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A note on QSPR Analysis of Leap Randić index of Octanes

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Abstract

Topological indices are used in QSPR studies modeling structural properties of molecules. Zagreb indices were used modeling π-electron energy levels of alternant hydrocarbons. Randić index was used modeling molecular branching which was defined after Zagreb indices. These both indices are the most used topological indices in chemical literature. Leap Zagreb indices have been defined recently as parallel to Zagreb indices by using 2-distance degree notion (connection number) in graph theory. Several QSPR studies show that leap Zagreb indices are possible tools in quantitative structure property relationship studies. Leap Randić index defined as "the product connectivity index" by using 2-distance degree notion (connection number). We firstly analyze the applicability of this index in view of QSPR studies by using some chemical properties of octanes. We show that leap Randić index give low correlation for the chemical properties of octanes. Also leap Randić index has low relationship with Randić index. We conclude that leap Randić index is not a possible tool for QSPR studies.

Keywords: QSPR studies, Leap Randić index, Leap Zagreb indices, Connection number

1. INTRODUCTION

Chemical graph theory is one of the branch of graph theory is considered as the intersections of graph theory, chemistry and information science. Pictorial representations of molecules in chemistry correspond graphs in graph theory. A topological index is a numerical value which derived the graph by using any graph invariant. Topological indices are used in QSPR studies for modeling physico-chemical and structural properties of chemical substances and networks. The first topological index is Wiener index which was defined by Harold Wiener as "path number" modeling paraffin's boiling points [1]. The first degree based topological indices are Zagreb and Randić indices which are the most used topological indices for QSPR studies. Especially modelling π-electron energy levels and molecular branching, respectively [2,3]. A novel topological index has been accepted valuable in view of chemistry if this topological index give better correlation modelling some physico-chemical properties of molecules compared to classical Zagreb and Randić indices. Detailed discussion of Wiener, Zagreb and Randić indices, we refer to [4-14] and references therein for interested reader. Zagreb indices have been defined independently in two different studies [15,16]. It was shown that leap Zagreb indices correlates well with the acentric factor and entropy of octane isomers [16]. The relationship between leap Zagreb indices and Zagreb indices were stated in [15]. Alkanes characterized with the first three maximal/minimal first leap Zagreb index in [16].

Kulli defined Leap product connectivity index and computed this index for helm graphs [17]. Product connectivity index is the less familiar name of the "Randić index". Due to this fact, we rename "leap product connectivity index" as "leap Randić index".

QSPR analysis of leap Randić index has not been investigated by now.

We firstly analyze the applicability of this index in view of QSPR studies by using some chemical properties of octanes in this paper.

2. PRELIMINARIES

Let $G = (V, E)$be a connected graph with n vertices and m edges and v be a vertex of G. For a positive integer k, the open k-neighborhood of v in the graph G, denoted by $N_k(v) = \{u \in V(G): d(u,v) = k\}$ where $d(u,v)$ (the distance between u and v) is the minimum number of edges connecting the vertices u and v. k-distance degree of a vertex v of G defined as; the number of vertices in the open k-neighborhood of v and denoted as; $d_k(v) = |N_k(v)|$ [1]. Notice that the degree of the vertex v is the 1-distance degree of v i.e. $d_1(v) = |N_1(v)|$. The 2-distance degree of the vertex v is also called as connection number of v [15,16]. The connection number was defined in order to find the electron energy of alternant hydrocarbons [2]. Wiener index index [1] of a simple connected graph were used as modelling boiling points of paraffins, defined as;

$$W(G) = \frac{1}{2}\sum_{u,v\in V(G)} d(u,v) \quad (1)$$

The first and second Zagreb and Randić indices [3] of a simple connected graph G defined as;

$$M_1(G) = \sum_{v\in V(G)} d_1(v)^2 \quad (2)$$

$$M_2(G) = \sum_{uv\in E(G)} d_1(u)d_1(v) \quad (3)$$

$$R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_1(u)d_1(v}} \quad (4)$$

2-distance degree (connection number) based Zagreb indices have been defined independently in two different studies [15,16]. Leap Zagreb indices defined as;

$$LM_1(G) = \sum_{v\in V(G)} d_2(v)^2 \quad (5)$$

$$LM_2(G) = \sum_{uv \in E(G)} d_2(u) d_2(v) \quad (6)$$
$$LM_3(G) = \sum_{v \in V(G)} d_1(v) d_2(v) \quad (7)$$

