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RESEARCH ARTICLE

DETERMINATION OF PHYSICAL-CHEMICAL PROPERTIES OF TITANIUM ORGANIC COMPOUNDS USING TOPOLOGICAL INDICES; QSPR TECHNIQUES

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ABSTRACT

Topological indices are defined based on graph theory and are the constants of graph, which are used to study quantitative structure activity relationship (QSAR) and quantitative structure Properties relationship (QSPR). This graph describes the simplest connection of atoms in a molecule (Zarrabian, 2000). In this article we will randomly choose a number of organic compounds of titanium and calculating four topological indices: Wiener, Harary, Balaban and Randic. Then we try to fit a model to predict the physical and chemical properties of some organic compounds of titanium. To offer this model, the physical and chemical properties of the samples were calculated using the Gaussian software. The results indicate good agreement on the application of topological indices Harary and Randic, to predict the physical and chemical properties.

INTRODUCTION

Today, the production and development of chemical compounds requires long time and a lot of financial costs. This process is more important, particularly in the pharmaceutical and use of new drugs because of the high financial costs over the long run; however, the success rate is very low (Zarrabian, 2000; Thayer, 2000; Wilson, 2000). Therefore, it is very important to use the techniques of (QSAR) and (QSPR) to predict physical and chemical properties. Topological indices are constant of graph, used to study quantitative structure activity relationship (QSAR) and quantitative structure Properties relationship (QSPR) (Consonni, 2009; Van de Waterbeemd, 1992; Van de Waterbeemd, 1993). In addition to mathematics, graph theory is used in physics, chemistry, pharmacology, genetics, and also some other sciences. In physics and chemistry the graph theory has been applied to a wide range of research fields (Bonchev, 1983). Topological indices in graph theory are defined based on distance and the simple descriptors that indicate the type of valances between the atoms in a molecule. They are independent of the molecule spatial structures. These indices are widely used to illustrate the relationship between molecular structure and physical and chemical properties (Trinajstic, 1992; Ezra, 1982).

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Topological indices were first used in chemistry and biology in 1947 by Wiener with the introduction of Wiener index (W) which described the relationship between thermodynamic properties and molecular structure (Wiener, 1947). Following Weiner, others (Randic 1975, Harary1991 and Balaban1982) tried to introduce various indices to describe the properties of a substance based on its molecular structure. In 1975, Randic introduced the index (χ), and demonstrated a good relationship between the graph of chemical compounds and some physical and chemical properties (Razinger, 1985; Randic, 1975). Harary index (H), introduced by Harary in 1991, influenced the development of chemical graphs (Plavsic, 1993). Balaban index (J), introduced in 1982, has high performance to describe the thermodynamic properties of molecules with benzene rings (Balaban, 1982).

Definitions

A graph is a non-empty set of objects called vertices (V) with the connected edges (E), to form G = G (V, E). A molecular graph is a simple graph. Those atoms of a molecule are vertices, and the bonds between the atoms are the edges of the graph. In chemical graphs, hydrogen atoms are removed and discarded (Bonchev, 1983). The Wiener number, W=W (G) of G, introduced as the path number, is defined as the half-sum of the elements of the distance matrix (Hosaya, 1971).

$$W = (\frac{1}{2}) \sum_{i=1}^{N} \sum_{J=1}^{N} d_{ij} \quad (1)$$

d_{ij} is the distance between vertices i and j, and N is the number of vertices. The Randic index χ is defined as (Seybold, 1987):

$$\chi = \sum_{all\ edges} [D(i)D(j)\ ]^{-1/2} \quad (2)$$

Where D (i) and D (j) are the bonds of the vertices i and j
The balaban index, J=J (G) of G, was introduced as the average - distance sum connectivity (Balaban, 1982):

$$J = \left(\frac{m}{\mu+1}\right) \sum_{all\ edges} [d_i d_j]^{-1/2} \quad (3)$$

That m is the total number of valences, μ is the number of loops (μ=m-N+1) and d_i is given by (Balaban, 1982):

$$d_i = \sum_{J=1}^{N} d_{ij} \quad (4)$$

And the Harary number, H=H (G) of G, is defined below (Razinger, 1985; Randic, 1975):

$$H = (\frac{1}{2}) \sum_{i=j}^{N} \sum_{j \neq i}^{N} d_{ij}^{-1}. \quad (5)$$

MATERIALS AND METHODS

Titanium and its compounds are known to be one of the most used elements, mostly in industries like: technology, medicine, pharmacy and Environmental Sciences.

