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Research article

On chemical and mathematical characteristics of generalized degree–based molecular descriptors

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Abstract: This paper deals with the properties of the generalized Gutman–Milovanović index, generalized elliptic–Sombor index, generalized Zagreb–Sombor index, and general Euler–Sombor index. These include, as special cases, several previously studied molecular descriptors and most of their general versions; for instance, the general Randić index, the general sum-connectivity index, the general Sombor index, etc. The aforementioned descriptors are examined for their applicability in predicting 13 properties of octane isomers, and the results are compared with the ones generated by a benchmark data set (proposed by the International Academy of Mathematical Chemistry), containing 102 descriptors of octane isomers, and also with variable and discrete Adriatic indices. Although these descriptors slightly outperform the descriptors considered for comparison in several cases, a considerable improvement is detected in the case of boiling point. Several fundamental bounds and optimal results of the above-said descriptors are also reported.

Keywords: molecular descriptor; topological index; degree of a vertex; degree-based topological index; chemical graph theory
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1. Introduction

Molecular descriptors are essential tools in the process of predicting physicochemical and biological properties of chemical compounds, as well as for virtual screening of molecular libraries [3]. According to Todeschini and Consonni [22], “the final result of a logic and mathematical procedure which transforms chemical information encoded within a symbolic representation of a molecule into a useful number or the result of some standardized experiment” is known as a molecular descriptor. Descriptors that are defined using the graph-based model of a molecule are usually referred to as topological indices [23, 26].

For a (molecular) graph G, define

$$\mathcal{GM}_{\alpha,\beta}(G) = \sum_{uv \in E(G)} (d_u\, d_v)^{\alpha} (d_u + d_v)^{\beta}\,, \tag{1.1}$$

where $E(G)$ represents the edge set of G, d_u denotes the degree of the vertex u in G, and both α, β are real numbers.

As far as we know, the molecular descriptor $\mathcal{GM}_{\alpha,\beta}$ was considered in [9] for the first time as a generalization of the well-known first and second Zagreb indices (see the most recent survey [4] on these two Zagreb indices). Nowadays, this descriptor is studied under the name "Gutman–Milovanović index" [10, 16, 17]. Since this index involves two arbitrary parameters, α and β, we propose to call it the generalized Gutman–Milovanović index. It is worth noting that it was studied also in [11] under the name "generalized inverse sum indeg index" as a generalization of the inverse sum indeg (ISI) index (see the survey [1] on the ISI index).

By using geometric representations of vertex degrees, the so-called Sombor index ($\mathcal{SO}$) was developed [6]. For a graph G, this index is defined as

$$\mathcal{SO}(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2}\,.$$

This index has been extensively studied (see the survey [14]), and several of its variants were put forward. One of these is the so-called elliptic Sombor index ($\mathcal{ESO}$),

$$\mathcal{ESO}(G) = \sum_{uv \in E(G)} (d_u + d_v) \sqrt{d_u^2 + d_v^2}\,,$$

introduced in [8] and later studied in [15,18,20]. In [8], a new geometric method for designing degree-based topological indices was proposed. The authors in [8] mentioned that numerous topological indices can be devised using the introduced method. The most significant among them is the Euler Sombor index ($\mathcal{EU}$),

$$\mathcal{EU}(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2 + d_u\, d_v}\,.$$

It was studied in recent articles [7,21]. A topological index, similar to the $\mathcal{ESO}$ and $\mathcal{EU}$, is the Zagreb–Sombor index ($\mathcal{ZSO}$),

$$\mathcal{ZSO}(G) = \sum_{uv \in E(G)} d_u\, d_v \sqrt{d_u^2 + d_v^2}\,.$$

This particular modification of the Sombor index is proposed here for the first time.

Anyway, all the aforementioned specified indices can be generalized in the same manner as $\mathcal{GM}_{\alpha,\beta}$ (see Eq (1.1)), and so we have:

$$\text{generalized elliptic Sombor index:} \quad \mathcal{ESO}_{\alpha,\beta}(G) = \sum_{uv \in E(G)} (d_u + d_v)^{\alpha} (d_u^2 + d_v^2)^{\beta},$$

$$\text{general Euler Sombor index:} \quad \mathcal{EU}_{\alpha}(G) = \sum_{uv \in E(G)} (d_u^2 + d_v^2 + d_u\, d_v)^{\alpha},$$

$$\text{generalized Zagreb–Sombor index:} \qquad \mathcal{ZSO}_{\alpha,\beta}(G) = \sum_{uv\in E(G)} (d_u\, d_v)^{\alpha}(d_u^2 + d_v^2)^{\beta}.$$

Here, we use the term "generalized" for a molecular descriptor when it contains two arbitrary parameters (e.g., α and β) and the word "general" for a descriptor containing only one arbitrary parameter. Many existing general or generalized topological indices are covered by the $\mathcal{GM}_{\alpha,\beta}$, $\mathcal{ESO}_{\alpha,\beta}$, $\mathcal{ZSO}_{\alpha,\beta}$, and $\mathcal{EU}_{\alpha}$ indices (e.g., the general Randić index [19] is covered by both the $\mathcal{GM}_{\alpha,\beta}$ and $\mathcal{ZSO}_{\alpha,\beta}$ indices for $\beta = 0$, and the general sum-connectively index [28] is obtained from either $\mathcal{GM}_{\alpha,\beta}$ index for $\alpha = 0$ or $\mathcal{ESO}_{\alpha,\beta}$ index for $\beta = 0$). Other special cases of these descriptors are the general Sombor index [12], ordinary generalized geometric-arithmetic index [5], general elliptic–Sombor index [17], general inverse sum indeg index (which is obtained from the $\mathcal{GM}_{\alpha,\beta}$ index by replacing β with $-\alpha$), and general symmetric division deg index (which is obtained from the $\mathcal{ZSO}_{\alpha,\beta}$ index by replacing α with $-\beta$). In this paper, some of the mathematical and chemical properties of the $\mathcal{GM}_{\alpha,\beta}$, $\mathcal{ESO}_{\alpha,\beta}$, $\mathcal{ZSO}_{\alpha,\beta}$, and $\mathcal{EU}_{\alpha}$ are presented.

The rest of this paper is organized as follows: In the next section, the $\mathcal{GM}_{\alpha,\beta}$, $\mathcal{ESO}_{\alpha,\beta}$, $\mathcal{ZSO}_{\alpha,\beta}$, and $\mathcal{EU}_{\alpha}$ indices are examined for their applicability in predicting 13 properties of octane isomers. The obtained results are compared with the ones generated by not only a benchmark data set—proposed by the International Academy of Mathematical Chemistry—containing 102 descriptors of octane isomers[*], but also discrete Adriatic indices [25] and variable Adriatic indices [24]. Section 3 studies the monotonicity of the functions associated with the $\mathcal{GM}_{\alpha,\beta}$, $\mathcal{ESO}_{\alpha,\beta}$, and $\mathcal{ZSO}_{\alpha,\beta}$ indices. Several bounds on the $\mathcal{GM}_{\alpha,\beta}$, $\mathcal{ESO}_{\alpha,\beta}$, and $\mathcal{ZSO}_{\alpha,\beta}$ indices are reported in Section 4. Finally, some optimal results concerning the $\mathcal{GM}_{\alpha,\beta}$, $\mathcal{ESO}_{\alpha,\beta}$, and $\mathcal{ZSO}_{\alpha,\beta}$ indices for molecular graphs are presented in Section 5.

