

**A note on QSPR analysis of 3-total Wiener Polarity Index**

Süleyman Ediz

Van Yüzüncü Yıl University, Turkey, E-mail: [suleymanediz@yyu.edu.tr](mailto:suleymanediz@yyu.edu.tr)

İdris Çiftçi

Van Yüzüncü Yıl University, Turkey, E-mail: [iciftci@yyu.edu.tr](mailto:iciftci@yyu.edu.tr)

Süleyman Soygüder

Van Yüzüncü Yıl University, Turkey, E-mail: [soyguder78@yyu.edu.tr](mailto:soyguder78@yyu.edu.tr)

Murat Cancan

Van Yüzüncü Yıl University, Turkey, E-mail: [mcancan@yyu.edu.tr](mailto:mcancan@yyu.edu.tr)

Mehmet Şerif Aldemir

Van Yüzüncü Yıl University, Turkey, E-mail: [msaldemir@yyu.edu.tr](mailto:msaldemir@yyu.edu.tr)**ABSTRACT**

Topological indices are used in QSPR/QSAR studies to modeling physico-chemical properties of molecules. Wiener polarity index, is one of the oldest topological index together with Wiener index, was used to modeling paraffin boiling points. Recently k-total Wiener polarity index has been defined by mathematically. In this study, we examine 3-total Wiener polarity index whether is a possible tool or not for QSPR/QSAR researches. We show that 3-total Wiener polarity index gives better correlation to modeling acentric factor of octane isomers compared with the well-known topological indices such as; Wiener, Zagreb and Randić indices.

**Keywords:** QSPR analysis, QSAR analysis, k-total distance degree, k-total Wiener polarity index, 3-total Wiener polarity index

**Introduction**

Chemical graph theory is considered as the intersection of graph theory and chemistry. Molecules in chemistry are corresponding graphs in chemical graph theory. Structural properties of molecules are examined in QSAR/QSPR studies in chemistry. Topological indices are graph invariants which are real numbers corresponding graphs. Topological indices are frequently used in QSAR/QSPR studies to modeling chemical properties of chemical substances. The first and oldest topological indices are Wiener and Wiener polarity indices which were used in modeling boiling points of paraffin [1]. Wiener and Wiener polarity indices are distance based topological indices. Zagreb indices which are degree based

topological indices were used in modeling total  $\pi$ -electron energy of atoms [2]. Another well-known degree based topological index is Randić index which were used in molecular branching [3]. These indices are the most used topological indices are used in QSAR/QSPR studies. Recently, Ilić and Ilić have defined k-total Wiener polarity index as the sum of generalized Wiener indices [4]. They suggested that examination of chemical and mathematical properties of this novel index were interesting problem in future studies. Some of the present authors have studied mathematical properties of the k-total Wiener polarity index and gave closed formula of the k-total Wiener polarity index by defining k-total distance degree notion [5]. In this study, we show that 3-total Wiener polarity index gives better correlation to modeling acentric factor of octane isomers compared with Wiener, Zagreb and Randić indices.

### 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;  $d_k(v) = |N_k(v)|$  [6]. 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  $v$  [2,6]. The connection number was defined in order to find the electron energy of alternant hydrocarbons [2]. 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  $G$  and denoted as  $D$  and minimum eccentricity is called the radius of  $G$  and denoted as  $r$ . Wiener index and Wiener polarity index [1] of a simple connected graph were used as modelling boiling points of paraffins, defined as;

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

$$W_p(G) = \frac{1}{2} \sum_{v \in V(G)} d_3(v) \quad (2)$$

The authors in [4], defined generalized Wiener polarity index as;

$$W_k(G) = \frac{1}{2} \sum_{v \in V(G)} d_k(v) \quad (3)$$

and developed a linear time algorithm for trees and characterized extremal trees. For other studies about generalized Wiener polarity index see [7-10]. Clearly from equations 2 and 3,  $W_3(G) = W_p(G)$  and  $W_1(G) = m$  for any connected graph  $G$ .

The first and second Zagreb indices [2] of a simple connected graph  $G$  defined as;

$$M_1(G) = \sum_{v \in V(G)} d_1(v)^2 \quad (4)$$

$$M_2(G) = \sum_{uv \in E(G)} d_1(u)d_1(v) \quad (5)$$

Randić index [3] of a simple connected graph  $G$  defined as;

$$R(G) = \sum_{uv \in E(G)} (d_1(u)d_1(v))^{-1/2} \quad (6)$$

In [5], some of the present authors firstly defined the k-total distance degree of a vertex  $v$  of  $G$  as; for  $k \leq D$ ,

$$d_{tk}(v) = \sum_{i=1}^k d_i(v) \quad (7)$$

and k-total Wiener polarity index as;

$$W_k^*(G) = \frac{1}{2} \sum_{v \in V(G)} d_{tk}(v) \quad (8)$$

We proved that;

$$W_3^*(T) = \frac{1}{2} M_1(T) + W_p(T) \quad (9)$$

in [5]. By using this useful equality and some physical properties of octane isomers we calculate 3-total Wiener polarity index is considered as a novel molecular descriptor in view of chemical graph theory in the next section.

