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**The Structural Relationship Between Topological Indices and Some  
Thermodynamic Properties**

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**ABSTRACT**

The fact that the properties of a molecule are tightly connected to its structural characteristics is one of the fundamental concepts in chemistry. In this connection, graph theory has been successfully applied in developing some relationships between topological indices and some thermodynamic properties. So, a novel method for computing the new descriptors to construct a quantitative relation between structure and properties is presented. At first, a brief review on the classical graph theories introduced and, then, the link with molecular similarity is drawn. In the applications section, molecular topological indices are calculated. Afterwards, the molecular descriptors, that include the necessary structural information for proper description of system are employed to derive a numerical correlation with thermodynamic properties. Finally, some useful topological indices for examination of the structure-property relationship are presented. In addition, the relationship between the Randić<sup>1</sup>, Wiener, Hosoya, Balaban and Schultz indices and Harray numbers and Distance matrix to the enthalpies of formation ( $\Delta H^{\circ}_f$ ), heat capacities, (Cp), enthalpies of combustion ( $\Delta H^{\circ}_c$ ), enthalpies of vaporization ( $\Delta H^{\circ}_{vap}$ ) and normal boiling points (*bpK*) for C<sub>2</sub> – C<sub>10</sub> normal alcohols is established.

**Keywords:** Thermodynamic properties; Topological indices; Alcohol; Graph theory; QSAR; QSPR

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## INTRODUCTION

Chemical graph theory is a branch of mathematical chemistry, and consequently of theoretical chemistry. It is concerned with handling chemical graphs, that represent chemical systems. Hence, chemical graph theory deals with analyses of all consequences of connectivity in a chemical system. In other words, chemical graph theory is concerned with all aspects of the application of graph theory to chemistry area.

Quantitative Structure- Activity Relationship (QSAR) research field has been widely developed, from its very beginnings when, in 1865, Crum-Brown and Fraser postulated a relationship between any physiological activity and the corresponding chemical structure [1]. Later, Richet[2] correlated toxicities with their solubility in water and, in 1900, Meyer and Overton [3,4] found linear relationships between the toxicity of organic compounds and their lipophilicity. Hammett also has reported the Linear Free Energy Relationship, applied to the description of electronic properties of aromatic systems [5]. However, the currently used QSAR methodology did not evolve since, in the 60s, when Hansch and Fujita published a free-energy related model to correlate biological activities with physicochemical properties [6]. The main assumption underlying in theoretical foundation [7-11] consists of considering that chemical structure contains necessary information about activities. Assuming this very first premise, QSAR model would be capable of quantifying the connection between the structure and molecular properties by means of a mathematical model. More recently, other widely developed field in QSAR studies is the inclusion of three-dimensional parameters in the description of compounds to predict biological properties [12-16].

In this paper, a variant of QSAR studies, the so-called Quantitative Structure-Property Relationships (QSPR), using topological indices as molecular descriptors [21-25], is used. The incredibly great number of works devoted to this has led to the appearance of hundreds of new indices, which are useful to

describe with more or less accuracy specific properties of given compounds.

In the last few years, also the necessity of describing the three – dimensional character of molecular structures has contributed to the development of three – dimensional indices [26]. The main application of topological descriptors is to quantitatively correlate structures and properties of biologically active compounds [27]. But it has to be taken into account that, whereas chemical structures are discrete entities, their properties show a continuous variation, expressed within a certain numerical range.

The classical topological approach [28, 29] relates the chemical structure constitution (the two – dimensional model of a molecule, which is represented by a structural formulae) with a non – dimensional numerical entity, the so – called topological index. In this correspondence, each structure has a single associated descriptor, but not vice versa; one index may correspond to more than a graph. Here arises the problem of the degeneracy; so it is desirable that the working indices present low degeneracy.

To translate chemical structures into a single number, the graph theory visualizes chemical structures as mathematical object sets consisting of vertices or points, which symbolize atoms, and vertices or lines, linking a pair of edges, which represent covalent bonds or shared electron pairs. In this notation, adjacent vertices stand for pairs of covalently linked atoms situated at a topological distance equal to unit.