2. Chemical applicability of $\mathcal{ESO}_{\alpha,\beta}$, $\mathcal{ZSO}_{\alpha,\beta}$, $\mathcal{GM}_{\alpha,\beta}$, and $\mathcal{EU}_{\alpha}$

In this section, we examine the applicability of the molecular descriptors $\mathcal{ESO}_{\alpha,\beta}$, $\mathcal{ZSO}_{\alpha,\beta}$, $\mathcal{GM}_{\alpha,\beta}$, and $\mathcal{EU}_{\alpha}$ in predicting 13 properties of octane isomers under the constraints $-3 \le \alpha \le 3$ and $-3 \le \beta \le 3$. The mentioned 13 properties are given as follows: BP (boiling point), CT (heat capacity at constant T), CP (heat capacity at constant P), S (standard entropy), DENS (density), HVAP (enthalpy of vaporization), DHVAP (standard enthalpy of vaporization), HFORM (enthalpy of formation), DHFORM (standard enthalpy of formation), AcenFac (acentric factor), TSA (total surface area), LogP (octanol-water partition coefficient), and MV (molar volume).

We calculated the maximum of the absolute correlation coefficients between each of the mentioned properties of octane isomers and each of the mentioned descriptors, with the constraints $-3 \le \alpha \le 3$ and $-3 \le \beta \le 3$, by using the tool "NMaximize" available in Mathematica [13] and used the following three methods: "SimulatedAnnealing", "DifferentialEvolution", "RandomSearch"; the obtained maximum correlation coefficients between the considered descriptors and 12 properties are given in Table 1; the symbol "—" indicates that the obtained absolute correlation coefficient is less than 0.8. Since the maximum absolute correlation coefficient between each considered descriptor and LogP is less than 0.8, we omitted these data from Table 1. We remark here that the maximum absolute correlation coefficient given in the table may or may not be unique. Namely, for any particular cell, say

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[*] This dataset was published at the website `https://moleculardescriptors.eu`, which ceased to exist. Now, it can be accessed using `https://web.archive.org` [27].

c_{ij}, of the considered table, it is possible that there exist values of α and β in the interval $[-3, 3]$, different from those given in c_{ij}, for which the corresponding correlation coefficient is approximately the same as that in the mentioned cell. The last column of Table 1 gives the highest correlation coefficients among each of the 12 considered properties and any of the (i) molecular descriptors of the benchmark data set for octane isomers, or (ii) discrete Adriatic indices [25], or (iii) variable Adriatic indices [24]. The last column of Table 1 is obtained from Table 1 of [24]. Although the examined descriptors slightly outperform those considered for comparison in several cases, we noticed a considerable improvement in the case of the boiling point.

Table 1. Absolute correlation coefficient between 4 descriptors and 12 properties of octane isomers.

	$\mathcal{ESO}_{\alpha,\beta}$	$\mathcal{ZSO}_{\alpha,\beta}$	$\mathcal{GM}_{\alpha,\beta}$	$\mathcal{EU}_{\alpha}$	Target Values
BP	**0.9387** $(0.7579, -0.3005)$	0.9208 $(-0.6334, 0.2506)$	0.9027 $(2.0033, -3.0000)$	0.8536 (-1.4781)	0.8832
CT	—	0.8559 $(-0.0819, 0.0342)$	0.8597 $(-0.1937, 0.2095)$	—	0.8718
CP	—	**0.8520** $(-1.4403, 0.5529)$	0.8410 $(-2.2397, 2.2987)$	—	0.8307
S	0.9630 $(3.0000, -0.3121)$	0.9621 $(0.5970, 0.6851)$	0.9628 $(0.1444, 2.2411)$	0.9605 (1.4625)	0.9644
DENS	0.8937 $(3.0000, 3.0000)$	0.9513 $(3.0000, 2.9427)$	0.9504 $(3.0000, 3.0000)$	0.8230 (3.0000)	0.9644
HVAP	**0.9782** $(-0.1168, 0.0474)$	0.9711 $(2.1385, -1.7146)$	0.9592 $(1.8046, -3.0000)$	0.9426 (-0.7636)	0.9539
DHVAP	0.9833 $(3.0000, -1.3433)$	**0.9858** $(2.4023, -2.1281)$	0.9734 $(1.6411, -3.0000)$	0.9629 (-0.3518)	0.9849
HFORM	**0.9536** $(2.6641, -1.0832)$	0.9535 $(0.9629, -0.5680)$	0.9501 $(2.0094, -3.0000)$	0.8682 (-1.3551)	0.9110
DHFORM	**0.8824** $(3.0000, -1.1447)$	0.8650 $(1.9417, -0.9779)$	0.8569 $(2.4234, -3.0000)$	—	0.8660
AcenFac	0.9919 $(3.0000, -0.8174)$	**0.9953** $(0.5751, 0.0313)$	**0.9953** $(0.5411, 0.0414)$	0.9772 (1.2172)	0.9950
TSA	—	**0.9625** $(-1.1701, 0.4477)$	—	—	0.9592
MV	0.8865 $(3.0000, 3.0000)$	0.9397 $(3.0000, 2.1853)$	0.9429 $(3.0000, 3.0000)$	0.8214 (3.0000)	0.9539

As an example, we compared the absolute value of the correlation coefficient obtained by correlating the boiling points of octanes with the $\mathcal{ESO}_{\alpha,\beta}$, where α and β are taken the optimal values ($(\alpha, \beta) = (0.7579, -0.3005)$), with those obtained by calculating $\mathcal{ESO}_{\alpha,\beta}$ where α and β are rounded to the closest rational numbers with denominator 2 to the aforementioned optimal values. Thus, $\mathcal{ESO}_{\alpha,\beta}$ values are calculated for the following four ordered (α,β) pairs: $(1/2, 0), (1/2, -1/2), (1, 0), (1, -1/2)$, and the obtained absolute values of the correlation coefficients with the boiling points are 0.7504, 0.8122, 0.7203, and 0.8281, respectively. It is evident that the absolute values of these correlation coefficients are significantly lower than the $|R| = 0.9387$ that is achieved using $\mathcal{ESO}_{0.7579,-0.3005}$.

3. Monotonicity of the functions associated with $\mathcal{ESO}_{\alpha,\beta}$, $\mathcal{ZSO}_{\alpha,\beta}$, and $\mathcal{GM}_{\alpha,\beta}$

Mathematical treatment of the $\mathcal{ESO}_{\alpha,\beta}$, $\mathcal{ZSO}_{\alpha,\beta}$, and $\mathcal{GM}_{\alpha,\beta}$ is narrowed to the sets of ordered pairs (α,β) containing those ordered pairs that correspond to the bolded numbers in Table 1. For example, we considered here $E_{BP} = \left\{(\alpha, \beta) : \alpha \geq \frac{3}{4} \text{ and } \beta \geq -\frac{31}{100}\right\}$ that encompasses $(\alpha, \beta) = (0.7579, -0.3005)$. $\mathcal{ESO}_{0.7579,-0.3005}$ correlates well with the boiling points of octanes (in Table 1 is shown that $|R| = 0.9387$).

