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Graph Irregularity Indices Used as Molecular Descriptors in QSPR Studies

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Abstract

A comparative study based on the structure-property regression analysis is performed in order to test and evaluate the application possibilities of various graph irregularity indices for the prediction of physico-chemical properties of octane isomers. By restricting attention to single-variable linear regressions, we investigate the stochastic relationships between 18 preselected irregularity indices and 5 physico-chemical properties of octane isomers. These are: Boiling point (Bp), Standard enthalpy of vaporization (DHVAP), Acentric factor (AcenFac), Enthalpy of vaporization (HVAP) and Entropy. The degree of the intercorrelation was evaluated by traditional correlation coefficients. In physico-chemical applications, it is a widely accepted but theoretically not verified belief is that the use of graph irregularity indices are not to be efficient in QSPR studies of molecular graphs. Our observations refute this preconception. Presenting demonstrative counter-examples it is shown that there exist several irregularity indices by which four octane isomer properties (DHVAP, Entropy, AcenFac and HVAP) can be predicted with a good accuracy.

1 Introduction, preliminary considerations

In this study, we are concerned with simple connected graphs G(V, E) denoting by V(G) and E(G) the set of vertices and edges of G, respectively. For a graph G with n vertices and m edges, the degree d_u of a vertex u of G is the number of first neighbors of u, and uv denotes an edge in G connecting the vertices u and v.

The total number of edges in G with end-vertex degrees i and j is denoted by $m_{i,j}$ where we suppose that $1 \leq i \leq j \leq n-1$. Using the standard terminology [1,2,3], let A=A(G) be the adjacency matrix of G. For a graph G, the largest eigenvalue ρ(G) of A(G) is referred to as the spectral radius of G. As usual, we denote by P_n the path and by S_n the star graph.

A graph is said to be regular (R-regular) if all its vertices have the same degree R. A connected bipartite graph is called *semiregular* if each vertex in the same part of bipartition has the same degree. A connected graph G is called *harmonic* (pseudo-regular) [3,4,5,6], if there exists a positive constant p(G) such that each vertex u of G has the same average neighbor degree number identical to p(G). The spectral radius ρ(G) of a harmonic graph G is equal to p(G). It is obvious that any connected R-regular graph G_R is a harmonic graph with $p(G_R)=\rho(G_R)=R$. A bipartite graph G called *pseudo-semiregular* [4] if each vertex in the same part of bipartition has the same average degree. From these definitions it follows that any semiregular graph is a bipartite pseudo-semiregular graph.

2 Irregularity indices selected for QSPR studies

Consider a topological invariant formulated as

$$TI(G) = \sum_{uv \in E} f(d_u, d_v) \ ,$$

where f(x,y) is an appropriately selected function. According to the traditional terminology, TI(G) belongs to the family of degree-based topological indices [7,8]. It is easy to see that the graph invariant TI(G) can be rewritten in the following alternative form:

$$TI(G) = \sum_{i \leq j} m_{i,j} f(i, j) \ .$$

For simplicity, the parameters $m_{i,j}$ will be called the edge-parameters of a graph G. From the previous considerations it follows that if graphs G_a and G_b are characterized by the same set of edge parameters $m_{i,j}$, then $TI(G_a)=TI(G_b)$ holds for any degree-based topological index TI.

In other words, using an arbitrary degree-based topological index TI, it is impossible to discriminate between graphs G_a and G_b.

For degree-based topological invariants (indices) the following general definition can be given: A topological invariant TOP(G) of a connected graph G is said to be degree-based, if for any two non-isomorphic graphs G_a and G_b characterized by the same set of edge parameters $\{m_{i,j} >0\}$ the equality $TOP(G_a)=TOP(G_b)$ holds.

A topological invariant TOP(G) is called an irregularity index of a graph G if $TOP(G) \geq 0$ and TOP(G)=0 if and only if G is a regular graph. It is worth noting that the irregularity indices have found almost no applications for predicting physico-chemical properties of organic molecules. This is explained by the fact that several researchers are convinced that discriminating and predicting power of irregularity indices are rather low [9].