For example, titanium dioxide nanoparticles are widely used due to the photo-catalytic and self-cleaning properties and can be easily produced from organic compounds of titanium (Khakpoor, 2013; Kavei, 2013). Therefore, predicting physical and chemical properties of organic compounds of titanium is very important. The purpose of this paper is to provide a simple method based on graph theory to predict the physical and chemical properties of these compounds. That's why 17 randomly organic compounds of titanium (titanium carboxide) were selected and four topological indices, Wiener, Randic, Balaban, and Harary were calculated for these compounds. Using the software, Gaussian, two properties of Exact Mass and Log (P) were calculated for these compounds. Following, the method of calculating, the four indices for one of the 17 samples are expressed.

Sample calculations

To calculate the topology indices, the molecule $C_6H_{14}O_2Ti$ was selected. Thus, consider the graph structure of the molecule $C_6H_{14}O_2Ti$, as shown in Fig.1.

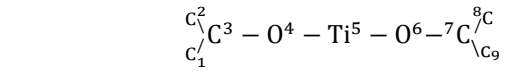

Fig.1. The graph structure of the molecule $C_6H_{14}O_2Ti$

Table 1 shows the distance matrix for these molecules. Using the matrix elements of Table 1, in the equations (1), Wiener number for graph C6H14O2Ti molecule is equal to W=108. The Inverse distance matrix elements have relationship for C6H14O2Ti, calculation, and are provided in Table 2. Using Table 2, the equation (5) gives 17.226 for Harary index value (H=17.226). Using the equations (2) and (3), Randic index for $C_6H_{14}O_2Ti$ molecule Fig.1, is equal to 4.13, and Balaban index is 2.91.

Table 1. The distance matrix for $C_6H_{14}O_2Ti$

	1	2	3	4	5	6	7	8	9	$d_i=\sum_{J=1}^{N} d_{ij}$
1	0	2	1	2	3	4	5	6	6	29
2	2	0	1	2	3	4	5	6	6	29
3	1	1	0	1	2	3	4	5	5	22
4	2	2	1	0	1	2	3	4	4	19
5	3	3	2	1	0	1	2	3	3	18
6	4	4	3	2	1	0	1	2	2	19
7	5	5	4	3	2	1	0	1	1	22
8	6	6	5	4	3	2	1	0	2	29
9	6	6	5	4	3	2	1	2	0	29

Table 2. The inverse distance matrix for $C_6H_{14}O_2Ti$

	1	2	3	4	5	6	7	8	9	$\sum_{J\neq i}^{N} d_{ij}^{-1}$
1	0	0.5	1	0.5	0.333	0.25	0.2	0.17	0.17	3.12
2	0.5	0	1	0.5	0.333	0.25	0.2	0.17	0.17	3.12
3	1	1	0	1	0.5	0.333	0.25	0.2	0.2	4.483
4	0.5	0.5	1	0	1	0.5	0.333	0.25	0.25	4.333
5	0.333	0.333	0.5	1	0	1	0.5	0.333	0.333	4.34
6	0.25	0.25	0.333	0.5	1	0	1	0.5	0.5	4.333
7	0.2	0.2	0.25	0.333	0.5	1	0	1	1	4.483
8	0.17	0.17	0.2	0.25	0.333	0.5	1	0	0.5	3.12
9	0.17	0.17	0.2	0,25	0.333	0.5	1	0.5	0	3.12

RESULTS

Seventeen different samples of titanium dioxide organic compounds were selected and for them, the Wiener (W), Harary (H), Randic (χ), and Balaban (J) indices were calculated. The results are summarized in Table 4. To study the physical and chemical properties, using the software Gaussian, and two properties of Exact Mass and Log (P) were calculated.

Table 3. The Wiener, Harary, Randic and Balaban indices for seventeen organic compounds of titanium dioxide