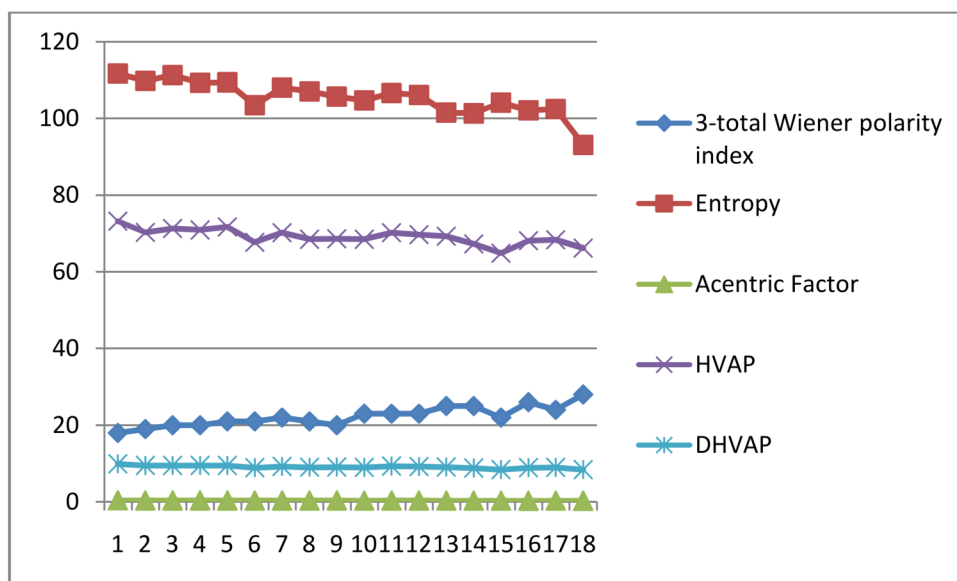
## Results

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 and regression analysis techniques to compare well-known topological indices such as Zagreb, Wiener, Randic indices with 3-total Wiener polarity index for modelling physical properties of octane isomers.

**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

We can summarize the information in Table 1 with the values of 3-total Wiener polarity index of octane isomers in Fig. 1

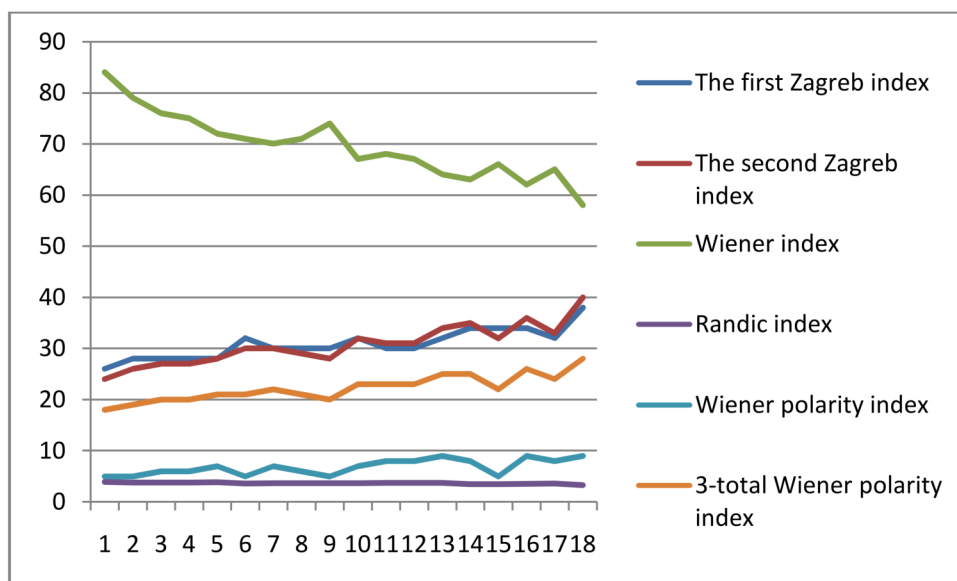


**Fig. 1.** Physical properties of octane isomers

**Table 2.** Topological indices of octane isomers

Molecule	$M_1$	$M_2$	W	R	$W_p$	$W_3^*$
n-octane	26	24	84	3,914	5	18
2-methyl-heptane	28	26	79	3,770	5	19
3-methyl-heptane	28	27	76	3,808	6	20
4-methyl-heptane	28	27	75	3,808	6	20
3-ethyl-hexane	28	28	72	3,846	7	21
2,2-dimethyl-hexane	32	30	71	3,561	5	21
2,3-dimethyl-hexane	30	30	70	3,681	7	22
2,4-dimethyl-hexane	30	29	71	3,664	6	21
2,5-dimethyl-hexane	30	28	74	3,626	5	20
3,3-dimethyl-hexane	32	32	67	3,621	7	23
3,4-dimethyl-hexane	30	31	68	3,719	8	23
2-methyl-3-ethyl-pentane	30	31	67	3,719	8	23
3-methyl-3-ethyl-pentane	32	34	64	3,682	9	25
2,2,3-trimethyl-pentane	34	35	63	3,481	8	25
2,2,4-trimethyl-pentane	34	32	66	3,417	5	22
2,3,3-trimethyl-pentane	34	36	62	3,504	9	26
2,3,4-trimethyl-pentane	32	33	65	3,553	8	24
2,2,3,3-tetramethylbutane	38	40	58	3,250	9	28

We can summarize the information in Table 2 in Figure 2.



