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Two physicochemical properties of benzenoid chains: solvent accessible molecular volume and molar refraction

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Abstract: Predicting physicochemical properties of molecules is one of the fundamental tasks in chemical physics. Many predictive methods have been development for correlating the molecular structures with their physicochemical properties. One of the simplest such methods involves topological indices. Edge connectivity index (or equivalently, reformulated Randić index), denoted by ε , seems to be a good topological index for predicting the solvent accessible molecular volume and molar refraction of polycyclic aromatic hydrocarbons. In this paper, a closed form formula for calculating the reformulated Randić index ε of benzenoid hydrocarbons chains (or simply, benzenoid chains which represent a type of polycyclic aromatic hydrocarbons) is derived. Benzenoid chains with maximum (and minimum) ε value are also determined from the collection of all benzenoid chains having fixed number of hexagonal rings. Moreover, an attempt is made to generalize the obtained results for reformulated bond incident degree indices.

Keywords: Solvent accessible molecular volume; molar refraction; benzenoid chain; reformulated Randić index; reformulated bond incident degree index.

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1. Introduction

Chemical compounds are associated with physical and chemical properties, and some of these compounds have biological activities. Actually, in the search for new antibacterial and various other medicinal drugs, pharmaceutical companies synthesize and test annually millions of new chemical compounds, characterizing in detail those compounds that show

some potential [1]. In 2017, the number of substances registered in the *Chemical Abstracts Service Registry* database reached 135 million [2]. Testing for biological activity is expensive, therefore many theoretical methods have been devised for correlating structures with their biological activities or physical-chemical properties. One of the simplest such methods involves topological indices [1, 3, 4].

Molecules can be represented by graphs (undefined notations and terminologies concerning graph theory can be found in [5]) in which vertices correspond to the atoms while edges represent the covalent bonds between atoms [6]. In this paper, we consider only hydrogen-depleted molecular graphs, that is, the molecular graphs with hydrogen atoms deleted. A number obtained from a molecular graph, reflecting certain structural features of the molecule is called a topological index (or, molecular descriptor) [7]. A great variety of such indices is studied and used in theoretical chemistry [6, 7]. Among them a considerable number of indices depend only on vertex degrees of the (molecular) graph [6-8], and most of them can be represented as the sum of edge contributions of the graph. The general form [9, 10] of these indices is:

$$BID(G) = \sum_{\delta(G) \leq i \leq j \leq \Delta(G)} \theta_{i,j} \cdot x_{i,j}(G) \quad (1)$$

where $\theta_{i,j}$ is a non-negative real valued function depending on i, j with $\theta_{i,j} = \theta_{j,i}$, $\Delta(G)$ is the maximum degree of the graph G , $\delta(G)$ is the minimum degree of G and $x_{i,j}(G)$ is the number of edges in G connecting the vertices of degrees i and j . These topological indices are known as bond incident degree indices (BID indices in short [11]). Many well-known topological indices, like Randić index [12], first Zagreb index [13], natural logarithm of multiplicative Zagreb indices [14, 15], can be obtained from Equation (1) by taking some suitable $\theta_{i,j}$.

Estrada [16] proposed the following topological index (known as the *edge connectivity index*) for predicting the molar volume and molar refraction of certain hydrocarbons:

$$\varepsilon(G) = \sum_{v \in V(G)} \sum_{\substack{uv, vw \in E(G) \\ u \neq w}} \frac{1}{\sqrt{(d_u + d_v - 2)(d_v + d_w - 2)}}, \tag{2}$$

where $E(G)$ is the edge set of the graph G (with at least three vertices), $V(G)$ is the vertex set of G , d_u is degree of the vertex $u \in V(G)$ and uv is the edge connecting the vertices u and v . Gutman and Estrada [16] introduced a concept of the topological indices based on a line graph: if $I(G)$ is a topological index that can be calculated from a graph G , then there is another topological index $i(G)$ such that $i(G) = I(L(G))$, where $L(G)$ is the line graph of G . We call such line graph-based topological indices as reformulated topological indices. It is clear that $\varepsilon(G) = R(L(G))$, where R is the (vertex) connectivity index [12], also known as the Randić index. Hence, the edge connectivity index ε is simply the reformulated Randić index. Possible applications of line graphs in (physical) chemistry can be found in the Refs. [16-20].