### Classical topological indices

A large number of topological indices have been defined and used. The majority of the topological indices are derived from the various matrices corresponding to the molecular graphs. The Adjacency matrix (A) and the Distance matrix (D) of the molecular graph have been most widely used in the definition of topological indices. Although a number of topological indices have been reported but only a handful of them have been

successfully employed in QSAR/QSPR studies.

In computing, a graph is stored by means of matrices that account for adjacency and distance. Particularly, the most commonly used indices in graph theoretical representation can be coded by means of an attached Adjacency matrix (A), whose elements are composed by one if the associated atoms are considered directly connected, and by zero otherwise. From the adjacency matrix elements, topological indices are mathematically derived in a direct and unambiguous manner. These indices account for molecular size and shape at the same time and, depending on the case, they can also include a simple kind of three-dimensional information. Also, the Distance matrix (D), which accounts for the topological length of the shortest path between two atoms, and the valence vector, calculated as the sum of entries in  $i$ -th row or  $j$ -th column of topological matrix, which indicates if an atom is primary, secondary, tertiary or quaternary, are essentially used. Table 1 shows the definition of the above-mentioned matrices, being  $n$  the number of atoms in the molecule and  $n_b$  the length of the shortest path between the vertices  $i$  and  $j$ .

**Table 1.** Classical matrices used in chemical graph theory

$$A_{ij} = \begin{cases} 1 & \text{if atoms } i \text{ and } j \text{ are bonded} \\ 0 & \text{if atoms } i \text{ and } j \text{ are not bonded} \end{cases} \quad A(n * n)$$

$$D_{ij} = \begin{cases} 0 & \text{if } i = j \\ n_b & \text{if } i \neq j \end{cases} \quad D(n * n)$$

From these basic definitions, a large number of Topological Indices has been formulated (30-36). Various definitions of topological indices have been used in order to obtain molecular descriptors. The most used ones are presented below:

**Wiener index:** The Wiener index (Wiener, 1947 a,b; Randić et al., 1993; Sardana and Madan, 2003), a well-known distance-based topological index is defined as:

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

where  $P_i$  is the length of the path that contains the least number of edges between vertex  $i$  and vertex  $j$  and  $N$  is the maximum possible number of  $i$  and  $j$  [5].

**Hosoya index:** The Hosoya index,  $Z = Z(G)$ , was defined in 1971 [2], for non-directed graphs, as follows:

$$Z = \sum_{i=0}^{N/2} P^{(G,i)} \quad (2)$$

where  $P^{(G,i)}$  is the number of selections of  $i$  mutually non-adjacent edges in  $G$ . By definition,  $P^{(G,0)} = 1$ , and  $P^{(G,i)}$  is the number of edges in  $G$ . The Hosoya index was firstly used to correlate several thermodynamic quantities of saturated hydrocarbons, such as the boiling point.

**Randić index:** The Randić index was introduced by Randić in 1975, as the connectivity index [9]. Based in the classification of bonds in molecular graphs, the Randić index is one of the most widely used topological indices in quantitative structure-reactivity relationship (QSAR) analysis [10]. Randić classified the kind of bond between atoms, depending on the number of atoms bonded to each terminal vertex. The Randić index is defined as [1,7,20,27]:

$$X = \sum_{\text{all edges}} \left( d(i) \cdot d(j) \right)^{-0.5} \quad (3)$$

where  $d(i)$  and  $d(j)$  are the valencies of the vertices  $i$  and  $j$  that define the edge  $ij$ .

**Balaban index:** The Balaban index,  $J = J(G)$  of  $G$  was introduced in 1982 [21] as one of the less degenerated indices. It calculates the average distance sum connectivity index, according to the equation:

$$J = \frac{M}{\mu + 1} \sum_{\text{all edges}} \left( (D)_i \cdot (D)_j \right)^{-0.5} \quad (4)$$

where  $M$  is the number of the edges in  $G$ ;  $\mu$  is the cyclomatic number of

$G$  ; and  $(D)_i$  is the distance sum where  $i = 1, 2, \dots, N$ .

