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Research article

On h-integral Sombor indices

Jorge Batanero[1], **Edil D. Molina**[2] **and José M. Rodríguez**[1,*]

[1] Universidad Carlos III de Madrid, Departamento de Matemáticas, Avenida de la Universidad, 30 (edificio Sabatini), 28911 Leganés (Madrid), Spain; ROR: https://ror.org/03ths8210

[2] Facultad de Matemáticas, Universidad Autónoma de Guerrero, Carlos E. Adame No.54 Col. Garita, 39650 Acalpulco Gro., Mexico

* **Correspondence:** Email: jomaro@math.uc3m.es.

Abstract: In 2021, Ivan Gutman introduced the Sombor index, a new vertex-degree-based topological index with significant geometric meaning. This index has shown remarkable growth in research activity in recent years. Following this geometric approach, in this paper we propose several generalizations of the Sombor integral indices. In addition, we study their properties and applications in modeling the enthalpy of vaporization of octane isomers.

Keywords: Sombor indices; integral Sombor indices; generalized Sombor indices; topological indices; vertex-degree-based topological indices
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1. Introduction

Topological indices have emerged as essential tools in the analysis of complex structures across various scientific disciplines, particularly in mathematical chemistry, bioinformatics, and network theory. These indices are numerical values that capture the intrinsic properties of a structure, regardless of its specific representation or the coordinates used. This characteristic makes them powerful tools for the characterization and classification of complex systems in multiple disciplines.

In chemistry, for example, topological indices have been fundamental for the prediction of physicochemical and biological properties of molecules, facilitating the rational design of new compounds. By providing a numerical representation of molecular structure, these indices allow researchers to correlate structural features with biological activities, physical properties, and chemical reactivity, see [1–3]. For more information on other important applications of topological indices to specific problems in physics, computer science, and environmental science, see [4–6].

Vertex-degree-based topological indices are an essential category within topological indices and have received considerable attention due to their simplicity and effectiveness in a wide range of applications (see [7] for the geometric-arithmetic index, [8] for the sum-connectivity index, [9] for the arithmetic-geometric index, [10–12] for variable indices, [13, 14] for extremal problems, [15] for spectral properties, and [16] for applications). Among these indices, the recently introduced Sombor index has proven to be a valuable tool in the characterization of molecular structure and the prediction of physicochemical properties. This index is defined in [17] for a graph G as

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

where d_u denotes the degree of the vertex u.

There is a lot of work regarding this index, studying generalizations [18, 19], inequalities [20–22], optimization problems [23–25], and random graphs [26, 27].

In [19], the geometric approach of the SO index is emphasized. Additionally, in the same paper two new indices are defined, called Sombor integral indices, also with a geometric approach. Following this line of research, the present article proposes generalizations of the Sombor integral indices, examines their mathematical properties, and explores their application in modeling the enthalpy of vaporization (ΔH°_{vap}) property of octane isomers.

2. Definitions

Throughout this work, $G = (V(G), E(G))$ denotes a finite simple graph without isolated vertices. The degree d_u of a vertex $u \in V(G)$ is the number of vertices adjacent to u. If there is an edge from vertex u to vertex v, we indicate this by uv (or vu).

Recall that a function $f : [a, b] \to \mathbb{R}$ is *absolutely continuous* if for every $\varepsilon > 0$, there is $\delta > 0$ such that whenever a finite sequence of pairwise disjoint intervals $(a_1, b_1), \dots, (a_N, b_N) \subset [a, b]$ satisfies

$$\sum_{n=1}^{N}(b_n - a_n) < \delta,$$

then

$$\sum_{n=1}^{N} |f(b_n) - f(a_n)| < \varepsilon.$$

If $I \subseteq \mathbb{R}$ is any interval, a function $f : I \to \mathbb{R}$ is *absolutely continuous* if it is absolutely continuous on each compact interval contained in I. It is well-known that $f : I \to \mathbb{R}$ is absolutely continuous if and only if there exists $f'(x)$ for a.e.$x \in I$ and $f(b) - f(a) = \int_a^b f'(x)\,dx$ for every $a, b \in I$.

The next definitions play a fundamental role in this work.

Given a function $h : [1, \infty) \to (0, \infty)$ which is bounded on each compact interval, we say that a set of functions $\mathcal{F} = \{f_\alpha\} = \{f_\alpha\}_{\alpha\in A}$ (where A is the set to which the parameter α belongs, usually $A = \mathbb{R}^+$) is *h-admissible* if each $f_\alpha : [0, \infty) \to [0, \infty)$ is an absolutely continuous function satisfying the following property: For each positive integers a, b with $a \geq b$ there exists a unique α such that $f_\alpha(h(a)) = h(b)$. Given positive integers a, b with $a \geq b$ and α such that $f_\alpha(h(a)) = h(b)$, define,

$$F_{\mathcal{F},h,1}(a,b) = F_{\mathcal{F},h,1}(b,a) = \int_0^{h(a)} \sqrt{1 + f'_\alpha(x)^2}\, dx,$$
$$F_{\mathcal{F},h,2}(a,b) = F_{\mathcal{F},h,2}(b,a) = \int_0^{h(a)} f_\alpha(x)\, dx.$$

Remark 1. *Note that $F_{\mathcal{F},h,1}(a,b)$ is the length of the graph of f_α for $0 \le x \le h(a)$, and, since $f_\alpha \ge 0$, $F_{\mathcal{F},h,2}(a,b)$ is the area under the graph of f_α for $0 \le x \le h(a)$. This shows the geometric meaning of these quantities.*

Also, define the *first and second h-integral Sombor indices* of a graph G as

$$ISO_{\mathcal{F},h,1}(G) = \sum_{uv\in E(G)} F_{\mathcal{F},h,1}(d_u, d_v),$$
$$ISO_{\mathcal{F},h,2}(G) = \sum_{uv\in E(G)} F_{\mathcal{F},h,2}(d_u, d_v).$$

Remark 2. *If we consider $h(x) = x$ and the h-admissible set of functions $\mathcal{F}_1 = \{f_\alpha(x) = \alpha x : \alpha > 0\}$, then*

$$ISO_{\mathcal{F}_1,h,1}(G) = SO(G)$$

for every graph G (see Proposition 4.2).

Note that for $h(x) = x$ we have $ISO_{\mathcal{F},h,1} = ISO_{\mathcal{F},1}$ and $ISO_{\mathcal{F},h,2} = ISO_{\mathcal{F},2}$, so these new indices generalize the integral Sombor indices $ISO_{\mathcal{F},1}$ and $ISO_{\mathcal{F},2}$ defined in [19].

For any graph G, we define

$$h\text{-}M_1(G) = \sum_{uv\in E(G)} (h(d_u) + h(d_v)) = \sum_{u\in V(G)} d_u h(d_u)\,,$$

$$h\text{-}M_2(G) = \sum_{uv\in E(G)} h(d_u)h(d_v)\,,$$

and

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

Note that if $h(x) = x$, the first and second Zagreb indices and the Sombor index are obtained, respectively. In this context, the following inequality chain naturally arises:

$$\sqrt{2\, h\text{-}M_2(G)} \le h\text{-}SO(G) \le h\text{-}M_1(G).$$

Next, we include a list summarizing the meanings of all symbols:
$\mathcal{F} = \{f_\alpha\}$: family of functions.
$\mathcal{F}_s = \{f_\alpha(x) = \alpha x^s \ : \ \alpha > 0\}$ for fixed $s > 0$.
$\mathcal{G}_s = \{g_\alpha(x) = \alpha e^{sx} \ : \ \alpha > 0\}$ for fixed $s \neq 0$.
$F_{\mathcal{F},h,1}(a,b) = \int_0^{h(a)} \sqrt{1 + f'_\alpha(x)^2}\, dx$.
$F_{\mathcal{F},h,2}(a,b) = \int_0^{h(a)} f_\alpha(x)\, dx$.
$ISO_{\mathcal{F},h,1}(G) = \sum_{uv\in E(G)} F_{\mathcal{F},h,1}(d_u, d_v)$: first h-integral Sombor index.

$ISO_{\mathcal{F},h,2}(G) = \sum_{uv\in E(G)} F_{\mathcal{F},h,2}(d_u, d_v)$: second h-integral Sombor index.
h-$M_1(G) = \sum_{uv\in E(G)}(h(d_u) + h(d_v))$.
h-$M_2(G) = \sum_{uv\in E(G)} h(d_u)h(d_v)$.
h-$SO(G) = \sum_{uv\in E(G)}\sqrt{h(d_u)^2 + h(d_v)^2}$.

Next, we compute the values of the h-integral Sombor indices for some particular types of graphs. We say that a graph G with maximum degree Δ and minimum degree δ is *biregular* if $\{d_u, d_v\} = \{\Delta, \delta\}$ for every $uv \in E(G)$ (in particular, every regular graph is biregular).

Proposition 2.1. *Let G be a biregular graph with m edges, minimum degree δ, and maximum degree Δ. Define the family of functions $\mathcal{F}_s = \{f_\alpha(x) = \alpha x^s : \alpha > 0\}$ for each fixed $s > 0$. Then, $\mathcal{F}_s$ is h-admissible for each $s > 0$, and*

$$ISO_{\mathcal{F}_s,h,2}(G) = \frac{m}{s+1}\, h(\Delta)h(\delta),$$
$$ISO_{\mathcal{F}_s,h,1}(G) = m\int_0^1 \sqrt{h(\Delta)^2 + h(\delta)^2 s^2 x^{2s-2}}\, dx.$$

In particular, if $s = 3/2$, then

$$ISO_{\mathcal{F}_{3/2},h,1}(G) = \frac{m}{27}\, h(\delta)^{-2}\left(4h(\Delta)^2 + 9h(\delta)^2\right)^{3/2}.$$

Proof. We have that $f_\alpha(x) : [0,\infty) \to [0,\infty)$ is a C^∞ function on $(0,\infty)$ for each $\alpha > 0$ and $s > 0$.

Let $a, b \in \mathbb{Z}^+$ such that $a \geq b$. If we take $\alpha = h(a)^{-s}h(b) > 0$, then $f_\alpha(h(a)) = h(a)^{-s}h(b)h(a)^s = h(b)$. Therefore, $\mathcal{F}_s$ is h-admissible and $f_{\alpha_0}(h(\Delta)) = h(\delta)$, with $\alpha_0 = h(\Delta)^{-s}h(\delta)$.