It was shown that leap Zagreb indices correlates well with the acentric factor and entropy of octane isomers [16]. The relationship between leap Zagreb indices and Zagreb indices were stated in [15].

Leap Randić index [17] defined as;

$$LR(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_2(u) d_2(v}} \quad (8)$$

3. MAIN RESULTS

We take the physical properties of octane isomers from the website of the international academy of mathematical chemistry (http://www.iamc-online.org/) and show in Table 1. We calculate the topological indices of octane isomers and give the results in Table 2. We will use correlation coefficients technique to compare topological indices for modelling physical properties of octane isomers such as ; Entropy , Acentric factor (Acen Fac), Enthalpy of vaporization (HVAP) and Standard enthalpy of vaporization (DHVAP).
Those physicochemical properties of octane isomers are selected for which give reasonably good correlations, i.e. the absolute value of correlation coefficients are larger than 0.8 except from the properties HVAP and DHVAP for the old topological indices as; Wiener, Zagreb and Randić indices (see Table 3).

Table 1. Some physical properties of octane isomers

Molecule	Entropy	Ac.Fac.	HVAP	DHVAP
n-octane	111,70	0,39790	73,19	9,915
2-methyl-heptane	109,80	0,37792	70,30	9,484
3-methyl-heptane	111,30	0,37100	71,30	9,521
4-methyl-heptane	109,30	0,37150	70,91	9,483
3-ethyl-hexane	109,40	0,36247	71,70	9,476
2,2-dimethyl-hexane	103,40	0,33943	67,70	8,915
2,3-dimethyl-hexane	108,00	0,34825	70,20	9,272
2,4-dimethyl-hexane	107,00	0,34422	68,50	9,029
2,5-dimethyl-hexane	105,70	0,35683	68,60	9,051
3,3-dimethyl-hexane	104,70	0,32260	68,50	8,973
3,4-dimethyl-hexane	106,60	0,34035	70,20	9,316
2-methyl-3-ethyl-pentane	106,10	0,33243	69,70	9,209
3-methyl-3-ethyl-pentane	101,50	0,30690	69,30	9,081
2,2,3-trimethyl-pentane	101,30	0,30082	67,30	8,826
2,2,4-trimethyl-pentane	104,10	0,30537	64,87	8,402
2,3,3-trimethyl-pentane	102,10	0,29318	68,10	8,897
2,3,4-trimethyl-pentane	102,40	0,31742	68,37	9,014
2,2,3,3-tetramethylbutane	93,06	0,25529	66,20	8,410

Table 2. Topological indices of octane isomers

Molecule	W	M_1	M_2	R	LR
n-octane	84	26	24	3,914	4,914
2-methyl-heptane	79	28	26	3,770	4,606
3-methyl-heptane	76	28	27	3,808	4,230
4-methyl-heptane	75	28	27	3,808	4,678
3-ethyl-hexane	72	28	28	3,846	3,934
2,2-dimethyl-hexane	71	32	30	3,561	5,560
2,3-dimethyl-hexane	70	30	30	3,681	3,727
2,4-dimethyl-hexane	71	30	29	3,664	3,618
2,5-dimethyl-hexane	74	30	28	3,626	4,316
3,3-dimethyl-hexane	67	32	32	3,621	3,655
3,4-dimethyl-hexane	68	30	31	3,719	3,380
2-methyl-3-ethyl-pentane	67	30	31	3,719	3,474
3-methyl-3-ethyl-pentane	64	32	34	3,682	3,065
2,2,3-trimethyl-pentane	63	34	35	3,481	2,992
2,2,4-trimethyl-pentane	66	34	32	3,417	4,626
2,3,3-trimethyl-pentane	62	34	36	3,504	3,190
2,3,4-trimethyl-pentane	65	32	33	3,553	3,060
2,2,3,3-tetramethylbutane	58	38	40	3,250	2,333