The main purpose of the present study is to establish results concerning the reformulated Randić index of benzenoid hydrocarbon chains (or simply, benzenoid chains), which represent a special type of polycyclic aromatic hydrocarbons. These results may be useful for predicting the solvent accessible molecular volume and molar refraction of any benzenoid chain, as well as for determining the benzenoid chains having maximum/minimum solvent accessible molecular volume and maximum/minimum molar refraction among all benzenoid chains with fixed number of hexagonal rings.

2. Results and discussion

Firstly, we check whether the reformulated Randić index is suitable for predicting the molar refraction (MR) and solvent accessible molecular volume (SAV) of polycyclic aromatic hydrocarbons.

Table 1. Molar refraction, solvent accessible molecular volume and ε values of some polycyclic aromatic hydrocarbons

Compound	Molar Refraction (MR)	Solvent Accessible Molecular Volume (SAV)	ε Value
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Naphthalene	41.92	489.1	5.4544
Biphenyl	50.72	570.0	6.4544
Fluorene	53.31	591.2	7.4424
Phenanthrene	57.46	607.2	7.9256
2-Methylphenanthrene	62.08	660.9	8.4087
Acenaphthene	49.16	485.4	6.9315
Benz[a]anthracene	73.00	673.7	10.4136
Pyrene	64.20	592.4	9.4087
9-Methylanthracene	62.08	589.6	8.3995
Benzene	26.39	316.7	3.0000
Anthracene	57.46	560.4	7.9424

We consider a set of 11 polycyclic aromatic hydrocarbons, whose MR and SAV values are taken from the Ref. [21], see Table 1. For this test data, the correlation between MR and ε is 0.993, while the correlation between SAV and ε is 0.910 (see Figure 1). Thereby, the reformulated Randić index may be useful in predicting the above-mentioned two properties of polycyclic aromatic hydrocarbons. The regression lines are given as

$$MR \approx 6.2042\varepsilon + 8.2177 \quad (2a)$$

and

$$SAV \approx 45.0602\varepsilon + 222.8659 \quad (2b)$$

Next, we derive a general expression for calculating the reformulated Randić index of benzenoid chains. In order to establish this expression, some definitions are needed, which are recalled in the following. A benzenoid hydrocarbon system (or simply, a benzenoid system) can be considered as a connected geometric figure obtained by concatenating congruent regular hexagons side to side in a plane in such a way that the figure divides the plane into one infinite (external) region and a number of finite (internal) regions, and all internal regions must be congruent regular hexagons. An example of a benzenoid system is given in Figure 2. In a benzenoid system, two hexagons are said to be adjacent if they share a side. The characteristic graph (or dualist or inner dual) of a given benzenoid system consists of vertices corresponding to hexagons of the system; two vertices are adjacent if and only if the corresponding hexagons are adjacent. A benzenoid system whose characteristic graph is the path graph is known as a benzenoid chain. A benzenoid chain can be represented by a graph (called a benzenoid chain graph) in which the edges represent

sides of a hexagon, while the vertices correspond to the points where two sides of a hexagon meet. In the rest of paper, by the term benzenoid chain, we actually mean benzenoid chain graph.

When going along the perimeter of a benzenoid system, then cove and fjord are paths with the degree sequences $(2,3,3,2)$ and $(2,3,3,3,2)$, respectively (see Figure 3). The number of coves and fjords in a benzenoid system will be denoted by C and F respectively.