Since $\{d_u, d_v\} = \{\Delta, \delta\}$ for every $uv \in E(G)$, we obtain

$$\begin{aligned} F_{\mathcal{F}_s,h,2}(d_u, d_v) = F_{\mathcal{F}_s,h,2}(\Delta, \delta) &= \int_0^{h(\Delta)} f_{\alpha_0}(x)\, dx = \int_0^{h(\Delta)} h(\Delta)^{-s}h(\delta)x^s\, dx \\ &= h(\Delta)^{-s}h(\delta)\, \frac{x^{s+1}}{s+1}\Bigg|_0^{h(\Delta)} = \frac{1}{s+1}\, h(\Delta)h(\delta), \end{aligned}$$

and

$$F_{\mathcal{F}_s,h,1}(d_u, d_v) = F_{\mathcal{F}_s,h,1}(\Delta, \delta) = \int_0^{h(\Delta)} \sqrt{1 + f'_{\alpha_0}(x)^2}\, dx = \int_0^{h(\Delta)} \sqrt{1 + h(\Delta)^{-2s}h(\delta)^2 s^2 x^{2s-2}}\, dx.$$

With the change of variable $t = x/h(\Delta)$, we obtain

$$F_{\mathcal{F}_s,h,1}(d_u, d_v) = \int_0^1 \sqrt{1 + h(\Delta)^{-2}h(\delta)^2 s^2 t^{2s-2}}\, h(\Delta)\, dt = \int_0^1 \sqrt{h(\Delta)^2 + h(\delta)^2 s^2 t^{2s-2}}\, dt.$$

In particular, if $s = 3/2$, then

$$\begin{aligned}
F_{\mathcal{F}_{3/2},h,1}(d_u, d_v) &= \int_0^1 \sqrt{h(\Delta)^2 + h(\delta)^2 s^2 x^{2s-2}}\, dx = \int_0^1 \left(h(\Delta)^2 + h(\delta)^2 \frac{9}{4}\, x \right)^{1/2} dx \\
&= \frac{2}{3}\, h(\delta)^{-2}\, \frac{4}{9} \left(h(\Delta)^2 + h(\delta)^2 \frac{9}{4}\, x \right)^{3/2} \Bigg|_0^1 \\
&= \frac{8}{27}\, h(\delta)^{-2} \left(h(\Delta)^2 + h(\delta)^2 \frac{9}{4} \right)^{3/2} \\
&= \frac{1}{27}\, h(\delta)^{-2} \left(4h(\Delta)^2 + 9h(\delta)^2 \right)^{3/2}.
\end{aligned}$$

Therefore, the desired equalities hold. □

Proposition 2.1 has the following consequences.

Corollary 2.2. *Let G be a δ-regular graph with m edges. If $\mathcal{F}_s = \{f_\alpha(x) = \alpha x^s \,:\, \alpha > 0\}$ with fixed $s > 0$, then*

$$\begin{aligned}
ISO_{\mathcal{F}_s,h,2}(G) &= \frac{m}{s+1}\, h(\delta)^2, \\
ISO_{\mathcal{F}_s,h,1}(G) &= m\, h(\delta) \int_0^1 \sqrt{1 + s^2 x^{2s-2}}\, dx.
\end{aligned}$$

In particular, if $s = 3/2$, then

$$ISO_{\mathcal{F}_{3/2},h,1}(G) = \frac{13\sqrt{13}}{27}\, h(\delta)\, m.$$

Corollary 2.3. *Let $\mathcal{F}_s = \{f_\alpha(x) = \alpha x^s \,:\, \alpha > 0\}$ with fixed $s > 0$.*

- *If K_n is the complete graph with n vertices ($n \ge 2$), then*

$$\begin{aligned}
ISO_{\mathcal{F}_s,h,2}(K_n) &= \frac{n(n-1)}{2s+2}\, h(n-1)^2, \\
ISO_{\mathcal{F}_{3/2},h,1}(K_n) &= \frac{13\sqrt{13}}{54}\, n(n-1)\, h(n-1).
\end{aligned}$$

- *If C_n is the cycle graph with n vertices ($n \ge 3$), then*

$$\begin{aligned}
ISO_{\mathcal{F}_s,h,2}(C_n) &= \frac{n}{s+1}\, h(2)^2, \\
ISO_{\mathcal{F}_{3/2},h,1}(C_n) &= \frac{13\sqrt{13}}{27}\, n\, h(2).
\end{aligned}$$

- *If K_{n_1,n_2} is the complete bipartite graph with $n_1 + n_2$ vertices ($n_1 \ge n_2 \ge 1$), then*

$$\begin{aligned}
ISO_{\mathcal{F}_s,h,2}(K_{n_1,n_2}) &= \frac{n_1 n_2}{s+1}\, h(n_1) h(n_2), \\
ISO_{\mathcal{F}_{3/2},h,1}(K_{n_1,n_2}) &= \frac{n_1 n_2}{27}\, h(n_2)^{-2} \left(4h(n_1)^2 + 9h(n_2)^2 \right)^{3/2}.
\end{aligned}$$

- *If S_n is the star graph with n vertices* ($n \geq 3$)*, then*

$$ISO_{\mathcal{F}_s,h,2}(S_n) = \frac{n-1}{s+1}\, h(n-1)h(1),$$
$$ISO_{\mathcal{F}_{3/2},h,1}(S_n) = \frac{n-1}{27}\, h(1)^{-2}\left(4h(n-1)^2 + 9h(1)^2\right)^{3/2}.$$

- *If W_n is the wheel graph with n vertices* ($n \geq 4$)*, then*

$$ISO_{\mathcal{F}_s,h,2}(W_n) = \frac{2n-2}{s+1}\, h(n-1)h(3),$$
$$ISO_{\mathcal{F}_{3/2},h,1}(W_n) = \frac{2n-2}{27}\, h(3)^{-2}\left(4h(n-1)^2 + 9h(3)^2\right)^{3/2}.$$

3. Background on integral inequalities

We collect in this section some integral inequalities that will be useful throughout the paper.

The following Hardy-Muckenhoupt inequality [28] will be used to establish a relationship between the first and second h-integral Sombor indices (see Theorem 4.4). As usual, we denote by $\|f\|_{L^p([a,b],\mu)}$ the L^p-norm ($1 \leq p < \infty$) of the function f with respect to the measure μ on $[a, b]$:

$$\|f\|_{L^p(X,\mu)} = \left(\int_a^b |f|^p \, d\mu\right)^{1/p}.$$

Also, denote by $d\mu_1/dx$ the Radon-Nikodym derivative of the measure μ with respect to the Lebesgue measure.

Lemma 3.1. *Let us consider* $1 \leq p \leq q < \infty$ *and measures* μ_0, μ_1 *on* $[a, b]$ *with* $\mu_0(\{b\}) = 0$*. Then, there exists a positive constant C such that*

$$\left\|\int_a^x u(t)\, dt\right\|_{L^q([a,b],\mu_0)} \leq C\, \|u\|_{L^p([a,b],\mu_1)}$$

for any measurable function u on $[a, b]$*, if and only if*

$$B := \sup_{a<x<b} \mu_0([x, b))^{1/q} \left\| (d\mu_1/dx)^{-1} \right\|^{1/p}_{L^{1/(p-1)}([a,x],\mu_1)} < \infty, \tag{3.1}$$

where we use the convention $0 \cdot \infty = 0$*. Moreover, we can choose*

$$C = \begin{cases} B\left(\dfrac{q}{q-1}\right)^{(p-1)/p} q^{1/q}, & \text{if } p > 1, \\ B, & \text{if } p = 1. \end{cases} \tag{3.2}$$

Remark 3. *Note that the Hardy-Muckenhoupt inequality is very useful since it allows us to bound the norm of the derivative of a function with respect to a measure in terms of the norm of the function with respect to a (possibly different) measure.*

The following results for the integral of convex functions will be useful in order to obtain bounds of the first and second h-integral Sombor indices (see Theorem 4.7). First, the Hermite-Hadamard inequality, which was first presented by Jacques Hadamard in 1893, and then Bullen's inequality, proved in [29] (see also [30]).

Lemma 3.2. *If f is a convex function on $[a,b]$, then*

$$f\left(\frac{a+b}{2}\right) \le \frac{1}{b-a}\int_a^b f(x)\,dx \le \frac{f(a)+f(b)}{2}.$$

Lemma 3.3. *If f is a convex function on $[a,b]$, then*

$$\frac{2}{b-a}\int_a^b f(x)\,dx \le \frac{f(a)+f(b)}{2} + f\left(\frac{a+b}{2}\right).$$

Finally, we will need the following integral inequality (see Lemma 4.10).

Lemma 3.4. *Let $g : [0,a] \to \mathbb{R}$ be an absolutely continuous function such that $g(0) = 0$. Then,*

$$\left|\int_0^a g(x)\,dx\right| \le \frac{a^2}{2}\,\|g'\|_{L^\infty[0,a]}\,.$$

Proof. We have

$$\int_0^a g(x)\,dx = ag(a) - \int_0^a xg'(x)\,dx = a\int_0^a g'(x)\,dx - \int_0^a xg'(x)\,dx = \int_0^a (a-x)g'(x)\,dx$$

and so,

$$\begin{aligned}\left|\int_0^a g(x)\,dx\right| &= \left|\int_0^a (a-x)g'(x)\,dx\right| \le \int_0^a (a-x)|g'(x)|\,dx \\ &\le \|g'\|_{L^\infty[0,a]}\int_0^a (a-x)\,dx = \frac{a^2}{2}\,\|g'\|_{L^\infty[0,a]}\,.\end{aligned}$$

□

4. Main properties of h-integral Sombor indices

In this section we include some inequalities for h-integral Sombor indices which are standard consequences of convexity or known integral bounds. The novelty of these inequalities lies in their careful application to h-integral Sombor indices.

Let us start with a lower bound for the first h-integral Sombor index.

We say that a graph G is $(\mathcal{F}, h, 1)$-*minimal* if for each $uv \in E(G)$ the function f_α such that $f_\alpha(h(\max\{d_u, d_v\})) = h(\min\{d_u, d_v\})$ is an affine function on the interval $[0, h(\max\{d_u, d_v\})]$.

Recall that a graph G with maximum degree Δ and minimum degree δ is *biregular* if $\{d_u, d_v\} = \{\Delta, \delta\}$ for every $uv \in E(G)$ (in particular, every regular graph is biregular). Then, a biregular graph is $(\mathcal{F}, h, 1)$-minimal if and only if the function f_{α_0} such that $f_{\alpha_0}(h(\Delta)) = h(\delta)$ is an affine function on the interval $[0, h(\Delta)]$.

