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CMMSE: Applications of the inverse degree index to molecular structures

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Abstract
The inverse degree index, also called inverse index, first attracted attention through numerous conjectures generated by the computer programme Graffiti. Since then its relationship with other graph invariants has been studied by several authors. In this paper we obtain new inequalities involving the inverse degree index, and we characterize graphs which are extremal with respect to them. In particular, we obtain several inequalities relating the inverse degree index with the first and second Zagreb indices, the general first and second Zagreb indices, the Forgotten index, the general sum-connectivity index, the Sombor index and the misbalance indeg index, and several parameters of the molecular graph as the number of vertices, the number of edges, the minimum degree and the maximum degree. Also, we compute the inverse degree index for some classes of chemical graphs. Furthermore, some applications are given to the study of the physicochemical properties of three classes of compounds: polyaromatic hydrocarbons, polychlorobiphenyls, and octane isomers.

Keywords: inverse topological index, inverse degree index, vertex-degree-based topological indices, molecular structures.

MSC Classification: 05C09, 92E10
1 Introduction

A topological descriptor is a single number that represents a chemical structure in graph-theoretical terms via the molecular graph, they play a significant role in mathematical chemistry especially in the QSPR/QSAR investigations. A topological descriptor is called a topological index if it correlates with a molecular property. Topological indices are used to understand physicochemical properties of chemical compounds, since they capture some properties of a molecule in a single number. Hundreds of topological indices have been introduced and studied, starting with the seminal work by Wiener [44].

Topological indices based on end-vertex degrees of edges have been used over 40 years. Among them, several indices are recognized to be useful tools in chemical researches. Probably, the best know such descriptor is the Randić connectivity index \((R)\) [33]. There are more than thousand papers and a couple of books dealing with this molecular descriptor (see, e.g., [15, 20, 21, 38, 39] and the references therein). During many years, scientists were trying to improve the predictive power of the Randić index. This led to the introduction of a large number of new topological descriptors resembling the original Randić index. Two of the main successors of the Randić index are the first and second Zagreb indices, denoted by \(M_1\) and \(M_2\), respectively, defined as

\[
M_1(G) = \sum_{uv \in E(G)} (d_u + d_v) = \sum_{u \in V(G)} d_u^2, \quad M_2(G) = \sum_{uv \in E(G)} d_u d_v,
\]

where \(uv\) denotes the edge of the graph \(G\) connecting the vertices \(u\) and \(v\), and \(d_u\) is the degree of the vertex \(u\). These indices have attracted growing interest, see e.g. [3, 6, 11, 24] (in particular, they are included in a number of programs used for the routine computation of topological indices).

The inverse degree index \(ID(G)\) of a graph \(G\) is defined by

\[
ID(G) = \sum_{u \in V(G)} \frac{1}{d_u} = \sum_{uv \in E(G)} \left( \frac{1}{d_u} + \frac{1}{d_v} \right) = \sum_{uv \in E(G)} \frac{d_u^2 + d_v^2}{d_u^2 d_v^2}.
\]

The inverse degree index first attracted attention through numerous conjectures generated by the computer programme Graffiti [10]. Since then its relationship with other graph invariants, such as diameter, edge-connectivity, matching number, Wiener index has been studied by several authors (see, e.g., [5, 7–9, 47]).

Miličević and Nikolić defined in [30] the variable first and second Zagreb indices as

\[
^\alpha M_1(G) = \sum_{u \in V(G)} d_u^{2\alpha}, \quad ^\alpha M_2(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha,
\]

with \(\alpha \in \mathbb{R}\). In [23] and [4] the general first and second Zagreb indices are introduced as

\[
M_1^\alpha(G) = \sum_{u \in V(G)} d_u^\alpha, \quad M_2^\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha,
\]
respectively. It is clear that these indices are equivalent to the previous ones, since 
\[ \alpha M_1(G) = M_2^{\alpha}(G) \] and \[ \alpha M_2(G) = M_2^\alpha(G) \]. We prefer to use \[ M_2^\alpha(G) \] instead of \[ \alpha M_2(G) \], for \( j = 1, 2 \), since the inequalities obtained in this paper become simpler with them.

Note that \( M_0^1 \) is \( n \), \( M_2^1 \) is \( 2m \), \( M_2^{-1} \) is the first Zagreb index \( M_1 \), \( M_2^{-1} \) is the inverse index \( ID \), \( M_2^3 \) is the forgotten index \( F \), etc.; also, \( M_0^2 \) is \( m \), \( M_2^{-1}/2 \) is the usual Randić index \( R \), \( M_2^2 \) is the second Zagreb index \( M_2 \), \( M_2^{-1} \) is the modified Zagreb index, etc.

The concept of the variable molecular descriptors was proposed as a new way of characterizing heteroatoms in molecules (see \([34, 35]\)), but also to assess the structural differences (e.g., the relative role of carbon atoms of acyclic and cyclic parts in alkylcycloalkanes \([36]\)). The idea behind the variable molecular descriptors is that the variables are determined during the regression so that the standard error of estimate for a studied property is as small as possible.

In the paper of Gutman and Tosovic \([16]\), the correlation abilities of 20 vertex-degree-based topological indices occurring in the chemical literature were tested for the case of standard heats of formation and normal boiling points of octane isomers. It is remarkable to realize that the general second Zagreb index \( M_2^\alpha \) with exponent \( \alpha = -1 \) (and to a lesser extent with exponent \( \alpha = -2 \)) performs significantly better than the Randić index \( R = M_2^{-1/2} \).

The variable second Zagreb index is used in the structure-boiling point modeling of benzenoid hydrocarbons \([32]\). Various properties and relations of these indices are discussed in several papers (see, e.g., \([2, 22, 25, 40, 45, 46]\)).

In this paper we obtain new inequalities involving the inverse degree index, and we characterize graphs which are extremal with respect to them. Also, some applications are given to the study of the physicochemical properties of three classes of compounds: polyaromatic hydrocarbons, polychlorobiphenyls, and octane isomers. The physicochemical properties of these compounds studied are melting point, relative retention time, octanol-water partition coefficient, total surface area, log Henry constant, log water solubility, log water activity coefficient, relative enthalpy of formation.

Throughout this paper, \( G = (V(G), E(G)) \) denotes a (non-oriented) finite simple (without multiple edges and loops) non-trivial (each vertex belongs to some edge) graph.

2 Main inequalities

The following result is a useful and well-known inequality (see, e.g., \([29]\), Lemma 3.4) for a proof of the statement of equality).