Chemical formula	IUPAC name	W	H	X	J
C_3H_7Oti	(propan-2-yloxy)titanium	18	6.67	2.27	2.54
$C_6H_{14}O_2Ti$	bis(propan-2-yloxy)titanium	108	17.22	4.13	2.91
$C_6H_{15}O_3Ti$	triethoxytitanium	138	20.45	4.85	3.30
$C_8H_{20}O_4Ti$	tetraethoxytitanium	256	32.23	6.24	4.19
$C_9H_{21}O_3Ti$	tris(propan-2-yloxy)titanium	270	31.65	5.91	3.87
$C_9H_{21}O_3Ti$	tripropoxytitanium	300	30.13	6.35	3.47
$C_{10}H_{24}O_3Ti$	Methyltris(propan-2-yloxy)titanium	310	36.65	6.25	4.32
$C_{12}H_{27}O_3Ti$	tris(tert-butoxy)titanium	444	45.35	6.79	4.53
$C_{12}H_{27}O_3Ti$	tris(2-methylpropoxy)titanium	516	42.06	42.06	3.85
$C_{12}H_{27}O_3Ti$	tributoxytitanium	555	40.56	40.56	3.58
$C_{12}H_{28}O_4Ti$	tetrakis(propan-2-yloxy)titanium	504	49.97	49.97	4.89
$C_{12}H_{28}O_4Ti$	dibutoxydiethoxytittanium	576	47.08	8.24	4.25
$C_{16}H_{36}O_4Ti$	tetrakis(2-methylpropoxy)titanium	968	66.13	9.67	4.85
$C_{16}H_{36}O_4Ti$	tetrabutoxytitanium	1041	63.71	10.24	4.52
$C_{30}H_{62}O_5Ti$	tributoxytitaniooctadecanoate	5856	128.73	17.64	4.06
$C_{32}H_{68}O_4Ti$	tetrakis((2-ethylhexyl)oxy)titanium	4560	148.86	17.97	5.79
$C_{72}H_{148}O_4Ti$	tetrakis(octadecyloxy)titanium	48640	345.69	38.24	4.97

Table 4. Exact Mass and Log (P) for seventeen organic compounds of titanium dioxide

Chemical formula	Log(P)	Exact. Mass(g/mol)
C_3H_7Oti	.95	106.997
$C_6H_{14}O_2Ti$	1.89	166.047
$C_6H_{15}O_3Ti$	1.6	183.050
$C_8H_{20}O_4Ti$	2.14	228.084
$C_9H_{21}O_3Ti$	2.84	225.128
$C_9H_{21}O_3Ti$	3.01	225.097
$C_{10}H_{24}O_3Ti$	2.85	240.120
$C_{12}H_{27}O_3Ti$	3.08	267.143
$C_{12}H_{27}O_3Ti$	4.22	267.143
$C_{12}H_{27}O_3Ti$	4.20	267.143
$C_{12}H_{28}O_4Ti$	3.79	284.146
$C_{12}H_{28}O_4Ti$	3.87	284.146
$C_{16}H_{36}O_4Ti$	5.62	340.209
$C_{16}H_{36}O_4Ti$	5.60	340.209
$C_{30}H_{62}O_5Ti$	10.71	550.440
$C_{32}H_{68}O_4Ti$	11.96	564.459
$C_{72}H_{148}O_4Ti$	27.79	1125.085

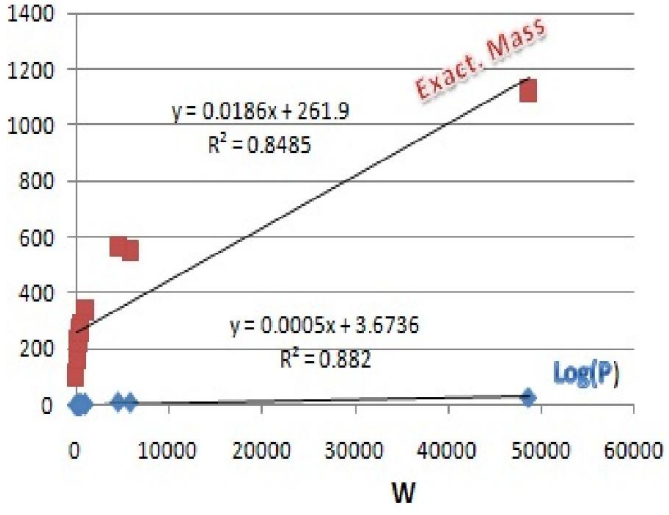

Fig. 2. The Exact Mass and Log (P) versus Wiener index

The values calculated by the Gaussian software are given in Table 4.

Fig. 2 shows, the changes Exact Mass and Log (P), versus Wiener index, based on data given in Table 4 and Table 4.

Fig. 2 shows that with the Wiener index, the properties of Exact Mass and Log (P) cannot be predicted. With The changes of exact mass and Log (P) versus Balaban index, shown in Fig.3, the same results were obtained.