Lemma 1. *Let*

$$\begin{aligned} E_{BP} &= \left\{(\alpha, \beta) : \alpha \geq \frac{3}{4} \textit{ and } \beta \geq -\frac{31}{100}\right\}, \\ E_{DHFORM} &= \left\{(3, \beta) : \beta \geq -\frac{6}{5}\right\}, \\ E_{HFORM} &= \left\{(\alpha, \beta) : \alpha \geq \frac{133}{50} \textit{ and } \beta \geq -\frac{11}{10}\right\} \quad \textit{and} \\ E_{HVAP} &= \left\{(\alpha, \beta) : \alpha \leq -\frac{29}{250} \textit{ and } \beta \leq \frac{6}{125}\right\}. \end{aligned}$$

For fixed real numbers α and β, define the function $\hbar$ as

$$\hbar(x_1, x_2) = (x_1 + x_2)^{\alpha}(x_1^2 + x_2^2)^{\beta}, \textit{ with } x_1 \geq 1 \textit{ and } x_2 \geq 1.$$

If $(\alpha, \beta) \in E_{BP} \cup E_{DHFORM} \cup E_{HFORM}$, then $\hbar$ is strictly increasing in both of its variables. However, if $(\alpha, \beta) \in E_{HVAP}$, then $\hbar$ is strictly decreasing in both of its variables.

Proof. Since

$$\alpha(x_1^2 + x_2^2) + 2\beta x_1(x_1 + x_2) \begin{cases} \geq \frac{1}{100}(13x_1^2 - 62x_1x_2 + 75x_2^2) > 0 & \text{if } (\alpha, \beta) \in E_{BP}, \\ \geq \frac{3}{5}(x_1^2 - 4x_1x_2 + 5x_2^2) > 0 & \text{if } (\alpha, \beta) \in E_{DHFORM}, \\ \geq \frac{1}{50}(23x_1^2 - 110x_1x_2 + 133x_2^2) > 0 & \text{if } (\alpha, \beta) \in E_{HFORM}, \\ \leq -\frac{1}{250}(5x_1^2 - 24x_1x_2 + 29x_2^2) < 0 & \text{if } (\alpha, \beta) \in E_{HVAP}, \end{cases}$$

we have

$$\begin{aligned} \frac{\partial}{\partial x_1}(\hbar(x_1, x_2)) &= (x_1 + x_2)^{\alpha-1}(x_1^2 + x_2^2)^{\beta-1}[\alpha(x_1^2 + x_2^2) + 2\beta x_1(x_1 + x_2)] \\ &\begin{cases} > 0 & \text{if } (\alpha, \beta) \in E_{BP} \cup E_{DHFORM} \cup E_{HFORM}, \\ < 0 & \text{if } (\alpha, \beta) \in E_{HVAP}. \end{cases} \end{aligned}$$

□

Lemma 2. *Let*

$$Z_{AcenFac} = \left\{(\alpha, \beta) : \alpha \geq 0 \textit{ and } \beta > -\frac{\alpha}{2}\right\},$$
$$Z_{TSA/CP} = \left\{(\alpha, \beta) : \alpha \leq 0 \textit{ and } \beta < -\frac{\alpha}{2}\right\} \quad \textit{and}$$
$$Z_{DHVAP} = \left\{\left(\frac{24023}{10000}, -\frac{21281}{10000}\right)\right\}.$$

For fixed real numbers α *and* β*, define the function* $\hbar$ *as*

$$\hbar(x_1, x_2) = (x_1x_2)^{\alpha}(x_1^2 + x_2^2)^{\beta}, \textit{ with } x_1 \geq 1 \textit{ and } x_2 \geq 1.$$

If $(\alpha, \beta) \in Z_{AcenFac}$ *(respectively,* $(\alpha, \beta) \in Z_{TSA/CP}$*), then* $\hbar$ *is strictly increasing (respectively, strictly decreasing) in both of its variables. However, if* $(\alpha, \beta) \in Z_{DHVAP}$*, then* $\hbar$ *is not monotone in either of its variables.*

Proof. Since

$$\frac{\partial}{\partial x_1}(\hbar(x_1, x_2)) = x_1^{\alpha-1}x_2^{\alpha}(x_1^2 + x_2^2)^{\beta-1}\Big[(\alpha + 2\beta)x_1^2 + \alpha x_2^2\Big],$$

we have the required conclusion. □

Lemma 3. *Let* $M_{AcenFac} = \{(\alpha, \beta) : \alpha \geq 0 \textit{ and } \beta > -\alpha\}$*. For fixed real numbers* α *and* β*, define the function* $\hbar$ *as*

$$\hbar(x_1, x_2) = (x_1x_2)^{\alpha}(x_1 + x_2)^{\beta}, \textit{ with } x_1 \geq 1 \textit{ and } x_2 \geq 1.$$

If $(\alpha, \beta) \in M_{AcenFac}$*, then* $\hbar$ *is strictly increasing in both of its variables.*

Proof. Since

$$\frac{\partial}{\partial x_1}(\hbar(x_1, x_2)) = x_1^{\alpha-1}x_2^{\alpha}(x_1 + x_2)^{\beta-1}\Big[(\alpha + \beta)x_1 + \alpha x_2\Big],$$

we have the required conclusion. □

4. Bounds on $\mathcal{ESO}_{\alpha,\beta}$, $\mathcal{ZSO}_{\alpha,\beta}$, and $\mathcal{GM}_{\alpha,\beta}$

In the preceding section, we have seen that the functions associated with $\mathcal{ESO}_{\alpha,\beta}$, $\mathcal{ZSO}_{\alpha,\beta}$, and $\mathcal{GM}_{\alpha,\beta}$ are strictly monotone in all considered cases, except one. Hence, instead of presenting bounds on $\mathcal{ESO}_{\alpha,\beta}$, $\mathcal{ZSO}_{\alpha,\beta}$, and $\mathcal{GM}_{\alpha,\beta}$ separately, in the next three propositions we give such bounds on the following descriptor (covering $\mathcal{ESO}_{\alpha,\beta}$, $\mathcal{ZSO}_{\alpha,\beta}$, and $\mathcal{GM}_{\alpha,\beta}$) when $\hbar$ is a strictly monotone function:

$$\mathcal{I}_{\hbar}(G) = \sum_{xy \in E(G)} \hbar(d_x(G), d_y(G)),$$

where $\hbar(r_1, r_2) = \hbar(r_2, r_1)$ for all r_1 and r_2 in the domain of $\hbar$.

Before going any further, we define some terms that will be used in the rest of this paper. If the degree of a vertex is equal to 1, it is referred to as a pendent vertex. A pendent edge in a graph is the one incident with a pendent vertex. By an m-size graph, we mean a graph of size m, i.e., containing m edges. Similarly, an n-order graph is a graph of order n, i.e., containing n vertices. The degree set of a graph G is the set consisting of all distinct members of the degree sequence of G.