The cyclomatic number  $\mu = \mu(G)$  of a polycyclic graph  $G$  is equal to the minimum number of edges that must be removed from  $G$  to transform it to the related acyclic graph. For trees,  $\mu = 0$  ; for monocycles ,  $\mu = 1$ .

The distance sum  $(D)_i$  for a vertex  $i$  of  $G$  represents a sum of all entries in the corresponding row of the distance matrix.

$$(D)_i = \sum_{j=1}^N (D)_{ij} \quad (i = 1, 2, \dots, N) \quad (5)$$

Clearly the Wiener number can also be expressed in terms of the distance sums.

$$W = \frac{1}{2} \sum_{i=1}^N (D)_i \quad (6)$$

**Schultz index:** The Schultz index (MTI) was introduced by Schultz in 1989, as the molecular topological index [22]. It takes into account the effect of adjacency and distance matrices and the valence vector, and it is computed as:

$$MTI = \sum_{i=1}^N e_i \quad (7)$$

Where the  $e_i$ 's ( $i = 1, 2, \dots, N$ ) represent the elements of the following row matrix of order  $N$ .

$$V[A + D] = [e_1 e_2 \dots e_N]$$

Where  $v$  is the valency row matrix ,  $A$  is the adjacency matrix , and  $D$  is the distance matrix.

**Harary number:** The Harary number ( $H$ ) was introduced in 1991 by Plavsic et al., [23] in honor of Professor Frank Harary , due to his influence on the development of graph theory and , especially , to its application in chemistry . This index is defined from the inverse of the squared elements of the distance matrix according to the expression:

$$H = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N (D_{ij})^{-2} \quad (8)$$

Where  $D^{-2}$  is the matrix whose elements are the squares of the reciprocal distances.

## Graphs

For drawing the graphs of our results, we used the Microsoft Office Excel – 2003 program.

## Mathematical methods

The values of the determinants of Distance matrixes ( $D$ ) and six molecular topological indices discussed in this report (equs1-8) were shown in Table 2. The determinants were solved by using MAPLE – 9.01 package implemented to a PC – computer.

The boiling Points ( in K) of the alcohols are taken from the CRC Hand book of Chemistry and Physics [37] and Beilstein [38].The thermodynamic values of Table 2 are from The NBS Tables of Chemical Thermodynamic Properties (1982), and NIST Chemistry Web Book.

## Discussion and Designing the QSPR Models

A graph –theoretical approach to QSPR is based on the use of topological indices for encoding the structural informations. The topological index term indicates a characterization of a molecule (or a corresponding molecular graph by a single number) .The need to represent molecular structure by a single number arises from the fact that most molecular properties are recorded as single numbers. Therefore, QSPR modeling reduces to a correlation between the two sets of numbers via an algebraic expression. (One set of numbers represents the properties, and the other set represents the structures of molecules under study.)

A novel method for computing the new descriptors to construct QSPR is presented. First, a brief review on the classical graph theory is presented and, then, the link with molecular similarity is drawn. In the applications section, molecular topological indices are calculated. After wards, the molecular descriptors, which include the structural information necessary to properly describe the system, are employed to derive numerical correlation with property.

The values of the determinant of the Distance matrixes of considered alcohols ( $C_2 - C_{10}$ ) increase with increasing number of carbons. According to the data of Tables 2&3 the

logarithmic values of the Distance matrixes and six topological indices increase by increasing the values of  $C_p$ ,  $\Delta H_{vap}^o$  and  $bp$  (K) while the values of  $\Delta H_f^o$  and  $\Delta H_c^o$  decrease by increasing the above topological indices.

In Figs. 1-6, two dimensional diagrams showing the relationship between appropriate characteristic parameters (such as Randic' index (X), Harary number (H), and the values of  $\Delta H_c^o$ ,  $\Delta H_{vap}^o$ ,  $C_p$ ,  $bp(K)$ ,  $\Delta H_f^o$  liquid,  $\Delta H_f^o$  gas of considered alcohols are illustrated). The resultant curves, show highly correlation between the respect values. It is noticeable that some relationship such as Distance matrix (D), Wiener index (W), Hosoya index (Z), Balaban index (J), against the values of  $\Delta H_c^o$ ,  $\Delta H_{vap}^o$ ,  $C_p$ ,  $bp(K)$ ,  $\Delta H_f^o$  liquid and  $\Delta H_f^o$  gas for the  $(C_2 - C_{10})$  alcohols are not linear. Now these nonlinear curves are not included.

