 2$ for any two adjacent vertices in the two partition sets R and S. Hence, $HM_1^{\mathcal{L}}(\varsigma) = rs(9(r+s-2)+2)$.
2. For any two locating vertices $\overrightarrow{v_i}$ and $\overrightarrow{u_j}$ corresponding two the adjacent vertices v_i and u_j in $K_{r,s}$ we have $\overrightarrow{v_i} \cdot \overrightarrow{u_j} = 2(r+s-2)$ Hence $HM_2^{\mathcal{L}}(\varsigma) = 4rs(r+s-2)^2$.
3. By part 2 we deduce that $R^{\mathcal{L}}(\varsigma) = \dfrac{rs}{\sqrt{2(r+s-2)}}$.
4. For any $i = 1, 2, \ldots, r$ we have $|\overrightarrow{v_i}|^2 = 4(r-1) + s$ and $|\overrightarrow{u_j}|^2 = 4(s-1) + r$ for all $j = 1, 2, \ldots, s$ hence $|\overrightarrow{v_i}|^2 + |\overrightarrow{u_j}|^2 = 5r + 5s - 8$. Hence $SO^{\mathcal{L}}(\varsigma) = rs\sqrt{5(r+s)-8}$.

□

Theorem 2. *Let ς be wheel graph W_r with $r+1$ vertices such that $(r \geq 4)$. Then*

1. $HM_1^{\mathcal{L}}(\varsigma) = r(4r-6)^2 + 9r(r-1)^2$.
2. $HM_2^{\mathcal{L}}(\varsigma) = r[(4r-11)^2 + (2r-4)^2]$.
3. $R^{\mathcal{L}}(\varsigma) = \dfrac{\sqrt{2r}}{(4r-11)(2r-4)}$.
4. $SO^{\mathcal{L}}(\varsigma) = r\sqrt{17r^2 - 72r + 81} - 9\sqrt{2}r + 4\sqrt{2}r^2$.

Proof. Let $\varsigma \cong W_r$ with $r+1$ vertices. Suppose that the vertices $v_1, v_2, \cdots, v_r, v_{r+1} \in V(\varsigma)$ are labeling in the counterclockwise direction and the center of the wheel is labeled v_{r+1}. Hence the locating vector $\overrightarrow{v_i}$ for each vertex v_i where $i = 1, 2, \ldots, r$ has 0 component in the ith position, three components of value one, and $(r-3)$ components of value two. Where the locating vector $\overrightarrow{v_{r+1}}$ that corresponds to the vertex v_{r+1} is equal to $(\overbrace{1, 1, \cdots, 1}^{r \text{ times}}, 0)$. It is straightforward to notice that the permutation components in each vector $\overrightarrow{v_i}$ where $i = 1, 2, \cdots, r$, is $\mathbf{1, 0, 1}$. Therefore

1. For any two adjacent vertices $v_i + v_j$ where $i, j \in \{1, 2, \ldots, r\}$, $(\overrightarrow{v_i} + \overrightarrow{v_j})$ vector has two components of value one, two components of value three, one component of value two, and $r-4$ components of value four. For any vertex v_i, where $i = 1, \ldots, r$ we have $\overrightarrow{v_i} + \overrightarrow{v_{r+1}}$ is a vector contains two components of value one, two components of value two, and $(r-3)$ components of value three. So

$$|\overrightarrow{v_i} + \overrightarrow{v_j}|^2 = \begin{cases} (4r-6)^2 & \text{for } i,j \in \{1,2,\ldots,r\} \\ 9(r-1)^2 & \text{for } i \in \{1,2,\ldots,r\} \;\; j = r+1 \end{cases}$$

Hence $HM_1^{\mathcal{L}}(\varsigma) = r(4r-6)^2 + 9r(r-1)^2$.

2. Keeping in mind the permutation of components 1, 0, 1 in each vector $\overrightarrow{v_i}$ where $i = 1, \ldots, r$. It is clear that for v_i and v_j any two adjacent vertices where $i, j \in \{1, 2, \ldots, r\}$, hence $(\overrightarrow{v_i} \cdot \overrightarrow{v_j})^2 = (4r-11)^2$ and $(\overrightarrow{v_i} \cdot \overrightarrow{v_{r+1}})^2 = (2r-4)^2$. Therefore

$$HM_2^{\mathcal{L}}(\varsigma) = \sum_{v_i v_j \in E(\varsigma)} (4r-11)^2 + \sum_{v_i v_{r+1} \in E(\varsigma)} (2r-4)^2 = r[(4r-11)^2 + (2r-4)^2].$$

3. From part 2 we deduce that $R^{\mathcal{L}}(\varsigma) = \dfrac{\sqrt{2r}}{(4r-11)(2r-4)}$.
4. $|\overrightarrow{v_i}|^2 = (4r-9)^2$ for each corresponding locating vector $\overrightarrow{v_i}$ with the vertex v_i (i = 1,2,...,r) and $|\overrightarrow{v_{r+1}}|^2 = r^2$. Hence

$$\begin{aligned} SO^{\mathcal{L}}(\varsigma) &= \sum_{v_iv_j\in E(\varsigma)} \sqrt{2(4r-9)^2} + \sum_{v_iv_{r+1}\in E(\varsigma)} \sqrt{r^2+(4r-9)^2} \\ &= r(\sqrt{2}(4r-9) + \sqrt{r^2+(4r-9)^2}) = r\sqrt{17r^2-72r+81} - 9\sqrt{2}r + 4\sqrt{2}r^2. \end{aligned}$$

Hence the result.

□

Theorem 3. *For any path P_r where $(r \geq 3)$. Then*

1. $HM_1^{\mathcal{L}}(\varsigma) = \frac{1}{3}r(r-1)\big(2r^2-2r-1\big)$.
2. $HM_2^{\mathcal{L}}(\varsigma) = \frac{1}{15}r(r-1)(r-2)(r+1)\big(r^2-r-1\big)$.
3. $R^{\mathcal{L}}(\varsigma) = \sum\limits_{i=1}^{r-1} \dfrac{\sqrt{3}}{\sqrt{3i^2r-3ir^2+r^3-r}}$.
4. $SO^{\mathcal{L}}(\varsigma) = \sum_{i=1}^{r-1} \sqrt{\sum\limits_{k=1}^{r-i} k^2 + \sum\limits_{k=1}^{i} (k-1)^2 + \sum\limits_{k=1}^{r-i-1} k^2 + \sum\limits_{k=1}^{i+1} (k-1)^2}$.