Table 3. The correlation coefficients between new and old topological indices and some physicochemical properties of octane isomers

Index	Entropy	AcenFac	HVAP	DHVAP
LR	0,6345	0,7096	0,2934	0,4036
W	0,8772	0,9656	0,7381	0,8202
M_1	-0,9543	-0,9731	-0,8860	-0,9361
M_2	-0,9410	-0,9864	-0,7281	-0,8118
R	0,9063	0,9043	0,9359	0,9580

We can see from Table 3 that leap Zagreb index is not possible tool which give reasonably low correlation less than 0.71 for modeling chemiacal properties of of octanes. We visualize these low relations in Figures 1 to 4. Stacked area displays the ternd of percentage each value contributes over categories.

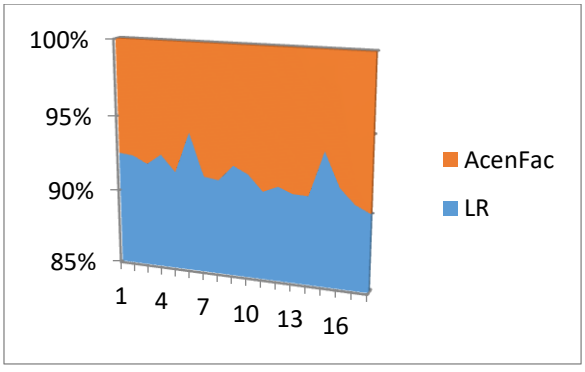

Figure 1. The stacked area graph between Acentric factor and leap Randić index

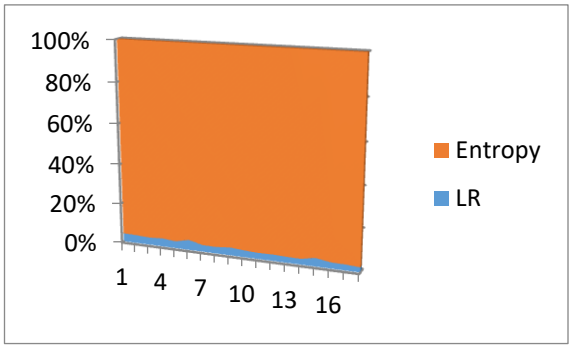

Figure 2. The stacked area graph between Entropy and leap Randić index

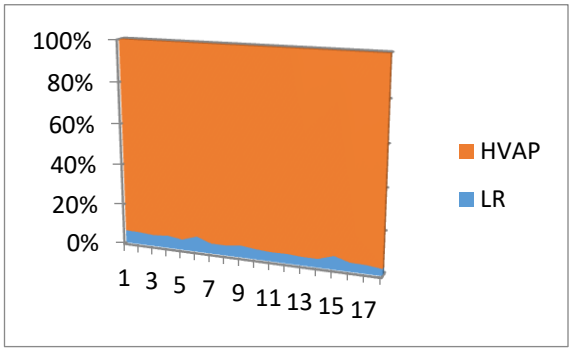

Figure 3. The stacked area graph between HVAP and leap Randić index

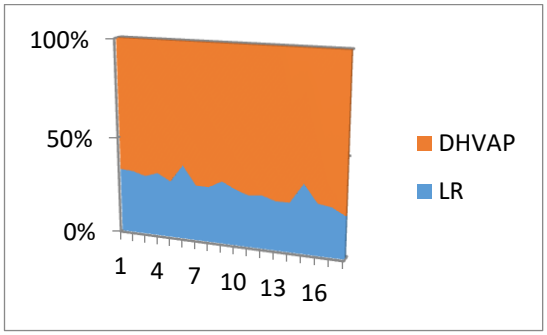

Figure 4. The stacked area graph between DHVAP and leap Randić index

The low relations between leap Zagreb index with chemical properties of octanes can bee seen visually clearly from the Figures 1-4.

