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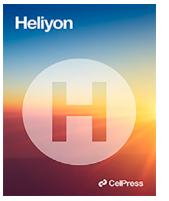

Research article

Predicting enthalpy of formation of benzenoid hydrocarbons and ordering molecular trees using general multiplicative Zagreb indices

Sadia Noureen [a], Akbar Ali [b,*], Akhlaq A. Bhatti [c], Abdulaziz M. Alanazi [d], Yilun Shang [e,*]

[a] *Faculty of Science, University of Gujrat, Gujrat, Pakistan*
[b] *College of Science, University of Ha'il, Ha'il, Saudi Arabia*
[c] *Department of Sciences and Humanities, National University of Computer and Emerging Sciences, Lahore Campus, B-Block, Faisal Town, Lahore, Pakistan*
[d] *Department of Mathematics, University of Tabuk, Tabuk 71491, Saudi Arabia*
[e] *Department of Computer and Information Sciences, Northumbria University, Newcastle upon Tyne, NE1 8ST, UK*

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ABSTRACT

Many existing studies show that there exists a strong relationship between structures and characteristics of molecules. Topological indices are often used in modeling the properties of chemical compounds and biological activities in theoretical chemistry. Topological indices are numerical values associated with structures of molecules in such a way that they remain constant under graph isomorphism. Multiplicative Zagreb indices are among the famous topological indices that have been explored by numerous researchers in the last few years. The first objective of the present paper is to examine the importance of general multiplicative Zagreb indices for forecasting the enthalpy of formation of hydrocarbons using a data set of 25 benzenoid hydrocarbons. The second objective of this paper is to study molecular trees with a given order and with a given number of branching vertices or segments using general multiplicative (first and second) Zagreb indices. Sharp lower/upper bounds on these Zagreb indices for the aforementioned molecular trees are obtained and the graphs attaining these bounds are determined. Bounds on the classical multiplicative Zagreb and Narumi-Katayama indices are corollaries of the obtained results.

1. Introduction

Let G be a simple connected graph (a graph without loops and multi-edges) with edge set $E(G)$ and vertex set $V(G)$. The number of edges incident with a vertex v in G is the degree $d_G(v)$ of v. A molecular tree is a connected graph containing no cycle and the maximum degree of whose vertices is at most 4, see for example [24,28]. A vertex v of a molecular tree T is said to be a branching vertex (pendent vertex, respectively) if $d_T(v) \geq 3$ ($d_T(v) = 1$, respectively). A segment S in a molecular tree T is a path in T such that end vertices of S have degrees different from 2 (in T), and every other vertex of S has degree 2 (in T).

* Corresponding authors.
E-mail addresses: sadia.tauseef@uog.edu.pk (S. Noureen), akbarali.maths@gmail.com (A. Ali), akhlaq.ahmad@nu.edu.pk (A.A. Bhatti), am.alenezi@ut.edu.sa (A.M. Alanazi), yilun.shang@northumbria.ac.uk (Y. Shang).

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Many existing studies show that there exists a strong relationship between structures and characteristics of chemical compounds. Topological indices are often used in modeling the properties of chemical compounds and biological activities in theoretical chemistry; for example, see [11,17,19,20,22,33]. Topological indices are numerical values associated with structures of chemical compounds in such a way that they remain constant under graph isomorphism. Multiplicative Zagreb indices are among of the famous topological indices that have been explored by numerous researchers in the last few years. For details, see [1,3,7–9,12,13,16,25,26,29–32,34] and the references cited therein.

For a real number α, general multiplicative first and second Zagreb indices, denoted P_1^α and P_2^α, were introduced in [15] and [26], respectively. For a graph G, they are defined as

$$P_1^\alpha(G) = \prod_{v\in V(G)} (d_G(v))^\alpha$$

and

$$P_2^\alpha(G) = \prod_{v\in V(G)} (d_G(v))^{\alpha d_G(v)}.$$

Some existing indices are can be recovered from these general indices: $P_1^1(G)$ is the Narumi-Katayama index $NK(G)$, $P_1^2(G)$ is the multiplicative first Zagreb index $\prod_1(G)$, and $P_2^1(G)$ is the multiplicative second Zagreb index $\prod_2(G)$.

The general multiplicative sum Zagreb index of G is defined by

$$\Pi_{1,\alpha}^*(G) = \prod_{uv\in E(G)} (d_G(u) + d_G(v))^\alpha.$$

Note that the index $\Pi_{1,\alpha}^*$ may be viewed also as a multiplicative version of the sum-connectivity index (see for example [4]); also, see [27] where $\Pi_{1,\alpha}^*$ was referred to as the general multiplicative third Zagreb index.

Based on the definitions of the above-mentioned multiplicative indices, we remark here that only one member from each of the sets $\{P_1^\alpha, \prod_1, NK\}$, $\{P_2^\alpha, \prod_2\}$ and $\{\Pi_{1,\alpha}^*, \Pi_{1,1}^*\}$ is sufficient to consider for studying any extremal problem.