Theorem 4.1. *If $\mathcal{F} = \{f_\alpha\}$ is an h-admissible set of functions such that $f_\alpha(0) = 0$ for each α, then*

$$ISO_{\mathcal{F},h,1}(G) \geq h\text{-}SO(G)$$

for every graph G. The equality holds in this inequality if and only if G is a $(\mathcal{F}, h, 1)$-minimal graph.

Proof. Since $f_\alpha(0) = 0$ for every α, $F_{\mathcal{F},h,1}(a, b)$ is the length of the curve $\gamma(t) = (t, f_\alpha(t))$ joining the points $(0, 0)$ and $(h(a), h(b))$, which is at least the Euclidean distance between these two points:

$$\sqrt{h(a)^2 + h(b)^2} = \text{dist}((0, 0), (h(a), h(b))) \leq F_{\mathcal{F},h,1}(a, b).$$

Hence, for every graph G and $uv \in E(G)$,

$$\begin{aligned} F_{\mathcal{F},h,1}(d_u, d_v) &\geq \sqrt{h(d_u)^2 + h(d_v)^2}\,, \\ ISO_{\mathcal{F},h,1}(G) &\geq \sum_{uv\in E(G)} \sqrt{h(d_u)^2 + h(d_v)^2}\,. \end{aligned}$$

The previous argument implies that the equality holds in this inequality if and only if for each $uv \in E(G)$ the function f_α such that $f_\alpha(h(\max\{d_u, d_v\})) = h(\min\{d_u, d_v\})$ is an affine function on the interval $[0, h(\max\{d_u, d_v\})]$, i.e., if and only if G is a $(\mathcal{F}, h, 1)$-minimal graph. □

Remark 4. *Let us fix an h-admissible set of functions $\mathcal{F} = \{f_\alpha\}$ such that $f_\alpha(0) = 0$ for each α and positive integer numbers $\delta \leq \Delta$. Assume that the function f_{α_0} such that $f_{\alpha_0}(h(\Delta)) = h(\delta)$ is an affine function on the interval $[0, h(\Delta)]$. As we have seen before Theorem 4.1, every biregular graph G with maximum degree Δ and minimum degree δ is $(\mathcal{F}, h, 1)$-minimal graph, and so it satisfies $ISO_{\mathcal{F},h,1}(G) = h\text{-}SO(G)$ by Theorem 4.1. Hence, under these assumptions, the complete graph K_n with n vertices ($n \geq 2$), the cycle graph C_n with n vertices ($n \geq 3$), the complete bipartite graph K_{n_1,n_2} with $n_1 + n_2$ vertices ($n_1, n_2 \geq 1$), the star graph S_n with n vertices ($n \geq 3$), the wheel graph W_n with n vertices ($n \geq 4$), the cube graph Q_n with 2^n vertices ($n \geq 1$), and the Petersen graph achieve the bound in Theorem 4.1.*

Proposition 4.2. *Let us consider the set $\mathcal{F}_1 = \{f_\alpha(x) = \alpha x : \alpha > 0\}$. Then, $\mathcal{F}_1$ is an h-admissible set of functions, and*

$$ISO_{\mathcal{F}_1,h,1}(G) = h\text{-}SO(G)$$

for every graph G. In particular, if $h(x) = x$, then

$$ISO_{\mathcal{F}_1,h,1}(G) = SO(G)$$

for every graph G.

Proof. Let $a, b \in \mathbb{Z}^+$ such that $a \geq b$. If we take $\alpha = h(b)/h(a) > 0$, then $f_\alpha(h(a)) = h(a)^{-1}h(b)h(a) = h(b)$. Therefore, $\mathcal{F}_1$ is h-admissible. Since $f_\alpha(x) = \alpha x$ is an affine function with $f_\alpha(0) = 0$ for each $\alpha > 0$, Theorem 4.2 implies that

$$ISO_{\mathcal{F}_1,h,1}(G) = h\text{-}SO(G)$$

for every graph G. Since $h\text{-}SO(G) = SO(G)$ for every graph G if $h(x) = x$, the last statement in the proposition holds. □

We also have the following upper bound for the first h-integral Sombor index.

We say that a graph G is $(\mathcal{F}, h, 1)$-*maximal* if for each $uv \in E(G)$ the function f_α such that $f_\alpha(h(\max\{d_u, d_v\})) = h(\min\{d_u, d_v\})$ is constant on the interval $[0, h(\max\{d_u, d_v\})]$.

Then, a biregular graph is $(\mathcal{F}, h, 1)$-maximal if and only if the function f_{α_0} such that $f_{\alpha_0}(h(\Delta)) = h(\delta)$ is constant on the interval $[0, h(\Delta)]$.

Theorem 4.3. *If $\mathcal{F} = \{f_\alpha\}$ is an h-admissible set of functions such that $f_\alpha(0) = 0$ and f_α is a non-decreasing function for each α, then*

$$ISO_{\mathcal{F},h,1}(G) \le h\text{-}M_1(G)$$

for every graph G. The equality holds in this inequality if and only if G is a $(\mathcal{F}, h, 1)$-maximal graph.

Proof. Since $f'_\alpha \ge 0$ for every α, we have

$$\begin{aligned} F_{\mathcal{F},h,1}(a,b) &= \int_0^{h(a)} \sqrt{1 + f'_\alpha(x)^2}\, dx \le \int_0^{h(a)} (1 + |f'_\alpha(x)|)\, dx = \int_0^{h(a)} (1 + f'_\alpha(x))\, dx \\ &= \left[x + f_\alpha(x)\right]_{x=0}^{x=h(a)} = h(a) + f_\alpha(h(a)) = h(a) + h(b). \end{aligned}$$

Therefore, for every graph G and $uv \in E(G)$,

$$\begin{aligned} F_{\mathcal{F},h,1}(d_u, d_v) &\le h(d_u) + h(d_v), \\ ISO_{\mathcal{F},h,1}(G) &\le \sum_{uv \in E(G)} (h(d_u) + h(d_v)) = h\text{-}M_1(G), \end{aligned}$$

for every graph G.

The previous argument implies that the equality holds in this inequality if and only if for each $uv \in E(G)$ the function f_α such that $f_\alpha(h(\max\{d_u, d_v\})) = h(\min\{d_u, d_v\})$ is constant on the interval $[0, h(\max\{d_u, d_v\})]$, i.e., if and only if G is an $(\mathcal{F}, h, 1)$-maximal graph. □

Remark 5. *Let us fix an h-admissible set of functions $\mathcal{F} = \{f_\alpha\}$ such that $f_\alpha(0) = 0$ and f_α is a non-decreasing function for each α and positive integers numbers $\delta \le \Delta$. Assume that the function f_{α_0} such that $f_{\alpha_0}(h(\Delta)) = h(\delta)$ is constant on the interval $[0, h(\Delta)]$. As we have seen before Theorem 4.3, every biregular graph G with maximum degree Δ and minimum degree δ is $(\mathcal{F}, h, 1)$-maximal graph, and so it satisfies $ISO_{\mathcal{F},h,1}(G) = h\text{-}M_1(G)$ by Theorem 4.3. Hence, under these assumptions, the complete graph K_n with n vertices ($n \ge 2$), the cycle graph C_n with n vertices ($n \ge 3$), the complete bipartite graph K_{n_1,n_2} with $n_1 + n_2$ vertices ($n_1, n_2 \ge 1$), the star graph S_n with n vertices ($n \ge 3$), the wheel graph W_n with n vertices ($n \ge 4$), the cube graph Q_n with 2^n vertices ($n \ge 1$), and the Petersen graph achieve the bound in Theorem 4.3.*

Our next result provides a relationship between the first and second h-integral Sombor indices.

Theorem 4.4. *Let G be a graph with maximum degree Δ and minimum degree δ. Let $\mathcal{F} = \{f_\alpha\}$ be an admissible set of functions with $f_\alpha(0) = 0$ for each α. Then,*

$$ISO_{\mathcal{F},h,2}(G) \le \sup_{x \in [\delta,\Delta]} \{h(x)\}\, ISO_{\mathcal{F},h,1}(G)\,.$$

Proof. Let $a, b \in \mathbb{Z}^+$ with $a \geq b$, and let α such that $f_\alpha(h(a)) = h(b)$.

If in Lemma 3.1 we take $p = q = 1$ and let $\mu_0 = \mu_1$ be the Lebesgue measure, then

$$C = B = \sup_{0<x<h(a)} \mu_0 ([x, h(a)))^{1/q} \left\| (d\mu_1/dx)^{-1} \right\|^{1/p}_{L^{1/(p-1)}([0,x])}$$
$$= \sup_{0<x<h(a)} (h(a) - x) \, \|1\|_{L^\infty([0,x])} = h(a) < \infty$$

and therefore, since $f_\alpha(0) = 0$ and $f_\alpha \geq 0$, Lemma 3.1 implies

$$\int_0^{h(a)} f_\alpha(x)\, dx = \int_0^{h(a)} |f_\alpha(x) - f_\alpha(0)|\, dx \leq h(a) \int_0^{h(a)} |f'_\alpha(x)|\, dx \leq h(a) \int_0^{h(a)} \sqrt{1 + f'_\alpha(x)^2}\, dx.$$

Thus, for each $uv \in E(G)$, we have

$$F_{\mathcal{F},h,2}(d_u, d_v) \leq h(\max\{d_u, d_v\})\, F_{\mathcal{F},h,1}(d_u, d_v)$$
$$\leq \sup_{x\in[\delta,\Delta]} \{h(x)\}\, F_{\mathcal{F},h,1}(d_u, d_v)\,.$$

Consequently, summing for each $uv \in E(G)$, we have

$$\sum_{uv\in E(G)} F_{\mathcal{F},h,2}(d_u, d_v) \leq \sup_{x\in[\delta,\Delta]} \{h(x)\} \sum_{uv\in E(G)} F_{\mathcal{F},h,1}(d_u, d_v),$$
$$ISO_{\mathcal{F},h,2}(G) \leq \sup_{x\in[\delta,\Delta]} \{h(x)\}\, ISO_{\mathcal{F},h,1}(G)\,.$$

□

Corollary 4.5. *Let G be a graph with maximum degree* Δ *and minimum degree* δ*. Let* $\mathcal{F} = \{f_\alpha\}$ *be an admissible set of functions with* $f_\alpha(0) = 0$ *for each* α*.*

(1) If h is a non-decreasing function on $[\delta, \Delta]$*, then*

$$ISO_{\mathcal{F},h,2}(G) \leq h(\Delta) ISO_{\mathcal{F},h,1}(G)\,.$$

(2) If h is a non-increasing function on $[\delta, \Delta]$*, then*

$$ISO_{\mathcal{F},h,2}(G) \leq h(\delta) ISO_{\mathcal{F},h,1}(G)\,.$$

Now we shall employ the Hermite-Hadamard and Bullen's inequalities to establish the following result for the functions $F_{\mathcal{F},h,1}$ and $F_{\mathcal{F},h,2}$.