Figs.7-12, show the relations of  $\log Z$  or  $\log (D)$  against  $\Delta H_c^o$ ,  $\Delta H_{vap}^o$ ,  $C_p$ ,  $bp(K)$ ,  $\Delta H_f^o$  liquid and  $\Delta H_f^o$  gas. These curves, show a good correlation between the considered values.

Fig.13, shows the three -dimensional relationship between Harary number (H), Randic index (X) and  $\Delta H_{vap}^o$ . Fig.14, shows the three -dimensional relationship between  $\log (D)$ ,  $\log (Z)$  and  $\Delta H_f^o$  gas. These three -dimensional plots demonstrate the comparative relations between  $\log(Z)$  and  $\log(D)$  versus  $\Delta H_f^o$  gas and Randic' index (X), Harary number (H) versus  $\Delta H_{vap}^o$  of the alcohols.

There are several ways to design the QSPR models. Here we outline one possible strategy which contains six steps:

**Step 1.** To get a reliable source of experimental data for a given set of molecules. This initial set of molecules is sometimes called the training set[39]. The data in this set must be reliable and accurate. The quality of the selected data is important because it will affect all the following steps.

**Step 2.** The topological index is selected and computed. This is also an important step because

selecting the appropriate topological index (or indices) can facilitate finding the most accurate model.

**Step 3.** The two sets of numbers are then statistically analyzed using a suitable algebraic expression.

The QSPR model is thus a regression model, and one must be careful about its statistical stability. Chance factors could yield spuriously accurate correlations[40]. The quality of the QSPR models can be conveniently measured by the correlation coefficient  $r$  and the standard deviation  $s$ . A good QSPR model must have  $r > 0.99$ , while  $s$  depends on the property. For example, for boiling point,  $s < 5^\circ C$ . Therefore, Step 3 is a central step in the design of the structure-property models.

**Step 4.** Predictions are made for the values of the molecular property for species that are not part of the training set via the obtained initial QSPR model. The unknown molecules are structurally related to the initial set of compounds.

**Step 5.** The predictions are tested with unknown molecules by experimental determination of the predicted properties. This step is rather involved because it requires acquiring or preparing the test molecules.

We will apply the procedure from the preceding section, to give an instructive example of the design of the QSPR model for predicting the boiling point of alcohols. As the initial set we will consider alcohols with up to 4 carbon atoms (11 molecules). The thermodynamic properties of these alcohols are taken from [37,38], and the molecular topological indices such as the Randic index (X), Harary number (H), logarithmic values of Hosoya indices (Z), Distance matrixes (D) of the above mentioned are calculated (see table 4).

The following structure-property models are the most successful for the Randic' index (X),

Harary number (H), logarithmic values of Distance matrixes (D) and Hosoya index (Z) considered:

$$\Delta H_{vap}^o = 0.001X^3 + 0.0381X^2 + 9.7543X + 32.638 \quad R^2=0.9986 \quad (9)$$

$$\Delta H_f^o gas = -0.0079X^3 - 0.0089X^2 + 4.3476X + 19.288 \quad R^2=0.9994 \quad (10)$$

$$\Delta H_f^o liquid = 0.4991X^3 - 4.8822X^2 + 65.134X + 217.21 \quad R^2=0.9998 \quad (11)$$

$$\Delta H_c^o = 1.2539X^3 - 12.244X^2 + 168.52X - 18.874 \quad R^2=0.9999 \quad (12)$$

$$bp = 0.4154X^3 - 4.5535X^2 + 53.585X + 302.15 \quad R^2=0.9999 \quad (13)$$

$$Cp = 1.0812X^3 - 9.7246X^2 + 91.456X + 29.978 \quad R^2=0.9998 \quad (14)$$

$$\Delta H_{vap}^o = -0.0003H^3 - 0.0067H^2 + 3.5303H + 38.791 \quad R^2=0.9989 \quad (15)$$