The sharp bounds on the indices P_1^α and P_2^α for trees with a fixed order and a given number of pendent vertices, segments, or branching vertices were investigated in [26]. The bounds were found on these indices for graphs with a given clique number in [27]. The problem of finding the sharp bounds for tetracyclic, tricyclic, and bicyclic graphs with a fixed order and with a given number of pendent vertices was solved in [5]. Furthermore, sharp bounds on the indices under consideration for graphs with a fixed number of vertices and with a given number of cut-edges were found in [6].

The first objective of the present paper is to examine the importance of general multiplicative Zagreb indices P_1^α, P_2^α and $\Pi_{1,\alpha}^*$ for forecasting the enthalpy of formation of hydrocarbons using a data set of 25 benzenoid hydrocarbons. Denote by $\mathcal{B}_{n,\beta}$ and $\mathcal{B}'_{n,s}$ the families of those n-vertex molecular trees that have exactly β branching vertices and s segments, respectively. The second objective of this paper is to present sharp upper and lower bounds on the indices P_1^α and P_2^α for molecular trees in the classes $\mathcal{B}_{n,\beta}$ and $\mathcal{B}'_{n,s}$.

2. Enthalpy of formation of benzenoid hydrocarbons

The present section examines the importance of P_1^α, P_2^α and $\Pi_{1,\alpha}^*$ for forecasting the enthalpy of formation ΔH_f of the specified hydrocarbons for $-2 \le \alpha \le 2$ using a data set of 25 benzenoid hydrocarbons (names are given in Table 1). The experimental information (shown in the mentioned table) for the chosen characteristic of these hydrocarbons comes from [10,23]. In Table 1, we also list the values of P_1^α, P_2^α and $\Pi_{1,\alpha}^*$ for all the considered hydrocarbons; these values are calculated by utilizing the Mathematica software.

The absolute value R of the correlation coefficient between the indices P_1^α, P_2^α, $\Pi_{1,\alpha}^*$ and the enthalpy of formation for the compounds listed in Table 1, when $-2 \le \alpha \le 2$, are given in Figs. 2, 3, 4, respectively. Table 2 provides the largest possible absolute value R of the correlation coefficient between the enthalpy of formation and each of the indices P_1^α, P_2^α, $\Pi_{1,\alpha}^*$ for the compounds listed in Table 1, when $-2 \le \alpha \le 2$; for the indices P_1^α, P_2^α, $\Pi_{1,\alpha}^*$, such values are approximately equal to 0.9806, 0.9773, 0.9797, respectively, which occur at $\alpha \approx 0.0062, 0.0028, 0.0034$, respectively. The corresponding regression lines at the mentioned values of α are given as follows:

$$\Delta H_f = -2706.78 + 2721.03 P_1^{0.0062},$$
$$\Delta H_f = -2244.46 + 2276.81 P_2^{0.0028},$$
$$\Delta H_f = -2104.2 + 2128.94 \Pi_{1,0.0034}^*,$$

respectively. This finding suggests that all these three indices deserve further studies on other data sets of compounds for $0 < \alpha < 0.5$. This is the main reason that, in the next sections, we pay particular attention to the positive values of α.

Next, we apply the above regression lines to a benzenoid hydrocarbon not included in the data set, predict its enthalpy of formation, and then compare the predicted values with the experimental data (as shown in the paper [2]). We consider the coronene (a benzenoid hydrocarbon different from the 25 benzenoid hydrocarbons mentioned in Table 1). The molecular graph of the coronene is depicted in Fig. 1. If we denote by C the molecular graph of the coronene, then we have

$$P_1^a(C) = 6^{12a}, \quad P_2^a(C) = 2^{24a}\, 3^{36a}, \quad \text{and} \quad \Pi_{1,a}^*(C) = 2^{24a}\, 15^{12a}.$$

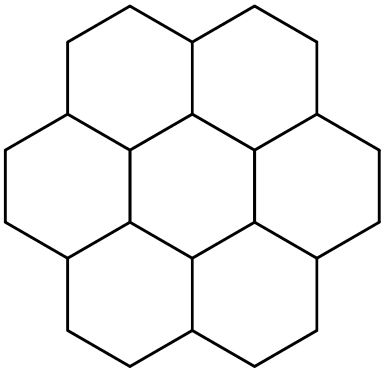

Fig. 1. Molecular graph of the coronene.

Table 1
The values of P_1^{α}, P_2^{α}, $\Pi_{1,\alpha}^{*}$, and the enthalpy of formation for the 25 hydrocarbons under consideration.