**Lemma 1.** If \( a_j, b_j \geq 0 \) and \( Mb_j \leq a_j \leq Nb_j \) for \( 1 \leq j \leq k \) and some positive constants \( M, N \), then

\[
\left( \sum_{j=1}^k a_j^2 \right)^{1/2} \left( \sum_{j=1}^k b_j^2 \right)^{1/2} \leq \frac{1}{2} \left( \sqrt{\frac{N}{M}} + \sqrt{\frac{M}{N}} \right) \sum_{j=1}^k a_j b_j.
\]

If \( a_j > 0 \) for some \( 1 \leq j \leq k \), then the equality holds if and only if \( M = N \) and \( a_j = Mb_j \) for every \( 1 \leq j \leq k \).
Lemma 1 allows to obtain the following result relating $M_1^{-4}$, the first Zagreb and the inverse degree indices.

**Theorem 2.** If $G$ is a graph, then

$$\frac{2}{\Delta^3 + \delta^3} \sqrt{\Delta^3 \delta^3 M_1(G)} M_1^{-4}(G) \leq ID(G) \leq \sqrt{M_1(G) M_1^{-4}(G)}.$$  

The equality is attained in each inequality if and only if $G$ is regular.

**Proof.** Cauchy-Schwarz inequality gives

$$ID(G)^2 = \left( \sum_{u \in V(G)} d_u d_u^{-2} \right)^2 \leq \left( \sum_{u \in V(G)} d_u^2 \right) \left( \sum_{u \in V(G)} d_u^{-4} \right) = M_1(G) M_1^{-4}(G).$$

On the other hand, since we have

$$\delta^3 \leq \frac{d_u}{d_u^2} = d_u^3 \leq \Delta^3,$$

Lemma 1 gives

$$ID(G)^2 = \left( \sum_{u \in V(G)} d_u d_u^{-2} \right)^2 \geq \frac{\left( \sum_{u \in V(G)} d_u^2 \right) \left( \sum_{u \in V(G)} d_u^{-4} \right)}{\frac{3}{2} \left( \frac{\Delta^3}{\delta^3} + \frac{\delta^3}{\Delta^3} \right)^2} = \frac{4 \Delta^3 \delta^3 M_1(G) M_1^{-4}(G)}{(\Delta^3 + \delta^3)^2}.$$

If the graph is regular, then both bounds are the same, and they are equal to $ID(G)$.

If the equality is attained in the upper bound, then Cauchy-Schwarz inequality gives that the vectors $(d_u)_{u \in V(G)}$ and $(d_u^{-2})_{u \in V(G)}$ are parallel; thus, $d_u = d_v$ for every $u, v \in V(G)$, and $G$ is regular. If the equality is attained in the lower bound, then Lemma 1 gives that $\delta^3 = \Delta^3$, and $G$ is regular.

We need the following technical result.

**Lemma 3.** We have for any $0 < \delta \leq x, y \leq \Delta$

$$\frac{2}{\Delta} \leq \frac{x + y}{xy} \leq \frac{2}{\delta}, \quad \frac{2}{\Delta^2} \leq \frac{x^2 + y^2}{x^2 y^2} \leq \frac{2}{\delta^2}.$$  

Each upper (respectively, lower) bound is attained if and only if $x = y = \delta$ (respectively, $x = y = \Delta$).

**Proof.** The proof is direct since $(x + y)/(xy) = x^{-1} + y^{-1}$ and $(x^2 + y^2)/(x^2 y^2) = x^{-2} + y^{-2}$ are strictly decreasing functions on each variable.
In the same paper, where Zagreb indices were introduced, the *forgotten topological index* (or *F-index*) is defined as

\[ F(G) = \sum_{u \in V(G)} d_u^3 = \sum_{uv \in E(G)} (d_u^2 + d_v^2). \]

Both the forgotten topological index and the first Zagreb index were employed in the formulas for total \(\pi\)-electron energy in [17], as a measure of branching extent of the carbon-atom skeleton of the underlying molecule. However, this index never got attention except recently, when Furtula and Gutman in [12] established some basic properties of the F-index and showed that its predictive ability is almost similar to that of first Zagreb index and for the entropy and acetic factor, both of them yield correlation coefficients greater than 0.95. Besides, [12] pointed out the importance of the F-index; it can be used to obtain a high accuracy of the prediction of logarithm of the octanol-water partition coefficient.

Lemma 3 allows to obtain the following result relating \(M_2^2\), the inverse degree and the forgotten indices.

**Theorem 4.** If \(G\) is a graph with minimum degree \(\delta\) and maximum degree \(\Delta\), then

\[
\frac{F(G)^2}{2\Delta^2 M_2^2(G)} \leq ID(G) \leq \frac{(\Delta^2 + \delta^2)^2 F(G)^2}{8\Delta^2 \delta^4 M_2^2(G)}.
\]

*Proof.* Cauchy-Schwarz inequality gives

\[
F(G)^2 = \left( \sum_{uv \in E(G)} \frac{d_u^2 + d_v^2}{d_u d_v} d_u d_v \right)^2 \leq \left( \sum_{uv \in E(G)} \frac{(d_u^2 + d_v^2)^2}{d_u^2 d_v^2} \right) \sum_{uv \in E(G)} (d_u d_v)^2 \leq \sum_{uv \in E(G)} 2\Delta^2 \frac{d_u^2 + d_v^2}{d_u^2 d_v^2} \sum_{uv \in E(G)} (d_u d_v)^2 = 2\Delta^2 ID(G) M_2^2(G).
\]

On the other hand, since Lemma 3 gives

\[
\frac{2}{\Delta^2} \leq \frac{d_u^2 + d_v^2}{d_u d_v} = \frac{d_u^2 + d_v^2}{\delta^2 d_u^2 d_v^2} \leq \frac{2}{\delta^2}, \quad \text{with} \quad \sqrt{\frac{2}{\Delta^2}} = \frac{\Delta}{\delta},
\]

Lemma 1 allows to conclude

\[
F(G)^2 = \left( \sum_{uv \in E(G)} \frac{d_u^2 + d_v^2}{d_u d_v} d_u d_v \right)^2 \geq \sum_{uv \in E(G)} \frac{(d_u^2 + d_v^2)^2}{d_u^2 d_v^2} \sum_{uv \in E(G)} (d_u d_v)^2 \geq \frac{2\Delta^2 \delta^2}{(\Delta^2 + \delta^2)^2} \sum_{uv \in E(G)} (d_u d_v)^2 = \frac{8\Delta^2 \delta^4 ID(G) M_2^2(G)}{(\Delta^2 + \delta^2)^2}.
\]
If the graph is regular, then the lower and upper bound are the same, and they are equal to $ID(G)$. If the equality is attained in the lower (respectively, upper) bound, then $d_u^2 + d_v^2 = 2\Delta^2$ (respectively, $d_u^2 + d_v^2 = 2\delta^2$) for every $uv \in E(G)$; hence, $d_u = \Delta$ (respectively, $d_u = \delta$) for every $u \in V(G)$ and the graph is regular.