Proof. Assume that P_r is the path with vertices $(r \geq 3)$. Suppose that the locating function is constructed by identify the vertices as $v_1, v_2, \cdots, v_r$ from left to right. Hence the corresponding vector for each vertex $v_i \in V(\varsigma)$ $(i = 1, \cdots, r)$ are given as in the following:

$$\begin{aligned} &\overrightarrow{v_1} = \langle 0,1,2,3,\cdots,r-1\rangle, &&\overrightarrow{v_2} = \langle 1,0,1,2,\cdots,r-2\rangle \\ &\overrightarrow{v_{r-1}} = \langle r-2,r-3,\cdots,0,1\rangle, &&\overrightarrow{v_r} = \langle r-1,r-2,r-3,\cdots,0\rangle. \end{aligned}$$

By notice the symmetry between the components of the vectors $\overrightarrow{v_1}$ and $\overrightarrow{v_r}$ and $\overrightarrow{v_2}$ and $\overrightarrow{v_{r-1}}$,....so on. Hence

1. For any two adjacent vertices v_i and v_{i+1} we have $|\overrightarrow{v_i} + \overrightarrow{v_{i+1}}|^2 = \sum\limits_{k=1}^{r-i}(2k-1)^2 + \sum\limits_{k=1}^{i}(2k-1)^2$ where $i = 2,\ldots,r-1$. Hence

$$HM_1^{\mathcal{L}}(\varsigma) = \sum_{i=1}^{r-1}\sum_{k=1}^{r-i}(2k-1)^2 + \sum_{i=1}^{r-1}\sum_{k=1}^{i}(2k-1)^2 = \frac{2r^4-4r^3+r^2+r}{3}.$$

2. For the other case $HM_2^{\mathcal{L}}(\varsigma)$ we have $\overrightarrow{v}_i \cdot \overrightarrow{v}_{i+1} = \sum\limits_{k=1}^{r-i} k(k-1) + \sum\limits_{k=1}^{i} k(k-1)$, hence

$$\begin{aligned} HM_2^{\mathcal{L}}(\varsigma) &= \sum_{i=1}^{r-1} \left(\overrightarrow{v}_i \cdot \overrightarrow{v}_{i+1}\right)^2 = \sum_{i=1}^{r-1}\sum_{k=1}^{r-i}[k(k-1)]^2 + \sum_{i=1}^{r-1}\sum_{k=1}^{i}[k(k-1)]^2 \\ &= \frac{1}{6}r^3 - \frac{1}{30}r^2 - \frac{1}{15}r - \frac{1}{10}r^5 + \frac{1}{30}r^6 - \frac{1}{30}r(r-1)(r+1)(r-2)\Big(-r^2+r+1\Big) \\ &= \frac{1}{15}r(r-1)(r-2)(r+1)\Big(-r+r^2-1\Big). \end{aligned}$$

Therefore, $HM_2^{\mathcal{L}}(\varsigma)$ is obtained as required in the statement of theorem.

3. From part 2, we have

$$R^{\mathcal{L}}(\varsigma) = \sum_{i=1}^{r-1} \frac{1}{\sqrt{\sum_{k=1}^{r-i} k(k-1) + \sum_{k=1}^{i} k(k-1)}} = \sum_{i=1}^{r-1} \frac{1}{\sqrt{\frac{3ri^2 - 3r^2 i + r^3 - r}{3}}} = \sum_{i=1}^{r-1} \frac{\sqrt{3}}{\sqrt{3i^2 r - 3ir^2 + r^3 - r}}.$$

4. With some calculation we conclude that $|\overrightarrow{v_i}|^2 = \sum_{k=1}^{r-i} k^2 + \sum_{k=1}^{i} (k-1)^2$ and $|\overrightarrow{v_{i+1}}|^2 = \sum_{k=1}^{r-i-1} k^2 + \sum_{k=1}^{i+1} (k-1)^2$. Hence

$$SO^{\mathcal{L}}(\varsigma) = \sum_{i=1}^{r-1} \sqrt{\sum_{k=1}^{r-i} k^2 + \sum_{k=1}^{i} (k-1)^2 + \sum_{k=1}^{r-i-1} k^2 + \sum_{k=1}^{i+1} (k-1)^2}.$$

Which is the required result.

□

Theorem 4. *For an even integer $r \geq 4$, let $\varsigma \cong C_r$. Then*

1. $HM_1^{\mathcal{L}}(\varsigma) = \dfrac{(r^2-1)(r^2+1)}{3}$.
2. $HM_2^{\mathcal{L}}(\varsigma) = \dfrac{r(r^3-4r)^2}{144}$.
3. $R^{\mathcal{L}}(\varsigma) = 2r\dfrac{\sqrt{r^3-4r}}{\sqrt{3}}$.
4. $SO^{\mathcal{L}}(\varsigma) = r\sqrt{\frac{1}{3}r + \frac{1}{6}r^3}$.

Proof. By identifying the vertices of the cycle C_r as $\{v_1, v_2, \cdots, v_r\}$ in the counterclockwise direction. Then the locating vector $\overrightarrow{v_i}$ correspond to the vertex v_i has zero component in the position i, one component of value $\frac{r}{2} - 1$, two components of values of value 1, two components of value 2, and two components of value 3. Hence, for any two adjacent vertices v_i and v_{i+1} where $i = 1, 2, \ldots, r-1$

1. For any two adjacent vertices v_i and v_{i+1} we have $|\overrightarrow{v_i} + \overrightarrow{v_{i+1}}|^2 = 2\sum_{k=1}^{\frac{r}{2}} (2k-1)^2$. Therefore

$$HM_1^{\mathcal{L}}(\varsigma) = 2r\sum_{k=1}^{\frac{r}{2}} (2k-1)^2 = \frac{r(r^3-r)}{3} = \frac{r^4-r^3}{3} = \frac{(r^2-1)(r^2+1)}{3}.$$

2. we have $\overrightarrow{v_i} \cdot \overrightarrow{v_{i+1}} = 2\sum_{i=2}^{\frac{r}{2}} i(i-1) = \frac{1}{12}r^3 - \frac{1}{3}r$. Therefore $HM_2^{\mathcal{L}}(\varsigma) = r\left(2\sum_{i=2}^{\frac{r}{2}} i(i-1)\right)^2$
$= \dfrac{r(r^3-4r)^2}{144}$.
3. By part 2, $R^{\mathcal{L}}(\varsigma) = \dfrac{r}{\left(2\sum_{i=2}^{\frac{r}{2}} i(i-1)\right)^{\frac{1}{2}}} = 2r\dfrac{\sqrt{r^3-4r}}{\sqrt{3}}$.