A benzenoid chain with $n \geq 3$ hexagons will be denoted by H_n . In a benzenoid chain H_n , a hexagon is said to be *terminal* (respectively, *non-terminal*) if it is adjacent with one (respectively, two) other hexagon(s). A non-terminal hexagon is said to be a *kink* if it contains an edge connecting the vertices of degree 2. Number of kinks of a benzenoid chain will be denoted by k . The line graph of H_n is denoted by $L(H_n)$. The line graph of the benzenoid chain, given in Figure 4, is depicted in Figure 5. Now, we are ready to state and prove our first main result.

Theorem 2.0. If H_n is a benzenoid chain with $n \geq 3$ hexagons, k kinks, C coves and F fjords, then the reformulated Randić index ε of H_n can be calculated using the following formula:

$$\varepsilon(H_n) = 4\left(\frac{1}{3} + \frac{1}{2\sqrt{3}}\right)n + \frac{2}{\sqrt{3}}(\sqrt{2} - 1) + k\left(\sqrt{\frac{2}{3}} - \frac{5}{6}\right) + \omega\left(\frac{7}{12} - \frac{1}{\sqrt{3}}\right),$$

where $\omega = C + 2F$.

Proof. The reformulated Randić index ε can be rewritten as

$$\varepsilon(H_n) = R(L(H_n)) = \sum_{\delta(L(H_n)) \leq i \leq j \leq \Delta(L(H_n))} \frac{x_{ij}(L(H_n))}{\sqrt{ij}}. \quad (3)$$

It can be easily observed that $\delta(L(H_n)) = 2$ and $\Delta(L(H_n)) = 4$ (for example, see Figure 5). Now, simple calculations yield:

$$\begin{aligned}
x_{2,2}(L(H_n)) &= 4, \\
x_{2,3}(L(H_n)) &= 2(k+2), \\
x_{2,4}(L(H_n)) &= 0, \\
x_{3,4}(L(H_n)) &= 4(n-1) - 2\omega, \\
x_{4,4}(L(H_n)) &= 2k + \omega.
\end{aligned}$$

where $\omega = C + 2F$. The number of edges of $L(H_n)$ is calculated as

$$|E(L(H_n))| = \frac{1}{2} \cdot M_1(H_n) - |E(H_n)| = 8n - 2,$$

where $M_1(H_n)$ is the first Zagreb index of H_n . Now, from the identity

$$|E(L(H_n))| = \sum_{2 \leq i \leq j \leq 4} x_{i,j}(L(H_n)),$$

it follows that

$$x_{3,3}(L(H_n)) = 4(n-k) + \omega - 6.$$

After substituting the values of $x_{2,2}(L(H_n))$, $x_{2,3}(L(H_n))$, $x_{2,4}(L(H_n))$, $x_{3,3}(L(H_n))$, $x_{3,4}(L(H_n))$, $x_{4,4}(L(H_n))$ in Equation (3), we get the desired formula. ■

Example 2.0: Let us consider the molecular graph P of the Picene whose molecular formula is $C_{22}H_{14}$. For P , we have $n = 5$, $k = 3$, $C = F = 0$ and hence by using the formula derived in Theorem 2.0, we get

$$\varepsilon(P) = 20\left(\frac{1}{3} + \frac{1}{2\sqrt{3}}\right) + \frac{2}{\sqrt{3}}(\sqrt{2} - 1) + 3\left(\sqrt{\frac{2}{3}} - \frac{5}{6}\right) \approx 12.868.$$

Now, by using (2a) and (2b), we have $MR \approx 88.053$ and $SAV \approx 802.698$. ■

A benzenoid chain with $n \geq 3$ hexagons is said to be linear (respectively, zigzag) benzenoid chain if $k = 0$ (respectively, if $k = n - 2$ and $C = F = 0$). A linear (respectively, zigzag) benzenoid chain with $n \geq 3$ hexagons is denoted by L_n (respectively, Z_n).