The sum-connectivity index was proposed in [48] and it is found that this index correlates well with the $\pi$-electronic energy of benzenoid hydrocarbons [27]. More applications of the sum-connectivity index can be found in [28]. Recently, this concept was extended to the general sum-connectivity index in [49], which is defined by

$$\chi_a(G) = \sum_{uv \in E(G)} (d_u + d_v)^a.$$  

Note that $\chi_{-1/2}$ is the sum-connectivity index, $\chi_1$ is the first Zagreb index and $\chi_{-1}$ is half the harmonic index.

The following result relates $\chi_a$ and the inverse degree index.

**Theorem 5.** Let $G$ be a graph with maximum degree $\Delta$ and minimum degree $\delta$. If $a \leq -2$, then

$$2^{1-a}\delta^{-a-2} \chi_a(G) \leq ID(G) \leq \max \{ (\Delta + \delta)^{-a}(\Delta^{-2} + \delta^{-2}), 2^{1-a}\Delta^{-a-2} \} \chi_a(G).$$

If $a < -2$, the equality in the lower bound is attained if and only if $G$ is regular.

**Proof.** For each $\delta \leq x, y \leq \Delta$, define the function

$$U(x, y) = \frac{x^2 + y^2}{(x+y)^a} = (x+y)^{-a}(x^2 + y^2).$$

A computation gives

$$\frac{\partial U}{\partial x}(x, y) = -a(x+y)^{-a-1}(x^2 + y^2) - 2(x+y)^{-a}x^{-3} = x^{-3}y^{-2}(x+y)^{-a-1}(-a(xy^2 + x^3) - 2xy^2 - 2y^3).$$

By symmetry, we can assume that $x \geq y$.

Since $a \leq -2$, we obtain

$$\frac{\partial U}{\partial x}(x, y) \geq x^{-3}y^{-2}(x+y)^{-a-1}(-a(xy^2 + x^3) - 2xy^2 - 2y^3) \geq x^{-3}y^{-2}(x+y)^{-a-1}(2x^3 - 2y^3) \geq 0.$$ 

Hence, $U(y, y) \leq U(x, y) \leq U(\Delta, y)$.

Consider the function

$$V(y) = U(y, y) = (y+y)^{-a}(y^{-2} + y^{-2}) = 2^{1-a}y^{-a-2}.$$
Since $a \leq -2$, $V$ is a non-decreasing function and

$$U(x, y) \geq U(y, y) = V(y) \geq V(\delta) = 2^{1-a}\delta^{-a-2}.$$ 

Consequently,

$$\frac{x^2 + y^2}{(x + y)^a} = U(x, y) \geq 2^{1-a}\delta^{-a-2},$$

$$\frac{x^2 + y^2}{x^2y^2} \geq 2^{1-a}\delta^{-a-2}(x + y)^a$$

$$\frac{d_u^2 + d_v^2}{d_u^2d_v^2} \geq 2^{1-a}\delta^{-a-2}(d_u + d_v)^a$$

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

$$\text{ID}(G) \geq 2^{1-a}\delta^{-a-2}\chi_a(G).$$

If $a < -2$ and $\text{ID}(G) = 2^{1-a}\delta^{-a-2}\chi_a(G)$, then the previous argument gives that $d_u = d_v = \delta$ for every $uv \in E(G)$, i.e., $G$ is a regular graph.

If $G$ is a regular graph with $m$ edges, then

$$\text{ID}(G) = 2m\delta^{-2} = 2^{1-a}\delta^{-a-2}m(2\delta)^a = 2^{1-a}\delta^{-a-2}\chi_a(G).$$

Consider now the function

$$W(y) = U(\Delta, y) = (\Delta + y)\delta^{-a}((\Delta^2 + y^2))$$

on $[\delta, \Delta]$. We have

$$W'(y) = y^{-3}\Delta^{-2}(\Delta + y)^{-a-1}(-a(y\Delta^2 + y^3) - 2y\Delta^2 - 2\Delta^3).$$

Let us consider the function

$$X(y) = -a(y\Delta^2 + y^3) - 2y\Delta^2 - 2\Delta^3$$

on $[\delta, \Delta]$. Since $a \leq -2$,

$$X'(y) = -a(\Delta^2 + 3y^2) - 2\Delta^2 \geq 2(\Delta^2 + 3y^2) - 2\Delta^2 = 6y^2 > 0.$$ 

Consequently, $X$ is an increasing function. Since

$$X(\Delta) = -2a\Delta^3 - 4\Delta^3 = -2\Delta^3(a + 2) \geq 0,$$

$X$ satisfies either: (a) $X \geq 0$ on $[\delta, \Delta]$ or (b) there exists $\alpha \in [\delta, \Delta]$ such that $X \leq 0$ on $[\delta, \alpha]$ and $X \geq 0$ on $[\alpha, \Delta]$. 

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Since $W'(y) = y^{-3}\Delta^{-2}(\Delta + y)^{\alpha - 1}X(y)$, the function $W$ also satisfies the above property and so,

$$W(y) \leq \max \{ W(\delta), W(\Delta) \} = \max \{ U(\Delta, \delta), U(\Delta, \Delta) \}$$

$$= \max \{ (\Delta + \delta)^{-a}(\Delta^{-2} + \delta^{-2}), 2^{1-a}\Delta^{-a-2} \}$$

for every $y \in [\delta, \Delta]$. Consequently,

$$\frac{x^{-2} + y^{-2}}{(x + y)^a} = U(x, y) \leq W(y) \leq \max \{ (\Delta + \delta)^{-a}(\Delta^{-2} + \delta^{-2}), 2^{1-a}\Delta^{-a-2} \},$$

$$\frac{x^2 + y^2}{x^2y^a} \leq \max \{ (\Delta + \delta)^{-a}(\Delta^{-2} + \delta^{-2}), 2^{1-a}\Delta^{-a-2} \}(x + y)^a$$

$$\frac{d_u^2 + d_v^2}{d_u^2d_v^2} \leq \max \{ (\Delta + \delta)^{-a}(\Delta^{-2} + \delta^{-2}), 2^{1-a}\Delta^{-a-2} \}(d_u + d_v)^a$$

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

$$ID(G) \leq \max \{ (\Delta + \delta)^{-a}(\Delta^{-2} + \delta^{-2}), 2^{1-a}\Delta^{-a-2} \} \chi_a(G).$$

\[\square\]

**Remark 1.** If $a > 0$, then we can obtain directly the inequalities

$$2^{1-a}\Delta^{-a-2} \chi_a(G) \leq ID(G) \leq 2^{1-a}\delta^{-a-2} \chi_a(G),$$

and the equality in each bound is attained if and only if $G$ is regular.