4. We can see that each $\overrightarrow{v_i}$ has equivalent components but in different location, hence each $|\overrightarrow{v_i}|^2$ has the same sum as the form of

$$|\overrightarrow{v_i}|^2 = \frac{r(r+1)(r+2) - 3r^2}{12}.$$

Hence

$$\begin{aligned} SO^{\mathcal{L}}(\varsigma) &= \sum_{v_iv_j \in E(\varsigma)} \sqrt{|\overrightarrow{v_i}|^2 + |\overrightarrow{v_j}|^2} \\ &= r\sqrt{\frac{r(r+1)(r+2) - 3r^2}{12} + \frac{r(r+1)(r+2) - 3r^2}{12}} \\ &= r\sqrt{\frac{1}{3}r + \frac{1}{6}r^3}. \end{aligned}$$

□

Theorem 5. *For an odd integer $r \geq 3$, let $\varsigma \cong C_r$. Then*

1. $HM_1^{\mathcal{L}}(\varsigma) = \dfrac{r\left(2r^3 - 3r^2 - 2r + 15\right)}{6}$.
2. $HM_2^{\mathcal{L}}(\varsigma) = \frac{1}{12}(r+3)(r-1)(r-2)$.
3. $R^{\mathcal{L}}(\varsigma) = \dfrac{2\sqrt{3}r}{\sqrt{(r-1)(r-2)(r+3)}}$.
4. $SO^{\mathcal{L}}(\varsigma) = r\sqrt{\frac{1}{6}r(r^2-1)}$.

Proof. We notice the following vectors in the cycle C_r

$$\begin{aligned} \overrightarrow{v_1} &= \left\langle 0, 1, 2, 3, \cdots, \frac{r-1}{2}, \frac{r-1}{2} - 1, \frac{r-1}{2} - 2, \cdots, 1 \right\rangle, \\ \overrightarrow{v_2} &= \left\langle 1, 0, 1, 2, \cdots, \frac{r-1}{2} - 1, \frac{r-1}{2}, \frac{r-1}{2} - 1, \cdots, 2 \right\rangle, \\ \overrightarrow{v_3} &= \left\langle 2, 1, 0, 1, \cdots, \frac{r-1}{2} - 2, \frac{r-1}{2} - 1, \frac{r-1}{2}, \cdots, 3 \right\rangle, \\ &\vdots \\ \overrightarrow{v_r} &= \left\langle 1, 2, 3, \cdots, \frac{r-1}{2}, \frac{r-1}{2} - 1, \frac{r-1}{2} - 2, \cdots, 0 \right\rangle. \end{aligned}$$

with some calculation we obtain

1. For any two adjacent vertices v_i and v_{i+1} we have $|\overrightarrow{v_i} + \overrightarrow{v_{i+1}}|^2 = 2\sum_{k=1}^{\frac{r-1}{2}}(2k-1)^2$ $+2\left(\frac{r-1}{2}\right)^2 = \frac{1}{3}r^3 - \frac{1}{2}r^2 - \frac{1}{3}r + \frac{1}{2}$, hence

$$HM_1^{\mathcal{L}}(\varsigma) = \frac{r\left(2r^3 - 3r^2 - 2r + 15\right)}{6}.$$

2. Additionally,

$$\begin{aligned}
\overrightarrow{v_i}\cdot\overrightarrow{v_{i+1}} &= 2\sum_{i=1}^{\frac{r-1}{2}} i(i-1)+\frac{(r-1)^2}{4}\\
&= \left(2\frac{\frac{r-1}{2}\left(\frac{r-1}{2}+1\right)\left(2\frac{r-1}{2}+1\right)}{6}\right)-1-\left(2\frac{\frac{r-1}{2}\left(\frac{r-1}{2}+1\right)}{2}-1\right)+\frac{(r-1)^2}{4}\\
&= \frac{1}{12}r^3-\frac{7}{12}r+\frac{1}{2}\\
&= \frac{1}{12}(r+3)(r-1)(r-2).
\end{aligned}$$

Hence $HM_2^{\mathcal{L}}(\varsigma)=\frac{1}{12}(r+3)(r-1)(r-2)$ as required.

3. By part 2, $R^{\mathcal{L}}(\varsigma)=\dfrac{2\sqrt{3}r}{\sqrt{(r-1)(r-2)(r+3)}}$.

4. For $SO^{\mathcal{L}}(\varsigma)$ we have$|\overrightarrow{v_i}|^2=2\sum_{i=1}^{\frac{r-1}{2}} i^2=\dfrac{r(r^2-1)}{12}$ which implies

$$SO^{\mathcal{L}}(\varsigma)=r\sqrt{\frac{r(r^2-1)}{12}+\frac{r(r^2-1)}{12}}=r\sqrt{\frac{1}{6}r(r^2-1)}.$$

□

3. New Versions of Locating Indices and Helm Graph

In this Section we will compute the exact value of new versions of locating indices of the Helm graph. Recall that [24] Helm graph (H_r) is a simple graph obtained from the r-wheel W_m graph next to the edge of the pendant at each vertex of the C_r cycle.

Theorem 6. *Given that H_r be a helm graph with $r\geq 3$. Then*

1. $HM_1^{\mathcal{L}}(\varsigma)=r(212r-431)^2$.
2. $HM_2^{\mathcal{L}}(\varsigma)=r(15r-49)^2+r(18r-36)^2+r(8r-14)^2$.
3. $R^{\mathcal{L}}(\varsigma)=\dfrac{r}{\sqrt{(15r-49)+(18r-36)+8r-14}}$.
4. $SO^{\mathcal{L}}(\varsigma)=\sqrt{2}r(13r-27)+r\sqrt{(13r-27)^2+(15r-14)^2}+r\sqrt{(13r-27)^2+25r^2}$.

Proof. Let H_r be the Helm graph obtained by attaching a pendant edge at each vertex of the cycle. Let $V(H_r)=\{v_0\}\cup\{v_1,v_2,\cdots,v_r\}\cup\{v_{r+1},v_{r+2},\cdots,v_{2r}\}$ where $v_i's$ are the vertices of cycles taken in cyclic order and $v'_{r+i}s$ are pendant vertices such that each v_iv_{r+i} is a pendant edge and v_0 is the center of the cycle. Therefore, we obtain the corresponding vectors $\overrightarrow{v_i}$ for each vertex $v_i\in V(H_r)$ where $i=1,2,\ldots,r$ as follows:

$$\begin{aligned}
\overrightarrow{v_1} &= \left\langle 0,1,\overbrace{2,\ldots,2}^{r-3},1,1,2,\overbrace{3,\ldots,3}^{r-3},2,1\right\rangle,\ \overrightarrow{v_2}=\left\langle 1,0,1,\overbrace{2,\ldots,2}^{r-2},1,2,\overbrace{3,\ldots,3}^{r-3},1\right\rangle,\\
,\ldots,\overrightarrow{v_r} &= \left\langle 1,\overbrace{2,\ldots,2}^{r-3},1,0,2,\overbrace{3,\ldots,3}^{r-3},2,1,1\right\rangle
\end{aligned}$$