$$\Delta H_f^o gas = 0.0147H^3 - 0.4315H^2 + 18.965H + 33.848 \quad R^2=0.9999 \quad (16)$$

$$\Delta H_f^o liquid = -0.0004H^3 - 0.0083H^2 + 1.5536H + 22.028 \quad R^2=0.99795 \quad (17)$$

$$\Delta H_c^o = 0.0443H^3 - 1.2515H^2 + 54.747H + 83.749 \quad R^2=1 \quad (18)$$

$$bp = 0.0154H^3 - 0.4778H^2 + 17.108H + 334.54 \quad R^2=0.9999 \quad (19)$$

$$Cp = 0.0397H^3 - 0.9307H^2 + 28.346H + 84.672 \quad R^2=0.9998 \quad (20)$$

$$\Delta H_{vap}^o = -0.3325(\log Z)^3 + 1.6528(\log Z)^2 + 21.52\log Z + 35.834 \quad R^2=0.9984 \quad (21)$$

$$\Delta H_f^o gas = -0.2575(\log Z)^3 + 0.5318(\log Z)^2 + 9.5857\log Z + 20.7 \quad R^2=0.9993 \quad (22)$$

$$\Delta H_f^o liquid = 4.8504(\log Z)^3 - 17.649(\log Z)^2 + 139.65\log Z + 237.47 \quad R^2=0.9998 \quad (23)$$

$$\Delta H_c^o = 11.944(\log Z)^3 - 43.253(\log Z)^2 + 361.35\log Z + 33.701 \quad R^2=0.9999 \quad (24)$$

$$bp = 4.0423(\log Z)^3 - 17.5441(\log Z)^2 + 114.26\log Z + 318.75 \quad R^2=0.9999 \quad (25)$$

$$Cp = 11.733(\log Z)^3 - 38.625(\log Z)^2 + 192.11\log Z + 58.293 \quad R^2=0.9997 \quad (26)$$

$$\Delta H_{vap}^o = 1.8247(\log D)^3 - 1.9881(\log D)^2 + 7.0556\log D + 38.172 \quad R^2=0.9991 \quad (27)$$

$$\Delta H_f^o gas = 0.3186(\log D)^3 + 1.1249(\log D)^2 + 0.4136\log D + 22.818 \quad R^2=0.9995 \quad (28)$$

$$\Delta H_f^o liquid = 7.6858(\log D)^3 - 4.2283(\log D)^2 + 31.481\log D + 257.82 \quad R^2=0.9999 \quad (29)$$

$$\Delta H_c^o = 18.791(\log D)^3 - 4.0047(\log D)^2 + 70.427\log D + 91.435 \quad R^2=1 \quad (30)$$

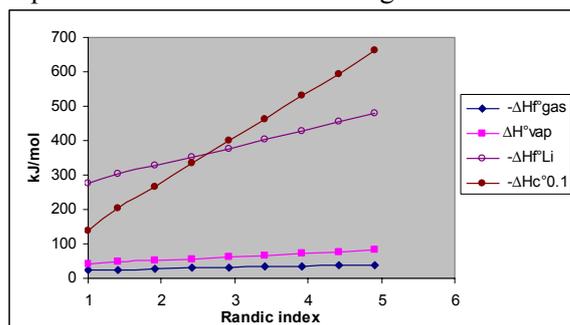
$$bp = -1.0117(\log D)^3 + 8.3456(\log D)^2 + 28.941\log D + 351.08 \quad R^2=0.9998 \quad (31)$$

$$Cp = -0.7864(\log D)^3 + 11.167(\log D)^2 + 48.844\log D + 111.88 \quad R^2=0.9997 \quad (32)$$