Let us show how to obtain the first inequality (the second one can be obtained in a similar way): if $G$ is a graph with $m$ edges, then

$$2^{1-a}\Delta^{-a-2} \chi_a(G) \leq 2^{1-a}\Delta^{-a-2}(2\Delta)^a m = 2\Delta^{-2} m \leq ID(G).$$

The following inequalities are known for $x_1, \ldots, x_n > 0$:

$$(x_1 + \cdots + x_n)^a \leq n^{a-1}(x_1^a + \cdots + x_n^a) \quad \text{if } a > 1 \text{ or } a < 0,$$

$$n^{a-1}(x_1^a + \cdots + x_n^a) \leq (x_1 + \cdots + x_n)^a \quad \text{if } 0 < a < 1,$$

and the equality in each bound is tight for some fixed $a$ if and only if $x_1 = \cdots = x_n$.

These inequalities allow to obtain the following results.

**Theorem 6.** Let $\alpha \in \mathbb{R} \setminus \{0\}$ and $G$ a graph with $n$ vertices. Then

$$ID(G) \leq n^{1-1/\alpha}M_1^{-\alpha}(G)^{1/\alpha}, \quad \text{if } \alpha > 1,$$

$$ID(G) \geq n^{1-1/\alpha}M_1^{-\alpha}(G)^{1/\alpha}, \quad \text{if } \alpha < 1,$$

and the equality in each bound is tight for some fixed $\alpha$ if and only if $G$ is regular.
Proof. Let us prove first the cases $\alpha > 1$ and $\alpha < 0$. The previous inequalities, with $x_i = 1/d_u$, give
\[
\left( \sum_{u \in V(G)} \frac{1}{d_u} \right)^\alpha \leq n^{\alpha-1} \sum_{u \in V(G)} d_u^{-\alpha},
\]
\[
ID(G)^\alpha \leq n^{\alpha-1} M_1^{-\alpha}(G).
\]
If $\alpha > 1$, we conclude
\[
ID(G) \leq n^{1-1/\alpha} M_1^{-\alpha}(G)^{1/\alpha}.
\]
If $\alpha < 0$, we have
\[
ID(G) \geq n^{1-1/\alpha} M_1^{-\alpha}(G)^{1/\alpha}.
\]
The equality in each bound is attained if and only if $1/d_u = 1/d_v$ for every $u, v \in V(G)$, i.e., $G$ is a regular graph.

The proof for $0 < \alpha < 1$ is similar.

Note that if we take $\alpha \to 1$ in Theorem 6, then the we obtain the trivial equality $M_1^{-1}(G) = ID(G)$ for every graph $G$.

The next result relates the inverse degree and the $M_2^{-1}$ indices.

**Theorem 7.** If $G$ is a graph with $n$ vertices, maximum degree $\Delta$ and minimum degree $\delta$, then
\[
\frac{2n}{\Delta} \leq ID(G) + 2M_2^{-1}(G) \leq \frac{2n}{\delta},
\]
and the equality in each bound is attained if and only if $G$ is regular.

**Proof.** Since
\[
\frac{1}{d_u^2} + \frac{1}{d_v^2} + \frac{2}{d_ud_v} = \left( \frac{1}{d_u} + \frac{1}{d_v} \right)^2,
\]
we obtain
\[
ID(G) + 2M_2^{-1}(G) = \sum_{uv \in E(G)} \left( \frac{1}{d_u^2} + \frac{1}{d_v^2} \right) + \sum_{uv \in E(G)} \frac{2}{d_ud_v} = \sum_{uv \in E(G)} \left( \frac{1}{d_u} + \frac{1}{d_v} \right)^2.
\]

Thus, the following results imply the desired inequalities
\[
\sum_{uv \in E(G)} \left( \frac{1}{d_u} + \frac{1}{d_v} \right)^2 \leq \sum_{uv \in E(G)} \left( \frac{1}{d_u} + \frac{1}{d_u} \right)^2 = \frac{2}{\delta} \sum_{u \in V(G)} 1 = \frac{2n}{\delta},
\]
\[
\sum_{uv \in E(G)} \left( \frac{1}{d_u} + \frac{1}{d_u} \right)^2 \geq \sum_{uv \in E(G)} \left( \frac{1}{d_u} + \frac{1}{d_u} \right)^2 \Delta = \frac{2}{\Delta} \sum_{u \in V(G)} 1 = \frac{2n}{\Delta}.
\]

If $G$ is a regular graph, then $\Delta = \delta$, and so, both bounds are equal and they are equal to $ID(G) + 2M_2^{-1}(G)$.

Assume now that the equality in the upper (respectively, lower) bound is attained. Then $d_u = d_v = \delta$ (respectively, $d_u = d_v = \Delta$) for every $uv \in E(G)$, and so, $G$ is a regular graph.
The known equality for \( a_i, b_i > 0 \):

\[
\sum_{i=1}^{n} a_i \cdot \sum_{i=1}^{n} b_i - \sum_{i=1}^{n} (a_i + b_i) \cdot \sum_{i=1}^{n} \frac{a_i b_i}{a_i + b_i} = \sum_{1 \leq i < j \leq n} \frac{(a_i b_j - a_j b_i)^2}{(a_i + b_i)(a_j + b_j)}
\]

gives the following result.

**Lemma 8.** The following inequality holds for every \( a_i, b_i > 0 \):

\[
\sum_{i=1}^{n} a_i \cdot \sum_{i=1}^{n} b_i \geq \sum_{i=1}^{n} (a_i + b_i) \cdot \sum_{i=1}^{n} \frac{a_i b_i}{a_i + b_i},
\]

and the equality holds if and only if \( a_i/b_i = a_j/b_j \) for every \( 1 \leq i, j \leq n \), i.e., there exists a positive constant \( k \) such that \( b_i = ka_i \) for every \( 1 \leq i \leq n \).

There exists a well-known lower bound of the inverse degree index depending on the maximum degree of the graph: \( ID(G) \geq n/\Delta \). The following inequality improves this bound for every graph which is not regular.

**Theorem 9.** If \( G \) is a graph with \( n \) vertices, \( m \) edges and maximum degree \( \Delta \), then

\[
\frac{2mn\Delta}{2m\Delta^2 - n\Delta + 2m},
\]

and the equality in this bound holds if and only if \( G \) is regular.

**Proof.** Lemma 8 gives

\[
2mID(G) = \sum_{u \in V(G)} \frac{1}{d_u} \sum_{v \in V(G)} d_u \geq \left( \sum_{u \in V(G)} \frac{1}{d_u} + \sum_{v \in V(G)} d_u \right) \sum_{v \in V(G)} \frac{1}{d_u + d_v}
\]

\[
= \left( ID(G) + 2m \right) \sum_{u \in V(G)} \frac{d_u}{1 + d_u} \geq \left( ID(G) + 2m \right) \sum_{u \in V(G)} \frac{\Delta}{1 + \Delta^2}
\]

\[
= \left( ID(G) + 2m \right) \frac{n\Delta}{1 + \Delta^2}
\]

and so,

\[
2mID(G) + 2m\Delta^2 ID(G) \geq n\Delta ID(G) + 2mn\Delta,
\]

\[
ID(G) \geq \frac{2mn\Delta}{2m\Delta^2 - n\Delta + 2m}.
\]

The equality in this bound holds if and only if

\[
\sum_{u \in V(G)} \frac{1}{d_u} \sum_{v \in V(G)} d_u = \left( \sum_{u \in V(G)} \frac{1}{d_u} + \sum_{v \in V(G)} d_u \right) \sum_{v \in V(G)} \frac{1}{d_u + d_v}
\]

and

\[
\frac{d_u}{1 + d_u^2} = \frac{\Delta}{1 + \Delta^2}
\]
for every $u \in V(G)$.