Hence, each $\overrightarrow{v_i}=\left\langle \overbrace{0}^{i^{th}\ position},\overbrace{2,\ldots,2}^{r-1},\overbrace{1,\ldots,1}^{4-times},\overbrace{3,\ldots,3}^{r-3}\right\rangle$, more clearly has 0 component in ith position, $(r-1)$ components of value two, $(r-3)$ components of value three, and four comonents of value one. Moreover, the corresponding vectors $\overrightarrow{v_{r+i}}$ for each vertex $v_{r+i}\in V(H_r)$ where $i=1,2,\ldots,r$ as follows:

$$\overrightarrow{v_{r+1}} = \left\langle 1,2,\overbrace{3\ldots,3}^{r-3},2,\overbrace{0}^{(r+1)\text{ position}},3,\overbrace{4,\ldots 4}^{r-3},3,2\right\rangle,\ \overrightarrow{v_{r+2}} = \left\langle 2,1,2,\overbrace{3,\ldots,3}^{r-2},\overbrace{0}^{(r+2)\text{ position}},3,\overbrace{4,\ldots 4}^{r-3},2\right\rangle,$$

$$,\ldots,\overrightarrow{v_{2r}} = \left\langle 2,\overbrace{3\ldots,3}^{r-3},2,1,3,\overbrace{4,\ldots 4}^{r-3},3,\overbrace{0}^{2r\text{ position}},2\right\rangle$$

Hence, each $\overrightarrow{v_{r+i}} = \left\langle \overbrace{0}^{(r+i)^{th}\ position},\overbrace{2,\ldots,2}^{3\ times},\overbrace{1}^{r^{th}\ position},\overbrace{3,\ldots,3}^{r-1},\overbrace{4,\ldots,4}^{r-3}\right\rangle$, more clearly has 0 component in $(r+i)^{th}$ position, $(r-1)$ components of value three, $(r-3)$ components of value four, and three competent of value two. Finally the corresponding vectors $\overrightarrow{v_0}$ for each vertex $v_0 \in V(H_r)$ is $\overrightarrow{v_0} = \left\langle \overbrace{1,\ldots,1}^{r\text{ times}},\overbrace{2,\ldots,2}^{r\text{ times}},0\right\rangle$. Now let $A,B,C \subset V(H_r)$ such that

$$A = \{v_1, v_2, \cdots, v_r\}, B = \{v_{r+1}, v_{r+2}, \cdots, v_{2r}\}, \text{ and } C = \{v_0\}.$$

Hence,

1. $HM_1^{\mathcal{L}}(\varsigma) = \overbrace{\sum_{\substack{v_i,v_{i+1}\in A\\ v_i\sim v_{i+1}}} |\overrightarrow{v_i} + \overrightarrow{v_{i+1}}|^2}^{(1)} + \overbrace{\sum_{\substack{v_i,\in A,\ v_{r+i}\in B\\ v_i\sim v_{r+i}}} |\overrightarrow{v_i} + \overrightarrow{v_{r+i}}|^2}^{(2)} + \overbrace{\sum_{\substack{v_i\in A, v_0\in C\\ v_i\sim v_0}} |\overrightarrow{v_i} + \overrightarrow{v_0}|^2}^{(3)}$. For the summation (1), we have

$$\overrightarrow{v_1} + \overrightarrow{v_2} = \left\langle 1,1,3,\overbrace{4,\ldots,4}^{r-4},3,3,3,5,\overbrace{6,\ldots,6}^{r-4},5,2\right\rangle,\ \overrightarrow{v_2} + \overrightarrow{v_3} = \left\langle 3,1,1,3,\overbrace{4,\ldots,4}^{r-4},5,3,3,5,\overbrace{6,\ldots,6}^{r-4},2\right\rangle$$

$$,\ldots,\overrightarrow{v_{r-1}} + \overrightarrow{v_r} = \left\langle 3,\overbrace{4,\ldots,4}^{r-4},3,1,1,5,\overbrace{6,\ldots,6}^{r-4},5,3,3,2\right\rangle$$

$$\overrightarrow{v_1} + \overrightarrow{v_r} = \left\langle 1,3,\overbrace{4,\ldots,4}^{r-4},3,1,2,5,\overbrace{6,\ldots,6}^{r-4},5,3,2\right\rangle$$

Hence, each $\overrightarrow{v_i} + \overrightarrow{v_{i+1}} = \left\langle \overbrace{1}^{2-times},\overbrace{2}^{1-times},\overbrace{3,\ldots,3}^{4-times},\overbrace{4,\ldots,4}^{r-4},\overbrace{5}^{2-times},\overbrace{6,\ldots,6}^{r-4}\right\rangle$, more clearly has 1 two times, 2 one time, 3 four times, $(r-4)$ components of value four, $(r-4)$ components of value six, and 5 two times. Also $\overrightarrow{v_1} + \overrightarrow{v_r} = \left\langle \overbrace{1}^{2-times},\overbrace{2}^{2-times},\overbrace{3,\ldots,3}^{3-times},\overbrace{4,\ldots,4}^{r-4},\overbrace{5}^{2-times},\overbrace{6,\ldots,6}^{r-4}\right\rangle$, more clearly has 1 two times, 2 two times, 3 three times, $(r-4)$ components of value four, $(r-4)$ components of value six, and 5 two times. Therefore

$$\sum_{\substack{v_i,v_{i+1}\in A\\ v_i\sim v_{i+1}}} |\overrightarrow{v_i} + \overrightarrow{v_{i+1}}|^2 = \sum_{\substack{v_i,v_{i+1}\in A\\ v_i\sim v_{i+1}}} (179 + 104r - 416)^2 = r(104r - 237)^2.$$

For summation in (2), we have

$$\overrightarrow{v_1} + \overrightarrow{v_{r+1}} = \left\langle 1,3,\overbrace{5,\ldots,5}^{r-2},3,1,5,\overbrace{7,\ldots,7}^{r-3},5,3 \right\rangle,\ \overrightarrow{v_2} + \overrightarrow{v_{r+2}} = \left\langle 3,1,3,\overbrace{5,\ldots,5}^{r-2},15,\overbrace{7,\ldots,7}^{r-3},3 \right\rangle$$

$$,\ldots,\overrightarrow{v_r} + \overrightarrow{v_{2r}} = \left\langle 3,\overbrace{5,\ldots,5}^{r-3},3,1,5,\overbrace{7,\ldots,7}^{r-3},5,1,3 \right\rangle$$