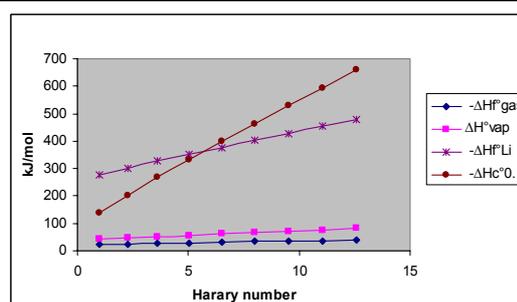
We used eqs 9-32 to predict  $\Delta H_c^o$ ,  $\Delta H_f^o$ ,  $\Delta H_{vap}^o$ ,  $C_p$ ,  $bp(K)$  of mentioned alcohols. The resultant boiling points are shown in table 5. Comparison of the predicted boiling points with the experimental values of the alcohols revealed that eqs 19 and 31 are not quite suitable for predicting the bp (K) of these alcohols, while the other equations are fairly adequate for predicting the respect thermodynamic properties.

## CONCLUSION

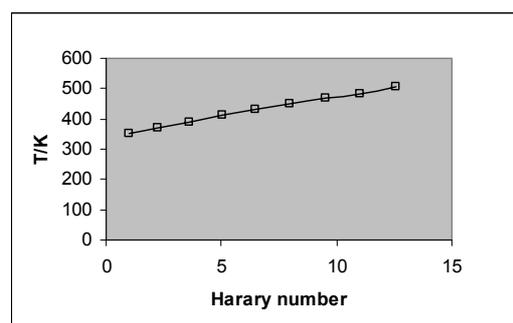
Graph theory has provided the chemists with a variety of very useful tools that can be used to predict many interesting physical and chemical properties of considered materials. Regarding this aspect we have presented a strategy for designing the quantitative structure – property relationships based on topological indices. The instructive example was directed to the design of the structure – property model for predicting the enthalpies of formation, heat capacities, enthalpies of combustion, enthalpies of vaporization and the boiling points of some alcohols. Six selected topological indices and distance matrix were tested. The correlation of the Randic index (x), Harary number (H), logarithm values distance matrix and Hosoya index (Z) with  $\Delta H_f^o$  liquid,  $\Delta H_f^o$  gas,  $\Delta H_{vap}^o$ ,  $\Delta H_c^o$ ,  $C_p$  and  $bp(K)$  appeared to have better results than the other indices. Meanwhile, the discussion of relationship between respected theoretical and experimental areas became straightforward.



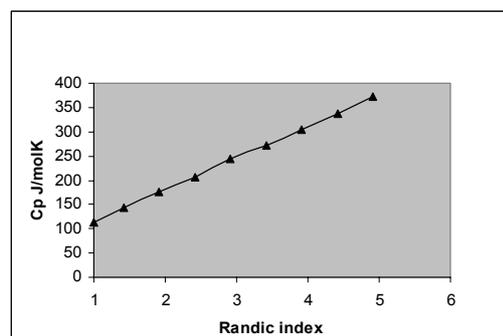
**Fig.1.** Plots of the Randic indices(X) versus  $\Delta H_{vap}^o$ ,  $\Delta H_f^o$  (gas,liquid),  $\Delta H_c^o$  for the  $C_2 - C_{10}$  normal alcohols.



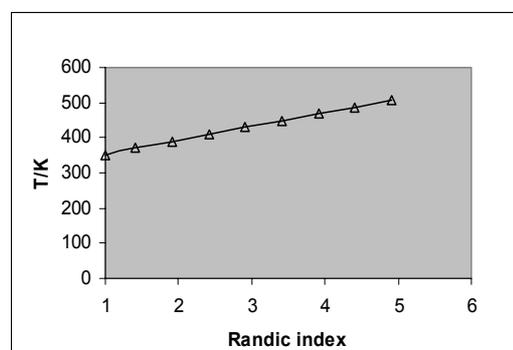
**Fig.2.** Plots of the Harary number(H) versus  $\Delta H_{vap}^o$ ,  $\Delta H_f^o$  ( gas,liquid),  $\Delta H_c^o$  for the  $C_2 - C_{10}$  normal alcohols.