The second condition holds if and only if $d_u = \Delta$ for every $u \in V(G)$, i.e., $G$ is regular. Lemma 8 gives that the first condition holds if and only if there exists a positive constant $k$ with $1/d_u = kd_u$ for every $u \in V(G)$, i.e., $d_u = k^{-1/2}$ for every $u \in V(G)$, that is, $G$ is regular.

Hence, the equality in the bound holds if and only if $G$ is regular.

**Remark 2.** Theorem 9 improves the bound $ID(G) \geq n/\Delta$ for every graph which is not regular:

This is a consequence of

$$n\Delta \geq 2m,$$

$$2m\Delta^2 \geq 2m\Delta^2 - n\Delta + 2m,$$

$$\frac{2mn\Delta}{2m\Delta^2 - n\Delta + 2m} \geq \frac{n}{\Delta}.$$

Since $n\Delta = 2m$ if and only if the graph is regular, the lower bound in Theorem 9 is greater than $n/\Delta$ for every non-regular graph.

The Sombor index of $G$ was defined in [14] as

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

Many papers have continued the study of the Sombor index. In [37] it is shown that this index have good predictive potential.

Our next result relates $M_2^2$, the Sombor and the inverse degree indices.

**Theorem 10.** If $G$ is a graph with maximum degree $\Delta$ and minimum degree $\delta$, then

$$\frac{SO(G)^2}{M_2^2(G)} \leq ID(G) \leq \frac{(\Delta^3 + \delta^3)^2}{4\Delta^3\delta^3} \frac{SO(G)^2}{M_2^2(G)}.$$

The equality in the upper bound is attained if and only if $G$ is regular. The equality in the lower bound is attained if $G$ is regular.

**Proof.** Cauchy-Schwarz inequality gives

$$SO(G)^2 = \left( \sum_{uv \in E(G)} \frac{\sqrt{d_u^2 + d_v^2}}{d_ud_v} d_ud_v \right)^2$$

$$\leq \left( \sum_{uv \in E(G)} \frac{d_u^2 + d_v^2}{d_u^2 d_v^2} \right) \left( \sum_{uv \in E(G)} d_u^2 d_v^2 \right) = ID(G) M_2^2(G).$$

Let us prove now the upper bound. Since

$$\frac{\sqrt{x^2+y^2}}{xy} = \frac{1}{xy} \sqrt{\frac{1}{x^2} + \frac{1}{y^2}}$$
is a decreasing function on each variable, we have
\[
\frac{\sqrt{2}}{\Lambda^3} = \frac{1}{\Lambda^2} \sqrt{2} \frac{\sqrt{d_u^2 + d_v^2}}{d_u d_v} \leq \frac{1}{\delta^2} \sqrt{2} \frac{\sqrt{\delta^2 + \delta^3}}{\delta^3} = \frac{\sqrt{\delta}}{\delta^3}.
\]

Hence, Lemma 1 gives
\[
SO(G)^2 = \left( \sum_{uv \in E(G)} \frac{\sqrt{d_u^2 + d_v^2}}{d_u d_v} \right)^2 \\
\geq \frac{1}{4} \left( \frac{\sqrt{\delta^2 + \delta^3}}{\delta^3} \right)^2 \left( \sum_{uv \in E(G)} \frac{d_u^2 + d_v^2}{d_u^2 d_v^2} \right) \left( \sum_{uv \in E(G)} d_u^2 d_v^2 \right) \\
= \frac{4\Delta^3 \delta^3}{(\Delta^3 + \delta^3)^2} ID(G) M^2(G).
\]

If \( G \) is a regular graph, then \( \Delta = \delta \) and so, both bounds are equal and they are equal to \( ID(G) \).

By Lemma 1, if the equality in the upper bound is attained, then \( \frac{\sqrt{2}}{\Lambda^3} = \frac{\sqrt{2}}{\delta^3} \).

Thus, \( \Delta = \delta \) and \( G \) is regular.

We are going to prove the following general type-Gibbs’s inequality.

**Theorem 11.** Let \((X, \mu)\) be a measure space, \( f, g : X \to \mathbb{R} \) be \( \mu \)-integrable functions such that \( g > 0 \ \mu\text{-a.e.} \) and \( f/g \) takes values on \( A \subseteq \mathbb{R} \) \( \mu\text{-a.e.} \). If \( \varphi : A \to \mathbb{R} \) is a convex function, then
\[
\int_X \varphi \left( \frac{f}{g} \right) g \, d\mu \geq \varphi \left( \int_X f \, d\mu / \int_X g \, d\mu \right) \int_X g \, d\mu.
\]

**Proof.** Note that \( ||g||_{L^1(X, \mu)} = \int_X g \, d\mu > 0 \), since \( g > 0 \ \mu\text{-a.e.} \). Thus, the measure \( g \, d\mu / \int_X g \, d\mu \) is a probability measure on \( X \) and, since \( f/g \) is an integrable function with respect to this probability measure \( g \, d\mu / (\int_X g \, d\mu) \), Jensen’s inequality gives
\[
\int_X \varphi \left( \frac{f}{g} \right) \frac{g \, d\mu}{\int_X g \, d\mu} \geq \varphi \left( \int_X \frac{f \, d\mu}{\int_X g \, d\mu} \right) = \varphi \left( \int_X \frac{f \, d\mu}{\int_X g \, d\mu} \right),
\]
and we obtain the desired result by multiplying by \( \int_X g \, d\mu > 0 \).

Theorem 11 has the following discrete consequence if \( \mu \) is the counting measure.

**Corollary 12.** Let us consider a convex function \( \varphi : A \to \mathbb{R} \), \( x_1, x_2, \ldots, x_n \in \mathbb{R} \) and positive weights \( a_1, a_2, \ldots, a_n \) with \( x_1/a_1, \ldots, x_n/a_n \in A \). Then
\[
\sum_{k=1}^n \varphi \left( \frac{x_k}{a_k} \right) a_k \geq \varphi \left( \frac{\sum_{k=1}^n x_k}{\sum_{k=1}^n a_k} \right) \sum_{k=1}^n a_k.
\]
Note that if we choose the convex function \( \varphi(t) = -\log t \) on \( \mathbb{R}^+ \), Corollary 12 gives the classical Gibbs’s inequality.