In our comparative study for testing purpose we selected the set of 18 octane isomers and their 5 physico-chemical properties. The graphs of octane isomers depicted in Fig.1 are tree graphs with 8 vertices and 7 edges. They belong to the family of molecular graphs because their maximum degree is not larger than four.

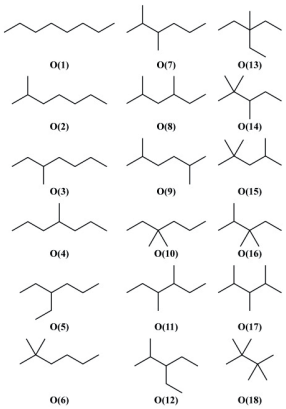

Fig 1. Graphs of octane isomers

The irregularity indices investigated are included in Table 1. Except IRM2(G), all of them belong to the family of degree-based irregularity indices.

Table 1. Irregularity indices selected for QSPR studies

Irregularity indices	
$VAR(G)=\sum_{u\in V}\left(d_u-\frac{2m}{n}\right)^2=\frac{M_1(G)}{n}-\left(\frac{2m}{n}\right)^2$	$IRDIF(G)=\sum_{uv\in E}\left\|\frac{d_u}{d_v}-\frac{d_v}{d_u}\right\|=\sum_{i<j}m_{i,j}\left(\frac{j}{i}-\frac{i}{j}\right)$
$AL(G)=\sum_{uv\in E}\left\|d_u-d_v\right\|$	$IRL(G)=\sum_{uv\in E}\left\|\ln d_u-\ln d_v\right\|=\sum_{i<j}m_{i,j}\ln\left(\frac{j}{i}\right)$
$IR1(G)=\sum_{u\in V}d_u^3-\frac{2m}{n}\sum_{u\in V}d_u^2=F(G)-\frac{2m}{n}M_1(G)$	$IRLU(G)=\sum_{uv\in E}\frac{\left\|d_u-d_v\right\|}{\min(d_u,d_v)}=\sum_{i<j}m_{i,j}\ln\left(\frac{j-i}{i}\right)$
$IR2(G)=\sqrt{\frac{\sum_{uv\in E}d_ud_v}{m}}-\frac{2m}{n}=\sqrt{\frac{M_2(G)}{m}}-\frac{2m}{n}$	$IRLF(G)=\sum_{uv\in E}\frac{\left\|d_v-d_u\right\|}{\sqrt{(d_vd_u)}}=\sum_{i<j}m_{i,j}\left(\frac{j-i}{\sqrt{ij}}\right)$
$IRF(G)=\sum_{uv\in E}\left(d_u-d_v\right)^2=F(G)-2M_2(G)$	$IRLA(G)=2\sum_{uv\in E}\frac{\left\|d_v-d_u\right\|}{d_v+d_u}=2\sum_{i<j}m_{i,j}\left(\frac{j-i}{j+i}\right)$
$IRFW(G)=\frac{IRF(G)}{M_2(G)}$	$IRD1=\sum_{uv\in E}\ln\left\{1+\left\|d_u-d_v\right\|\right\}=\sum_{i<j}m_{i,j}\ln(1+j-i)$
$IRA(G)=\sum_{uv\in E}\left(d_u^{-1/2}-d_v^{-1/2}\right)^2=n-2Ra(G)$	$IRGA(G)=\sum_{uv\in E}\ln\left(\frac{d_u+d_v}{2\sqrt{d_ud_v}}\right)=\sum_{i<j}m_{i,j}\ln\left(\frac{i+j}{2\sqrt{ij}}\right)$
$IRB(G)=\sum_{uv\in E}\left(d_u^{1/2}-d_v^{1/2}\right)^2=M_1(G)-2RR(G)$	$IRM1(G)=\frac{1}{n}\sum_{u\in V}\mu_u-\frac{2m}{n}$
$IRC(G)=\frac{\sum_{uv\in E}\sqrt{d_ud_v}}{m}-\frac{2m}{n}=\frac{RR(G)}{m}-\frac{2m}{n}$	$IRM2(G)=\sum_{u\in V}\left\|d_u-\mu_u\right\|$