Proposition 1. *Let $\hbar$ be a strictly increasing function (in both of its variables) defined on the Cartesian square of the set of real numbers greater than or equal to 1 such that $\hbar(x_1, x_2) = \hbar(x_2, x_1) \geq 0$ for all x_1 and x_2 belonging to the domain of $\hbar$ and $\hbar(x_1, x_2) > 0$ for $x_1 \neq x_2$. If G is an m-size connected graph with p pendent vertices, then*

$$p \cdot \hbar(1, 2) + (m - p)\hbar(2, 2) \leq \mathcal{I}_{\hbar}(G) \leq p \cdot \hbar(1, \Delta) + (m - p)\hbar(\Delta, \Delta) \tag{4.1}$$

with the right equality iff either G is Δ-regular or the degree set of G is $\{1, \Delta\}$, while the left equality holds iff G is either the cycle graph or the path graph, where Δ is G's maximum degree and $m \geq 2$. If the function $\hbar$ is strictly decreasing (in both of its variables), then the inequality signs in (4.1) *are reversed.*

Proof. Since the proofs of the chain of inequalities (4.1) and its reverse version are fully similar to each other, we prove only this shown in (4.1). So, we assume that the function $\hbar$ is strictly increasing. Let E_p denote the set consisting of all pendent edges of G. Then, we have

$$\begin{aligned}\mathcal{I}_{\hbar}(G) &= \sum_{xy \in E_p} \hbar(d_x(G), d_y(G)) + \sum_{x'y' \in E(G) \setminus E_p} \hbar(d_{x'}(G), d_{y'}(G)) \\ &\leq \sum_{xy \in E_p} \hbar(1, \Delta) + \sum_{x'y' \in E(G) \setminus E_p} \hbar(\Delta, \Delta) \qquad (4.2) \\ &= p \cdot \hbar(1, \Delta) + (m - p)\hbar(\Delta, \Delta).\end{aligned}$$

We note that the equality in (4.2) holds iff one end vertex of every pendent edge (if it exists) has degree Δ and both end vertices of every non-pendent edge (if it exists) have degree Δ. Similarly, we have

$$\mathcal{I}_{\hbar}(G) \geq p \cdot \hbar(1, 2) + (m - p)\hbar(2, 2)$$

with equality iff one end vertex of every pendent edge (if it exists) has degree 2 and both end vertices of every non-pendent edge (if it exists) have 2. □

Proposition 2. *Let $\hbar$ be the strictly increasing function (in both of its variables) defined in Proposition 1. If G is an n-order tree of maximum degree Δ, then*

$$\mathcal{I}_{\hbar}(G) \leq \Delta \cdot \hbar(1, \Delta) + (n - \Delta - 1)\hbar(\Delta, \Delta) \tag{4.3}$$

with equality iff G is the star graph. If the function $\hbar$ is strictly decreasing (in both of its variables), then the inequality sign in (4.3) *is reversed.*

Proof. As the proofs of (4.3) and its reverse version are fully similar to each other, we prove only this shown in (4.3). So, we assume that $\hbar$ is strictly increasing. Since the number of pendent vertices in a tree is always greater than or equal to its maximum degree, by (4.1) we have

$$\mathcal{I}_{\hbar}(G) \leq \Delta \cdot \hbar(1, \Delta) + (n - \Delta - 1)\hbar(\Delta, \Delta)$$

with equality iff the number of pendent vertices of G is Δ and the degree set of G is $\{1, \Delta\}$; that is, iff G is the star graph. □

Proposition 3. *Let $\hbar$ be the strictly increasing function (in both of its variables) defined in Proposition 1. If G is an m-size connected graph of maximum degree Δ and minimum degree δ, then*

$$m \cdot \hbar(\delta, \delta) \le \mathcal{I}_{\hbar}(G) \le m \cdot \hbar(\Delta, \Delta), \tag{4.4}$$

where either of the equalities holds iff G is regular. If the function $\hbar$ is strictly decreasing (in both of its variables), then the inequality sign in (4.4) *is reversed.*

Proof. The result follows from the fact that $\delta \le d_x(G) \le \Delta$ for every vertex x of G. □

The following result is one of the notable consequences of Proposition 3:

Corollary 1. *Let $\hbar$ be the strictly increasing function (in both of its variables) defined in Proposition 1. For every n-order non-trivial graph G,*

$$\mathcal{I}_{\hbar}(G) \le \frac{n(n-1)}{2}\hbar(n-1, n-1)$$

with equality iff G is the complete graph K_n.

Proof. Assume that Δ is the maximum degree of G. Then, by Proposition 3, we have

$$\mathcal{I}_{\hbar}(G) \le |E(G)| \cdot \hbar(\Delta, \Delta) \le \frac{n(n-1)}{2}\hbar(n-1, n-1),$$

where the first equality holds iff G is Δ-regular while the second equality holds iff $|E(G)| = \frac{n(n-1)}{2}$ and $\Delta = n-1$. □

Molecular graphs pertaining to carbon-atom skeletons have vertices of degree 4 or less. Therefore, the size of a molecular graph of order n is at most $2n$. Thus, from Proposition 3, we also have the next result.

Corollary 2. *Let $\hbar$ be the strictly increasing function (in both of its variables) defined in Proposition 1. If G is an n-order connected graph, then $\mathcal{I}_{\hbar}(G) \le 2n \cdot \hbar(4, 4)$ with equality iff G is a 4-regular graph.*

Next, we present a bound on $\mathcal{I}_{\hbar}$ when $\hbar$ may or may not be monotone.

Theorem 1. *Let G be an n-order connected graph of size $m \ge 2$. Let $\hbar$ be the function defined in Proposition 1, not necessarily monotone. Define the function Φ on the set of positive integers as*

$$\Phi(r_1, r_2) := \hbar(r_1, r_2) + \frac{2\hbar(1,2)(r_1 r_2 - r_1 - r_2)}{r_1 r_2} + \frac{\hbar(2,2)(2r_1 + 2r_2 - 3r_1 r_2)}{r_1 r_2}. \tag{4.5}$$

For $n-1 \ge r_2 \ge r_1 \ge 1$ such that $(r_1, r_2) \notin \{(1,1), (1,2), (2,2)\}$, if $\Phi(r_1, r_2) > 0$, then

$$\mathcal{I}_{\hbar}(G) \ge 2[\hbar(1,2) - \hbar(2,2)]n + [3\hbar(2,2) - 2\hbar(1,2)]m, \tag{4.6}$$

with equality iff either G is the path graph P_n or G is the cycle graph C_n. If $\Phi(r_1, r_2) < 0$ with the above-mentioned constraints, then the inequality in (4.6) *is reversed.*

Proof. We prove the result when $\Phi(r_1, r_2) > 0$. If n_p is the number of vertices of G that have degree p, and $m_{p,q}$ is the number of edges of G whose one end vertex is of degree p and the other end vertex is of degree q, then

$$\begin{cases} m_{1,2} + m_{1,3} + \cdots + m_{1,n-1} = n_1 \\ m_{2,1} + 2m_{2,2} + m_{2,3} + \cdots + m_{2,n-1} = 2n_2 \\ m_{3,1} + m_{3,2} + 2m_{3,3} + \cdots + m_{3,n-1} = 3n_3 \\ \vdots \\ m_{n-1,1} + m_{n-1,2} + m_{n-1,3} + \cdots + 2m_{n-1,n-1} = (n-1)n_{n-1} \\ n_1 + n_2 + n_3 + \cdots + n_{n-1} = n \\ n_1 + 2n_2 + 3n_3 + \cdots + (n-1)n_{n-1} = 2m\,. \end{cases} \tag{4.7}$$