**Corollary 13.** For positive numbers \( x_1, x_2, \ldots, x_n \) and \( a_1, a_2, \ldots, a_n \), we have

\[
\sum_{k=1}^{n} a_k \log \left( \frac{a_k}{x_k} \right) \geq \log \left( \frac{\sum_{k=1}^{n} a_k}{\sum_{k=1}^{n} x_k} \right) \sum_{k=1}^{n} a_k.
\]

Corollary 12 allows to prove the following inequalities.

**Theorem 14.** Consider a graph \( G \) with \( m \) edges and \( c \in \mathbb{R} \setminus \{1\} \).

1. If \( c > 0 \), then

\[
ID(G) \geq \left( \frac{(2m)^c}{M_1^{2c-1}(G)} \right)^{1/(c-1)}.
\]

2. If \( c < 0 \), then

\[
ID(G) \leq \left( \frac{(2m)^c}{M_1^{2c-1}(G)} \right)^{1/(c-1)}.
\]

**Proof.** Assume first that \( c > 1 \) or \( c < 0 \). If we choose the convex function \( \varphi(t) = t^c \) on \( (0, \infty) \), \( a_k = d_u^{-1} \) and \( x_k = d_u \), then \( \sum_{k=1}^{n} x_k = \sum_{u \in V(G)} d_u = 2m \) and Corollary 12 gives

\[
M_1^{2c-1}(G) = \sum_{u \in V(G)} d_u^c d_u^{-1} \geq \left( \frac{2m}{\sum_{u \in V(G)} d_u^{-1}} \right)^c \sum_{u \in V(G)} d_u^{-1} = \frac{(2m)^c}{ID(G)^{c-1}}.
\]

Hence,

\[
ID(G) \geq \left( \frac{(2m)^c}{M_1^{2c-1}(G)} \right)^{1/(c-1)}
\]

if \( c > 1 \), and

\[
ID(G) \leq \left( \frac{(2m)^c}{M_1^{2c-1}(G)} \right)^{1/(c-1)}
\]

if \( c < 0 \).

Assume now that \( 0 < c < 1 \). If we choose the convex function \( \varphi(t) = -t^c \) on \( [0, \infty) \), \( a_k = d_u^{-1} \) and \( x_k = d_u \), then Corollary 12 gives

\[
-M_1^{2c-1}(G) = -\sum_{u \in V(G)} d_u^c d_u^{-1} \geq - \left( \frac{2m}{\sum_{u \in V(G)} d_u^{-1}} \right)^c \sum_{u \in V(G)} d_u^{-1} = - \frac{(2m)^c}{ID(G)^{c-1}}.
\]

Hence,

\[
ID(G) \geq \left( \frac{(2m)^c}{M_1^{2c-1}(G)} \right)^{1/(c-1)}.
\]

\( \square \)
Discrete Adriatic indices are the family of 148 topological indices defined in [43] by

\[
Adr(G) = \sum_{uv \in E(G)} \gamma_j(\phi_{i,a}(t_u), \phi_{i,a}(t_v)),
\]

where \( t_u \) is a function of the vertex \( u \), and \( \gamma_j \) and \( \phi_{i,a} \) are appropriate functions of two and one variables, respectively.

If we choose \( \gamma_4(x, y) = |x - y| \), \( t_u = d_u \) and \( \phi_{2,a}(x) = x^a \) with \( a \in \mathbb{R} \setminus \{0\} \), then the misbalance indeg index is defined as

\[
MII(G) = \sum_{uv \in E(G)} \gamma_4(\phi_{2,-1}(d_u), \phi_{2,-1}(d_v)) = \sum_{uv \in E(G)} \left| \frac{1}{d_u} - \frac{1}{d_v} \right|.
\]

This index is a significant predictor of enthalpy of vaporization and of standard enthalpy of vaporization for octane isomers, see [26]. Also, since \( MII(G) = 0 \) if and only if \( G \) is a regular graph, the misbalance indeg index is a measure of the irregularity of a graph. Recall that one of the most famous irregularity indices is the Albertson index, defined in [1] as

\[
Alb(G) = \sum_{uv \in E(G)} |d_u - d_v|.
\]

Note that

\[
\frac{1}{\Delta^2} Alb(G) \leq MII(G) \leq \frac{1}{\delta^2} Alb(G)
\]

for every graph \( G \) with minimum degree \( \delta \) and maximum degree \( \Delta \).

**Theorem 15.** If \( G \) is a graph with \( m \) edges, then

\[
ID(G) \geq 2M_2^{-1}(G) + \frac{1}{m} MII(G)^2.
\]

**Proof.** We have

\[
\frac{d_u^2 + d_v^2}{d_0^2d_0^2} - \frac{2d_ud_v}{d_0^2d_0^2} = \frac{(d_u + d_v)^2}{d_0^2d_0^2} = \left( \frac{1}{d_u} - \frac{1}{d_v} \right)^2,
\]

\[
ID(G) - 2M_2^{-1}(G) = \sum_{uv \in E(G)} \left( \frac{1}{d_u} - \frac{1}{d_v} \right)^2.
\]

Cauchy-Schwarz inequality gives

\[
MII(G)^2 = \left( \sum_{uv \in E(G)} \left| \frac{1}{d_u} - \frac{1}{d_v} \right| \right)^2 \leq \sum_{uv \in E(G)} \left( \frac{1}{d_u} - \frac{1}{d_v} \right)^2 \sum_{uv \in E(G)} 1^2
\]

\[
\leq m \sum_{uv \in E(G)} \left( \frac{1}{d_u} - \frac{1}{d_v} \right)^2
\]

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and so,

\[ ID(G) - 2M^{-1}_2(G) = \sum_{uv \in E(G)} \left( \frac{1}{d_u} - \frac{1}{d_v} \right)^2 \geq \frac{1}{m} \text{MII}(G)^2. \]

\[ \square \]

### 3 Results for some classes of chemical graphs

In [31] Nandargi and Kulli obtained closed formulas for the \((a, b)\)-Nirmala index for the families of jagged rectangle benzenoid systems \((B_{m,n})\) and the families of polycyclic aromatic hydrocarbons \((PAH_n)\). Also, in [18, 19] Kulli obtained closed formulas for the F-Revan index in the families of triangular benzenoid \((T_n)\), rhombus benzenoid \((R_n)\) and hourglass benzenoid \((X_n)\); and for the Revan index in the families of oxide networks \((OX_n)\) and honeycomb networks \((HC_n)\). For more information on these families of chemical graphs refer to the articles cited above. In the next results we compute the \(M^\alpha\) index of each this families.