As can be seen, the most indices are constructed from well-known graph invariants [10 - 19]. Topological invariants denoted by $M_1(G)$ and $M_2(G)$ are the first and the second Zagreb indices [7-15], while Ra(G) and RR(G) are identical to the ordinary Randić index and the so-called reciprocal Randić index [20-23]. The graph invariant denoted by F(G) is referred to as the forgotten topological index [24].

3 Some properties of selected irregulariy indices

Due to their simple computation, the degree-variance VAR(G) and the Albertson index AL(G) belong to the family of the widely used irregularity indices [25,26,27].

The degree-variance proposed by Bell [25] is formulated as

$$VAR(G)=\sum_{u\in V}\left(d_u-\frac{2m}{n}\right)^2=\frac{M_1(G)}{n}-\left(\frac{2m}{n}\right)^2=\left(\sqrt{\frac{M_1(G)}{n}}-\frac{2m}{n}\right)\left(\sqrt{\frac{M_1(G)}{n}}+\frac{2m}{n}\right),$$

while the Albertson index is defined by [26]

$$AL(G) = \sum_{uv \in E} |d_u - d_v|.$$

The majority of irregularity indices listed in Table 1 is characterized in Refs. [9,19, 27]. In what follows some fundamental properties of irregularity indices and relations between them are discussed.

i) Analyzing the topological structure of octane isomer graphs we can observe the known phenomena related to the discrimination ability (discriminativity) and degeneracy of topological indices [28,29,30].

Among octane isomers there exist two pairs of graphs, namely graph pairs (O(3), O(4)) and (O(11), O(12)) which are characterized by identical edge-parameter sets. For graphs O(3), O(4) we have $m_{1,2}=2$, $m_{1,3}=1$, $m_{2,2}=2$ and $m_{2,3}=2$, and for graphs O(11), O(12) one obtains that $m_{1,2}=2$, $m_{1,3}=2$, $m_{2,3}=2$ and $m_{3,3}=1$. This observation implies that by using an arbitrary degree-based topological index TI, the computed values of TI will be the same for graph pairs O(3), O(4) and O(11), O(12), respectively. It is worth noting that the diameter of O(11) is equal to 5, while the diameter of O(12) is equal to 4.

In connection with the discriminativity of topological indices, an interesting problem is to decide whether an arbitrary topological invariant TOP(G) can be considered as a degree-based topological index or not. In some cases checking our hypothesis can be facilitated by using the following simple decision rule: If there exist connected graphs G_a and G_b with identical set of edge parameters $m_{i,j}$, but $TOP(G_a)$ is not equal to $TOP(G_b)$, then TOP cannot be considered as a degree-based topological index. This concept is demonstrated by the following examples.

Lemma 1 Let μ_u be the average degree of the vertices adjacent to vertex u in G. In [31] it was proved that for a connected graph G

$$\frac{1}{n}\sum_{u \in V} \mu_u = \frac{1}{n}\sum_{i \le j} m_{i,j}\left(\frac{i}{j}+\frac{j}{i}\right) \ge \frac{2m}{n},$$

with equality if and only if G is a regular graph.

Consider the irregularity indices IRM1(G) and IRM2(G) defined as

$$IRM1(G) = \frac{1}{n}\sum_{u\in V}\left(\mu_u - \frac{2m}{n}\right) = \frac{1}{n}\sum_{u\in V}\mu_u - \frac{2m}{n},$$

$$IRM2(G) = \sum_{u\in V}\left|d_u - \mu_u\right|.$$

From Lemma 1 one obtains that

$$IRM1(G) = \frac{1}{n}\sum_{i\le j} m_{i,j}\left(\frac{i}{j}+\frac{j}{i}\right) - \frac{2m}{n} = \frac{1}{n}\sum_{i\le j} m_{i,j}\left(\frac{(i-j)^2}{ij}\right) \ge 0.$$

From this identity it follows that IRM1(G) is a degree-based irregularity index.