Compound Name	P_1^{α}	P_2^{α}	$\Pi_{1,\alpha}^{*}$	ΔH_f
benzene	64^{α}	$4^{6\alpha}$	$4^{6\alpha}$	82.9
naphthalene	2304^{α}	$6912^{2\alpha}$	15360000^{α}	150.6
anthracene	82944^{α}	$864^{4\alpha}$	$240000^{2\alpha}$	227.7
phenanthrene	82944^{α}	$864^{4\alpha}$	55296000000^{α}	207.1
pyrene	$864^{2\alpha}$	$20155392^{2\alpha}$	12441600000000^{α}	225.7
benzo[a]anthracene	$12^{6\alpha}$	$432^{6\alpha}$	$14400000^{2\alpha}$	291.0
benzo[c]phenanthrene	$12^{6\alpha}$	$432^{6\alpha}$	$20^{8\alpha}7776^{\alpha}$	302.4
chrysene	$12^{6\alpha}$	$432^{6\alpha}$	$20^{8\alpha}7776^{\alpha}$	262.8
naphthacene	$12^{6\alpha}$	$432^{6\alpha}$	$60000^{3\alpha}$	291.4
triphenylene	$12^{6\alpha}$	$432^{6\alpha}$	$240^{6\alpha}$	269.8
benzo[a]pyrene	$72^{4\alpha}$	$6^{24\alpha}$	$5^{10\alpha}24^{7\alpha}$	301.0
benzo[e]pyrene	$72^{4\alpha}$	$6^{24\alpha}$	$120^{8\alpha}$	304.0
perylene	$72^{4\alpha}$	$6^{24\alpha}$	$120^{8\alpha}$	324.0
benzo[b]chrysene	$10368^{2\alpha}$	$93312^{4\alpha}$	$864000000^{2\alpha}$	346.0
benzo[c]chrysene	$10368^{2\alpha}$	$93312^{4\alpha}$	$4^{9\alpha}5^{10\alpha}6^{7\alpha}$	334.0
benzo[g]chrysene	$10368^{2\alpha}$	$93312^{4\alpha}$	$28800^{4\alpha}$	333.0
benzo[a]tetracene	$10368^{2\alpha}$	$93312^{4\alpha}$	$4^{7\alpha}5^{14\alpha}6^{5\alpha}$	359.0
dibenzo[a,c]anthracene	$10368^{2\alpha}$	$93312^{4\alpha}$	$4^{9\alpha}5^{10\alpha}6^{7\alpha}$	345.0
dibenzo[a,h]anthracene	$10368^{2\alpha}$	$93312^{4\alpha}$	$864000000^{2\alpha}$	343.0
dibenzo[a,j]anthracene	$10368^{2\alpha}$	$93312^{4\alpha}$	$864000000^{2\alpha}$	343.0
dibenzo[b,g]phenanthrene	$10368^{2\alpha}$	$93312^{4\alpha}$	$864000000^{2\alpha}$	347.0
dibenzo[c,g]phenanthrene	$10368^{2\alpha}$	$93312^{4\alpha}$	$4^{9\alpha}5^{10\alpha}6^{9\alpha}$	335.0
pentacene	$10368^{2\alpha}$	$93312^{4\alpha}$	$30000^{4\alpha}$	374.5
pentaphene	$10368^{2\alpha}$	$93312^{4\alpha}$	$4^{7\alpha}5^{14\alpha}6^{5\alpha}$	359.0
picene	$10368^{2\alpha}$	$93312^{4\alpha}$	$4^{9\alpha}5^{10\alpha}6^{7\alpha}$	334.0

Thus, by using the above regression lines, the predicted values of the coronene are 402.271, 420.249, and 411.808, when we use the indices P_1^{α}, P_2^{α}, and $\Pi_{1,\alpha}^{*}$, respectively. On the other hand, the experimental value of the coronene is 295 ± 11, which is taken from [14]. Among the predicted values, the one (that is, 402.271) predicted by P_1^{α} is closest to the experimental value.

We close this section by discussing the efficacy of the proposed models with two existing studies [18,21]. In both the papers [18,21], none of the general multiplicative Zagreb indices was considered. It is however observed that among the topological indices considered in [21], none of them has the correlation (with the enthalpy of formation) greater than 0.9773 (that is, the least correlation among the ones given in Table 2). However, in [18], only two of the many considered topological indices have the correlation (with the enthalpy of formation) greater than 0.9773 (that is, the least correlation among the ones given in Table 2). These two values of the correlation are 0.9801 and 0.9808, which correspond to the scalar multiplicative harmonic (SMH) index and scalar multiplicative Randić (SMR) index. Consequently, based on the findings of [18] and those presented in the current study, it is appropriate to say that the SMH index, SMR index, and general multiplicative Zagreb indices have approximately the same but nice predictive ability for the case of the enthalpy of formation of benzenoid hydrocarbons. Thus, these indices deserve additional studies.