**Theorem 16.** Let \(m, n \in \mathbb{N}\) and \(\alpha \in \mathbb{R}\), then

1. \(M^\alpha(B_{m,n}) = 2^{n+1}(m + 2n + 1) + 3^\alpha(4mn + 2m - 2n - 4)\),
2. \(M^\alpha(PAH_n) = 6n + 3^{n+1}(2n^2)\),
3. \(M^\alpha(T_n) = 3(n + 1)2^n + 3^\alpha(n^2 + n - 2)\),
4. \(M^\alpha(R_n) = 2^{n+2}(n + 1) + 3^\alpha(2n^2 - 4)\),
5. \(M^\alpha(X_n) = 2^{n+1}(3n) + 3^\alpha(2n^2 + 2n - 4)\),
6. \(M^\alpha(OX_n) = 2^{n+1}(3n) + 4^\alpha(9n^2 - 3n)\),
7. \(M^\alpha(HC_n) = 2^{n+1}(3n) + 3^{n+1}(2n^2 - 2)\).

**Proof.** Let \(V_k = u \in V(G)\); \(d_u = k\) the sets of vertices of \(G\) with degree \(k\). Table 1 shows some data extracted from [18, 19, 31] about the classes of chemical graphs \(B_{m,n}, PAH_n, T_n, R_n, X_n, OX_n\) and \(HC_n\), the remaining data were obtained by calculation.

<table>
<thead>
<tr>
<th>(G)</th>
<th>([V(G)])</th>
<th>([V_1(G)])</th>
<th>([V_2(G)])</th>
<th>([V_3(G)])</th>
<th>([V_4(G)])</th>
</tr>
</thead>
<tbody>
<tr>
<td>(B_{m,n})</td>
<td>(4mn + 4m + 2n - 2)</td>
<td>(0)</td>
<td>(2m + 4n + 2)</td>
<td>(4mn + 2m - 2n - 4)</td>
<td>(0)</td>
</tr>
<tr>
<td>(PAH_n)</td>
<td>(6n^2 + 6n)</td>
<td>(6n)</td>
<td>(0)</td>
<td>(6n^2)</td>
<td>(0)</td>
</tr>
<tr>
<td>(T_n)</td>
<td>(n^2 + 4n + 1)</td>
<td>(0)</td>
<td>(3(n + 1))</td>
<td>(n^2 + n - 2)</td>
<td>(0)</td>
</tr>
<tr>
<td>(R_n)</td>
<td>(2n^2 + 4n)</td>
<td>(0)</td>
<td>(4(n + 1))</td>
<td>(2n^2 - 4)</td>
<td>(0)</td>
</tr>
<tr>
<td>(X_n)</td>
<td>(2(n^2 + 4n - 2))</td>
<td>(0)</td>
<td>(6n)</td>
<td>(2(n^2 + n - 2))</td>
<td>(0)</td>
</tr>
<tr>
<td>(OX_n)</td>
<td>(9n^2 + 3n)</td>
<td>(0)</td>
<td>(6n)</td>
<td>(0)</td>
<td>(9n^2 - 3n)</td>
</tr>
<tr>
<td>(HC_n)</td>
<td>(6n^2)</td>
<td>(0)</td>
<td>(6n)</td>
<td>(6n^2 - 6n)</td>
<td>(0)</td>
</tr>
</tbody>
</table>

Let \(G\) be a chemical graph, then we have

\[ M^\alpha(G) = \sum_{u \in V(G)} d_u^\alpha = |V_1(G)| + 2\alpha|V_2(G)| + 3\alpha|V_3(G)| + 4\alpha|V_4(G)|. \]
From these and Table 1 we obtain

\[ M_1^\alpha(B_{m,n}) = 2^{\alpha+1}(m + 2n + 1) + 3^\alpha(4mn + 2m - 2n - 4), \]
\[ M_1^\alpha(PAH_n) = 6n + 3^{\alpha+1}(2n^2), \]
\[ M_1^\alpha(T_n) = 3(n + 1)2^\alpha + 3^\alpha(n^2 + n - 2), \]
\[ M_1^\alpha(R_n) = 2^{\alpha+2}(n + 1) + 3^\alpha(2n^2 - 4), \]
\[ M_1^\alpha(X_n) = 2^{\alpha+1}(3n) + 3^\alpha(2n^2 + 2n - 4), \]
\[ M_1^\alpha(OX_n) = 2^{\alpha+1}(3n) + 4^\alpha(9n^2 - 3n), \]
\[ M_1^\alpha(HC_n) = 2^{\alpha+1}(3n) + 3^\alpha+1(2n^2 - 2). \]

These gives items (1)-(7).

As a consequence of Theorem 16 we have the next result for the ID index.

Corollary 17. Let \( m, n \in \mathbb{N} \), then

1. \( ID(B_{m,n}) = m + 2n + 1 + \frac{4mn+2m-2n-4}{3} \),
2. \( ID(PAH_n) = 6n + 2n^2 \),
3. \( ID(T_n) = \frac{3}{2}(n + 1) + \frac{n^2+n-2}{3} \),
4. \( ID(R_n) = 2(n + 1) + \frac{2n^2-4}{3} \),
5. \( ID(X_n) = 3n + \frac{2n^2+2n-4}{3} \),
6. \( ID(OX_n) = 3n + \frac{9n^2-3n}{4} \),
7. \( ID(OX_n) = 3n + 2n^2 - 2 \).

4 Comparison between the ID index and other known vertex-degree-based topological indices

In this section we compare the predictive power of the ID index and the following well-known topological indices:

- \( M_1(G) = \sum_{u,v \in E(G)} d_u + d_v = \sum_{u \in V(G)} d_u^2 \),
- \( M_2(G) = \sum_{u,v \in E(G)} d_u d_v \),
- \( R(G) = \sum_{u,v \in E(G)} \frac{1}{d_u d_v} \),
- \( \chi(G) = \sum_{u,v \in E(G)} \frac{1}{\sqrt{d_u + d_v}} \),
- \( H(G) = \sum_{u,v \in E(G)} \frac{1}{d_u + d_v} \),
- \( ABC(G) = \sum_{u,v \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \),
- \( GA(G) = \sum_{u,v \in E(G)} \frac{d_u d_v}{d_u + d_v} \),
- \( SO(G) = \sum_{u,v \in E(G)} \sqrt{d_u^2 + d_v^2} \).

We performed this comparison by studying the coefficient of determination \( r^2 \) between these indices and some physicochemical properties of three classes of molecules: polynuclear aromatic hydrocarbons, polychlorobiphenyls, and octane isomers. The topological indices and the coefficient of determination were calculated by a self-developed program.
Polycyclic aromatic hydrocarbons (PAHs) are a class of organic compounds consisting of multiple aromatic (carbon-based) rings. They are typically found in fossil fuels, coal, oil and natural gas, and are also produced by the burning of organic matter (see [41]).

The physicochemical properties of these compounds studied are melting point (MP), boiling point (BP) and octanol-water partition coefficient (LogP); the data were obtained from [41]. In Table 2 we show the $r^2$ values calculated for each property and each index, for each property we highlight the highest $r^2$ value.