Lemma 4.6. *Let* $\mathcal{F} = \{f_\alpha\}$ *be an h-admissible set of functions. Let* $a, b \in \mathbb{Z}^+$ *with* $a \geq b$*.*

(1) If $f'_\alpha(x) f'''_\alpha(x) \geq 0$ *for any* $x \in (0, \infty)$ *and any* α*, then*

$$h(a) \sqrt{1 + f'_\alpha\left(\frac{h(a)}{2}\right)^2} \leq F_{\mathcal{F},h,1}(a, b) \leq \frac{h(a)}{4} \left(\sqrt{1 + f'_\alpha(h(a))^2} + \sqrt{1 + f'_\alpha(0)^2}\right) + \frac{h(a)}{2} \sqrt{1 + f'_\alpha\left(\frac{h(a)}{2}\right)^2}\,.$$

(2) If f_α *is a convex function for each* α*, then*

$$h(a) f_\alpha\left(\frac{h(a)}{2}\right) \leq F_{\mathcal{F},h,2}(a, b) \leq \frac{h(a)}{4} (h(b) + f_\alpha(0)) + \frac{h(a)}{2} f_\alpha\left(\frac{h(a)}{2}\right).$$

Proof. Assume first that $f_\alpha'(x)f_\alpha'''(x) \geq 0$ for any $x \in (0,\infty)$ and any α.

Let $g(x) := \sqrt{1 + f_\alpha'(x)^2}$. We have

$$\begin{aligned}
g'(x) &= f_\alpha'(x)f_\alpha''(x)\left(1 + f_\alpha'(x)^2\right)^{-1/2}, \\
g''(x) &= (f_\alpha''(x)^2 + f_\alpha'(x)f_\alpha'''(x))\left(1 + f_\alpha'(x)^2\right)^{-1/2} - f_\alpha'(x)^2 f_\alpha''(x)^2\left(1 + f_\alpha'(x)^2\right)^{-3/2} \\
&= \frac{f_\alpha''(x)^2 + f_\alpha'(x)f_\alpha'''(x) + f_\alpha'(x)^2 f_\alpha''(x)^2 + f_\alpha'(x)^3 f_\alpha'''(x) - f_\alpha'(x)^2 f_\alpha''(x)^2}{(1 + f_\alpha'(x)^2)^{3/2}} \\
&= \frac{f_\alpha''(x)^2 + f_\alpha'(x)f_\alpha'''(x) + f_\alpha'(x)^3 f_\alpha'''(x)}{(1 + f_\alpha'(x)^2)^{3/2}} \\
&= \frac{f_\alpha''(x)^2 + f_\alpha'(x)f_\alpha'''(x)(1 + f_\alpha'(x)^2)}{(1 + f_\alpha'(x)^2)^{3/2}} \geq 0,
\end{aligned}$$

since $f_\alpha'(x)f_\alpha'''(x) \geq 0$ for any $x \in (0,\infty)$. Hence, $g(x)$ is a convex function on $[0,h(a)]$ and, by Lemma 3.2, it follows that

$$\frac{1}{h(a)}\int_0^{h(a)} g(x)\,dx \geq g\left(\frac{h(a)}{2}\right),$$

$$F_{\mathcal{F},h,1}(a,b) = \int_0^{h(a)} \sqrt{1 + f_\alpha'(x)^2}\,dx \geq h(a)\sqrt{1 + f_\alpha'\left(\frac{h(a)}{2}\right)^2}.$$

In addition, Lemma 3.3 gives

$$\frac{2}{h(a)}\int_0^{h(a)} g(x)\,dx \leq \frac{g(h(a)) + g(0)}{2} + g\left(\frac{h(a)}{2}\right),$$

$$\int_0^{h(a)} \sqrt{1 + f_\alpha'(x)^2}\,dx \leq \frac{h(a)}{4}\left(\sqrt{1 + f_\alpha'(h(a))^2} + \sqrt{1 + f_\alpha'(0)^2}\right) + \frac{h(a)}{2}\sqrt{1 + f_\alpha'\left(\frac{h(a)}{2}\right)^2}.$$

Assume now that f_α is a convex function for each α. Then, Lemma 3.2 gives

$$F_{\mathcal{F},h,2}(a,b) = \int_0^{h(a)} f_\alpha(x)\,dx \geq h(a) f_\alpha\left(\frac{h(a)}{2}\right).$$

Also, Lemma 3.3 implies

$$\begin{aligned}
\int_0^{h(a)} f_\alpha(x)\,dx &\leq \frac{h(a)}{4}\left(f_\alpha(h(a)) + f_\alpha(0)\right) + \frac{h(a)}{2} f_\alpha\left(\frac{h(a)}{2}\right) \\
&= \frac{h(a)}{4}\left(h(b) + f_\alpha(0)\right) + \frac{h(a)}{2} f_\alpha\left(\frac{h(a)}{2}\right).
\end{aligned}$$

□

Lemma 4.6 has the following consequence for the first and second h-integral Sombor indices.

Recall that h is bounded on each compact interval. Then, $\sup_{x\in K} h(x) < \infty$ for any compact set $K \subset [1,\infty)$.

Theorem 4.7. *Let G be a graph with m edges, minimum degree δ, and maximum degree Δ. Define $\Omega = \sup_{x\in[\delta,\Delta]} h(x)$ and $\omega = \inf_{x\in[\delta,\Delta]} h(x)$, and consider the family of functions $\mathcal{F}_s = \{f_\alpha(x) = \alpha x^s \,:\, \alpha > 0\}$ for each fixed $s > 0$. Then, the following inequalities hold:*

(1) We have, for every $s \geq 2$,

$$m\omega\sqrt{1+\frac{s^2}{2^{2s-2}}} \leq ISO_{\mathcal{F}_s,h,1}(G) \leq \frac{1}{4}m\Omega\left(\sqrt{1+s^2}+1+2\sqrt{1+\frac{s^2}{2^{2s-2}}}\right).$$

(2) We have, for every $s > 0$,

$$\frac{m\omega^2}{s+1} \leq ISO_{\mathcal{F}_s,h,2}(G) = \frac{h\text{-}M_2(G)}{s+1} \leq \frac{m\Omega^2}{s+1}.$$

Proof. Recall that Proposition 2.1 implies that $\mathcal{F}_s$ is h-admissible.

If $s \geq 2$, then we have $f_\alpha'(x)f_\alpha'''(x) = \alpha^2 s^2(s-1)(s-2)x^{2s-4} > 0$ for every $x > 0$. By Lemma 4.6, we have

$$F_{\mathcal{F}_s,h,1}(a,b) \geq h(a)\sqrt{1+\left(h(a)^{-s}h(b)s\left(\frac{h(a)}{2}\right)^{s-1}\right)^2} = \sqrt{h(a)^2+\frac{s^2}{2^{2s-2}}h(b)^2},$$

and

$$\begin{aligned} F_{\mathcal{F}_s,h,1}(a,b) &\leq \frac{h(a)}{4}\left(\sqrt{1+(h(a)^{-s}h(b)sh(a)^{s-1})^2}+1\right)+\frac{1}{2}\sqrt{h(a)^2+\frac{s^2}{2^{2s-2}}h(b)^2} \\ &= \frac{1}{4}\sqrt{h(a)^2+s^2h(b)^2}+\frac{1}{4}h(a)+\frac{1}{2}\sqrt{h(a)^2+\frac{s^2}{2^{2s-2}}h(b)^2}. \end{aligned}$$

So, for any $uv \in E(G)$, we have

$$\begin{aligned} F_{\mathcal{F}_s,h,1}(d_u,d_v) &\geq \sqrt{h(\max\{d_u,d_v\})^2+\frac{s^2}{2^{2s-2}}h(\min\{d_u,d_v\})^2} \\ &\geq \sqrt{\omega^2+\frac{s^2}{2^{2s-2}}\omega^2} \\ &= \omega\sqrt{1+\frac{s^2}{2^{2s-2}}}, \end{aligned}$$

and

$$\begin{aligned} F_{\mathcal{F}_s,h,1}(d_u,d_v) &\leq \frac{1}{4}\sqrt{h(\max\{d_u,d_v\})^2+s^2h(\min\{d_u,d_v\})^2}+\frac{1}{4}h(\max\{d_u,d_v\}) \\ &\quad+\frac{1}{2}\sqrt{h(\max\{d_u,d_v\})^2+\frac{s^2}{2^{2s-2}}h(\min\{d_u,d_v\})^2} \\ &\leq \frac{1}{4}\sqrt{\Omega^2+s^2\Omega^2}+\frac{1}{4}\Omega+\frac{1}{2}\sqrt{\Omega^2+\frac{s^2}{2^{2s-2}}\Omega^2} \\ &= \frac{1}{4}\Omega\left(\sqrt{1+s^2}+1+2\sqrt{1+\frac{s^2}{2^{2s-2}}}\right). \end{aligned}$$

Therefore, summing for all $uv \in E(G)$, we get

$$m\omega\sqrt{1+\frac{s^2}{2^{2s-2}}} \le ISO_{\mathcal{F}_s,h,1}(G) \le \frac{1}{4}m\Omega\left(\sqrt{1+s^2}+1+2\sqrt{1+\frac{s^2}{2^{2s-2}}}\right).$$

If $s > 0$, then we have

$$F_{\mathcal{F}_s,h,2}(a,b) = \int_0^{h(a)} \alpha x^s\,dx = \frac{h(b)h(a)^{-s}x^{s+1}}{s+1}\Bigg|_0^{h(a)} = \frac{h(b)h(a)}{s+1}.$$

Thus, for any $uv \in E(G)$, we have

$$\frac{\omega^2}{s+1} \le F_{\mathcal{F}_s,h,2}(d_u,d_v) = \frac{h(d_u)h(d_v)}{s+1} \le \frac{\Omega^2}{s+1}.$$

So, summing for all $uv \in E(G)$, we get

$$\frac{m\omega^2}{s+1} \le ISO_{\mathcal{F}_s,h,2} = \frac{1}{s+1}\sum_{uv\in E(G)} h(d_u)h(d_v) \le \frac{m\Omega^2}{s+1}.$$

□

The next result will be useful in the proof of Theorem 4.9 below.

