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A note on QSPR analysis of total Zagreb and total Randić İndices of octanes

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Topological indices are important tools for QSPR researches. Wiener, Zagreb, and Randić indices are pioneers of topological indices as the most used topological indices in view of chemistry and chemical graph theory. These three topological indices have been used for modeling physical properties of octanes and other chemical molecules. We firstly define k-total distance degree notion, k-total Zagreb and k-total Randić indices in graph theory. We investigated the prediction power of 3-total Zagreb indices and 3-total Randić index by using some physical properties of octanes such as entropy, acentric factor, enthalpy of vaporizatian and standard enthalpy of vaporization. We showed that these 3-total distance degree based novel indices are possible tools for QSPR studies, which they give a reasonably good correlation greater than 0.92 for modeling acentric factor of octanes. We also showed that 3-total indices give a strong correlation with Wiener index and the second Zagreb index.

KEYWORDS

QSPR analysis; Zagreb indices; randić index; k-total Zagreb indices; k-total Randić index.

Introduction

Chemical graph theory has been accepted a bridge between chemistry and graph theory. Pictorial representations of molecules are corresponding chemical graphs. Topological indices are real numbers derived from chemical graphs *via* using mathematical formulas. Many QSPR studies are conducted by using topological indices. The first distance based topological index is Wiener index which was used for modelling boiling point of paraffins. The first degree based topological indices are Zagreb and Randić indices that are the most used topological indices for QSPR studies, especially modeling π-electron energy levels and molecular branching, respectively. A novel topological index has been accepted valuable in view of chemistry, if this topological index gives better correlation modelling; some physico-chemical properties of molecules are compared with classical Zagreb and Randić indices. We can give basic definitions which are necessary for our computations. 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-neighbourhood 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 [1, 3]. The ve-degree of a vertex v, $d_{ve}(v)$, is the number of different edges incident to vertices in $N_1(v)$ [2]. The ev-degree of an edge $e = uv$, $d_{ev}(e)$, is $d_{ev}(e) = d_1(u) + d_1(v) - n(e)$, where $n(e)$ denotes the number of triangles in G containing the edge e. For a vertex v, $e(v)$ denotes the number of edges in the shortest path between the vertex v and the farthest vertex from v. $e(v)$ is called the eccentricity of v. For a graph G, maximum eccentricity is called the diameter of G denoted as D and minimum eccentricity is called the radius of G denoted as r.

In this study, we firstly defined the k-total distance degree of a vertex v of G as; for $k \leq D$,

$$d_{tk}(v) = \sum_{i=1}^{k} d_i(v) \quad (1)$$

For $k = r$, k-total distance degree can be called as "total radius distance degree" and $k = D$, k-total distance degree can be called as "total diameter distance degree". Clearly for any vertex v of G, $\sum_{i=1}^{e(v)} d_i(v) = n - 1$ and for $e(v) < k$, $d_k(v) = 0$.

Wiener, the first and second Zagreb and Randić indices [3-5] of a simple connected graph G are defined as;

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

$$M_1(G) = \sum_{v \in V(G)} d(v)^2 \quad (3)$$

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v) \quad (4)$$

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}} \quad (5)$$

For a detailed discussion of Wiener, Zagreb and Randić indices, we refer to [6-16] and references therein for interested readers.

We now firstly define k-total first Zagreb index, k-total second Zagreb index, k-total third Zagreb index and k-total Randić index by using the k-total distance degree notion as parallel of the definitions of Zagreb and Randić indices as follows:

k-total first Zagreb index:

$$T_kM_1(G) = \sum_{v \in V(G)} d_{tk}(v)^2 \quad (6)$$

k-total second Zagreb index:

$$T_kM_2(G) = \sum_{uv \in E(G)} d_{tk}(u)d_{tk}(v) \quad (7)$$

k-total third Zagreb index:

$$T_kM_3(G) = \sum_{uv \in E(G)} (d_{tk}(u) + d_{tk}(v)) \quad (8)$$

k-total Randić index:

$$T_kR(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_{tk}(u)d_{tk}(v)}} \quad (9)$$

For $k = 1$:

- 1-total first Zagreb index and 1-total third Zagreb index are the same as the first Zagreb index,
- 1-total second Zagreb index is the same as the second Zagreb index,
- 1-total Randić index is the same as Randić index.