**Fig.3.** Plots of the Harary number(H) versus bp(K) for the  $C_2 - C_{10}$  normal alcohols.



**Fig.4.** Plots of the Randic indices(X) versus  $C_p$  for the  $C_2 - C_{10}$  normal alcohols.



**Fig.5.** Plots of the Randic indices(X) versus bp(K) for the  $C_2 - C_{10}$  normal alcohols.

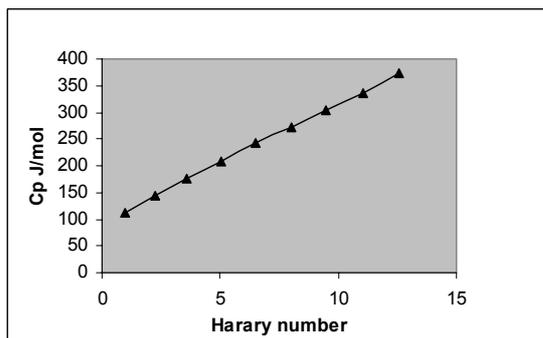


Fig.6. Plots of the Harary number(H) versus Cp for the  $C_2 - C_{10}$  normal alcohols.

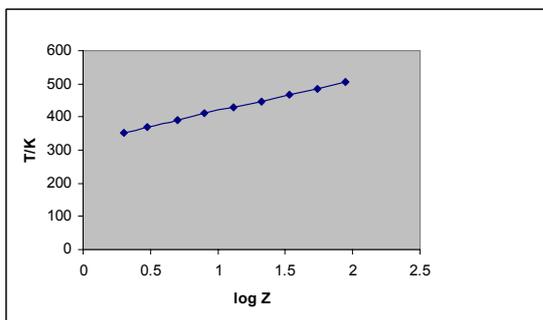


Fig.7. Plots of the log (Z) versus bp(K) for the  $C_2 - C_{10}$  normal alcohols.

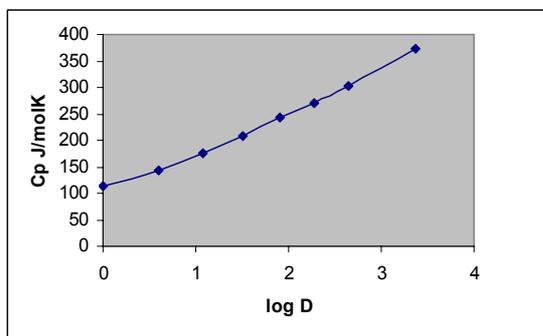


Fig.8. Plots of the log (D) versus Cp for the  $C_2 - C_{10}$  normal alcohols.

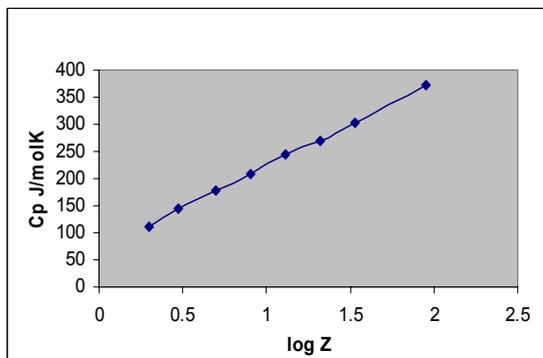


Fig.9. Plots of the log (Z) versus Cp for the  $C_2 - C_{10}$  normal alcohols.

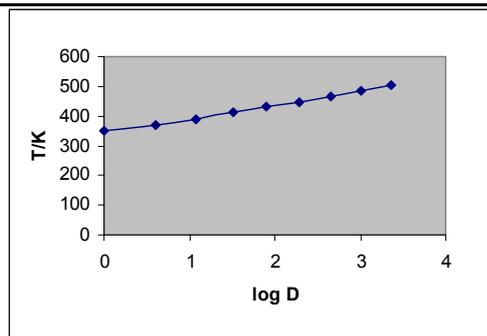


Fig.10. Plots of the log (D) versus bp(K) for the  $C_2 - C_{10}$  normal alcohols.