3. A useful lemma

Throughout this section, α is assumed to be a positive real number. In the rest of the paper, let $T(C_4^{b_4}, C_3^{b_3}, C_2^{b_2}, C_1^{b_1})$ denote the class of molecular trees with b_i vertices of degree i, where $1 \leq i \leq 4$. Denote by $|\, T_{(i)} \,|$ the number of vertices of degree i in a molecular tree T on n vertices, then

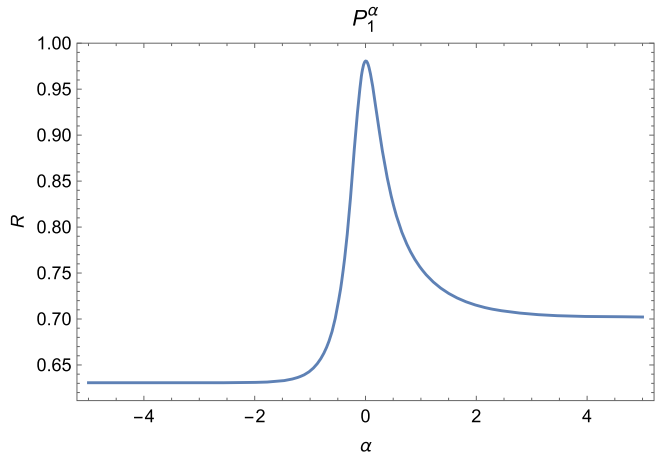

Fig. 2. The absolute value R of the correlation coefficient between the index P_1^α and enthalpy of formation for the compounds listed in Table 1, when $-2 \leq \alpha \leq 2$.

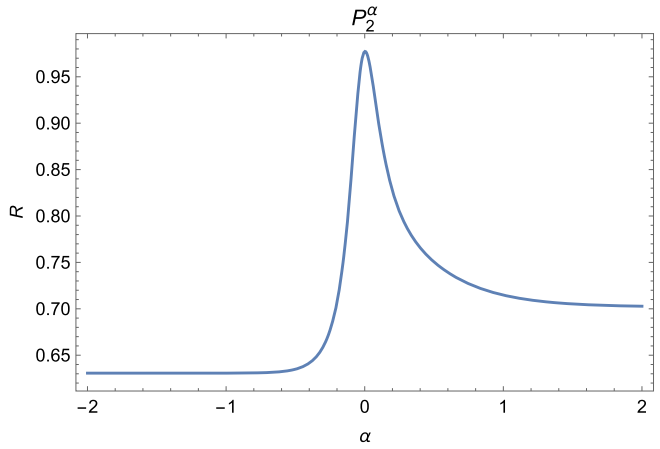

Fig. 3. The absolute value R of the correlation coefficient between the index P_2^α and enthalpy of formation for the compounds listed in Table 1, when $-2 \leq \alpha \leq 2$.

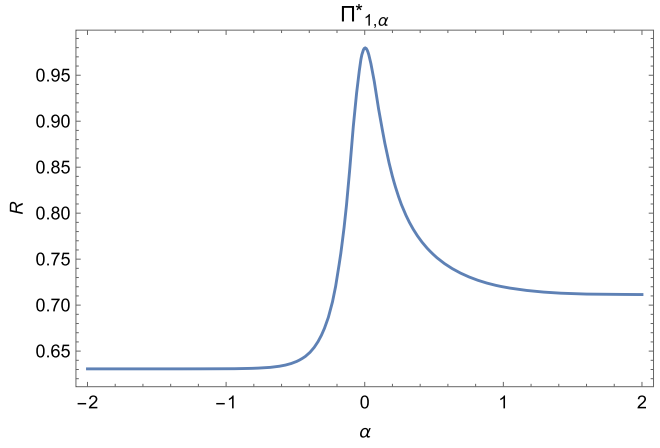

Fig. 4. The absolute value R of the correlation coefficient between the index $\Pi^*_{1,\alpha}$ and enthalpy of formation for the compounds listed in Table 1, when $-2 \leq \alpha \leq 2$.

Table 2
The largest possible absolute value R of the correlation coefficient between the enthalpy of formation and each of the indices P_1^α, P_2^α, $\Pi_{1,\alpha}^*$ for the compounds listed in Table 1, when $-2 \le \alpha \le 2$.