<table>
<thead>
<tr>
<th>Property</th>
<th>ID</th>
<th>M1</th>
<th>M2</th>
<th>R</th>
<th>Xi</th>
<th>H</th>
<th>ABC</th>
<th>GA</th>
<th>SO</th>
</tr>
</thead>
<tbody>
<tr>
<td>MP</td>
<td>0.697</td>
<td>0.73</td>
<td>0.715</td>
<td>0.73</td>
<td>0.732</td>
<td>0.727</td>
<td>0.737</td>
<td>0.73</td>
<td>0.732</td>
</tr>
<tr>
<td>BP</td>
<td>0.822</td>
<td>0.971</td>
<td>0.961</td>
<td>0.976</td>
<td>0.975</td>
<td>0.977</td>
<td>0.976</td>
<td>0.969</td>
<td></td>
</tr>
<tr>
<td>logP</td>
<td><strong>0.937</strong></td>
<td>0.878</td>
<td>0.86</td>
<td>0.899</td>
<td>0.887</td>
<td>0.888</td>
<td>0.894</td>
<td>0.877</td>
<td>0.883</td>
</tr>
</tbody>
</table>

From Table 2 we can conclude that for the MP and BP properties the ID index is a worse predictor than the other studied indices. However, for the logP property the ID index is a better predictor than the other indices with a value $r^2 = 0.937$.

Polychlorinated biphenyls (PCBs) are a group of synthetic organic compounds consisting of a central biphenyl structure with one or more chlorine atoms attached to the benzene rings. They are stable compounds and resistant to heat, light and chemical reactions, so many industrial applications used them. Also, these compounds are non-combustible, non-volatile and have high electrical insulating properties. Due to their persistence in the environment and toxicity to human health, they were banned by many countries (see [13, 42]).

The physicochemical properties of these compounds studied are melting point (MP), relative retention time (RTT), octanol-water partition coefficient (logP), total surface area (TSA), log Henry constant (logH), log water solubility (logSw), log water activity coefficient (logYw), relative enthalpy of formation (dHf); the data were obtained from [13, 42]. In Table 3 we show the $r^2$ values calculated for each property and each index, for each property we highlight the highest $r^2$ value.

<table>
<thead>
<tr>
<th>Property</th>
<th>ID</th>
<th>M1</th>
<th>M2</th>
<th>R</th>
<th>Xi</th>
<th>H</th>
<th>ABC</th>
<th>GA</th>
<th>SO</th>
</tr>
</thead>
<tbody>
<tr>
<td>MP</td>
<td>0.668</td>
<td>0.608</td>
<td>0.602</td>
<td>0.607</td>
<td>0.607</td>
<td>0.603</td>
<td><strong>0.610</strong></td>
<td>0.606</td>
<td>0.609</td>
</tr>
<tr>
<td>RRT</td>
<td>0.903</td>
<td>0.903</td>
<td>0.888</td>
<td>0.898</td>
<td>0.899</td>
<td>0.891</td>
<td><strong>0.907</strong></td>
<td>0.898</td>
<td>0.905</td>
</tr>
<tr>
<td>logP</td>
<td>0.848</td>
<td>0.848</td>
<td>0.828</td>
<td>0.842</td>
<td>0.843</td>
<td>0.832</td>
<td><strong>0.855</strong></td>
<td>0.841</td>
<td>0.853</td>
</tr>
<tr>
<td>TSA</td>
<td>0.995</td>
<td>0.995</td>
<td>0.986</td>
<td>0.993</td>
<td>0.993</td>
<td>0.988</td>
<td><strong>0.997</strong></td>
<td>0.992</td>
<td>0.996</td>
</tr>
<tr>
<td>logH</td>
<td>0.014</td>
<td>0.014</td>
<td><strong>0.016</strong></td>
<td>0.015</td>
<td>0.015</td>
<td>0.015</td>
<td>0.014</td>
<td>0.015</td>
<td>0.014</td>
</tr>
<tr>
<td>logSw</td>
<td>0.924</td>
<td>0.924</td>
<td>0.912</td>
<td>0.921</td>
<td>0.922</td>
<td>0.915</td>
<td><strong>0.928</strong></td>
<td>0.920</td>
<td>0.927</td>
</tr>
<tr>
<td>logYw</td>
<td>0.809</td>
<td>0.809</td>
<td>0.798</td>
<td>0.804</td>
<td>0.805</td>
<td>0.796</td>
<td><strong>0.814</strong></td>
<td>0.803</td>
<td>0.812</td>
</tr>
<tr>
<td>dHf</td>
<td>0.455</td>
<td>0.455</td>
<td><strong>0.459</strong></td>
<td>0.457</td>
<td>0.456</td>
<td>0.458</td>
<td>0.453</td>
<td>0.457</td>
<td>0.454</td>
</tr>
</tbody>
</table>
In Table 3 we can observe that, although the ID index is not the best predictor for any of the studied properties, for all of them the calculated $r^2$ value remains relatively close to the highest $r^2$ value found. In particular, it presents a high predictive power for the properties RTT, TSA and logSw. In addition, note that, for this family of compounds and the studied properties, the value of $r^2$ for the ID index is equal to that of the $M1$ index.

Now, with the ID index we build linear regression models of the form

$$P = aID(G) + b,$$

where $P$ is a physicochemical property (only those with a coefficient of determination $r^2 > 0.9$ were selected).

For the compounds polycyclic aromatic hydrocarbons, we have

$$\log P = 0.665 ID(G) + 0.315. \quad (1)$$

In Figure 1 we plot the ID index vs. the logP property of polycyclic aromatic hydrocarbons. Also, we test the linear regression model above (red dashed line).

**Fig. 1** Inverse degree index vs. the physicochemical property logP of polycyclic aromatic hydrocarbons. Red dashed line is the liner regression model of Eq. 1.

For the compounds polychlorinated biphenyls we have

$$RTT = 0.119ID(G) - 0.572, \quad TSA = 18.491ID(G) + 90.525, \quad (2)$$
$$\log Sw = 0.738ID(G) + 0.294.$$  

In Figure 2 we plot the ID index vs. the RTT, TSA and logSw properties of polycyclic aromatic hydrocarbons. Also we test the linear regression models above (red dashed lines).
Fig. 2 Inverse degree index vs. the physicochemical property (a) R TT, (b) TSA, and (c) logSw of polychlorinated biphenyls. Red dashed lines are the linear regression models of Eq. 2.

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Declarations

- Ethical Approval
  Not applicable.
- Competing interests
  The authors confirm that the content of this article has no conflict of interest or competing interests.
- Authors’ contributions
  The authors contributed equally to this work.
- Funding
  Agencia Estatal de Investigación (PID2019-106433GB-I00 / AEI / 10.13039/501100011033), Spain.
- Availability of data and materials
Some data in Table 1 were extracted from [18, 19, 31]. The remaining data in Table 1 were obtained by calculation. The data on physicochemical properties of the studied compounds were obtained from [13, 41, 42].

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