And now, we compare leap Randić index with Wiener, Zagreb and Randić indices. We calculate and show the correlation efficients between indices in Table 4.

Table 4. The correlation coefficients between new and old topological indices

Index	W	M_1	M_2	R
LM	0,7673	-0,5779	-0,7711	0,4646

The correlation efficients, r, between leap Zagreb index and Wiener, Zagreb and Randić indices lie in the interval $0{,}45 < r < 0{,}77$ which indicates low correlation (Table 4). We display these low relations between leap Zagreb index and Wiener, Zagreb and Randić indices in the following Figures 5-8.

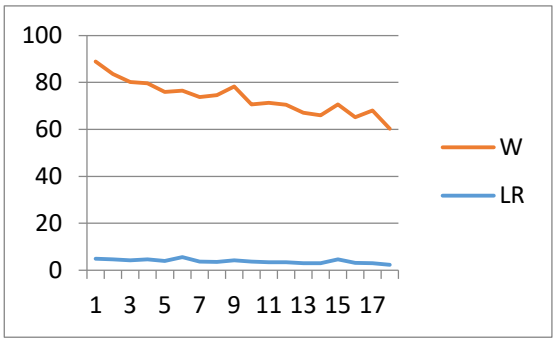

Figure 5. The relation of leap Randić index with Wiener index

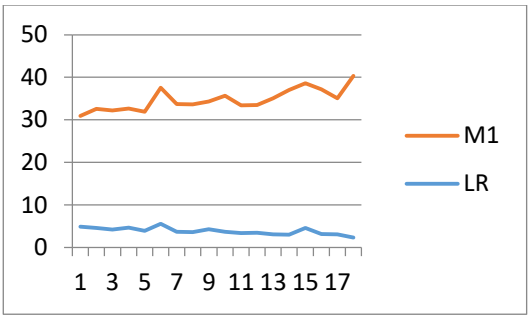

Figure 6. The relation of leap Randić index with the first Zagreb index

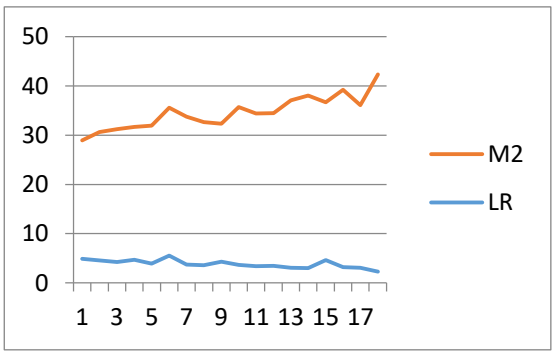

Figure 7. The relation of leap Randić index with the second Zagreb index

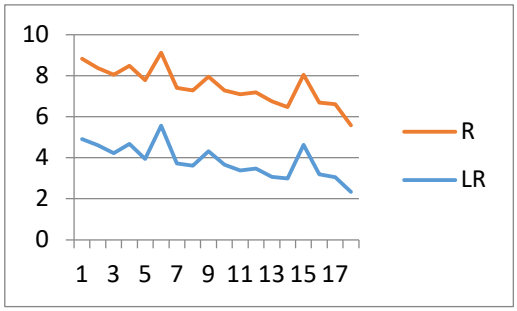

Figure 8. The relation of leap Randić index with Randić index

The low relations between leap Randić index with Wiener Zagreb and Randić indices can bee seen visually clearly from the Figures 5-8.

4. CONCLUSION

We firstly analyze the applicability of leap Randić index in view of QSPR studies by using entropy, acentric factor, enthalpy of vaporization and standard enthalpy of vaporization of octanes. We show that leap Randić index give low correlation for the chemical properties of octanes. Also leap Randić index has low relationship with Randić, Wiener and Zagreb indices. We conclude that leap Randić index is not a possible tool for QSPR studies.

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