Let

$$\begin{cases} \xi_1 = n_1 - m_{1,2} \\ \xi_2 = 2n_2 - m_{1,2} - 2m_{2,2} \\ \xi_j = jn_j \quad \text{when } 3 \le j \le n-1. \end{cases} \tag{4.8}$$

By using (4.7) and (4.8), we have

$$\sum_{i=1}^{n-1} \xi_i = 2(m - m_{1,2} - m_{2,2}) \tag{4.9}$$

and

$$\sum_{i=1}^{n-1} \frac{\xi_i}{i} = n - \frac{3m_{1,2}}{2} - m_{2,2}\,. \tag{4.10}$$

By solving (4.9) and (4.10) for $m_{1,2}$ and $m_{2,2}$, we obtain

$$m_{1,2} = 2\left(n - m - \sum_{i=1}^{n-1}\left(\frac{1}{i} - \frac{1}{2}\right)\xi_i\right) \tag{4.11}$$

and

$$m_{2,2} = 3m - 2n + \sum_{i=1}^{n-1}\left(\frac{2}{i} - \frac{3}{2}\right)\xi_i\,. \tag{4.12}$$

Define $S := \{(j,k) : 1 \le j \le k \le n-1\} \setminus \{(1,1),(1,2),(2,2)\}$. Using (4.7) and (4.8) in (4.11) and (4.12), we obtain

$$m_{1,2} = 2\left(n - m - \sum_{(j,k)\in S}\left(\frac{1}{j} + \frac{1}{k} - 1\right)m_{j,k}\right) \tag{4.13}$$

and

$$m_{2,2} = 3m - 2n + \sum_{(j,k)\in S} \left(\frac{2}{j} + \frac{2}{k} - 3\right) m_{j,k}\,. \tag{4.14}$$

Now, using (4.13) and (4.14) in the definition of $\mathcal{I}_{\hbar}$, we obtain

$$\begin{aligned} \mathcal{I}_{\hbar}(G) = \sum_{1\le j\le k\le n-1} \hbar(j,k)m_{j,k} &= 2[\hbar(1,2) - \hbar(2,2)]n + [3\hbar(2,2) - 2\hbar(1,2)]m \\ &\quad + \sum_{(j,k)\in S} m_{j,k}\,\Phi(j,k) \\ &\ge 2[\hbar(1,2) - \hbar(2,2)]n + [3\hbar(2,2) - 2\hbar(1,2)]m, \end{aligned} \tag{4.15}$$

where the equality in (4.15) holds iff $\sum_{(j,k)\in S} m_{j,k}\,\Phi(j,k) = 0$. □

The proof of the next result (which is a variant of Theorem 1 and is restricted to molecular graphs) is fully analogous to that of Theorem 1.

Theorem 2. *Let G be an n-order (connected) molecular graph of size $m \ge 2$. Let $\hbar$ be the function defined in Proposition 1, not necessarily monotone. Define the function Φ on the set of positive integers as*

$$\Phi(r_1, r_2) := \hbar(r_1, r_2) + \frac{2\hbar(1,2)(r_1 r_2 - r_1 - r_2)}{r_1 r_2} + \frac{\hbar(2,2)(2r_1 + 2r_2 - 3r_1 r_2)}{r_1 r_2}. \tag{4.16}$$

For $4 \ge r_2 \ge r_1 \ge 1$ such that $(r_1, r_2) \notin \{(1,1),(1,2),(2,2)\}$, if $\Phi(r_1, r_2) > 0$, then

$$\mathcal{I}_{\hbar}(G) \ge 2[\hbar(1,2) - \hbar(2,2)]n + [3\hbar(2,2) - 2\hbar(1,2)]m, \tag{4.17}$$

with equality iff either G is the path graph P_n or G is the cycle graph C_n. If $\Phi(r_1, r_2) < 0$ with the above-mentioned constraints, then the inequality in (4.17) is reversed.

5. Optimal results for $\mathcal{ESO}_{\alpha,\beta}$, $\mathcal{ZSO}_{\alpha,\beta}$, and $\mathcal{GM}_{\alpha,\beta}$

This section is concerned with the optimality study of $\mathcal{ESO}_{\alpha,\beta}$, $\mathcal{ZSO}_{\alpha,\beta}$, and $\mathcal{GM}_{\alpha,\beta}$ for molecular graphs. From Lemmas 1–3 and Corollary 2, the next result follows.

Proposition 4. *Among all n-order molecular graphs with $n \ge 5$, only the 4-regular graph(s) has/have the maximum value of $\mathcal{ESO}_{\alpha,\beta}$ for $(\alpha, \beta) \in E_{BP} \cup E_{DHFORM} \cup E_{HFORM}$, $\mathcal{ZSO}_{\alpha,\beta}$ for $(\alpha, \beta) \in Z_{AcenFac}$, and $\mathcal{GM}_{\alpha,\beta}$ for $(\alpha, \beta) \in M_{AcenFac}$.*

We note that by Lemmas 1–3 and Corollary 1, among all non-trivial n-order graphs, only the complete graph K_n has the maximum values of $\mathcal{ESO}_{\alpha,\beta}$, $\mathcal{ZSO}_{\alpha,\beta}$, and $\mathcal{GM}_{\alpha,\beta}$ for $(\alpha, \beta) \in E_{BP} \cup E_{DHFORM} \cup E_{HFORM}$, $(\alpha, \beta) \in Z_{AcenFac}$, and $(\alpha, \beta) \in M_{AcenFac}$, respectively. Next, we study the fixed-order molecular graphs with minimum values of $\mathcal{ZSO}_{\alpha,\beta}$ and $\mathcal{GM}_{\alpha,\beta}$ for $(\alpha, \beta) \in Z^{\star}_{AcenFac} \subset Z_{AcenFac}$ and $(\alpha, \beta) \in M^{\star}_{AcenFac} \subset M_{AcenFac}$, respectively, where $Z^{\star}_{AcenFac} = \left\{(\alpha, \beta) : \frac{57}{100} \le \alpha \le 1 \text{ and } \frac{3}{100} \le \beta \le \frac{1}{2}\right\}$ and $M^{\star}_{AcenFac} = \left\{(\alpha, \beta) : \frac{53}{100} \le \alpha \le 1 \text{ and } \frac{3}{100} \le \beta \le \frac{1}{2}\right\}$. The set $Z^{\star}_{AcenFac}$ (respectively, $M^{\star}_{AcenFac}$) contains the ordered pair corresponding to the correlation coefficient between $\mathcal{ZSO}_{\alpha,\beta}$ (respectively, $\mathcal{GM}_{\alpha,\beta}$) and AcenFac mentioned in Table 1.