Hence each $\overrightarrow{v_i} + \overrightarrow{v_{r+i}} = \left\langle \overbrace{1}^{2-times}, \overbrace{3,\ldots,3}^{3-times}, \overbrace{5}^{r-1}, \overbrace{7,\ldots,7}^{r-3} \right\rangle$, more clearly has 1 two times, 3 three times, $(r-1)$ components of value five, and $(r-3)$ competent of value seven. Therefore

$$\sum_{\substack{v_i, \in A,\, v_{r+i} \in B \\ v_i \sim v_{r+i}}} |\overrightarrow{v_i} + \overrightarrow{v_{r+i}}|^2 = \sum_{\substack{v_i, \in A,\, v_{r+i} \in B \\ v_i \sim v_{r+i}}} (74r-143)^2 = r(74r-143)^2.$$

For summation in (3)

$$\overrightarrow{v_1} + \overrightarrow{v_0} = \left\langle 1,2,\overbrace{3,\ldots,3}^{r-1},2,3,4,\overbrace{5,\ldots,5}^{r-3},4,1 \right\rangle, \overrightarrow{v_2} + \overrightarrow{v_0} = \left\langle 1,2,\overbrace{3,\ldots,3}^{r-1},2,3,4,\overbrace{5,\ldots,5}^{r-3},4,1 \right\rangle$$

$$,\ldots,\overrightarrow{v_r} + \overrightarrow{v_0} = \left\langle 2,\overbrace{3,\ldots,3}^{r-1},2,1,4,\overbrace{5,\ldots,5}^{r-3},4,3,1 \right\rangle$$

Hence, each $\overrightarrow{v_i} + \overrightarrow{v_0} = \left\langle \overbrace{1}^{2-times}, \overbrace{2}^{2-times}, \overbrace{3,\ldots,3}^{r-2}, \overbrace{4}^{2-times}, \overbrace{5,\ldots,5}^{r-3} \right\rangle$, more clearly has 1 two times, 2 two times, $(r-2)$ components of value three, 2 times of value 4, and $(r-3)$ competent of value five. Therefore $\sum\limits_{\substack{v_i \in A, v_0 \in C \\ v_i \sim v_0}} |\overrightarrow{v_i} + \overrightarrow{v_0}|^2 = \sum\limits_{\substack{v_i \in A, v_0 \in C \\ v_i \sim v_0}} (34r-51)^2$ $= r(34r-51)^2$. Hence

$$HM_1^{\mathcal{L}}(\varsigma) = r\Big[(104r-237)^2 + (74r-143)^2 + (34r-51)^2\Big] = r(212r-431)^2.$$

2. $HM_2^{\mathcal{L}}(\varsigma) = \overbrace{\sum\limits_{\substack{v_i, v_{i+1} \in A \\ v_i \sim v_{i+1}}} \left(\overrightarrow{v_i} \cdot \overrightarrow{v_{i+1}}\right)^2}^{(1)} + \overbrace{\sum\limits_{\substack{v_i, \in A,\, v_{r+i} \in B \\ v_i \sim v_{r+i}}} \left(\overrightarrow{v_i} \cdot \overrightarrow{v_{r+i}}\right)^2}^{(2)} + \overbrace{\sum\limits_{\substack{v_i \in A, v_0 \in C \\ v_i \sim v_0}} \left(\overrightarrow{v_i} \cdot \overrightarrow{v_0}\right)^2}^{(3)}$. For summation (1), we have $\sum\limits_{\substack{v_i, v_{i+1} \in A \\ v_i \sim v_{i+1}}} \left(\overrightarrow{v_i} \cdot \overrightarrow{v_{i+1}}\right)^2 = r[4(r-4) + 2(r-5) + 9(r-4) + 13]^2$ $= r(15r-49)^2$. For summation (2), we have $\sum\limits_{\substack{v_i, \in A,\, v_{r+i} \in B \\ v_i \sim v_{r+i}}} \left(\overrightarrow{v_i} \cdot \overrightarrow{v_{r+i}}\right)^2 = r[6(r-1)+$ $12(r-3) + 6]^2 = r(18r-36)^2$. For summation (3), we have $\sum\limits_{\substack{v_i \in A, v_0 \in C \\ v_i \sim v_0}} \left(\overrightarrow{v_i} \cdot \overrightarrow{v_0}\right)^2 =$ $r[6(r-3) + 2(r-3) + 10]^2 = r(8r-14)^2$. Hence $HM_2^{\mathcal{L}}(\varsigma) = r(15r-49)^2$ $+ r(18r-36)^2 + r(8r-14)^2$.
3. It is clear from part 2 that $R^{\mathcal{L}}(\varsigma) = \dfrac{r}{\sqrt{(15r-49) + (18r-36) + 8r - 14}}$.

4. $SO^{\mathcal{L}}(\varsigma) = \overbrace{\sum_{\substack{v_i, v_{i+1} \in A \\ v_i \sim v_{i+1}}} \sqrt{|\overrightarrow{v_i}|^2 + |\overrightarrow{v_{i+1}}|^2}}^{(1)} + \overbrace{\sum_{\substack{v_i, \in A,\, v_{r+i} \in B \\ v_i \sim v_{r+i}}} \sqrt{|\overrightarrow{v_i}|^2 + |\overrightarrow{v_{r+i}}|^2}}^{(2)} + \overbrace{\sum_{\substack{v_i \in A, v_0 \in C \\ v_i \sim v_0}} \sqrt{|\overrightarrow{v_i}|^2 + |\overrightarrow{v_0}|^2}}^{(3)}$. For summation in (1)

$$\sum_{\substack{v_i, v_{i+1} \in A \\ v_i \sim v_{i+1}}} \sqrt{|\overrightarrow{v_i}|^2 + |\overrightarrow{v_{i+1}}|^2} = r\sqrt{2[(4(r-1) + 9(r-3) + 4)]^2} = r\sqrt{2(13r-27)^2} = \sqrt{2}r(13r-27).$$

For summation in (2)

$$\begin{aligned} \sum_{\substack{v_i, \in A,\, v_{r+i} \in B \\ v_i \sim v_{r+i}}} \sqrt{|\overrightarrow{v_i}|^2 + |\overrightarrow{v_{r+i}}|^2} &= r\sqrt{[(4(r-1) + 9(r-3) + 4)]^2 + [9(r-1) + 6(r-3) + 13]^2} \\ &= r\sqrt{(13r-27)^2 + (15r-14)^2} \end{aligned}$$

For summation in (3)

$$\sum_{\substack{v_i \in A, v_0 \in C \\ v_i \sim v_0}} \sqrt{|\overrightarrow{v_i}|^2 + |\overrightarrow{v_0}|^2} = r\sqrt{(13r-27)^2 + 25r^2}.$$

Hence, $SO^{\mathcal{L}}(\varsigma) = \sqrt{2}r(13r-27) + r\sqrt{(13r-27)^2 + (15r-14)^2} + r\sqrt{(13r-27)^2 + 25r^2}$.