For $k = 2$:

- 2-total first Zagreb index is the sum of forgotten topological index with two times of the second Zagreb index,
- 2-total second Zagreb index of any triangle free graph is the same as the second ve-degree Zagreb index,
- 2-total third Zagreb index of any triangle free graph is the same as the first ve-degree Zagreb beta index,
- 2-total Randić index of any triangle free graph is the same as ve-degree Randić index.

For detailed discussions of ev-degree and ve-degree indices, see [17-43]. The prediction power of ev-degree and ve-degree indices is better than those of Zagreb and Randić [17-19].

Since for $k = 3$, these parameters are novel, we investigated the prediction power of 3-total Zagreb indices, 3-total Randić index by using some physical properties of octanes and compared these novel indices with Wiener, Zagreb and Randić indices in the next section.

Results

We took the physical properties of octane isomers from the website of the international academy of mathematical chemistry (http://www.iamc-online.org/) as shown in

Table 1. We calculated the topological indices of octane isomers and showed the results in Table 2. We will use correlation coefficients and regression analysis techniques to compare topological indices for modeling 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 there are reasonably good correlations, i.e. the absolute value of correlation coefficients is larger than 0.8 except from the properties HVAP and DHVAP (Table 3).

TABLE 1 Some physical properties of octane isomers

Molecule	Entropy	AcenFac	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	T_3M_1	T_3M_2	T_3M_3	T_3R
n-octane	84	26	24	3,914	238	223	78	1,333
2-methyl-heptane	79	28	26	3,770	297	251	83	1,238
3-methyl-heptane	76	28	27	3,808	300	281	88	1,151
4-methyl-heptane	75	28	27	3,808	302	292	90	1,128
3-ethyl-hexane	72	28	28	3,846	315	305	92	1,103
2,2-dimethyl-hexane	71	32	30	3,561	326	306	92	1,103
2,3-dimethyl-hexane	70	30	30	3,681	350	332	98	1,049
2,4-dimethyl-hexane	71	30	29	3,664	324	316	94	1,067
2,5-dimethyl-hexane	74	30	28	3,626	300	280	88	1,143
3,3-dimethyl-hexane	67	32	32	3,621	376	358	100	1,002
3,4-dimethyl-hexane	68	30	31	3,719	374	358	100	0,997
2-methyl-3-ethyl-pentane	67	30	31	3,719	378	368	102	0,979
3-methyl-3-ethyl-pentane	64	32	34	3,682	428	400	106	0,933
2,2,3-trimethyl-pentane	63	34	35	3,481	428	400	106	0,934
2,2,4-trimethyl-pentane	66	34	32	3,417	350	352	100	0,999
2,3,3-trimethyl-pentane	62	34	36	3,504	454	416	108	0,911
2,3,4-trimethyl-pentane	65	32	33	3,553	400	384	104	0,952
2,2,3,3-tetramethylbutane	58	38	40	3,250	512	448	112	0,875

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

Index	Entropy	Acen Fac	HVAP	DHVAP
T_3M_1	-0.8978	-0.9492	-0.6241	-0.7145
T_3M_2	-0.8614	-0.9510	-0.6483	-0.7369
T_3M_3	-0.8360	-0.9397	-0.6554	-0.7420
T_3R	0.8124	0.9242	0.6760	0.7574
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

TABLE 4 The correlation coefficients between new and old topological indices

Index	W	M_1	M_2	R
T_3M_1	-0.9531	0.8826	0.9832	-0.7742
T_3M_2	-0.9852	0.8668	0.9714	-0.7557
T_3M_3	-0.9880	0.8535	0.9564	-0.7466
T_3R	0.9885	-0.8376	-0.9335	0.7369

We can see from Table 3 that all these 3-total distance degree based novel indices are possible tools which give reasonably good correlation greater than 0.92 for modeling acentric factor of octanes. We visualize these strong relations in Figures 1 to 4. Stacked area displays the ternd of percentage each value contributes over categories.