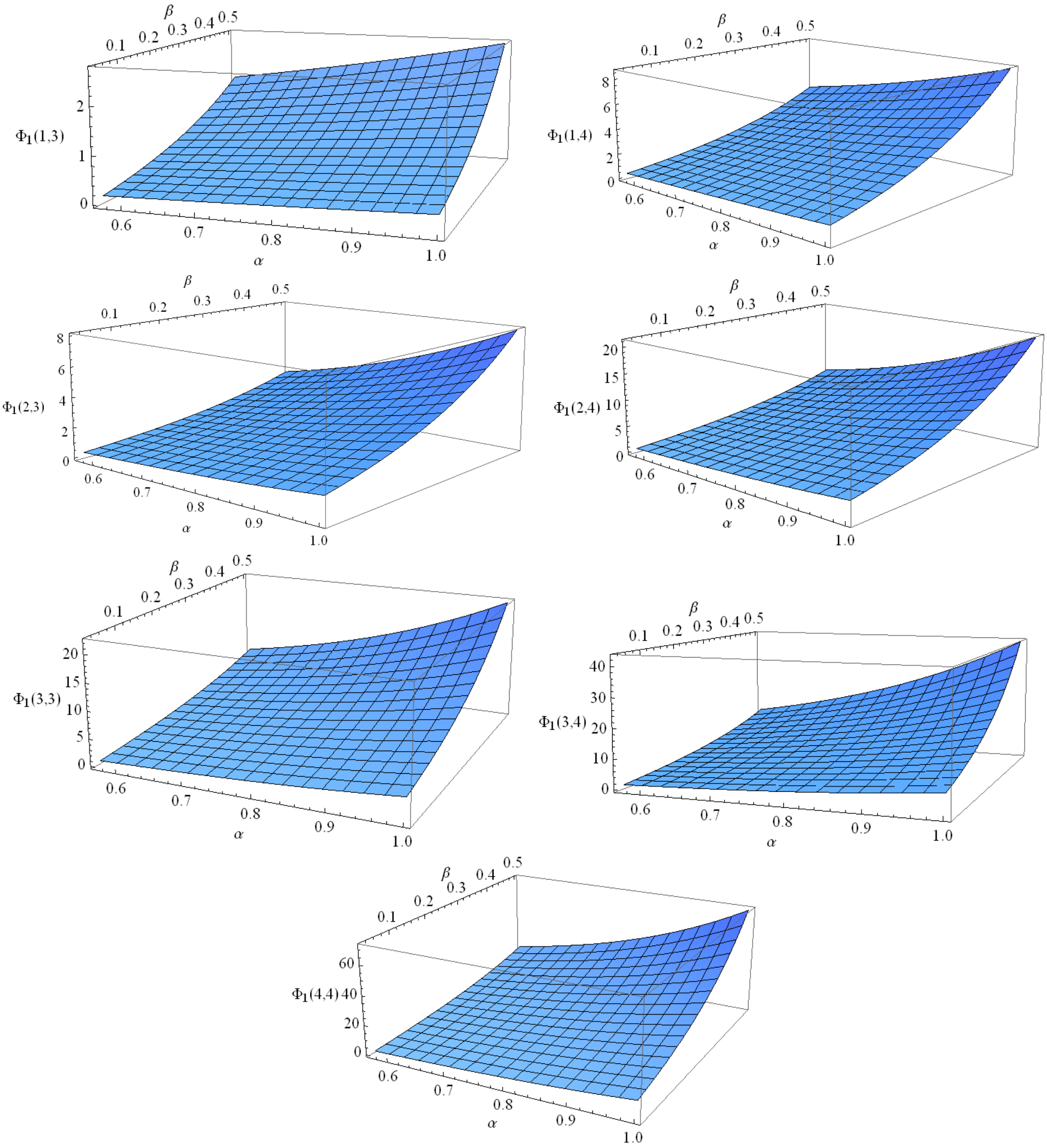

Figure 1. The graphs of the function $\Phi_1(r_1, r_2)$ for (r_1, r_2) belonging to the set $\{(1,3),(1,4),(2,3),(2,4),(3,3),(3,4),(4,4)\}$ when $\frac{57}{100} \le \alpha \le 1$ and $\frac{3}{100} \le \beta \le \frac{1}{2}$.

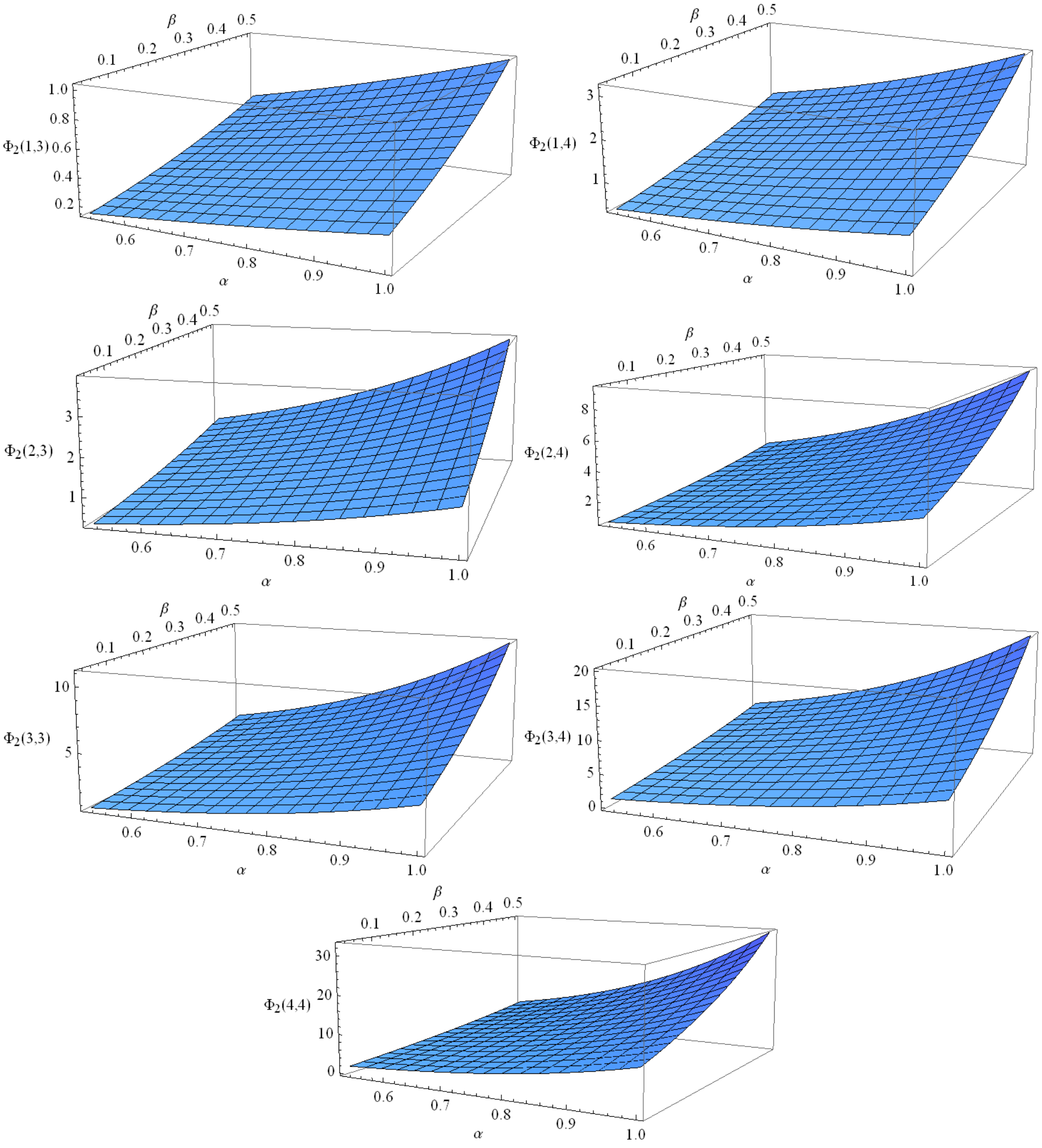

Figure 2. The graphs of the function $\Phi_2(r_1, r_2)$ for (r_1, r_2) belonging to the set $\{(1,3),(1,4),(2,3),(2,4),(3,3),(3,4),(4,4)\}$ when $\frac{53}{100} \le \alpha \le 1$ and $\frac{3}{100} \le \beta \le \frac{1}{2}$.