Lemma 4.8. *Let $\mathcal{F} = \{f_\alpha\}$ be an h-admissible set of functions such that f_α' is a non-decreasing absolutely continuous function with $f_\alpha' \ge 0$ on $[0,\infty)$ for each α, and $a,b \in \mathbb{Z}_+$ with $a \ge b$.*

(1) If f_α'' is a non-decreasing function, then

$$F_{\mathcal{F},h,1}(a,b) \le \frac{h(a)\left[f_\alpha'(h(a))\sqrt{1+f_\alpha'(h(a))^2} - f_\alpha'(0)\sqrt{1+f_\alpha'(0)^2} + \ln\left(\frac{f_\alpha'(h(a))+\sqrt{1+f_\alpha'(h(a))^2}}{f_\alpha'(0)+\sqrt{1+f_\alpha'(0)^2}}\right)\right]}{2\left(f_\alpha'(h(a)) - f_\alpha'(0)\right)}.$$

(2) If f_α'' is a non-increasing function, then

$$F_{\mathcal{F},h,1}(a,b) \ge \frac{h(a)\left[f_\alpha'(h(a))\sqrt{1+f_\alpha'(h(a))^2} - f_\alpha'(0)\sqrt{1+f_\alpha'(0)^2} + \ln\left(\frac{f_\alpha'(h(a))+\sqrt{1+f_\alpha'(h(a))^2}}{f_\alpha'(0)+\sqrt{1+f_\alpha'(0)^2}}\right)\right]}{2\left(f_\alpha'(h(a)) - f_\alpha'(0)\right)}.$$

Proof. Since there exists f_α'', we have that f_α' is continuous on $[0,h(a)]$, and so $\sqrt{1+(f_\alpha')^2}$ is bounded on $[0,h(a)]$. Since f_α' is an absolutely continuous function on $[0,\infty)$, f_α'' is integrable on $[0,h(a)]$. Then, $\sqrt{1+(f_\alpha')^2}\,f_\alpha''$ is integrable on $[0,h(a)]$ and

$$\begin{aligned}\int_0^{h(a)}\sqrt{1+f_\alpha'(x)^2}\,f_\alpha''(x)\,dx &= \int_{f_\alpha'(0)}^{f_\alpha'(h(a))}\sqrt{1+u^2}\,du = \frac{u}{2}\sqrt{1+u^2}+\frac{1}{2}\ln\left(u+\sqrt{1+u^2}\right)\Bigg|_{f_\alpha'(0)}^{f_\alpha'(h(a))} \\ &= \frac{f_\alpha'(h(a))}{2}\sqrt{1+f_\alpha'(h(a))^2} - \frac{f_\alpha'(0)}{2}\sqrt{1+f_\alpha'(0)^2} + \frac{1}{2}\ln\left(\frac{f_\alpha'(h(a))+\sqrt{1+f_\alpha'(h(a))^2}}{f_\alpha'(0)+\sqrt{1+f_\alpha'(0)^2}}\right). \end{aligned} \tag{4.1}$$

Since f_α' is non-decreasing and $f_\alpha' \geq 0$, the function $\sqrt{1 + f_\alpha'(x)^2}$ is also non-decreasing.

If f_α'' is also a non-decreasing function, Chebyshev's inequality gives

$$\frac{1}{h(a)} \int_0^{h(a)} \sqrt{1 + f_\alpha'(x)^2}\, dx \int_0^{h(a)} f_\alpha''(x)\, dx \leq \int_0^{h(a)} \sqrt{1 + f_\alpha'(x)^2}\, f_\alpha''(x)\, dx.$$

Consequently,

$$F_{\mathcal{F},h,1}(a,b) \leq \frac{h(a)\left[f_\alpha'(h(a)) \sqrt{1 + f_\alpha'(h(a))^2} - f_\alpha'(0) \sqrt{1 + f_\alpha'(0)^2} + \ln\left(\frac{f_\alpha'(h(a)) + \sqrt{1 + f_\alpha'(h(a))^2}}{f_\alpha'(0) + \sqrt{1 + f_\alpha'(0)^2}} \right) \right]}{2\left(f_\alpha'(h(a)) - f_\alpha'(0)\right)}.$$

If f_α'' is a non-increasing function, Chebyshev's inequality also gives

$$\frac{1}{h(a)} \int_0^{h(a)} \sqrt{1 + f_\alpha'(x)^2}\, dx \int_0^{h(a)} f_\alpha''(x)\, dx \geq \int_0^{h(a)} \sqrt{1 + f_\alpha'(x)^2}\, f_\alpha''(x)\, dx.$$

Consequently,

$$F_{\mathcal{F},h,1}(a,b) \geq \frac{h(a)\left[f_\alpha'(h(a)) \sqrt{1 + f_\alpha'(h(a))^2} - f_\alpha'(0) \sqrt{1 + f_\alpha'(0)^2} + \ln\left(\frac{f_\alpha'(h(a)) + \sqrt{1 + f_\alpha'(h(a))^2}}{f_\alpha'(0) + \sqrt{1 + f_\alpha'(0)^2}} \right) \right]}{2\left(f_\alpha'(h(a)) - f_\alpha'(0)\right)}.$$

□

Lemma 4.8 allows us to prove the following inequalities when we consider the set of functions $\mathcal{F}_s$ with $s \geq 1$.

Theorem 4.9. *Let G be a graph with m edges, maximum degree Δ, and minimum degree δ. Define $\Omega = \sup_{x \in [\delta,\Delta]} h(x)$ and $\omega = \inf_{x \in [\delta,\Delta]} h(x)$. Consider the h-admissible set of functions $\mathcal{F}_s = \{f_\alpha(x) = \alpha x^s \,:\, \alpha > 0\}$ with $s \geq 1$.*

(1) If $s \geq 2$, then

$$ISO_{\mathcal{F}_s,h,1}(G) \leq \frac{1}{2} m\Omega \left[\sqrt{1 + s^2} + \frac{\Omega}{s\omega} \ln\left(\frac{s\Omega}{\omega} + \sqrt{1 + \frac{s^2\Omega^2}{\omega^2}} \right) \right].$$

(2) If $1 \leq s \leq 2$, then

$$ISO_{\mathcal{F}_s,h,1}(G) \geq \frac{1}{2} m\omega \left[\sqrt{1 + s^2} + \frac{\omega}{s\Omega} \ln\left(\frac{s\omega}{\Omega} + \sqrt{1 + \frac{s^2\omega^2}{\Omega^2}} \right) \right].$$

Proof. Fix $a, b \in \mathbb{Z}^+$ with $a \geq b$. We have that $f_\alpha'(x) = s\alpha x^{s-1}$ and $f_\alpha''(x) = s(s-1)\alpha x^{s-2}$. Also, f_α' is a non-decreasing function and $f_\alpha' \geq 0$ on $[0, h(a)]$ since $s \geq 1$.

If $s \geq 2$, then f_α'' is a non-decreasing function on $[0, h(a)]$. Since $f_\alpha'(h(a)) = s\frac{h(b)}{h(a)}$, Lemma 4.8 gives

$$F_{\mathcal{F},h,1}(a,b) \leq \frac{1}{2} \sqrt{h(a)^2 + s^2 h(b)^2} + \frac{h(a)^2}{2sh(b)} \ln\left(\frac{sh(b)}{h(a)} + \sqrt{1 + \frac{s^2 h(b)^2}{h(a)^2}} \right).$$

So, for every $uv \in E(G)$, we have

$$F_{\mathcal{F},h,1}(d_u, d_v) \leq \frac{1}{2}\,\Omega\left[\sqrt{1+s^2} + \frac{\Omega}{s\omega}\ln\left(\frac{s\Omega}{\omega} + \sqrt{1+\frac{s^2\Omega^2}{\omega^2}}\right)\right].$$

If $1 \leq s \leq 2$, then f_α'' is a non-increasing function on $[0, h(a)]$. Lemma 4.8 gives

$$F_{\mathcal{F},h,1}(a,b) \geq \frac{1}{2}\sqrt{h(a)^2 + s^2h(b)^2} + \frac{h(a)^2}{2sh(b)}\ln\left(\frac{sh(b)}{h(a)} + \sqrt{1+\frac{s^2h(b)^2}{h(a)^2}}\right).$$

So, for every $uv \in E(G)$, we have

$$F_{\mathcal{F},h,1}(d_u, d_v) \geq \frac{1}{2}\omega\left[\sqrt{1+s^2} + \frac{\omega}{s\Omega}\ln\left(\frac{s\omega}{\Omega} + \sqrt{1+\frac{s^2\omega^2}{\Omega^2}}\right)\right].$$

□

We need the following results.

Lemma 4.10. *Let $\mathcal{F} = \{f_\alpha\}$ be an h-admissible set of functions such that f_α' is absolutely continuous for any α. Let $a, b \in \mathbb{Z}_+$ with $a \geq b$. Then,*

$$F_{\mathcal{F},h,1}(a,b) \leq h(a)\sqrt{1+f_\alpha'(0)^2} + \frac{1}{2}h(a)^2\left\|\frac{f_\alpha' f_\alpha''}{\sqrt{1+(f_\alpha')^2}}\right\|_{L^\infty[0,h(a)]},$$

$$F_{\mathcal{F},h,1}(a,b) \geq h(a)\sqrt{1+f_\alpha'(0)^2} - \frac{1}{2}h(a)^2\left\|\frac{f_\alpha' f_\alpha''}{\sqrt{1+(f_\alpha')^2}}\right\|_{L^\infty[0,h(a)]},$$

$$F_{\mathcal{F},h,2}(a,b) \leq h(a)f_\alpha(0) + \frac{1}{2}h(a)^2\left\|f_\alpha'\right\|_{L^\infty[0,h(a)]},$$

$$F_{\mathcal{F},h,2}(a,b) \geq h(a)f_\alpha(0) - \frac{1}{2}h(a)^2\left\|f_\alpha'\right\|_{L^\infty[0,h(a)]}.$$

Proof. Define $g(x) = \sqrt{1+f_\alpha'(x)^2} - \sqrt{1+f_\alpha'(0)^2}$. Then, $g(0) = 0$ and Lemma 3.4 give

$$\int_0^{h(a)} g(x)\,dx \leq \frac{1}{2}h(a)^2\,\|g'\|_{L^\infty[0,h(a)]},$$

$$F_{\mathcal{F},h,1}(a,b) - h(a)\sqrt{1+f_\alpha'(0)^2} \leq \frac{1}{2}h(a)^2\left\|\frac{f_\alpha' f_\alpha''}{\sqrt{1+(f_\alpha')^2}}\right\|_{L^\infty[0,h(a)]}.$$

If we replace g by $-g$, then we obtain

$$-\int_0^{h(a)} g(x)\,dx \leq \frac{1}{2}h(a)^2\,\|-g'\|_{L^\infty[0,h(a)]},$$

$$F_{\mathcal{F},h,1}(a,b) - h(a)\sqrt{1+f_\alpha'(0)^2} \geq -\frac{1}{2}h(a)^2\left\|\frac{f_\alpha' f_\alpha''}{\sqrt{1+(f_\alpha')^2}}\right\|_{L^\infty[0,h(a)]}.$$

Let us define $y(x) = f_\alpha(x) - f_\alpha(0)$. Then, $y(0) = 0$ and Lemma 3.4 imply

$$\int_0^{h(a)} y(x)\,dx \le \frac{1}{2}\,h(a)^2\,\|y'\|_{L^\infty[0,h(a)]}\,,$$
$$F_{\mathcal{F},h,2}(a,b) - h(a)f_\alpha(0) \le \frac{1}{2}\,h(a)^2\,\left\|f'_\alpha\right\|_{L^\infty[0,h(a)]}\,.$$

If we replace y with $-y$, then we obtain

$$-\int_0^{h(a)} y(x)\,dx \le \frac{1}{2}\,h(a)^2\,\|-y'\|_{L^\infty[0,h(a)]}\,,$$
$$F_{\mathcal{F},h,2}(a,b) - h(a)f_\alpha(0) \ge -\frac{1}{2}\,h(a)^2\,\left\|f'_\alpha\right\|_{L^\infty[0,h(a)]}\,.$$

□

Next, let us consider a new set of functions $\mathcal{G}_s$.