It is easy to show that the irregularity index IRM2(G) does not belong to the family of degree-based irregularity indices. Although graphs O(3), O(4) have identical edge-parameter set, ($m_{1,2}$=2, $m_{1,3}$=1, $m_{2,2}$=2 and $m_{2,3}$=2) the computed values of index IRM2(G) for the two octane isomer graphs are different, namely IRM2(O(3))= 6,3333 and IRM2(O(4))= 7,3333. We can conclude that IRM2(G) does not belong to the class of degree-based irregularity indices.

ii) There exists a broad class of connected graph for which the identity $\rho(G) = \sqrt{M_2(G)/m}$ is fulfilled. These graphs are called *Z_2 graphs*, because they are defined on the basis of the second Zagreb index [32]. It is a fundamental property of Z_2 graphs is that $\rho^2(G)=M_2(G)/m$ is a positive integer. The harmonic, semiregular and bipartite pseudo-semiregular graphs form subsets of Z_2 graphs [32]. From the previous considerations it follows that if G is a Z_2 graph then

$$IR2G) = CS(G) = \rho(G) - \frac{2m}{n},$$

where CS(G) is the Collatz–Sinogowitz irregularity index [33].

It is worth noting that the topological invariant $\sqrt{M_2(G)/m}$ is a good estimation of the spectral radius for molecular graphs, where the maximum degree of graph G is not larger than four [32]. The correspondence between CS(G) and IR2(G) for 18 octane isomer graphs is illustrated in Fig.2. As can be observed, there exists a strong linear correlation between them (r =0,987).

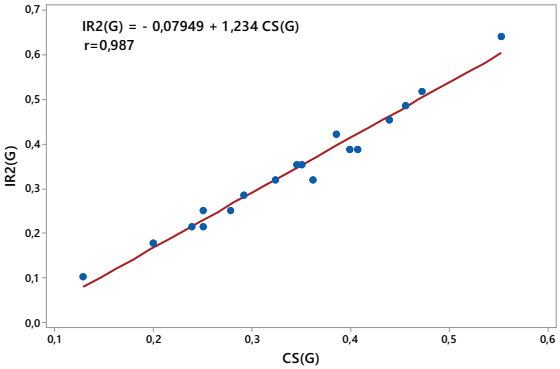

Fig 2. Relation between irregularity indices CS(G) and IR2(G) for 18 octane isomers

An interesting observation is that among 18 octane isomer graphs only the tree O(9) belongs to the family of Z_2 graphs. Its spectral radius is equal to 2.

iii) If G is a connected n-vertex graph, then inequality $|d_u - d_v| \le n - 2$ is fulfilled for any uv edge in G. According to Ref. [24] this implies that

$$IRF(G) = F(G) - 2M_2(G) \le m(n-2)^2$$

with equality if and only if G is the star S_n. It is verified that $IRF(G)=F(G)-2M_2(G) \le n^2VAR(G)$ and equality holds if G is a regular or a well-stabilized graph [34]. Additionally, in our comparative study we tested a weighted version of the irregularity index IRF(G) which is defined by $IRFW(G)= IRF(G)/M_2(G)$.

iv) Consider the irregularity index IRL(G) introduced by Vukičević and Gašperov [8].

$$IRL(G) = \sum_{uv \in E} |\ln d_v - \ln d_u| = \sum_{i<j} m_{i,j} \ln\left(\frac{j}{i}\right).$$

Based on the following two lemmas we can establish upper and lower bounds for IRL(G).

Lemma 2 [35]: Let d_v and d_u be positive integers where $d_v \ge d_u$. Then

$$\frac{d_v - d_u}{d_u} \ge \ln d_v - \ln d_u \ge \frac{d_v - d_u}{d_v}$$

with equality in both sides if and only if $d_v \ge d_u$.