	P_1^α	P_2^α	$\Pi_{1,\alpha}^*$
α	0.0062	0.0028	0.0034
R	0.9806	0.9773	0.9797

$$n = \sum_{i=1}^{4} | T_{(i)} | \tag{1}$$

and

$$\sum_{i=1}^{4} i| T_{(i)} | = 2(n-1). \tag{2}$$

From (1) and (2), it is easy to observe that

$$| T_{(2)} | +2 | T_{(3)} | +3 | T_{(4)} | = n-2. \tag{3}$$

Also, if T has s segments and β branching vertices (see Section 1 for the definitions of segments and branching vertices in a tree), then

$$| T_{(2)} | = n-s-1, \tag{4}$$

and

$$| T_{(3)} | + | T_{(4)} | = \beta. \tag{5}$$

Lemma 1. *Let $T \in \mathcal{B}_{n,\beta}$ be the molecular tree graph with minimum $P_1^\alpha(T)$ or maximum $P_2^\alpha(T)$ value, then at most one of the numbers $| T_{(2)} |$ and $| T_{(3)} |$ is non-zero.*

Proof. Suppose on contrary that $| T_{(2)} | \neq 0$ and $| T_{(3)} | \neq 0$, and there are vertices u and v in T such that $d_u = 2$ and $d_v = 3$. If we suppose that $N_v(T) = \{w, z\}$, then a molecular graph (say) T' exists among $\mathcal{B}_{n,\beta}$ which is obtained by deleting the edges wu and uz and adding new edges wz and uv in T that gives

$$\frac{P_1^\alpha(T)}{P_1^\alpha(T')} = \frac{6^\alpha}{4^\alpha} > 1$$

and

$$\frac{P_2^\alpha(T)}{P_2^\alpha(T')} = \left(\frac{3}{4}\right)^{3\alpha} < 1.$$

That is,

$$P_1^\alpha(T) > P_1^\alpha(T')$$

and

$$P_2^\alpha(T) < P_2^\alpha(T'),$$

a contradictory result. □

4. Extremal molecular trees

Throughout this section, α is assumed to be a positive real number. The results given in Theorem 1 and 2 can be observed directly from the results obtained for the class of trees in [26].

Theorem 1 *(see [26]). Let T be a molecular tree from the class $\mathcal{B}'_{n,s}$. Then*

$$P_1^\alpha(T) \le \begin{cases} 3^{\frac{\alpha(s-1)}{2}} 2^{\alpha(n-s-1)} & \text{if } s \text{ is odd,} \\ 4^\alpha 3^{\alpha(\frac{s}{2}-2)} 2^{\alpha(n-s-1)} & \text{if } s \text{ is even,} \end{cases}$$

and

$$P_2^{\alpha}(T) \geq \begin{cases} 3^{\frac{3\alpha(s-1)}{2}} 2^{2\alpha(n-s-1)} & \text{if } s \text{ is odd,} \\ 4^{4\alpha} 3^{3\alpha(\frac{s}{2}-2)} 2^{2\alpha(n-s-1)} & \text{if } s \text{ is even.} \end{cases}$$

The sufficient and necessary condition of equalities is $T \cong T(C_4^0, C_3^{\frac{s-1}{2}}, C_2^{n-s-1}, C_1^{\frac{s+3}{2}})$ *for odd* s*, and* $T \cong T(C_4^1, C_3^{\frac{s}{2}-2}, C_2^{n-s-1}, C_1^{\frac{s}{2}+2})$ *for even* s*.*

Theorem 2 *(see [26]). For* $1 \leq \beta < \frac{n-2}{3}$*, let* T *be a molecular tree among the class* $\mathcal{B}_{n,\beta}$*, then*

$$P_1^{\alpha}(T) \leq 3^{\alpha\beta} 2^{(n-2\beta-2)}$$

and

$$P_2^{\alpha}(T) \geq 3^{\alpha\beta} 2^{2\alpha(n-2\beta-2)},$$

with the sufficient and necessary condition of equalities is $T \cong T(C_4^0, C_3^{\beta}, C_2^{n-2\beta-2}, C_1^{\beta+2})$*.*

Theorem 3. *Let* T *be a molecular tree from the class* $\mathcal{B}'_{n,s}$*. Then*

$$P_1^{\alpha}(T) \geq 3^{p\alpha} 2^{\frac{\alpha}{3}(3n-s-5-4p)}$$

and

$$P_2^{\alpha}(T) \leq 3^{3p\alpha} 4^{\frac{\alpha}{3}(3n+s-7-8p)},$$

where $p \in \{0, 1, 2\}$*. The sufficient and necessary condition of equalities is* $T \cong T\left(C_4^{\frac{s-1-2p}{3}}, C_3^p, C_2^{n-s-1}, C_1^{\frac{2s+4-p}{3}}\right)$*.*

Proof. Let $T' \in \mathcal{B}'_{n,s}$ be the molecular tree possessing the minimum P_1^{α} and maximum P_2^{α} value. Then have the following possibilities:

Claim 3.1. *For a non-negative integer* p*,* $|\, T'_{(3)} \,| = p$ *if and only if*

$$s - 2p - 1 \equiv 0 \pmod 3.$$

By using $|\, T'_{(3)} \,| = p$ and (4) in (3), it is easy to obtain $3 \mid |\, T'_{(4)} \,| + 2p + 1 = s$ or $s - 2p - 1 \equiv 0 \pmod 3$.

Claim 3.2. $|\, T'_{(3)} \,| = p \leq 2$.