Proposition 4.11. *The family* $\mathcal{G}_s = \{g_\alpha(x) = \alpha e^{sx} \;:\; \alpha > 0\}$ *for* $s \neq 0$ *is h-admissible.*

(1) If $s > 0$*, we have*

$$\max_{x\in[0,h(a)]}\left|\frac{g'_\alpha(x)g''_\alpha(x)}{\sqrt{1+g'_a(x)^2}}\right| = \frac{s^3h(b)^2}{\sqrt{1+s^2h(b)^2}}\,.$$

(2) If $s < 0$*, we have*

$$\max_{x\in[0,h(a)]}\left|\frac{g'_\alpha(x)g''_\alpha(x)}{\sqrt{1+g'_a(x)^2}}\right| = \frac{|s|^3h(b)^2e^{-2sh(a)}}{\sqrt{1+s^2h(b)^2e^{-2sh(a)}}}\,.$$

Proof. Let $a, b \in \mathbb{Z}^+$ with $a \ge b$. If we take $\alpha = h(b)e^{-sh(a)}$, then $g_\alpha(h(a)) = h(b)e^{-sh(a)}e^{sh(a)} = h(b)$. Also, g_α is a positive C^∞ function for each α. Therefore, $\mathcal{G}_s$ is h-admissible.

Note that $g'_\alpha(x) = sg_\alpha(x)$ and $g''_\alpha(x) = s^2g_\alpha(x)$. For each fixed $s \neq 0$, let us define

$$\phi_s(x) = \frac{g'_\alpha(x)g''_\alpha(x)}{\sqrt{1+g'_a(x)^2}} = \frac{s^3g_\alpha(x)^2}{\sqrt{1+s^2g_\alpha(x)^2}}\,.$$

We have that ϕ_s is positive or negative if s is positive or negative, respectively. Also, we have

$$\frac{d}{dx}\phi_s(x) = \frac{2s^4g_\alpha(x)^2\sqrt{1+s^2g_\alpha(x)^2} - \frac{s^6g_\alpha(x)^4}{\sqrt{1+s^2g_\alpha(x)^2}}}{1+s^2g_\alpha(x)^2}$$
$$= \frac{2s^4g_\alpha(x)^2 + s^6g_\alpha(x)^4}{(1+s^2g_\alpha(x)^2)^{\frac{3}{2}}} > 0.$$

So, the function $|\phi_s|$ is decreasing or increasing if $s < 0$ or $s > 0$, respectively.

Therefore, if $s < 0$, we have

$$\max_{x\in[0,h(a)]}|\phi_s(x)| = |\phi_s(0)| = \frac{|s|^3h(b)^2e^{-2sh(a)}}{\sqrt{1+s^2h(b)^2e^{-2sh(a)}}}$$

and if $s > 0$, we have

$$\max_{x\in[0,h(a)]} |\phi_s(x)| = |\phi_s(h(a))| = \phi_s(h(a)) = \frac{s^3 h(b)^2}{\sqrt{1+s^2h(b)^2}}\,.$$

□

Lemma 4.10 and Proposition 4.11 allow us to prove the following inequalities for the h-integral Sombor indices.

Theorem 4.12. *Let G be a graph with m edges, maximum degree Δ, and minimum degree δ. Define $\Omega = \sup_{x\in[\delta,\Delta]} h(x)$ and $\omega = \inf_{x\in[\delta,\Delta]} h(x)$. Let $\mathcal{G}_s$ be the h-admissible set of functions $\mathcal{G}_s = \{\alpha e^{sx} \,:\, \alpha > 0\}$ with $s \neq 0$. The following facts hold:*

(1) If $s > 0$, then we have

$$m\left(\omega\sqrt{1+s^2\omega^2 e^{-2s\Omega}} - \frac{s^3\Omega^4}{2\sqrt{1+s^2\Omega^2}}\right) \le ISO_{\mathcal{G}_s,h,1}(G) \le m\left(\Omega\sqrt{1+s^2\Omega^2 e^{-2s\omega}} + \frac{s^3\Omega^4}{2\sqrt{1+s^2\Omega^2}}\right).$$

(2) If $s < 0$, then we have

$$m\left(\omega\sqrt{1+s^2\omega^2 e^{-2s\Omega}} - \frac{s^3\Omega^4 e^{-2s\omega}}{2\sqrt{1+s^2\Omega^2 e^{-2s\omega}}}\right) \le ISO_{\mathcal{G}_s,h,1}(G) \le m\,\frac{2\Omega + s^2\Omega^3 e^{-2s\omega}(2+s\Omega)}{2\sqrt{1+s^2\Omega^2 e^{-2s\omega}}}\,.$$

(3) We have

$$ISO_{\mathcal{G}_s,h,2}(G) = \frac{1}{s}\sum_{uv\in E(G)} h(\min\{d_u,d_v\})\left(1 - e^{-sh(\max\{d_u,d_v\})}\right)$$

and

$$\frac{m\omega}{s}(1-e^{-s\omega}) \le ISO_{\mathcal{G}_s,h,2}(G) \le \frac{m\Omega}{s}(1-e^{-s\Omega}).$$

Proof. If $s > 0$, then Lemma 4.10 and Proposition 4.11 give

$$\begin{aligned} F_{\mathcal{G}_s,h,1}(a,b) &\le h(a)\sqrt{1+g_\alpha'(0)^2} + \frac{1}{2}\,h(a)^2 \max_{x\in[0,h(a)]}\left|\frac{g_\alpha'(x)g_\alpha''(x)}{\sqrt{1+g_\alpha'(x)^2}}\right| \\ &= h(a)\sqrt{1+s^2h(b)^2e^{-2sh(a)}} + \frac{s^3h(a)^2h(b)^2}{2\sqrt{1+s^2h(b)^2}}\,, \\ F_{\mathcal{G}_s,h,1}(a,b) &\ge h(a)\sqrt{1+g_\alpha'(0)^2} - \frac{1}{2}\,h(a)^2 \max_{x\in[0,h(a)]}\left|\frac{g_\alpha'(x)g_\alpha''(x)}{\sqrt{1+g_\alpha'(x)^2}}\right| \\ &= h(a)\sqrt{1+s^2h(b)^2e^{-2sh(a)}} - \frac{s^3h(a)^2h(b)^2}{2\sqrt{1+s^2h(b)^2}}\,. \end{aligned}$$

Since the function $\frac{x^2}{\sqrt{1+s^2x^2}}$ is increasing for $x > 0$, we have, for every $uv \in E(G)$,

$$\omega\sqrt{1+s^2\omega^2e^{-2s\Omega}} - \frac{s^3\Omega^4}{2\sqrt{1+s^2\Omega^2}} \le F_{\mathcal{G}_s,h,1}(d_u,d_v) \le \Omega\sqrt{1+s^2\Omega^2e^{-2s\omega}} + \frac{s^3\Omega^4}{2\sqrt{1+s^2\Omega^2}}\,.$$

The first result follows by summing for each $uv \in E(G)$.

Now, suppose $s < 0$. Lemma 4.10 and Proposition 4.11 give

$$\begin{aligned} F_{\mathcal{G}_s,h,1}(a,b) &\le h(a)\sqrt{1+g'_\alpha(0)^2} + \frac{1}{2}h(a)^2 \max_{x\in[0,h(a)]}\left|\frac{g'_\alpha(x)g''_\alpha(x)}{\sqrt{1+g'_\alpha(x)^2}}\right| \\ &= h(a)\sqrt{1+s^2h(b)^2e^{-2sh(a)}} + \frac{s^3h(a)^2h(b)^2e^{-2sh(a)}}{2\sqrt{1+s^2h(b)^2e^{-2sh(a)}}}, \\ F_{\mathcal{G}_s,h,1}(a,b) &\ge h(a)\sqrt{1+g'_\alpha(0)^2} - \frac{1}{2}h(a)^2 \max_{x\in[0,h(a)]}\left|\frac{g'_\alpha(x)g''_\alpha(x)}{\sqrt{1+g'_\alpha(x)^2}}\right| \\ &= h(a)\sqrt{1+s^2h(b)^2e^{-2sh(a)}} - \frac{s^3h(a)^2h(b)^2e^{-2sh(a)}}{2\sqrt{1+s^2h(b)^2e^{-2sh(a)}}}. \end{aligned}$$

So, for every $uv \in E(G)$, we have

$$F_{\mathcal{G}_s,h,1}(d_u,d_v) \le \Omega\sqrt{1+s^2\Omega^2e^{-2s\omega}} + \frac{s^3\Omega^4e^{-2s\omega}}{2\sqrt{1+s^2\Omega^2e^{-2s\omega}}} = \frac{2\Omega + s^2\Omega^3e^{-2s\omega}(2+s\Omega)}{2\sqrt{1+s^2\Omega^2e^{-2s\omega}}},$$

and

$$F_{\mathcal{G}_s,h,1}(d_u,d_v) \ge \omega\sqrt{1+s^2\omega^2e^{-2s\Omega}} - \frac{s^3\Omega^4e^{-2s\omega}}{2\sqrt{1+s^2\Omega^2e^{-2s\omega}}}.$$

Then, the second result follows by summing for each $uv \in E(G)$.