**Fig. 2.** Topological indices of octane isomers

We calculate and show the correlation coefficients between the properties and topological indices in Table 3.

**Table 3.** The correlation coefficients between the properties and topological indices

Index	Entropy	AcenFac	HVAP	DHVAP
3-total Wiener Polarity Index	-0.8906	-0.9488	-0.6062	-0.7049
Wiener Polarity Index	-0.6148	-0.6975	-0.1885	-0.3107
Wiener Index	0.8772	0.9656	0.7381	0.8202
The First Zagreb Index	-0.9543	-0.9731	-0.8860	-0.9361
The Second Zagreb Index	-0.9410	-0.9864	-0.7281	-0.8118
Randić Index	0.9063	0.9043	0.9359	0.9580

We see from the Table 3 that 3-total Wiener polarity index give second good correlation with the property acentric factor. This information enables us to consider 3-total Wiener polarity index as novel topological index in QSAR/QSPR studies.

We calculate and show the correlation coefficients between the 3-total Wiener polarity index and topological indices in Table 4.

**Table 4.** The correlation coefficients between the 3-total Wiener polarity index and topological indices

Index	W	M <sub>1</sub>	M <sub>2</sub>	R	W <sub>p</sub>
3-total Wiener Polarity Index	-0.9609	0.8747	0.9838	-0.7596	0.8818

We can see from the Table 4 that 3-total Wiener polarity index gives very good correlation with the second Zagreb index and Wiener index.

We calculate and show the regression equations between the properties and 3-total Wiener Polarity index in Table 5.

**Table 5.** The regression equations of 3-total Wiener Polarity index and physical properties of octane isomers (X denotes 3-total Wiener Polarity index)

Index	Entropy	AcenFac	HVAP	DHVAP
3-total Wiener Polarity Index	-1,542X+139,774	-0,013X+0,623	-0,471X+79,656	-0,103X+11,434

We calculate and show the regression equations between the 3-total Wiener polarity index and topological indices in Table 6.

**Table 6.** The regression equations of the 3-total Wiener polarity index and topological indices X denotes 3-total Wiener Polarity index)

Index	W	M <sub>1</sub>	M <sub>2</sub>	R	W <sub>p</sub>
3-total Wiener Polarity Index	-2,385X +122,696	0,982X +9,007	1,491X +2,496	-0,048X +4,721	0,508X +4,503

## Conclusion

We show that 3-total Wiener polarity index is a novel molecular descriptor to modelling chemical properties of octane isomers. Also, we analyze that 3-total Wiener polarity index gives very good correlation with the well-known topological indices such as; Wiener, Wiener polarity, Randić and Zagreb indices. Studying mathematical and chemical properties of k-total Wiener index are interesting problems for future studies for specific values of k.

## References

- 1) H. Wiener, Structural determination of paraffin boiling points, J. Amer. Chem. Soc. 69, (1947), pp. 17–20.
- 2) I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. III. total  $\pi$ -electron energy of alternant hydrocarbons. Chem. Phys. Lett. 17, (1972), pp. 535–538.
- 3) M. Randić, On characterization of molecular branching. J. Am. Chem. Soc. 97 (1975), pp. 6609–6615.
- 4) A. Ilić and M. Ilić, Generalizations of Wiener polarity index and terminal Wiener index, Graphs and Combinatorics, 29(5), (2013), pp.1403-1416.
- 5) S. Ediz, İ. Çiftçi, M. Cancan, M.R. Farahani, On k-total Distance Degrees and k-total Wiener polarity index (Submitted)

- 6) A. M. Naji, N. D. Soner, I. Gutman, The first leap Zagreb index of some graph operations. *Communications in Combinatorics and Optimization*, 3(2), (2017), pp.179-194
- 7) Y. Wu, F. Wei, B. Liu, Z. Jia , The generalized (terminal) Wiener polarity index of generalized Bethe trees and coalescence of rooted trees, *MATCH Commun. Math. Comput. Chem* 70(2),(2013): pp. 603-620.
- 8) Y. Wu, F. Wei, Z. Jia, The generalized Wiener polarity index of some graph operations. *Iranian Journal of Mathematical Chemistry*, 4(2), (2013), pp. 177-183.
- 9) H. Bielak, K. Dąbrowska, K. Wolska, On the generalized Wiener polarity index for some classes of graphs, *Federated Conference on Computer Science and Information Systems (FedCSIS) 2015*, IEEE.
- 10) J. Yue, H. Lei, Y. Shi, On the generalized Wiener polarity index of trees with a given diameter. *Discrete Applied Mathematics*, 243, (2018), pp.279-285.