Corollary 2.0. If H_n is any benzenoid chain with $n \geq 3$ hexagons, then

$$\varepsilon(Z_n) \leq \varepsilon(H_n) \leq \varepsilon(L_n).$$

Left (respectively, right) equality holds if and only if $H_n \cong Z_n$ (respectively, $H_n \cong L_n$).

Proof. Suppose that H_n has k kinks, C coves and F fjords. From Theorem 2.0, it follows that

$$\varepsilon(H_n) = 4\left(\frac{1}{3} + \frac{1}{2\sqrt{3}}\right)n + \frac{2}{\sqrt{3}}(\sqrt{2} - 1) + k\left(\sqrt{\frac{2}{3}} - \frac{5}{6}\right) + \omega\left(\frac{7}{12} - \frac{1}{\sqrt{3}}\right),$$

which implies that $\varepsilon(H_n)$ is maximum or minimum if and only if

$$\Gamma(H_n) = k\left(\sqrt{\frac{2}{3}} - \frac{5}{6}\right) + \omega\left(\frac{7}{12} - \frac{1}{\sqrt{3}}\right)$$

is maximum or minimum, respectively. Due to the facts $k \geq \omega \geq 0$ and $\frac{7}{12} - \frac{1}{\sqrt{3}} > 0$, we have

$$\Gamma(H_n) = k\left(\sqrt{\frac{2}{3}} - \frac{5}{6}\right) + \omega\left(\frac{7}{12} - \frac{1}{\sqrt{3}}\right) \leq k\left(\sqrt{\frac{2}{3}} - \frac{5}{6}\right) + k\left(\frac{7}{12} - \frac{1}{\sqrt{3}}\right) \leq 0.$$

It is evident that the equation $\Gamma(H_n) = 0$ holds if and only if $\omega = k = 0$, that is, if and only if $H_n \cong L_n$. On the other hand, bearing in mind the facts $k \leq n - 2$ and $\sqrt{\frac{2}{3}} - \frac{5}{6} < 0$, we have

$$\Gamma(H_n) = k\left(\sqrt{\frac{2}{3}} - \frac{5}{6}\right) + \omega\left(\frac{7}{12} - \frac{1}{\sqrt{3}}\right) \geq k\left(\sqrt{\frac{2}{3}} - \frac{5}{6}\right) \geq (n - 2)\left(\sqrt{\frac{2}{3}} - \frac{5}{6}\right).$$

We note that the equation $\Gamma(H_n) = (n - 2)\left(\sqrt{\frac{2}{3}} - \frac{5}{6}\right)$ holds if and only if $\omega = 0$, $k = n - 2$, that is, if and only if $H_n \cong Z_n$. This completes the proof. ■

Remark 2.0. Corollary 2.0 may be useful for determining the benzenoid hydrocarbon chains having maximum/minimum solvent accessible molecular volume and maximum/minimum molar refraction from all benzenoid hydrocarbon chains with fixed number of hexagonal rings.

Now, we derive a formula for calculating the reformulated BID indices of benzenoid chains (and thereby generalize Theorem 2.0) and characterize the extremal benzenoid chains with respect to some reformulated Zagreb indices.

Theorem 2.1. If H_n is any benzenoid chain with $n \geq 3$ hexagons, k kinks, C coves and F fjords, then the reformulated BID indices of H_n can be calculated using the following formula:

$$\begin{aligned} BID(L(H_n)) = & 4n(\theta_{3,3} + \theta_{3,4}) + 2(2\theta_{2,2} + 2\theta_{2,3} - 3\theta_{3,3} - 2\theta_{3,4}) \\ & + 2k(\theta_{2,3} - 2\theta_{3,3} + \theta_{4,4}) \\ & + \omega(\theta_{3,3} - 2\theta_{3,4} + \theta_{4,4}), \quad \text{where } \omega = C + 2F. \end{aligned}$$