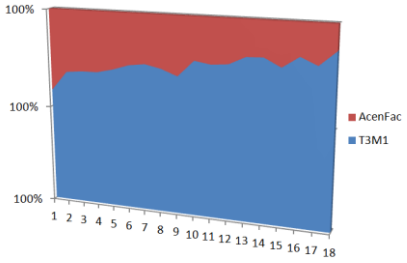

FIGURE 1 The stacked area graph between Acentric factor and 3-total first Zagreb index

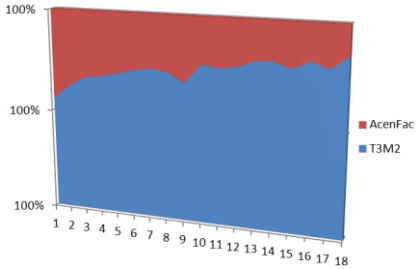

FIGURE 2 The stacked area graph between Acentric factor and 3-total second Zagreb index

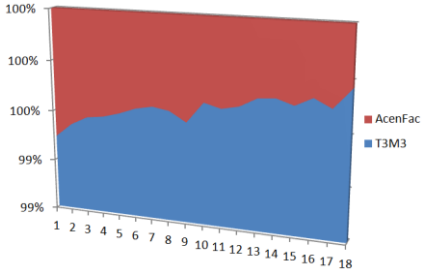

FIGURE 3 The stacked area graph between Acentric factor and 3-total third Zagreb index

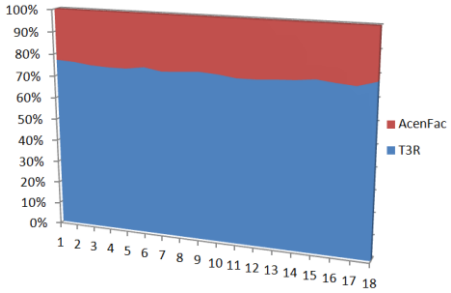

FIGURE 4 The stacked area graph between Acentric factor and 3-total Randić index

And now, we can investigate the relations between the old topological indices and the novel topological indices. The correlation coefficients between the Wiener, Zagreb, Randić indices and the 3-total Zagreb and Randić indices are shown in Table 4.

The correlation efficients between 3-total Zagreb and Randić indices and famous Wiener index is greater than 0.95, indicating very strong correlation (Table 4). This correlation may be expected due to total indices considered as distance based degree indices like Wiener index.

Also the correlation efficients between 3-total Zagreb and Randić indices and the second Zagreb index is greater than 0.93, also indicating a strong correlation (Table 4).

We display some of the these strong relations between 3-total indices and Wiener and the second Zagreb index in Figures 5-10 below.

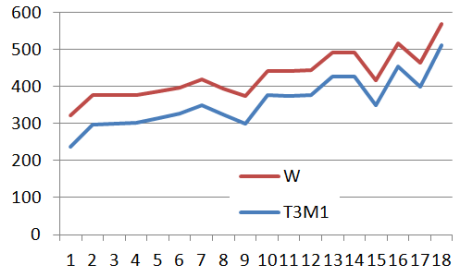

FIGURE 5 The relation of 3-total first Zagreb index with Wiener index.