Finally, we have

$$F_{\mathcal{G}_s,h,2}(a,b) = \int_0^{h(a)} \alpha e^{sx}\,dx = \frac{1}{s}\alpha e^{sx}\Big|_0^{h(a)} = \frac{1}{s}h(b) - \frac{1}{s}h(b)e^{-sh(a)}.$$

Thus, for each $uv \in E(G)$, we have

$$F_{\mathcal{G}_s,h,2}(d_u,d_v) = \frac{1}{s}h(\min\{d_u,d_v\})\left(1 - e^{-sh(\max\{d_u,d_v\})}\right)$$

and

$$\frac{\omega}{s}\left(1-e^{-s\omega}\right) \le F_{\mathcal{G}_s,h,2}(d_u,d_v) \le \frac{\Omega}{s}\left(1-e^{-s\Omega}\right).$$

Note that these inequalities also hold if $s < 0$. □

5. Modeling ΔH°_{vap} of octane isomers

This section examines the applicability of the proposed h-integral Sombor indices within the framework of Quantitative Structure–Property Relationship (QSPR) analysis. To this end, we assess the predictive performance of these indices, across four families of functions, in modeling the standard enthalpy of vaporization (ΔH°_{vap}) of octane isomers.

The dataset used in this study comprises all 18 structural isomers of octane, with their respective experimental values of standard enthalpy of vaporization (ΔH°_{vap}) sourced directly from the NIST

Chemistry WebBook. No additional preprocessing was required as the data had already been standardized and validated in previous literature. Measurement uncertainties reported by NIST are typically within ±0.024, a range considered acceptable for modeling purposes.

The specific families of functions employed in this study are listed below:

- $\mathcal{F}_p = \{\alpha x^p\}$.
- $\mathcal{G}_p = \{\alpha e^{px}\}$.
- $\mathcal{H}_p = \{\alpha(\sin(px) + 1.1)\}$.
- $\mathcal{I}_p = \{\alpha(\cos(px) + 1.1)\}$.

It can be easily shown that these families of functions are indeed h-admissible. After testing several h-admissible families, we have chosen these four families because of their good predictive properties. Note that the use of polynomials, exponential, and trigonometric functions is natural for its regular use in many mathematical problems.

Figure 1 presents color maps displaying the absolute value of the Pearson correlation coefficient ($|r|$) between the standard enthalpy of vaporization (ΔH°_{vap}) and the first (left) and second (right) h-integral Sombor indices, evaluated at the four families of h-admissible functions. For the $\mathcal{F}_p$ (panels (a) and (b)) and the $\mathcal{G}_p$ (panels (c) and (d)) families, the parameter grid spans $p, q \in (0, 10]$ with a step size of 0.1, using $h(x) = x^q$ and $h(x) = q \ln x$, respectively. For the trigonometric families $\mathcal{H}_p$ (panels (e) and (f)) and $\mathcal{I}_p$ (panels (g) and (h)), we consider $p, q \in (0, 2]$ with increments of 0.02, using the transformation $h(x) = qx$. Each subplot marks the optimal pair (p, q) that maximizes $|r|$ with a red dot. Darker regions in the color scale correspond to higher correlation values.

We constructed linear regression models of the form $\Delta H^\circ_{vap} = c_1 ISO_{\mathcal{F},h,i} + c_2$ with $i = 1, 2$. The simple linear regression method was used for this purpose, and the following models were obtained:

$$
\begin{aligned}
\Delta H^\circ_{vap} &= -0.188\, ISO_{\mathcal{F}_1, h(x)=x^{0.8}, 1} + 12.938,\\
\Delta H^\circ_{vap} &= -5.018\, ISO_{\mathcal{F}_{0.2}, h(x)=x^{0.2}, 2} + 45.752,\\
\Delta H^\circ_{vap} &= -0.762\, ISO_{\mathcal{G}_{0.5}, h(x)=0.4\ln x, 1} + 11.494,\\
\Delta H^\circ_{vap} &= 0.805\, ISO_{\mathcal{G}_{2.2}, h(x)=2.1\ln x, 2} + 7.354,\\
\Delta H^\circ_{vap} &= -0.866\, ISO_{\mathcal{H}_{0.14}, h(x)=0.12x, 1} + 11.342,\\
\Delta H^\circ_{vap} &= 0.00955\, ISO_{\mathcal{H}_{1.58}, h(x)=1.24x, 2} + 8.07,\\
\Delta H^\circ_{vap} &= -0.866\, ISO_{\mathcal{I}_{0.14}, h(x)=0.12x, 1} + 11.342,\\
\Delta H^\circ_{vap} &= 0.00437\, ISO_{\mathcal{I}_{1.26}, h(x)=1.04x, 2} + 8.27.
\end{aligned}
\tag{5.1}
$$

Figure 2 displays the fitted models compared with experimental data. Blue dots represent experimental values, red lines denote the predicted models.

Table 1 presents the highest values of $|r|$ and the corresponding optimal combinations of the parameters p and q for each family of functions considered in this study. Also, the table includes the regression and statistical parameters of the above models.

In addition to the correlation coefficient, we computed regression metrics including the root mean squared error (RMSE), mean absolute error (MAE), and coefficient of determination (R^2), summarized in Table 2.

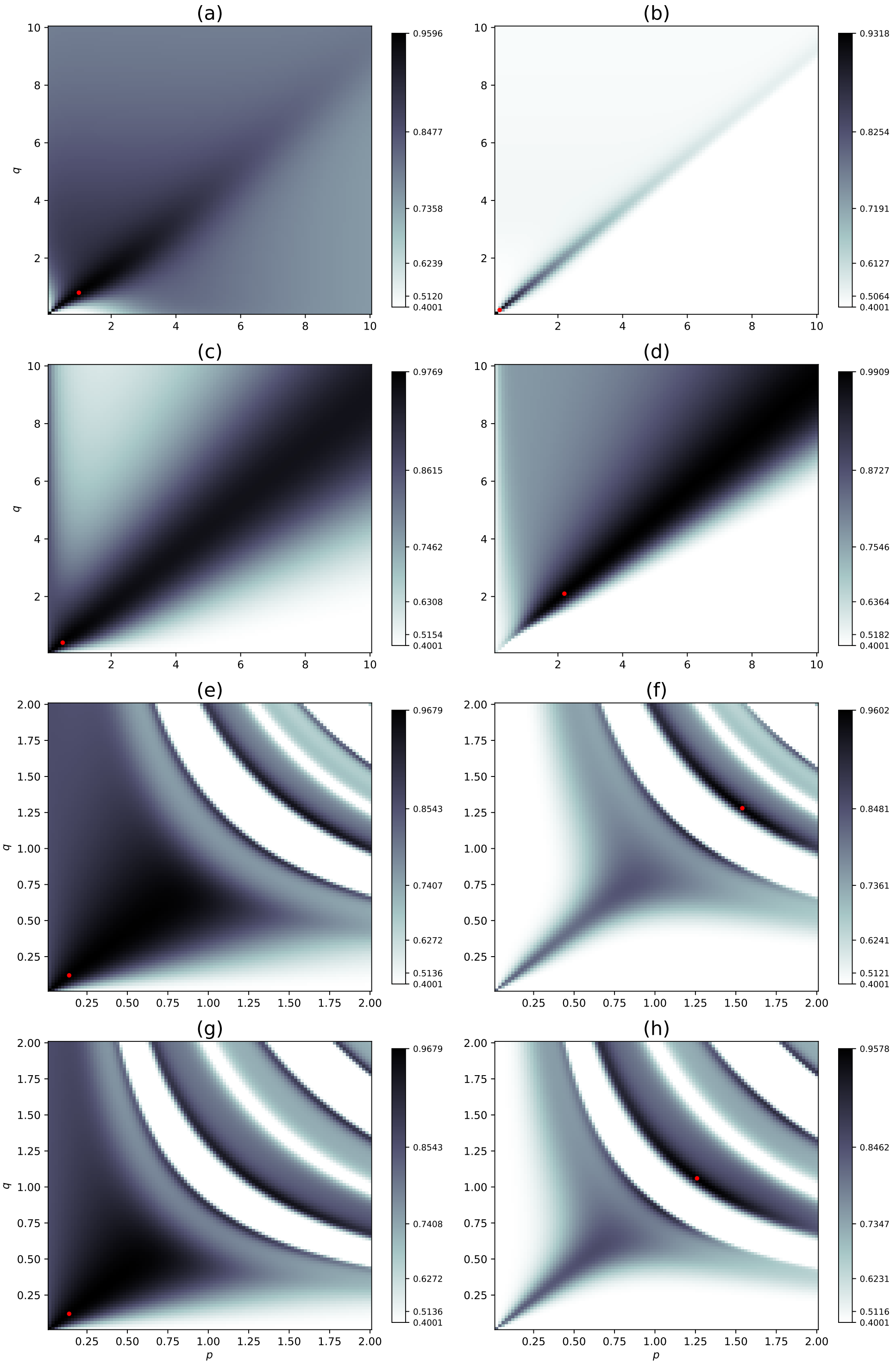

Figure 1. Absolute Pearson correlation coefficient ($|r|$) between the standard enthalpy of vaporization (ΔH°_{vap}) and the first (left column) and second (right column) h-integral Sombor indices, computed for four families of h-admissible functions. Each panel corresponds to a specific index family: (a)–(b) $\mathcal{F}_p$ with $h(x) = x^q$, (c)–(d) $\mathcal{G}_p$ with $h(x) = q \ln x$, (e)–(f) $\mathcal{H}_p$ and (g)–(h) $\mathcal{I}_p$ with $h(x) = qx$. Red dots mark the parameter pairs (p, q) yielding maximum $|r|$.