Proof. By substituting the values of $x_{2,2}(L(H_n))$, $x_{2,3}(L(H_n))$, $x_{2,4}(L(H_n))$, $x_{3,3}(L(H_n))$, $x_{3,4}(L(H_n))$, $x_{4,4}(L(H_n))$, calculated in the proof of Theorem 2.0, in Eq. (1), we get the required formula. ■

If we take $\Phi_1 = 2(\theta_{2,3} - 2\theta_{3,3} + \theta_{4,4})$ and $\Phi_2 = \theta_{3,3} - 2\theta_{3,4} + \theta_{4,4}$ then the formula given in Theorem 2.1, can be rewritten as

$$BID(L(H_n)) = 4n(\theta_{3,3} + \theta_{3,4}) + 2(2\theta_{2,2} + 2\theta_{2,3} - 3\theta_{3,3} - 2\theta_{3,4}) + k\Phi_1 + \omega\Phi_2.$$

Further, the substitution

$$k\Phi_1 + \omega\Phi_2 = \Gamma_{BID}(L(H_n)) \quad (4)$$

in the above equation gives

$$BID(L(H_n)) = 4n(\theta_{3,3} + \theta_{3,4}) + 2(2\theta_{2,2} + 2\theta_{2,3} - 3\theta_{3,3} - 2\theta_{3,4}) + \Gamma_{BID}(L(H_n)),$$

which yield the following result:

Theorem 2.2. Among all the benzenoid chains with $n \geq 3$ hexagons, the benzenoid chain H_n has the maximum or minimum reformulated BID index if and only if $\Gamma_{BID}(L(H_n))$ is maximum or minimum, respectively.

The substitutions $\theta_{i,j} = i + j, 2\left(\frac{\ln i}{i} + \frac{\ln j}{j}\right), \ln i + \ln j$ in Equation (1), correspond to the *first Zagreb index* (M_1), natural logarithm of the *first multiplicative Zagreb index* (Π_1), natural logarithm of the *second multiplicative Zagreb index* (Π_2), respectively, where “ $\ln$ ” denotes the natural logarithm. The following theorem gives the characterization of the extremal benzenoid chains with respect to the reformulated first Zagreb index, reformulated first multiplicative Zagreb index and reformulated second multiplicative Zagreb index.

Theorem 2.3. For $n \geq 3$, let H_n be any benzenoid chain with n hexagons. It holds that

a). $\Pi_1(L(Z_n)) \leq \Pi_1(L(H_n)) \leq \Pi_1(L(L_n)),$

with left (respectively right) equality if and only if $H_n \cong Z_n$ (respectively $H_n \cong L_n$).

b). $\Pi_2(L(L_n)) \leq \Pi_2(L(H_n)) \leq \Pi_2(L(Z_n)).$

$$M_1(L(L_n)) \leq M_1(L(H_n)) \leq M_1(L(Z_n)).$$

Left (respectively right) equality in both the above inequalities hold if and only if $H_n \cong L_n$ (respectively $H_n \cong Z_n$).

Proof. a). Suppose that H_n has k kinks. From Equation (4), it follows that

$$\Gamma_{\ln(\Pi_1)}(L(H_n)) \approx -0.2356k,$$

which, together with the inequality $0 \leq k \leq n - 2$, implies that $\Gamma_{\ln(\Pi_1)}(L(H_n))$ is maximum or minimum if and only if $H_n \cong L_n$ or $H_n \cong Z_n$, respectively. Since the exponential function is an increasing function and it is also the inverse function of the natural logarithm function. Hence, from Theorem 2.2, the desired result follows.

b). Again by using Equation (4), we have

$$\Gamma_{\ln(\Pi_2)}(L(H_n)) = 0.3398k$$

and

$$\Gamma_{M_1}(L(H_n)) = 2k,$$

which imply that both $\Gamma_{ln(\Pi_2)}(L(H_n))$ and $\Gamma_{M_1}(L(H_n))$ are maximum or minimum if and only if $H_n \cong Z_n$ or $H_n \cong L_n$, respectively. Now, by using Theorem 2.2, we get the required result. ■