Suppose on the contrary that there are vertices $u, v, w \in V(T')$ of degree 3 with the assumption that the vertex v lies on the uw-path. It is obvious that two neighbors say w_1 and w_2 of w do not lie on the aforementioned path. If a molecular tree T'' is formed by deleting the edges w_1w and ww_2 and then adding the new edges uw_1 and vw_2, we observe that T'' belongs to the class $\mathcal{B}'_{n,s}$ such that

$$\frac{P_1^{\alpha}(T')}{P_1^{\alpha}(T'')} = \frac{3^{3\alpha}}{4^{2\alpha}} = \left(\frac{27}{16}\right)^{\alpha} < 1,$$

and

$$\frac{P_2^{\alpha}(T')}{P_2^{\alpha}(T'')} = \frac{3^{9\alpha}}{4^{8\alpha}} = \left(\frac{3^9}{4^8}\right)^{\alpha} > 1,$$

which implies that $P_1^{\alpha}(T') > P_1^{\alpha}(T'')$ and $P_2^{\alpha}(T') < P_2^{\alpha}(T'')$. Hence, T' do not have the minimum P_1^{α} and maximum P_2^{α} value, which contradicts our assumption.
Now using the values $|\, T'_{(3)} \,| = p$ and $|\, T'_{(2)} \,| = n - s - 1$ in (1)-(3), we find that for the result $s - 2p - 1 \equiv 0 \pmod 3$, $T' \cong T(C_4^{\frac{s-1-2p}{3}}, C_3^p, C_2^{n-s-1}, C_1^{\frac{2s+4-p}{3}})$. Hence,

$$P_1^{\alpha}(T') = 3^{p\alpha} 2^{\frac{\alpha}{3}(3n-s-5-4p)}$$

and

$$P_2^{\alpha}(T') = 3^{3p\alpha} 4^{\frac{\alpha}{3}(3n+s-7-8p)},$$

which completes the proof. □

Theorem 4. *For $1 \leq \beta < \frac{n-2}{3}$, let T be a molecular tree among the class $\mathcal{B}_{n,\beta}$, then*

$$P_1^{\alpha}(T) \geq 4^{\frac{\alpha}{2}(n-\beta-2)}$$

and

$$P_2^{\alpha}(T) \leq 4^{\alpha(n+\beta-2)},$$

with the sufficient and necessary condition of equalities is $T \cong T(C_4^{\beta}, C_3^0, C_2^{n-3\beta-2}, C_1^{2\beta+2})$.

Proof. We assume that, for $\beta < \frac{n-2}{3}$, T^b denotes the tree that has minimum P_1^{α} and maximum P_2^{α} value among the trees in the class $\mathcal{B}_{n,\beta}$.

Claim 4.1. $| T^b{}_{(2)} | \geq 1$

If $| T^b{}_{(2)} | = 0$, Equations (1) and (2) conclude that

$$| T^b{}_{(4)} | = n - 2 - 2\beta \tag{6}$$

and using the result $3\beta < n - 2$ which is obtained from $\beta < \frac{n-2}{3}$, in (6), we get $| T^b{}_{(4)} | > \beta$, a contradiction.

For $| T^b{}_{(2)} | \geq 1$, Lemma 1 concludes that

$$| T^b{}_{(3)} | = 0. \tag{7}$$

By using equations (6), (7) in (4), (2) and (3) it is easy to check that
$T^b \cong T(C_4^{\beta}, C_3^0, C_2^{n-3\beta-2}, C_1^{2\beta+2})$. Hence, $P_1^{\alpha}(T^b) = 4^{\frac{\alpha}{2}(n-\beta-2)}$ and $P_2^{\alpha}(T^b) = 4^{\alpha(n+\beta-2)}$, which completes the proof. □

Theorem 5. *For $\beta = \frac{n-2}{3}$, let T be a molecular tree among the class $\mathcal{B}_{n,\beta}$ such that $P_1^{\alpha}(T)$ is minimum or $P_2^{\alpha}(T)$ is maximum, then*

$$P_1^{\alpha}(T) = 4^{\alpha\beta} \quad \textit{and} \quad P_2^{\alpha}(T) = (4)^{4\alpha\beta}.$$

Proof. By Lemma 1, at most one of the numbers $| T_{(2)} |$ and $| T_{(3)} |$ is non-zero. First, we prove the following claim.