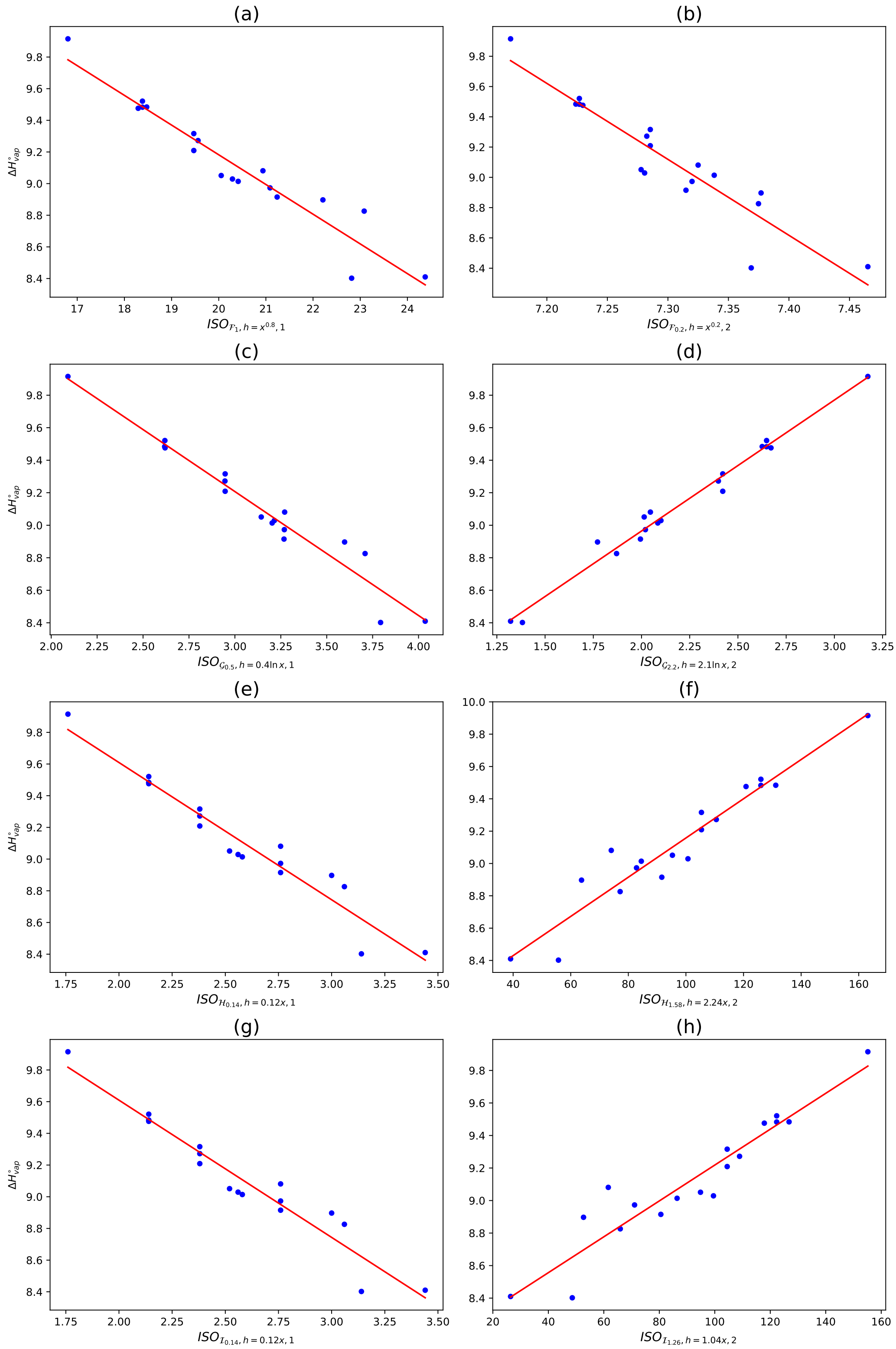

Figure 2. Linear regression of ΔH°_{vap} against the first (left) and second (right) h-integral Sombor indices for the optimal parameter combinations (p, q) maximizing $|r|$. Panels (a)–(h) correspond to the four index families as in Figure 1. Blue dots indicate experimental values, red lines show the fitted models from Eq (5.1).

Table 1. Regression parameters for the models in Eq. (5.1), including optimal values of (p, q) for each function family. r denotes the Pearson correlation coefficient, c_1 and c_2 are the slope and intercept, respectively, SE is the standard error, F is the F-statistic, and SF is the corresponding p-value.

$h(x)$	Family	Index	p	q	r	c_1	c_2	SE	F	SF
x^q	$\mathcal{F}_p$	$ISO_{\mathcal{F}_p,h,1}$	1.0	0.8	−0.96	−0.188	12.938	0.111	186.16	3.14×10^{-10}
		$ISO_{\mathcal{F}_p,h,2}$	0.2	0.2	−0.932	−5.018	45.752	0.143	105.4	1.9×10^{-8}
$q\ln(x)$	$\mathcal{G}_p$	$ISO_{\mathcal{G}_p,h,1}$	0.5	0.4	−0.977	−0.762	11.494	0.084	334.6	3.77×10^{-12}
		$ISO_{\mathcal{G}_p,h,2}$	2.2	2.1	0.991	0.805	7.354	0.053	866.6	2.31×10^{-15}
qx	$\mathcal{H}_p$	$ISO_{\mathcal{H}_p,h,1}$	0.14	0.12	−0.968	−0.866	11.342	0.099	237	5.17×10^{-11}
		$ISO_{\mathcal{H}_p,h,2}$	1.58	1.24	0.958	0.00955	8.07	0.113	179.7	4.07×10^{-10}
qx	$\mathcal{I}_p$	$ISO_{\mathcal{I}_p,h,1}$	0.14	0.12	−0.968	−0.866	11.342	0.099	237.2	5.14×10^{-11}
		$ISO_{\mathcal{I}_p,h,2}$	1.26	1.04	0.947	0.00437	8.27	0.127	137.7	2.85×10^{-9}

Table 2. Performance metrics for the linear regression models in Eq (5.1). RMSE: root mean squared error; MAE: mean absolute error; R^2: coefficient of determination.

Index	RMSE	MAE	R^2
$ISO_{\mathcal{F}_p,h,1}$	0.105	0.078	0.921
$ISO_{\mathcal{F}_p,h,2}$	0.135	0.103	0.868
$ISO_{\mathcal{G}_p,h,1}$	0.080	0.057	0.954
$ISO_{\mathcal{G}_p,h,2}$	0.050	0.037	0.982
$ISO_{\mathcal{H}_p,h,1}$	0.094	0.073	0.937
$ISO_{\mathcal{H}_p,h,2}$	0.106	0.078	0.919
$ISO_{\mathcal{I}_p,h,1}$	0.094	0.073	0.937
$ISO_{\mathcal{I}_p,h,2}$	0.123	0.093	0.892

Table 3. Leave-one-out cross validation (LOOCV) performance metrics for the models in Eq (5.1). LOOCV-RMSE: root mean squared error; LOOCV-MAE: mean absolute error; LOOCV-R^2: coefficient of determination computed on validation predictions.

Index	LOOCV-RMSE	LOOCV-MAE	LOOCV-R^2
$ISO_{\mathcal{F}_p,h,1}$	0.123	0.090	0.891
$ISO_{\mathcal{F}_p,h,2}$	0.155	0.119	0.827
$ISO_{\mathcal{G}_p,h,1}$	0.092	0.065	0.939
$ISO_{\mathcal{G}_p,h,2}$	0.056	0.042	0.978
$ISO_{\mathcal{H}_p,h,1}$	0.108	0.083	0.916
$ISO_{\mathcal{H}_p,h,2}$	0.125	0.095	0.887
$ISO_{\mathcal{I}_p,h,1}$	0.108	0.083	0.916
$ISO_{\mathcal{I}_p,h,2}$	0.139	0.105	0.860

To complement the standard regression analysis, we performed a leave-one-out cross validation (LOOCV) procedure for all models described in Eq (5.1). This validation technique provides an estimate of the predictive performance of the models when applied to unseen data, offering a more rigorous evaluation than training-set statistics alone. For each model, we computed the root mean squared error (LOOCV-RMSE), mean absolute error (LOOCV-MAE), and coefficient of determination (LOOCV-R^2) across the validation iterations. The results of this analysis are summarized in Table 3.

The results obtained in this study underscore the substantial predictive capacity of the proposed h-integral Sombor indices, whose performance is governed by the choice of parameters p and q within the corresponding families of functions. The fitted models reported in Eq (5.1) exhibit consistently strong linear associations between the indices and the standard enthalpy of vaporization (ΔH°_{vap}), as evidenced by the high absolute values of the Pearson correlation coefficient across all tested families. Moreover, the cross-validated metrics obtained through LOOCV indicate that the models retain high predictive accuracy when applied to unseen data, thereby confirming their statistical robustness and generalizability.

Among the four families explored, the exponential-based functions $\mathcal{G}_p$, in combination with the logarithmic transformation $h(x) = q \ln x$, delivered the most accurate results. Specifically, the model $ISO_{\mathcal{G}_{2.2},h(x)=2.1 \ln x,2}$ achieved $|r| = 0.991$, an RMSE of 0.05, an MAE of 0.037, and the highest coefficient of determination ($R^2 = 0.982$) in the training phase (Table 2). This model also demonstrated superior performance under LOOCV, with an RMSE of 0.056, MAE of 0.042, and $R^2 = 0.978$ (Table 3), reflecting minimal overfitting and strong predictive reliability.

The remaining function families, $\mathcal{F}_p$ (power-law), $\mathcal{H}_p$ (sine), and $\mathcal{I}_p$ (cosine), also produced statistically significant models, with slightly lower but still robust performance metrics. Notably, the first index variant for both trigonometric families achieved their maximum predictive accuracy at the same optimal parameter values ($p = 0.14, q = 0.12$) and yielded nearly identical regression outcomes. For instance, the models $ISO_{\mathcal{H}_{0.14},h(x)=0.12x,1}$ and $ISO_{\mathcal{I}_{0.14},h(x)=0.12x,1}$ both attained $|r| = 0.968$, RMSE $= 0.094$, and LOOCV-$R^2 = 0.916$, indicating that the sine and cosine transformations, despite their distinct functional forms, can encode topologically equivalent information when applied within this framework.

6. Conclusions

Ivan Gutman introduced the Sombor index in 2021, a new topological index with an important geometric meaning. This index has demonstrated remarkable growth in research activity over recent years.

In [19], the geometric approach of the SO index is emphasized, and two new indices (the Sombor integral indices) are defined. In this paper, following this geometric idea, we propose some generalizations of the Sombor integral indices: the h-integral Sombor indices.

Besides, we study the properties of these indices, proving several lower and upper bounds, and some relations between them.

Also, we show their application in modeling the enthalpy of vaporization property of octane isomers. Recall that octane isomers are widely recognized for their wide range of applications.

Finally, we would like to propose two open problems in which we are very interested: to compare the predictive capability of the h-integral Sombor indices with that of the known Kirchhoff and resistance-based indices, and to find relations between these indices and the h-integral Sombor indices. See [31–33] and the references therein for background about these indices.

Author contributions

All the authors contributed equally to this work. 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

Prof. José M. Rodríguez is the Guest Editor of special issue "Graph theory and its applications, 2nd Edition" for AIMS Mathematics. Prof. José M. Rodríguez was not involved in the editorial review and the decision to publish this article.

The authors confirm that the content of this article has no conflict of interest or competing interests.

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