Lemma 3 [36]: Let t, d_v and d_u be positive integers where $d_v \geq d_u$. Then

$$\frac{d_v^t - d_u^t}{t(d_v d_u)^{t/2}} \geq \ln d_v - \ln d_u \geq \frac{2(d_v^t - d_u^t)}{t(d_v^t + d_u^t)}$$

with equality in both sides if and only if G is regular.

Proposition 1 Starting with Lemma 2, define the irregularity indices IRLU(G) and IRLL(G) as

$$IRLU(G) = \sum_{uv \in E} \frac{|d_v - d_u|}{\min(d_v, d_u)} = \sum_{i<j} m_{i,j} \left(\frac{j-i}{i} \right)$$

$$IRLL(G) = \sum_{uv \in E} \frac{|d_v - d_u|}{\max(d_v, d_u)} = \sum_{i<j} m_{i,j} \left(\frac{j-i}{j} \right)$$

It is easy to see that

$$IRLU(G) \geq IRL(G) = \sum_{uv \in E} |\ln d_v - \ln d_u| \geq IRLL(G),$$

where equality holds in both sides if and only if G is regular.

Proposition 2 Using Lemma 3, and assuming that t=1, consider the irregularity indices IRLF(G) and IRLA(G) defined by

$$IRLF(G) = \sum_{uv \in E} \frac{|d_v - d_u|}{\sqrt{(d_v d_u)}} = \sum_{i<j} m_{i,j} \left(\frac{j-i}{\sqrt{ij}} \right)$$

and

$$IRLA(G) = 2 \sum_{uv \in E} \frac{|d_v - d_u|}{d_v + d_u} = 2 \sum_{i<j} m_{i,j} \left(\frac{j-i}{j+i} \right)$$

It follows that

$$IRLF(G) \geq IRL(G) = \sum_{uv \in E} |\ln d_v - \ln d_u| \geq IRLA(G)$$

where equalities hold in both sides if and only if G is regular.

v) Let T_n be an n-vertex tree. As can be observed, there exist several topological indices TOP for which the following inequalities hold:

$$TOP(P_n) \le TOP(T_n) \le TOP(S_n)$$

For example, the irregularity indices IR2(G), IRA(G) and IRC(G) are characterized by the above extremal property.

Lemma 4 [37]: If T_n is an n-vertex tree, then

$$4n-8 \le M_2(T_n) \le (n-1)^2$$

and the left equality holds if and only if T_n is the path P_n and the right equality holds if and only if T_n is the star S_n. As a consequence of above inequalities the following proposition yields:

Proposition 3 If T_n is an n-vertex tree then

$$IR2(P_n) = \sqrt{\frac{4n-8}{n-1}} - \frac{2(n-1)}{n} \le IR2(T_n) = \sqrt{\frac{M_2(T_n)}{n-1}} - \frac{2(n-1)}{n} \le IR2(S_n) = \sqrt{n-1} - \frac{2(n-1)}{n}$$

and the left equality holds if and only if T_n is the path P_n and the right equality holds if and only if T_n is the star S_n.

Lemma 5 [22]: Among trees with n vertices, the star S_n has the minimum and the path P_n has the maximum Randić index. This observation implies the following proposition:

Proposition 4 If T_n is an n-vertex tree, then

$$IRA(P_n) \le IRA(T_n) = n - 2Ra(T_n) \le IRA(S_n)$$

and the left equality holds if and only if T_n is the path P_n and the right equality holds if and only if T_n is the star S_n.

Lemma 6 [23]: Let T_n be an n-vertex tree. Then for the reciprocal Randić index $RR(T_n)$ one obtains that

$$RR(P_n) \le RR(T_n) = \sum_{uv \in E} \sqrt{d_u d_v} \le RR(S_n)$$

and the left equality holds if and only if T_n is the path P_n and the right equality holds if and only if T_n is the star S_n.