Claim 5.1. *$\beta = \frac{n-2}{3}$ if and only if $| T_{(2)} | = 0 = | T_{(3)} |$.*

If $\beta = \frac{n-2}{3}$ then using (1) and (5), we get

$$| T_{(1)} | + | T_{(2)} | = \frac{2n+2}{3} \tag{8}$$

Now, using (2), (5), and (8), we get

$$| T_{(2)} | = | T_{(3)} | = 0 \tag{9}$$

If $| T_{(2)} | = | T_{(3)} | = 0$, then the result $\beta = \frac{n-2}{3}$ can be easily obtained from (1) and (2).
The claim leads us to the fact that $T \cong T(C_4^{\beta}, C_3^0, C_2^0, C_1^{n-\beta})$. Hence, $P_1^{\alpha}(T) = 4^{\alpha\beta}$ and $P_2^{\alpha}(T) = (4)^{4\alpha\beta}$. □

Theorem 6. *For $\frac{n-2}{3} < \beta \leq \frac{n}{2} - 1$, let T be a molecular tree among the class $\mathcal{B}_{n,\beta}$, then*

$$P_1^{\alpha}(T) \geq 3^{\alpha(3\beta-n+2)} 4^{\alpha(n-2\beta-2)}$$

and

$$P_2^{\alpha}(T) \leq 3^{\alpha(9\beta-3n+6)} 4^{\alpha(4n-8\beta-8)}.$$

The sufficient and necessary condition of equalities is $T \cong T(C_4^{n-2\beta-2}, C_3^{3\beta-n+2}, C_2^0, C_1^{n-\beta})$.

Proof. We assume that, for $\frac{n-2}{3} < \beta \leq \frac{n}{2} - 1$, T^c denotes the tree that has minimum P_1^{α} and maximum P_2^{α} value among the trees in the class $\mathcal{B}_{n,\beta}$.

Claim 6.1. $| T^c{}_{(3)} | \geq 1$
If $| T^c{}_{(3)} | = 0$, then

$$| T^c{}_{(4)} | = \beta. \tag{10}$$

Now, using Equations (1), (2) *and* (10), *we get*

$$|T^c{}_{(2)}| = n - 3\beta - 2, \tag{11}$$

and the fact $\beta > \frac{n-2}{3}$ *along with* (11) *gives* $|T^c{}_{(2)}| < 0$, *which is a contradiction.*

Furthermore Lemma 1 helps us to proceed with the result

$$|T^c{}_{(2)}| = 0. \tag{12}$$

The results $|T^c{}_{(4)}| = n - 2\beta - 2$, $|T^c{}_{(3)}| = 3\beta - n + 2$ and $|T^c{}_{(1)}| = n - \beta$ are directly followed from the equations (1), (2), (10), (11) and (12). Hence,

$$T^c \cong T(C_4^{n-2\beta-2}, C_3^{3\beta-n+2}, C_2^0, C_1^{n-\beta})$$

with

$$P_1^\alpha(T^c) = 3^{\alpha(3\beta-n+2)}4^{\alpha(n-2\beta-2)} \quad \text{and} \quad P_2^\alpha(T^c) = 3^{\alpha(9\beta-3n+6)}4^{\alpha(4n-8\beta-8)}. \quad \square$$

5. Additional results

In the previous two sections, we obtained sharp bounds on the indices P_1^α and P_2^α for molecular trees. By setting $\alpha = 1$ in Theorems 3-6, we arrive at the following corollaries for the Narumi-Katayama index and multiplicative second Zagreb index.

Corollary 1. *Let* T *be a molecular tree from the class* $\mathcal{B}'_{n,s}$. *Then*

$$NK(T) \geq 3^p 2^{\frac{1}{3}(3n-s-5-4p)} \quad \textit{and} \quad \Pi_2(T) \leq 3^{3p}4^{\frac{1}{3}(3n+s-7-8p)},$$

where $p \in \{0, 1, 2\}$. *The sufficient and necessary condition of equalities is*

$$T \cong T(C_4^{\frac{s-1-2p}{3}}, C_3^p, C_2^{n-s-1}, C_1^{\frac{2s+4-p}{3}}).$$

Corollary 2. *For* $1 \leq \beta < \frac{n-2}{3}$, *let* T *be a molecular tree among the class* $\mathcal{B}_{n,\beta}$, *then*

$$NK(T) \geq 4^{\frac{1}{2}(n-\beta-2)} \quad \textit{and} \quad \Pi_2(T) \leq 4^{(n+\beta-2)},$$

with the sufficient and necessary condition of equalities is $T \cong T(C_4^\beta, C_3^0, C_2^{n-3\beta-2}, C_1^{2\beta+2})$.

Corollary 3. *For* $\beta = \frac{n-2}{3}$, *let* T *be a molecular tree among the class* $\mathcal{B}_{n,\beta}$ *such that* $NK(T)$ *is minimum or* $\Pi_2(T)$ *is maximum, then*

$$NK(T) = 4^\beta \quad \textit{and} \quad \Pi_2(T) = (4)^{4\beta}.$$

Corollary 4. *For* $\frac{n-2}{3} < \beta \leq \frac{n}{2} - 1$, *let* T *be a molecular tree among the class* $\mathcal{B}_{n,\beta}$, *then*

$$NK(T) \geq 3^{(3\beta-n+2)}4^{(n-2\beta-2)} \quad \textit{and} \quad \Pi_2(T) \leq 3^{(9\beta-3n+6)}4^{(4n-8\beta-8)}.$$

The sufficient and necessary condition of equalities is $T \cong T(C_4^{n-2\beta-2}, C_3^{3\beta-n+2}, C_2^0, C_1^{n-\beta})$.