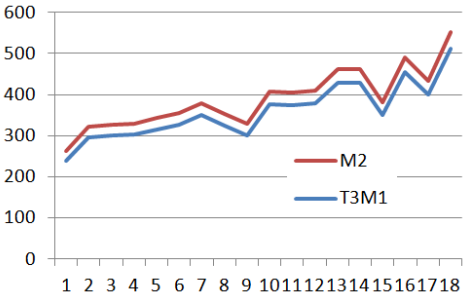

FIGURE 6 The relation of 3-total first Zagreb index with the second Zagreb index

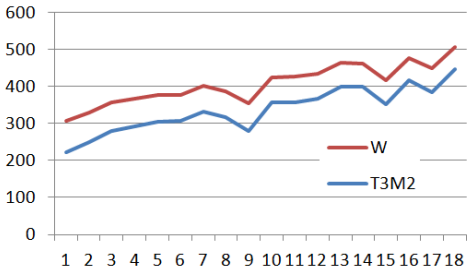

FIGURE 7 The relation of 3-total second Zagreb index with the Wiener index

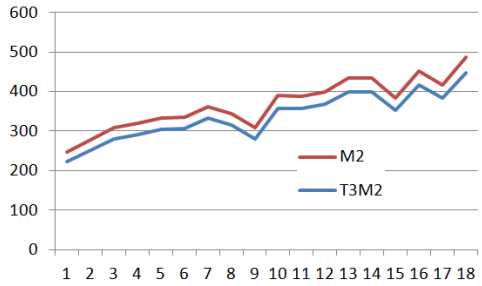

FIGURE 8 The relation of 3-total second Zagreb index with the second Zagreb index.

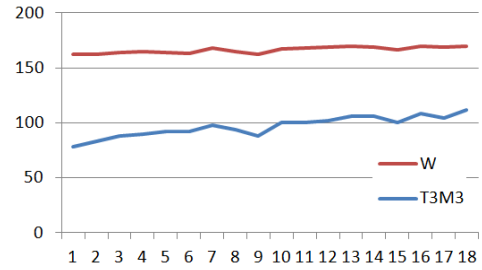

FIGURE 9 The relation of 3-total third Zagreb index with Wiener index

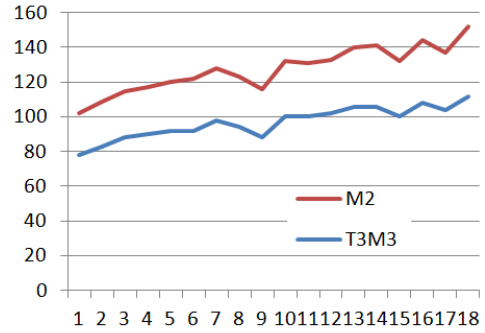

FIGURE 10 The relation of 3-total third Zagreb index with the second Zagreb index

The strong relations between 3-total indices with Wiener and the second Zagreb index can be clearly seen visually from the Figures 5-10.

Conclusion

We initially defined k-total distance degree notion as the sum of k-distance degrees ($k = 1,2,\dots,n$). By using this novel degree definition, we defined k-total first Zagreb index, k-total second Zagreb index, k-total third Zagreb index and k-total Randić index. We showed that these novel total indices are generalization of their classical degree-based

counterparts: Zagreb and Randić indices. For $k = 1$, these total indices are corresponding to Zagreb and Randić indices. For $k = 2$, these total indices are corresponding to ev-degree Zagreb and ev-degree Randić indices. For $k = 3$, these total indices are corresponding to novel graph invariants: 3-total Zagreb and 3-total Randić indices. We analysed predicting power of 3-total Zagreb and 3-total Randić indices by using some physico-chemical properties of octanes. Total indices gave strong correlations greater than 0.92 for modelling acentric factor of octanes. We showed that the correlation efficients between 3-total Zagreb and 3-total Randić indices with Wiener index is greater than 0.95 which indicates a very strong correlation. We also show that the correlation efficients between 3-total Zagreb and Randić indices with the second Zagreb index is greater than 0.93 that also indicates a strong correlation. Relying on these findings, we conclude that the 3-total indices are possible tools for QSPR studies. The following suggestions can be addressed by future studies about k-total indices:

- QSPR studies for other molecules for different values of *k*,
- Mathematical properties of k-total indices,
- Relations between total indices and other classical degree based topological indices,
- Total indices of drug structures and nanotubes,
- Other total type indices such as total geometric-arithmetic index, total sum-connectivity index, total harmonic index, total atom bond connectivity index.

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