Proposition 5 If T_n is an n-vertex tree, then from Lemma 6 one obtains that

$$IRC(P_n) \le IRC(T_n) = \frac{RR(T_n)}{m} - \frac{2m}{n} \le IRC(S_n)$$

and the left equality holds if and only if T_n is the path P_n and the right equality holds if and only if T_n is the star S_n.

4 Relations between selected irregularity indices and some physico-chemical properties of octane isomers

We tested the applicability of the preselected irregularity indices for predicting five physico-chemical properties of octane isomers. These are: Boiling point (Bp), Standard enthalpy of vaporization (DHVAP), Entropy, Acentric factor (AcenFac) and Enthalpy of vaporization (HVAP). All data were taken from the database www.moleculardescriptors.eu.

Table 2 summarizes the results of statistical structure-property analysis. It contains only the computed correlation coefficients (r) whose absolute values are not less than 0.8. Additionally, for comparison, in Table 2 the correlation coefficients related to Randić index (Ra) and the spectral radius (ρ) of octane isomer graphs are also included.

It should be noted that from the definitions of topological invariants Ra(G) and IRA(G) it follows that their absolute values of their correlation coefficients are identical.

Some computed results of structure-property correlation analysis are illustrated in Fig.3.

Table 2 The correlation coefficients between irregularity indices and 5 preselected physico-chemical properties of octane isomers

Topological invariant	Bp	DHVAP	Entropy	AcenFac	HVAP
VAR(G)	_	-0.936	**-0.954**	**-0.973**	-0.886
AL(G)	-0.816	**-0.976**	-0.897	-0.933	-0.944
IR1(G)	_	-0.919	**-0.951**	-0.961	-0.866
IR2(G)	_	-0.818	-0.936	**-0.987**	_
IRF(G)	_	-0.938	-0.907	-0.900	-0.906
IRFW(G)	**-0.855**	-0.952	-0.847	-0.844	-0.943
IRA(G)	-0.820	-0.958	-0.906	-0.904	-0.936
IRB(G)	-0.805	-0.953	-0.912	-0.906	-0.925
IRC(G)	_	-0.881	**-0.954**	**-0.995**	-0.812
IRDIF(G)	-0.830	-0.939	-0.863	-0.872	-0.915
IRL(G)	-0.837	**-0.987**	-0.893	-0.935	**-0.956**
IRLU(G)	-0.825	**-0.973**	-0.914	-0.924	-0.945
IRLF(G)	-0.829	**-0.984**	-0.902	-0.959	**-0.953**
IRLA(G)	-0.822	**-0.980**	-0.885	-0.937	-0.948
IRD1(G)	-0.804	-0.963	-0.851	-0.920	-0.928
IRGA(G)	-0.819	-0.962	-0.911	-0.909	-0.937
IRM1(G)	-0.812	-0.953	-0.910	-0.901	-0.928
IRM2G)	**-0.862**	-0.961	-0.863	-0.854	-0.944
Ra(G)	0.820	0.958	0.906	0.904	0.936
ρ(G)	_	-0.840	-0.916	**-0.980**	_