Proposition 5. *Among all n-order (connected) molecular graphs with* $n \ge 3$*, the path graph* P_n *uniquely attains the minimum values of* $\mathcal{ZSO}_{\alpha,\beta}$ *and* $\mathcal{GM}_{\alpha,\beta}$ *for* $(\alpha, \beta) \in Z^{\star}_{AcenFac}$ *and* $(\alpha, \beta) \in M^{\star}_{AcenFac}$*, respectively.*

Proof. Let G be an n-order (connected) molecular graph of size m such that $n \ge 3$. We take $\hbar(r_1, r_2) = (r_1\, r_2)^{\alpha}(r_1^2 + r_2^2)^{\beta}$ in (4.16) with $(\alpha, \beta) \in Z_{AcenFac}$, and to avoid confusion, we denote the resulting function by $\Phi_1(r_1, r_2)$ instead of $\Phi(r_1, r_2)$. Similarly, we substitute $\hbar(r_1, r_2) = (r_1 r_2)^\alpha (r_1 + r_2)^\beta$ in (4.16) with the assumption $(\alpha, \beta) \in M_{AcenFac}$ and denote the resulting function by $\Phi_2(r_1, r_2)$. Figures 1 and 2 show that $\Phi_i(r_1, r_2) > 0$ for every $(r_1, r_2) \in \{(1, 3), (1, 4), (2, 3), (2, 4), (3, 3), (3, 4), (4, 4)\}$ and $i \in \{1, 2\}$. In the following, we assume that $\mathcal{I}_\hbar \in \{\mathcal{ZSO}_{\alpha,\beta}, \mathcal{GM}_{\alpha,\beta}\}$. Hence, either by Theorem 2 and Lemma 2 or by Theorem 2 and Lemma 3, we have

$$\mathcal{I}_\hbar(G) \geq 2[\hbar(1, 2) - \hbar(2, 2)]n + [3\hbar(2, 2) - 2\hbar(1, 2)]m \geq (n - 3)\hbar(2, 2) + 2\hbar(1, 2), \tag{5.1}$$

where the first equality in (5.1) holds iff either G is the path graph P_n or G is the cycle graph C_n; while, the second equality in (5.1) holds iff G is the path graph P_n. □

Next, we discuss the graphs having the minimum value of $\mathcal{ESO}_{\alpha,\beta}$ among all n-order molecular (connected) graphs for $n \geq 5$ and $(\alpha, \beta) \in E^\star_{BP} \cup E^\star_{DHFORM} \cup E^\star_{HFORM}$, where $E^\star_{DHFORM} = \left\{(3, \beta) : -\frac{6}{5} \leq \beta \leq -\frac{28}{25}\right\}$, $E^\star_{BP} = \left\{(\alpha, \beta) : \frac{3}{4} \leq \alpha \leq \frac{4}{5} \text{ and } -\frac{31}{100} \leq \beta \leq -\frac{3}{10}\right\}$ and

$$E^\star_{HFORM} = \left\{(\alpha, \beta) : \frac{133}{50} \leq \alpha \leq \frac{27}{10} \text{ and } -\frac{11}{10} \leq \beta \leq -1\right\}.$$

The set $E^\star_{BP}$ (respectively, $E^\star_{HFORM}$ and $E^\star_{DHFORM}$) contains the ordered pair corresponding to the correlation coefficient between $\mathcal{ESO}_{\alpha,\beta}$ and BP (respectively, HFORM and DHFORM) mentioned in Table 1. Lemma 1 and the following known result confirm that the graphs attaining the minimum value of $\mathcal{ESO}_{\alpha,\beta}$ among all n-order molecular (connected) graphs for $n \geq 5$ and $(\alpha, \beta) \in E^\star_{BP} \cup E^\star_{DHFORM} \cup E^\star_{HFORM}$ must be trees:

Proposition 6. [2] *Let $\hbar$ be the strictly increasing function (in both of its variables) defined in Proposition 1. Let G be a graph, and let $v, w \in V(G)$ be its two non-adjacent vertices such that* $\max\{d_v(G), d_w(G)\} \geq 1$. *If $G + wv$ denotes the graph formed from G by adding an edge between v and w, then $\mathcal{I}_\hbar(G) < \mathcal{I}_\hbar(G + wv)$.*

Proposition 7. *Let $\hbar$ be the function defined in Proposition 1, not necessarily monotone. If* $2\hbar(2, 2) + \hbar(1, 2) - 2\hbar(1, 3) - \hbar(2, 3) > 0$ *(*$2\hbar(2, 2) + \hbar(1, 2) - 2\hbar(1, 3) - \hbar(2, 3) < 0$*, respectively), then any graph attaining the minimum value (maximum value, respectively) of $\mathcal{I}_\hbar$ among all n-order trees is different from the path graph P_n, where $n \geq 5$.*

Proof. Let $P^\star_n$ denote the n-order tree formed from the path graph P_{n-1} of order $n - 1$ by attaching a pendent vertex to a neighbor of a pendent vertex of P_{n-1}. Then

$$\mathcal{I}_\hbar(P_n) - \mathcal{I}_\hbar(P^\star_n) = 2\hbar(2, 2) + \hbar(1, 2) - 2\hbar(1, 3) - \hbar(2, 3).$$

□

Proposition 8. *Any graph attaining the minimum value of $\mathcal{ESO}_{\alpha,\beta}$ among all n-order molecular (connected) graphs is a tree but different from the path graph P_n, where $n \geq 5$ and $(\alpha, \beta) \in E^\star_{BP} \cup E^\star_{DHFORM} \cup E^\star_{HFORM}$.*

Proof. Let $G^\star$ be a graph attaining the minimum value of $\mathcal{ESO}_{\alpha,\beta}$ among all n-order molecular (connected) graphs, where $n \geq 5$ and $(\alpha, \beta) \in E^\star_{BP} \cup E^\star_{DHFORM} \cup E^\star_{HFORM}$. By Lemma 1 and

Proposition 6, the graph $G^\star$ must be a tree. If $\hbar(r_1, r_2) = (r_1 + r_2)^\alpha (r_1^2 + r_2^2)^\beta$, then from Figure 3 we have

$$2\hbar(2,2) + \hbar(1,2) - 2\hbar(1,3) - \hbar(2,3) = 2^{2\alpha+\beta+1}\left(4^\beta - 5^\beta\right) + 3^\alpha\, 5^\beta - 5^\alpha\, 13^\beta > 0$$

for $(\alpha, \beta) \in E^\star_{BP} \cup E^\star_{DHFORM} \cup E^\star_{HFORM}$. Hence, by Proposition 7, the graph $G^\star$ is different from the path graph P_n. □