If we put $\theta_{ij} = i \cdot j$ in Equation (1), we get the *second Zagreb index* (M_2). Now, we characterize the extremal benzenoid chains with respect to the reformulated second Zagreb index. Elementary computations gives,

$$\Gamma_{M_2}(L(H_n)) = 8k + 2F + C,$$

which, together with Theorem 2.1, Theorem 2.2 and the inequalities $0 \leq k \leq n - 2$,

$$F \leq \begin{cases} \frac{n-3}{3} & \text{for } n \equiv 0 \pmod{3}, \\ \frac{n-4}{3} & \text{for } n \equiv 1 \pmod{3}, \\ \frac{n-2}{3} & \text{for } n \equiv 2 \pmod{3}, \end{cases}$$

imply the next result.

Theorem 2.4. For $n \geq 4$, let H_n be any benzenoid chain with n hexagons. It holds that

$$M_2(L(H_n)) \geq M_2(L(L_n)),$$

with equality if and only if $H_n \cong L_n$. Also,

$$M_2(L(H_n)) \leq \begin{cases} \frac{278n-240}{3} & \text{for } n \equiv 0 \pmod{3}, \\ \frac{278n-239}{3} & \text{for } n \equiv 1 \pmod{3}, \\ \frac{278n-238}{3} & \text{for } n \equiv 2 \pmod{3}, \end{cases}$$

with equality if and only if H_n (for $n \not\equiv 0 \pmod{3}$) satisfies the following conditions

$$F = \begin{cases} \frac{n-4}{3} & \text{for } n \equiv 1 \pmod{3}, \\ \frac{n-2}{3} & \text{for } n \equiv 2 \pmod{3}, \end{cases}$$

$$C = \begin{cases} 1 & \text{for } n \equiv 1 \pmod{3}, \\ 0 & \text{for } n \equiv 2 \pmod{3}, \end{cases}$$

and $k = n - 2$. For $n \equiv 0 \pmod{3}$, the equality $M_2(L(H_n)) = \frac{278n - 240}{3}$ holds if and only if H_n satisfies either of the following two set of conditions (for example, see Figure 6 where a benzenoid chain is depicted satisfying the following first set of conditions):

- i. $F = \frac{n-3}{3}$, $C = 0$, $k = n - 2$,
- ii. $F = \frac{n-6}{3}$, $C = 2$, $k = n - 2$, $n \geq 6$.

3. Conclusion

We have established a general formula for calculating any reformulated bond incident degree index, including the reformulated Randić index which may be useful for predicting the solvent accessible molecular volume and molar refraction of benzenoid hydrocarbon chains. We have also determined the benzenoid chains having maximum and minimum reformulated Randić index as well as maximum and minimum reformulated Zagreb indices. The extremal result concerning reformulated Randić index may be used to identify the benzenoid hydrocarbon chains having maximum/minimum solvent accessible molecular volume and maximum/minimum molar refraction among all the benzenoid hydrocarbon chains having fixed number of hexagonal rings. It would be interesting in future to establish the related extremal results concerning benzenoid hydrocarbon chains for those reformulated bond incident degree indices which have some physicochemical applicability. Also, it seems that the reformulated Randić index has not yet gained a considerable attention from the mathematical chemistry community and hence it may be interesting to explore some properties of the reformulated Randić index in future.

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Figure 1. Molar refraction and solvent accessible molecular volume plotted versus ϵ values for the compounds given in Table 1.

Figure 2. An example of a benzenoid system.

Figure 3. The cove and fjord in a benzenoid system.

Figure 4. An example of a benzenoid chain.

Figure 5. Line graph of the benzenoid chain, given in Figure 4.

Figure 6. A benzenoid chain with the maximum reformulated second Zagreb index, mentioned in Theorem 2.4, for the case $n \equiv 0 \pmod{3}$.