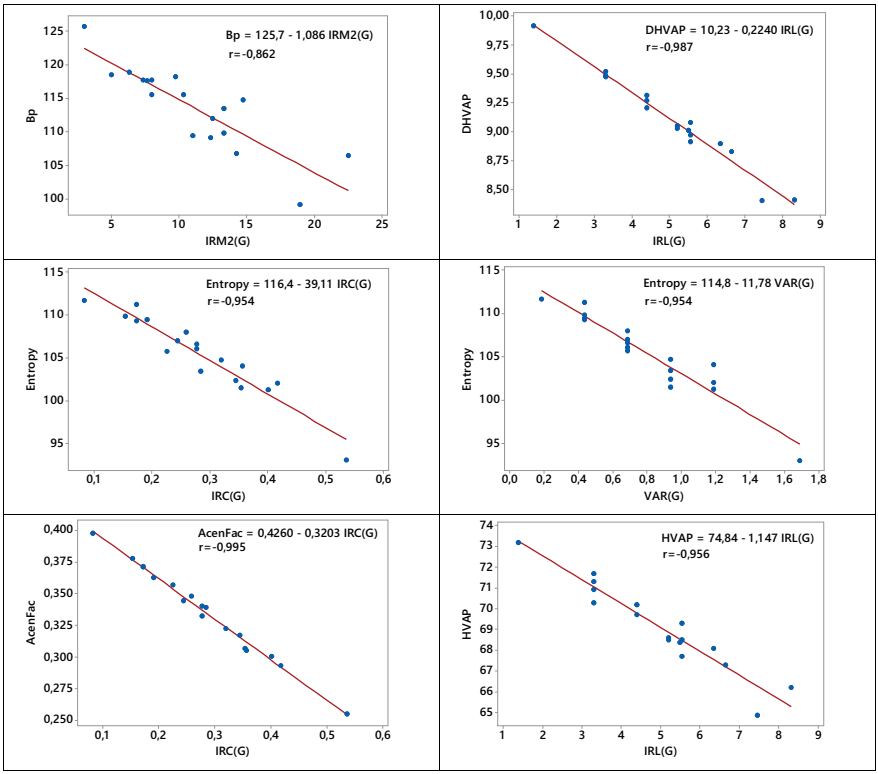

Fig. 3 Relations between irregularity indices and five physico-chemical properties of octane isomers.

Evaluating the predictive power of various topological indices on the basis of corresponding correlation coefficients listed in Table 2, we arrive at the following conclusions.

1) Considering the property prediction power (predictive ability), there exist irregularity indices which perform significantly better than the classical Randić index (Ra) or the spectral radius ρ(G) of octane isomer graphs. By inspection of the data given in Table 2, we see that the majority of selected irregularity indices is characterized by a good predictive power, and in several cases the absolute values of correlation coefficients are over 0,9.

2) It is an interesting observation is that all calculated correlation coefficients are negative numbers. Comparing the computed correlation coefficients it can be concluded that the most convenient irregularity indices for predicting

Bp are IRM2(G) with r = - 0.862 and IRFW(G) with r = - 0.855,
DHVAP are IRL(G) with r = - 0.987 and IRLF(G) with r = - 0.984,
Entropy are VAR(G) with r = - 0.954 and IRC(G) with r = - 0.954,
AcenFac are IRC(G) with r = - 0.995 and IR2(G) with r = - 0.987,
HVAP(G) are IRL(G) with r = - 0.956 and IRLF(G) with r = - 0.953.

As can be seen, the greatest correlation coefficients belong to DHVAP and AcenFac properties, while the prediction of the boiling point (Bp) is characterized by relatively lower correlation coefficients [40].

3) All irregularity indices investigated in this study, except topological index IRM2(G) belong to the family of degree-based molecular descriptors. The main advantage of using degree-based irregularity indices is that their computation is easy comparing them to distance-based and spectrum-based topological descriptors [8]. The practical application of distance-based and spectrum-based topological indices is more complicated, because they cannot be directly deduced from the structure of graphs.

5 Final remarks

Although several attempts have been made for the exact distinction of degree-based and non-degree-based topological invariants, their classification belongs to open problems [8,38].
A paradox phenomenon related to the characterization and categorization of various graph invariants (including irregularity indices as well) is demonstrated by the following example. Denote by Ω the set of connected graphs and consider the degree-based topological index defined by

$$IM(G) = 2(n-1)^2 - M_2(G)$$

where $G \in \Omega$. Let Ω_T be a subset of Ω including n-vertex trees T of diameter less than 5.

According to the identity published in [39]:

$$IM(T) = 2(n-1)^2 - M_2(T) = W(T)$$

where W(T) is the Wiener index of $T \in \Omega_T$. It is known that the Wiener index belongs to the family of most popular distance-based topological indices for $G \in \Omega$ [8, 39, 40]. But as we can conclude, in this particular case, (i.e. for trees included in Ω_T) the corresponding Wiener index can be considered as a degree-based topological invariant.

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