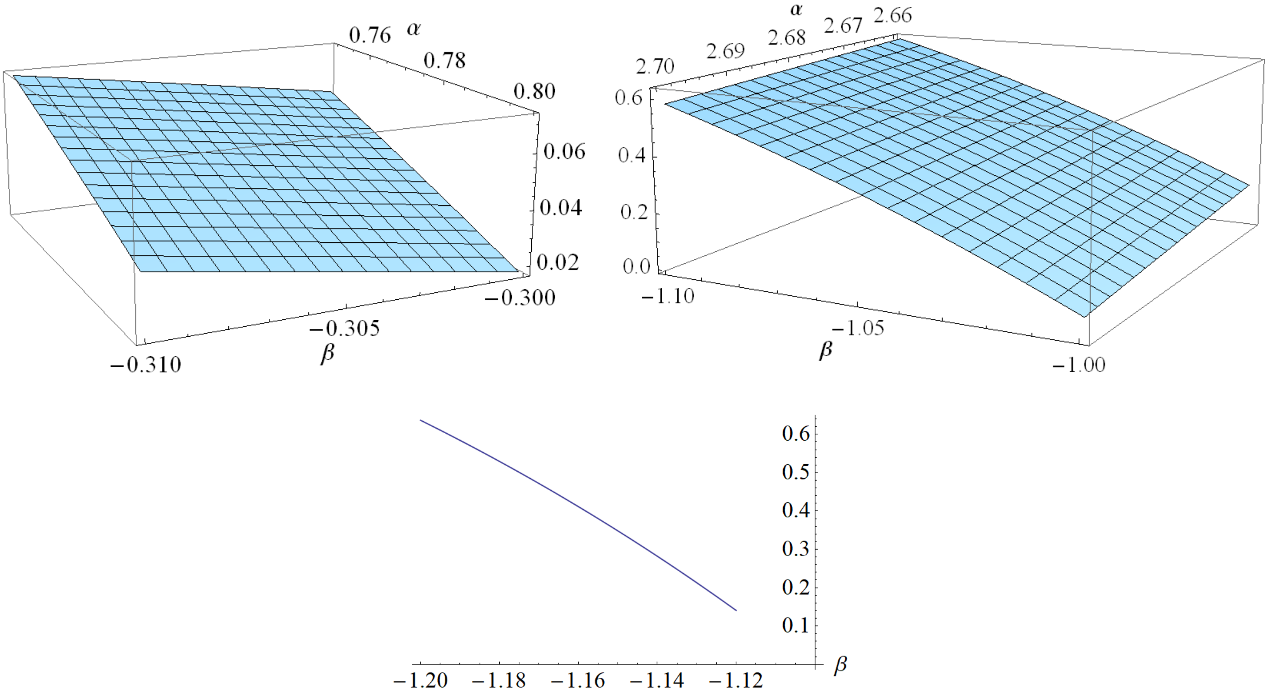

Figure 3. The graphs of $2^{2\alpha+\beta+1}\left(4^\beta - 5^\beta\right) + 3^\alpha\, 5^\beta - 5^\alpha\, 13^\beta$ when $(\alpha, \beta) \in E^\star_{BP}$, $(\alpha, \beta) \in E^\star_{HFORM}$ and $(\alpha, \beta) \in E^\star_{DHFORM}$, respectively.

We end this paper with the following open problem related to Proposition 8:

Problem 1. *Find graph(s) attaining the minimum value of* $\mathcal{ESO}_{\alpha,\beta}$ *among all n-order (molecular) trees, where* $n \geq 5$ *and* $(\alpha, \beta) \in E^\star_{BP} \cup E^\star_{DHFORM} \cup E^\star_{HFORM}$.

6. Conclusions

In this paper, we have examined the generalized Gutman–Milovanović index $\mathcal{GM}_{\alpha,\beta}$, generalized elliptic–Sombor $\mathcal{ESO}_{\alpha,\beta}$ index, generalized Zagreb–Sombor index $\mathcal{ZSO}_{\alpha,\beta}$, and general Euler–Sombor index $\mathcal{EU}_\alpha$ for their applicability in predicting 13 properties of octane isomers. We have compared the obtained results with the ones generated by not only a benchmark data set—proposed by the International Academy of Mathematical Chemistry—containing 102 descriptors of octane isomers, but also discrete Adriatic indices [25] and variable Adriatic indices [24]. We conclude from Table 1 that $\mathcal{ESO}_{\alpha,\beta}$ is a good predictor for the following properties of the octane isomers: (i) boiling point when $(\alpha, \beta) = (0.7579, -0.3005)$, (ii) enthalpy of vaporization when $(\alpha, \beta) = (-0.1168, 0.0474)$,

(iii) enthalpy of formation when $(\alpha, \beta) = (2.6641, -1.0832)$, and (iv) standard enthalpy of formation when $(\alpha, \beta) = (3.0000, -1.1447)$. Also, we conclude from Table 1 that $\mathcal{ZSO}_{\alpha,\beta}$ is a good predictor for the following properties of the octane isomers: (i) heat capacity at constant P when $(\alpha, \beta) = (-1.4403, 0.5529)$, (ii) standard enthalpy of vaporization when $(\alpha, \beta) = (2.4023, -2.1281)$, (iii) total surface area when $(\alpha, \beta) = (-1.1701, 0.4477)$, and (iv) acentric factor when $(\alpha, \beta) = (0.5751, 0.0313)$. Finally, Table 1 suggests that $\mathcal{GM}_{\alpha,\beta}$ with $(\alpha, \beta) = (0.5411, 0.0414)$ is a good predictor for the acentric factor of the aforementioned isomers. We have also reported some basic mathematical aspects of the indices $\mathcal{GM}_{\alpha,\beta}$, $\mathcal{ESO}_{\alpha,\beta}$ index, and $\mathcal{ZSO}_{\alpha,\beta}$, covering the aforementioned particular ordered pairs (α,β). Based on the obtained findings and keeping in mind the last paragraph of Section 2, we propose to further (i) examine the indices $\mathcal{GM}_{\alpha,\beta}$, $\mathcal{ESO}_{\alpha,\beta}$, $\mathcal{ZSO}_{\alpha,\beta}$, and $\mathcal{EU}_{\alpha}$ for their chemical applicability on other datasets, and (ii) establish mathematical properties of the indices $\mathcal{GM}_{\alpha,\beta}$, $\mathcal{ESO}_{\alpha,\beta}$, and $\mathcal{ZSO}_{\alpha,\beta}$, covering the above-mentioned aforementioned particular ordered pairs (α,β).

Author contributions

Investigation: AMA, AEH; Methodology: AA, IG, BF; Writing – original draft: AA, IG, BF, AMA, AEH; Validation: AMA, AEH; Writing – review & editing: AA, IG, BF; Funding Acquisition: AA, AMA, AEH. All authors have read and approved the final version of the manuscript for publication.

Use of Generative-AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The authors have no conflicts of interest to declare.

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