Also, by taking $\alpha = 2$ in Theorems 3-6, we get the following results regarding the multiplicative first Zagreb index.

Corollary 5. *Let* T *be a molecular tree from the class* $\mathcal{B}'_{n,s}$. *Then*

$$\Pi_1(T) \geq 3^{2p}2^{\frac{2}{3}(3n-s-5-4p)},$$

where $p \in \{0, 1, 2\}$. *The sufficient and necessary condition of equality is*

$$T \cong T(C_4^{\frac{s-1-2p}{3}}, C_3^p, C_2^{n-s-1}, C_1^{\frac{2s+4-p}{3}}).$$

Corollary 6. *For* $1 \leq \beta < \frac{n-2}{3}$, *let* T *be a molecular tree among the class* $\mathcal{B}_{n,\beta}$, *then*

$$\Pi_1(T) \geq 4^{(n-\beta-2)},$$

where the sufficient and necessary condition for the equality is $T \cong T(C_4^\beta, C_3^0, C_2^{n-3\beta-2}, C_1^{2\beta+2})$.

Corollary 7. *For $\beta = \frac{n-2}{3}$, let T be a molecular tree among the class $\mathcal{B}_{n,\beta}$ such that $\Pi_1(T)$ is minimum, then*

$$\Pi_1(T) = 4^{2\beta}.$$

Corollary 8. *For $\frac{n-2}{3} < \beta \leq \frac{n}{2} - 1$, let T be a molecular tree among the class $\mathcal{B}_{n,\beta}$, then*

$$\Pi_1(T) \geq 3^{2(3\beta-n+2)} 4^{2(n-2\beta-2)}.$$

The sufficient and necessary condition for the equality is $T \cong T(C_4^{n-2\beta-2}, C_3^{3\beta-n+2}, C_2^0, C_1^{n-\beta})$.

6. Conclusion

We have examined the predictive ability of general multiplicative Zagreb indices P_1^α, P_2^α, $\Pi_{1,\alpha}^*$, for forecasting the enthalpy of formation of hydrocarbons using a data set of 25 benzenoid hydrocarbons, when $-2 \leq \alpha \leq 2$. It has been found that the largest absolute value of the correlation coefficient between every considered index and the enthalpy of formation of the compounds listed in Table 1, when $-2 \leq \alpha \leq 2$, is greater than 0.97 (see Table 2 and Figs. 2–4. These three absolute values occurred at $\alpha \approx 0.0062, 0.0028, 0.0034$. This finding suggests that all the considered indices deserve further studies on other data sets of compounds for $0 < \alpha < 0.5$. This is the main reason that, in Sections 3 and 4, we have paid particular attention to the positive values of α and studied molecular trees with a given order and with a given number of branching vertices or segments using general multiplicative (first and second) Zagreb indices. We have obtained sharp lower/upper bounds on these Zagreb indices for the aforementioned molecular trees and determined the graphs attaining these bounds. Finally, we have obtained bounds on the classical multiplicative Zagreb and Narumi-Katayama indices as corollaries of our results (see the previous section).

The results given in Sections 4 and 5 may help to find suitable candidates with the maximum or minimum value of a certain physicochemical property among all molecules of a fixed number of atoms and a given number of branching atoms or segments. For instance, let a, b, and $\alpha_1 > 0$ be fixed non-zero real numbers corresponding to a considered property P of alkanes such that the general multiplicative first Zagreb index $P_1^{\alpha_1}$ has the following regression line:

$$P = a + bP_1^{\alpha_1}, \tag{13}$$

then by Equation (13) and Theorem 6, among all heptane isomers with two branching atoms, 2, 2, 3-Trimethylbutane uniquely attains the minimum (maximum, respectively) value of P when $b > 0$ (when $b < 0$, respectively), where a branching atom is any atom of valency greater than 2.

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CRediT authorship contribution statement

Sadia Noureen: Writing – original draft, Validation, Methodology, Conceptualization. **Akbar Ali:** Supervision, Software, Methodology. **Akhlaq A. Bhatti:** Writing – review & editing, Supervision, Formal analysis, Conceptualization. **Abdulaziz M. Alanazi:** Writing – review & editing, Validation, Investigation. **Yilun Shang:** Writing – review & editing, Validation, Funding acquisition.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Yilun Shang is a Section Editor for Heliyon.

Data availability

The experimental values (shown in Table 1) for the enthalpy of formation of the considered 25 benzenoid hydrocarbons come from [10,23]. No other data was used for the research described in this article.

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