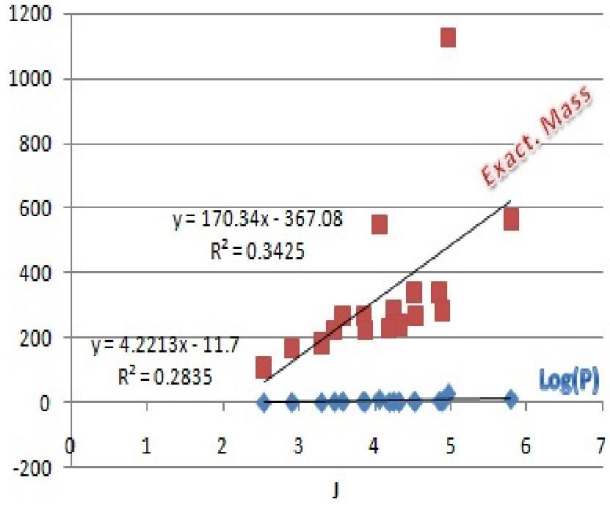

Fig.3. The Exact Mass and Log (P) versus Balaban index

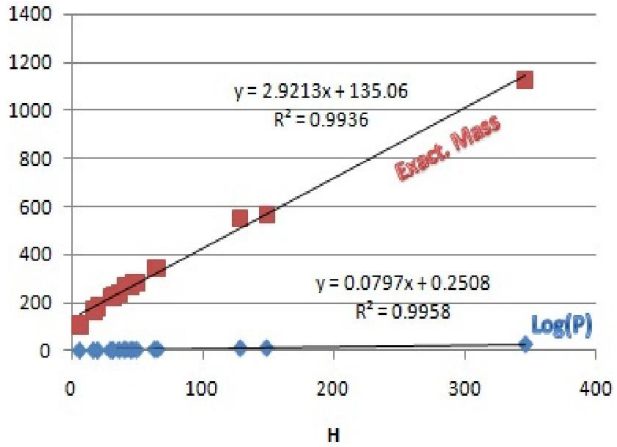

Fig. 4. The Exact Mass and Log (P) versus Harary index

Therefore, we conclude that the Balaban index, similar to Wiener index, isn't a good criterion to predict these properties.

In Fig. 4 and Fig. 5, using Table 4, the Changes of Log (P) and Exact Mass, versus Harary index (H), and Randic index (χ) is shown. As shown in Fig. 4, the Harary index of carboxide titanium can be predicted very carefully for Log (P) and Exact Mass.

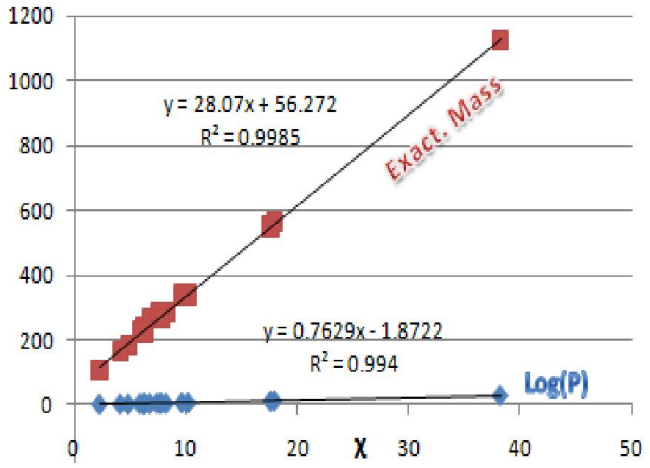

Fig. 5. The Exact Mass and Log (P) versus Randic index

The Log (P) and Exact Mass for these compounds versus Harary index (H), gives by:

$$\text{Log (P)} = 0.0797\ H + 0.2508 \quad (6)$$
$$\text{Exact Mass} = 2.9213\ H + 135.06 \quad (7)$$

In Fig. 5, with Table 4, the changes of exact mass and log (P) are drawn versus the index Randic. Fig. 5 shows that the Randics index, as well as Harary index, can be used to predict these properties. The equations describing these properties are as follows:

$$\text{Log (P)} = 0.7629\ \chi - 1.8722 \quad (8)$$
$$\text{Exact Mass} = 28.07\ \chi + 56.272 \quad (9)$$

Conclusion

The results of
Fig. 2, Fig.3, Fig. 4 and Fig. 5, show that the two indices, Wieners, and Balaban, cannot be used to determine Log (P), and Exact Mass, of titanium organic compounds.

Although both indices, Harary and Randic, can predict these properties, but Harary index determines the Log (P) more carefully. In contrast, the index Randic, can be a better predictor for exact mass measurements.

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