□

4. Significance of New Versions of Locating Indices

Accordant to Milan Randić [25] in order to consider a topological index as an acceptable index, it must satisfy some of the following conditions: have positive correlation with at least one property; have structural interpretation; preferably contradistinguish; be generalizable to more advanced analogues; be elementary; not be established based on properties; not be trivially related to other descriptors; be possible to compose effectively; and be based on organizable structural abstractions. In this section, we considered 11 benzenoid hydrocarbons to test the anticipating capability of these new indices. The experimental data of 11 benzenoid hydrocarbons are found in references [26–28], and also https://pubchem.ncbi.nlm.nih.gov (accessed on 26 March 2022). Table 1 indicates the experimental data of benzenoid hydrocarbons. Table 2 shows the new index-values of benzenoid hydrocarbons. Molecular graphs of benzenoid hydrocarbons are depicted in Figure 1. We have seen that these indices play a crucial part in evaluation the boiling point (BP), molar entropy (S), acentric factor (ϖ), octanol–water partition coefficient $(logP)$, complexity (C), and Kovats retention index (RI) of these 11 benzenoid hydrocarbons. Table 3 shows the correlation coefficient (R) of the these indices with some physicochemical properties of 11 benzenoid hydrocarbons (where the significance of bold numbers denote highest correlation value).

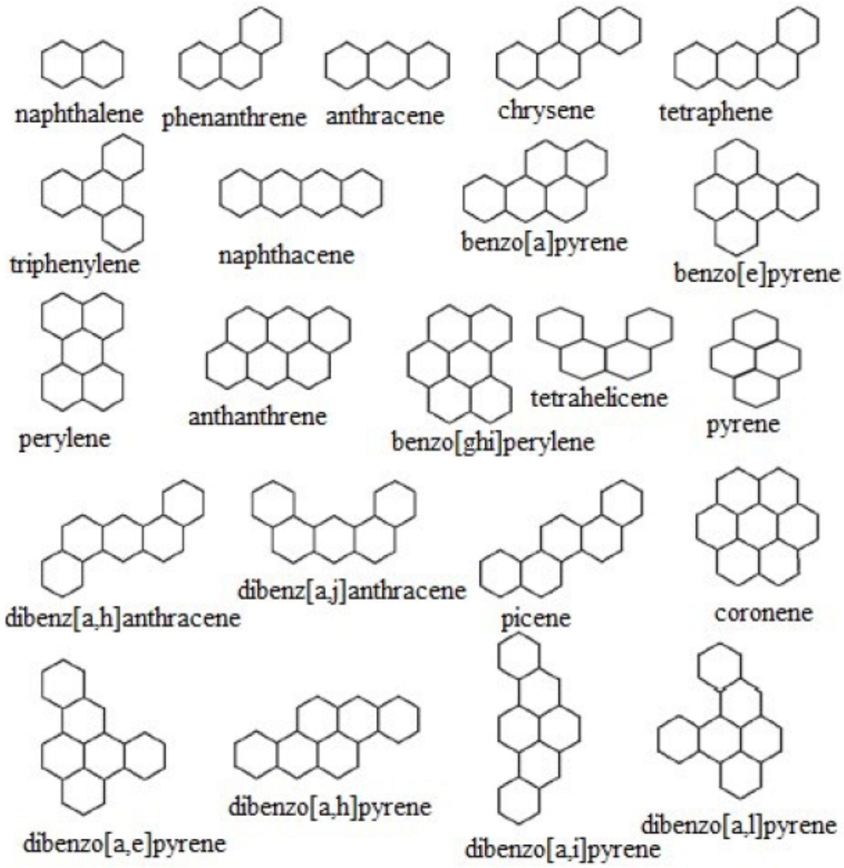

Figure 1. Molecular graphs of benzenoid hydrocarbons.

Table 1. Experimental values of some physicochemical properties of benzenoid hydrocarbons.

Benzenoid Hydrocarbons	(BP)	(S)	(ϖ)	$LogP$	(RI)	(C)
naphthalene	218	79.38	0.302	3.3	200	80.6
phenanthrene	338	93.79	0.39	4.46	300	335
chrysene	431	106.83	0.46	5.81	400	264
tetraphene	425	108.22	0.46	5.76	398.5	294
triphenylene	429	104.66	0.46	5.49	400	217
tetrahelicene	436	–	0.47	5.7	391.12	266
perylene	497	109.10	0.49	6.25	456.22	217
naphthacene	440	105.47	0.46	5.76	408.3	304
pyrene	404	96.06	0.41	4.88	351.22	236
benzo[a]pyrene	496	111.85	–	6.13	453.44	372
benzo[e]pyrene	493	110.46	–	6.44	450.73	336

Table 2. New locating indices of benzenoid hydrocarbons.

Benzenoid Hydrocarbons	$HM_1^{\mathcal{L}}(\varsigma)$	$HM_2^{\mathcal{L}}(\varsigma)$	$R^{\mathcal{L}}(\varsigma)$	$SO^{\mathcal{L}}(\varsigma)$
naphthalene	2857	412,483	1.4826	37.7094
phenanthene	8834	300,968	1.4640	261.804
chrysene	21,738	155,303	1.3854	474.224
tetraphene	22,490	165,133	1.3583	416.911
triphenylene	17,963	101,068	1.5071	375.695
tetrahelicene	20,446	134,949	1.4325	399.556
naphthacene	24,314	193,765	1.3058	429.787
pyrene	11,696	462,142	1.6024	328.713
perylene	24,699	163,161	1.5707	531.393
benzo[a]pyrene	27,576	215,760	1.4943	575.456
benzo[e]pyrene	24,158	159,451	1.5832	537.929

Table 3. Correlation coefficients (R) between versions of new locating indices and some physiochemical properties of benzenoid hydrocarbons.

Locating Index	(BP)	(S)	(ϖ)	$(LogP)$	(RI)	(C)
$HM_1^{\mathcal{L}}(\varsigma)$	0.930	0.967	0.945	0.964	0.955	0.669
$HM_2^{\mathcal{L}}(\varsigma)$	0.843	0.905	0.859	0.894	0.878	0.602
$R^{\mathcal{L}}(\varsigma)$	0.112	−0.080	−0.194	−0.013	0.052	0.069
$SO^{\mathcal{L}}(\varsigma)$	**0.980**	**0.975**	**0.972**	**0.978**	**0.982**	**0.788**

4.1. Regression Model

Using the data in Tables 1 and 2, linear regression models were obtained for boiling point (BP), molar entropy (S), acentric factor (ϖ), octanol–water partition coefficient $(logP)$, complexity (C), and Kovats retention index (RI). The corresponding R were calculated. Where, N, R^2, Se, F, and SF denote the population, coefficient of determination, standard error of estimate, Fischer F-values, F-significance, respectively. We have tested the following linear regression model $P = A + B(LI)$ where $P =$ physical property, LI= locating index. We have obtained the following different linear models for each of the locating indices, which are listed below:

1. First Hyper Locating Index $HM_1^{\mathcal{L}}(\varsigma)$:

$$BP = 235.916 + 0.01[HM_1^{\mathcal{L}}(\varsigma)] \tag{5}$$

$$\varpi = 0.312 + \left(7.1 \times 10^{(-6)}\right)[HM_1^{\mathcal{L}}(\varsigma)] \tag{6}$$

$$LogP = 3.31 + \left(1.1 \times 10^{(-4)}\right)[HM_1^{\mathcal{L}}(\varsigma)] \tag{7}$$

$$RI = 206.488 + 0.009[HM_1^{\mathcal{L}}(\varsigma)] \tag{8}$$

$$C = 136.682 + 0.007[HM_1^{\mathcal{L}}(\varsigma)] \tag{9}$$

$$S = 80.340 + 0.001[HM_1^{\mathcal{L}}(\varsigma)] \tag{10}$$

2. Second Hyper Locating Index $HM_2^{\mathcal{L}}(\varsigma)$:

$$BP = 296.857 + \left(9.8 \times 10^{(-5)}\right)[HM_2^{\mathcal{L}}(\varsigma)] \tag{11}$$

$$\varpi = 0.354 + \left(7.28 \times 10^{(-8)}\right)[HM_2^{\mathcal{L}}(\varsigma)] \quad (12)$$

$$LogP = 3.991 + \left(1.2 \times 10^{(-6)}\right)[HM_2^{\mathcal{L}}(\varsigma)] \quad (13)$$

$$RI = 263.502 + \left(9.6 \times 10^{(-5)}\right)[HM_2^{\mathcal{L}}(\varsigma)] \quad (14)$$

$$C = 180.186 + \left(6.9 \times 10^{(-5)}\right)[HM_2^{\mathcal{L}}(\varsigma)] \quad (15)$$

$$S = 87.27 + 1.24 \times 10^{(-5)}[HM_2^{\mathcal{L}}(\varsigma)] \quad (16)$$

3. Randić Locating Index $R^{\mathcal{L}}(\varsigma)$:

$$BP = 278.037 + 95.673[R^{\mathcal{L}}(\varsigma)] \quad (17)$$

$$\varpi = 0.602 - 0.115[R^{\mathcal{L}}(\varsigma)] \quad (18)$$

$$LogP = 5.638 - 0.126[R^{\mathcal{L}}(\varsigma)] \quad (19)$$

$$RI = 321.911 + 41.301[R^{\mathcal{L}}(\varsigma)] \quad (20)$$

$$C = 180.445 + 57.871[R^{\mathcal{L}}(\varsigma)] \quad (21)$$

$$S = 114.458 - 8.049[R^{\mathcal{L}}(\varsigma)] \quad (22)$$

4. Sombor Locating Index $SO^{\mathcal{L}}(\varsigma)$:

$$BP = 210.599 + 0.524[SO^{\mathcal{L}}(\varsigma)] \quad (23)$$

$$\varpi = 0.293 + 0.00039[SO^{\mathcal{L}}(\varsigma)] \quad (24)$$

$$LogP = 3.105 + 0.006[SO^{\mathcal{L}}(\varsigma)] \quad (25)$$

$$RI = 186.921 + 0.493[SO^{\mathcal{L}}(\varsigma)] \quad (26)$$

$$C = 101.352 + 0.414[SO^{\mathcal{L}}(\varsigma)] \quad (27)$$

$$S = 78.212 + 0.061[SO^{\mathcal{L}}(\varsigma)] \quad (28)$$

4.2. Results and Discussion

Using the regression models, we calculated the correlation coefficients (R) between versions of new locating indices and some physiochemical properties of benzenoid hydrocarbons shown in Table 3. Scatter plots between the boiling point (BP), molar entropy (S), acentric factor (ϖ), octanol–water partition coefficient $(logP)$, and Kovats retention index (RI) with new locating indices are shown in Figure 2.

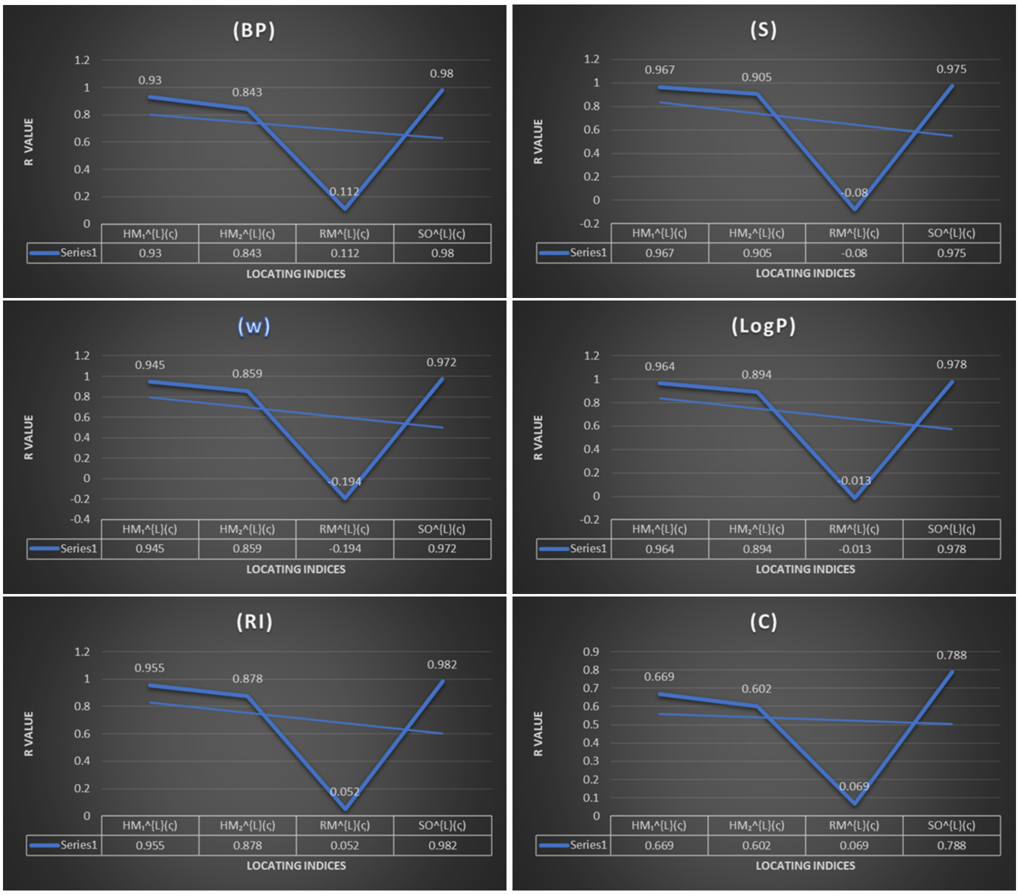

Figure 2. Physicochemical properties of benzoid hydrocarbons with topological indices.

4.3. Concluding Remarks

By analyzing the data given in Tables 4–7, it is possible to derive some results for the given new locating indices (expect for the Randić locating index which will be excluded from our discussion). These tables show the regression model of various physicochemical properties. It can be observed that the regression model value R is more than 0.6 and significance F is less than 0.05. Hence, it can be observed that all the physical and chemical properties of benzenoid hydrocarbons are positively correlated with the defined new locating indices. First, the Randić locating index was found to be completely inadequate for any structure–property correlation, although many models have been tested to validate this index it did not pass these tests. Second, the Sombor locating index, Table 7, depicts that this index is a beneficial tool in deriving the physical and chemical properties for benzenoid hydrocarbons with correlation coefficient values lying between 0.972 to 0.982 except for the complexity of benzenoid hydrocarbons, where the correlation coefficient value of the Sombor locating index with complexity is 0.788. More clearly, when examining the table correlation coefficients horizontally for physical properties, we see that $SO^{\mathcal{L}}(\varsigma)$ index gives highest correlation coefficient for boiling point (BP) $(R = 0.980)$, molar entropy (S) $(R = 0.975)$, acentric factor (ϖ) $(R = 0.972)$, octanol–water partition coefficient $(logP)$ $(R = 0.978)$, complexity (C) $(R = 0.788)$, and Kovats retention index (RI) $(R = 0.982)$. Sombor locating index is highly recommended for predicting the $QSPR$ of benzenoid hydrocarbons. The first Hyper locating index shows good correlation properties. The $QSPR$ study in Table 4 shows that the predicting power of this index is quite satisfactory, with range of $0.930 \leq R \leq 0.967$, excluding the complexity value of 0.669. On the other hand, the second Hyper locating index has a positive and highly significant correlation coefficient for molar entropy (S) $(R = 0.905)$ and for others, and for the physical and chemical properties for benzenoid hydrocarbons, the range of the correlation coefficient is between 0.843 and 0.894.

Table 4. Statical parameters for the linear *QSPR* model for first Hyper locating index.

Physical Properties	***N***	R^2	***Se***	***F***	***SF***
boiling point (BP)	11	0.866	31.317	57.973	$3 \times 10^{(-5)}$
molar entropy (S)	10	**0.935**	2.729	114.332	$5.1 \times 10^{(-6)}$
octanol partition coefficient $(logP)$	11	0.930	0.256	119.359	$1.7 \times 10^{(-7)}$
complexity (C)	11	0.447	62.32	7.273	0.025
Kovats retention index (RI)	11	0.913	23.7	93.939	$4.6 \times 10^{(-6)}$
acentric factor (ϖ)	9	0.892	0.02	57.864	0.0001

Table 5. Statical parameters for the linear *QSPR* model for second Hyper locating index.

Physical Properties	***N***	R^2	***Se***	***F***	***SF***
boiling point (BP)	11	0.711	45.928	22.14	0.001
molar entropy (S)	10	**0.819**	4.5335	36.295	0.0003
octanol partition coefficient $(logP)$	11	0.799	0.433	35.865	0.0002
complexity (C)	11	0.771	38.333	30.351	0.0004
Kovats retention index (RI)	11	0.362	66.914	5.116	0.05
acentric factor (ϖ)	9	0.738	0.032	19.7533	0.003

Table 6. Statical parameters for the linear *QSPR* model for Randić locating index.

Physical Properties	***N***	R^2	***Se***	***F***	***SF***
boiling point (BP)	11	0.013	84.890	0.115	0.742
molar entropy (S)	10	0.006	10.63802	0.051	0.827
octanol partition coefficient $(logP)$	11	0.001	0.96577	0.002	0.970
complexity (C)	11	0.005	80.04642	0.024	0.880
Kovats retention index (RI)	11	0.003	83.5988	0.043	0.840
acentric factor (ϖ)	9	**0.038**	0.061	0.274	0.067

Table 7. Statical parameters for the linear *QSPR* model for Sombor locating index.

Physical Properties	***N***	R^2	***Se***	***F***	***SF***
boiling point (BP)	11	0.961	16.879	221.565	$1.2 \times 10^{(-7)}$
molar entropy (S)	10	0.950	2.382	152.546	$1.7 \times 10^{(-6)}$
octanol partition coefficient $(logP)$	11	0.956	0.203	193.882	$2.1 \times 10^{(-7)}$
complexity (C)	11	0.621	51.56	14.775	0.004
Kovats retention index (RI)	11	**0.965**	15.003	247.879	$7.4 \times 10^{(-8)}$
acentric factor (ϖ)	9	0.945	0.014	120.011	$1.1 \times 10^{(-5)}$

In this paper, we introduce four new versions of locating indices, and find their exact values for some families of known graphs and for the Helm graph. We examined the efficiency of predicting the physicochemical properties of benzenoid hydrocarbons. Raw data from the chemistry literature and a mathematical effort to find new topological indices are joined in this study to introduce these novel indices which will encourage its utilization prospects in pharmacological and chemical fields. The cases in which satisfactory correlations were gained proposed the effectiveness of the computed topological indices to be useful in predicting the physicochemical properties of numerous intricate chemical compounds. For instance, they can be used in the characterization of nanotubes and graphene structures. This study predicted the validity new versions of locating indices. They have been applied for a series of polycyclic aromatic hydrocarbons. The study is reliable since it tested eleven polycyclic aromatic hydrocarbons. Accordingly, we can suggest applying these new indices to other types of compounds such as the linear and branched alkanes.

4.4. Comparative Analysis

To grasp the significance of these new indices, we will compare the results obtained from the new versions of locating indices and some known indices in the literature. The efficiency and applicability measured by comparable correlation coefficient (R) of the new versions of locating indices and those of other known indices is shown in Table 8. The R values of each index are very similar, range from 0.972 to 0.980. The unavailable data in the table inspires more questions for future investigation to compare different topological indices with our calculations of the new locating indices and to conduct more research into the different types of benzenoid hydrocarbons.

Table 8. Correlation coefficients (R) between some topological indices and the physiochemical properties of benzenoid hydrocarbons.

Topolgical Index	(BP)	(S)	(ϖ)	$(LogP)$	(RI)	(C)
$M_1(\varsigma)$ [First Zagreb index]						
$M_2(\varsigma)$ [Second Zagreb index]	0.980 [29]					
$R(\varsigma)$ [Randić Index]	0.975 [30]			0.972 [30]		
$H(\varsigma)$ [hyper Index]	0.974 [31]			0.972 [30]		
$SO(\varsigma)$ [Sombor index]						

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