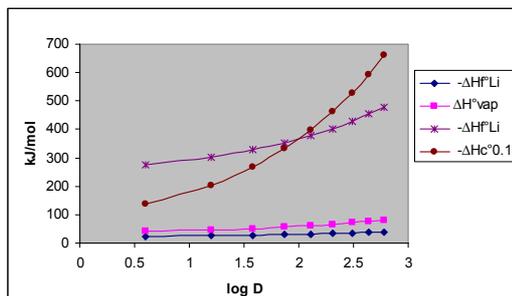


Fig.11. Plots of the log (D) versus  $\Delta H_{vap}^o$ ,  $\Delta H_f^o$  (gas,liquid),  $\Delta H_c^o$  for the  $C_2 - C_{10}$  normal alcohols.

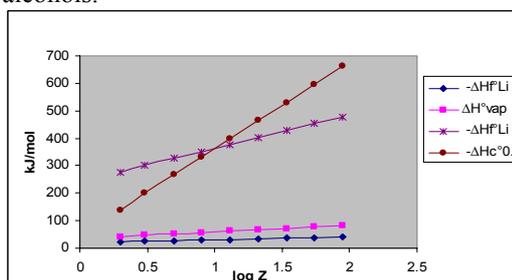


Fig.12. Plots of the log (Z) versus  $\Delta H_{vap}^o$ ,  $\Delta H_f^o$  (gas, liquid),  $\Delta H_c^o$  for the  $C_2 - C_{10}$  normal alcohols.

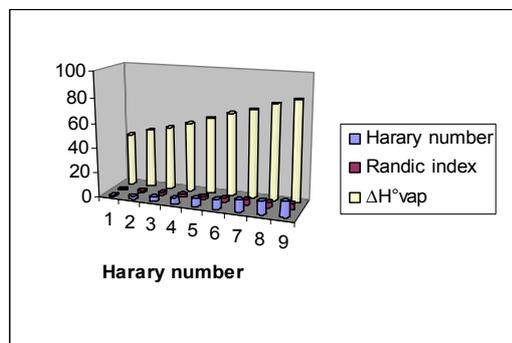
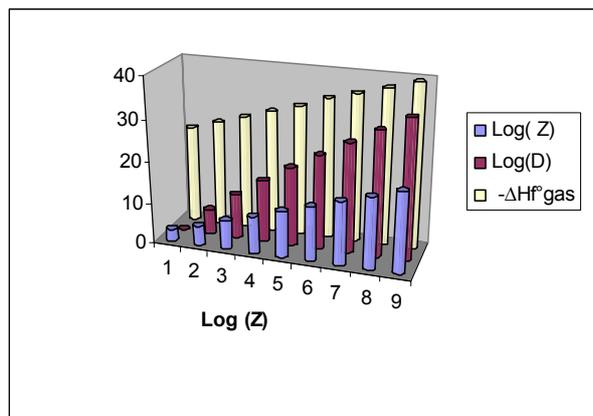


Fig.13. The three dimensional relationship between the Harary number (H), Randic index (X) and  $\Delta H_{vap}^o$  for the  $C_2 - C_{10}$  normal alcohols.



**Fig.14.** The three dimensional relationship between  $\log(Z)$ ,  $\log(D)$  and  $-\Delta H_f^\circ \text{ gas}$  for  $C_2 - C_{10}$  normal alcohols.

Table 2. The value of Randic indices(X), Distance matrixs (D), Wiener numbers(W), Hosoya indices(Z), Balaban indices(J), Schultz indices (MTI), Harary numbers(H) and  $\Delta H_f^\circ \text{ liquid}$ ,  $\Delta H_f^\circ \text{ gas}$ ,  $\Delta H^\circ_c$ ,  $C_p$ ,  $\Delta H^\circ_{\text{vap}}$  and Boiling points(bp in K) of Alcohols ( $C_2 - C_{10}$ ) (at Pressure of 1 bar & at 298K)

Alcohol	X	D	W	Z	J	MTI	H	$\frac{\Delta H_f^\circ \text{ gas}}{\text{kJmol}^{-1}}$	$\frac{\Delta H_f^\circ \text{ liquid}}{\text{kJmol}^{-1}}$	$\frac{C_p}{\text{Jmol}^{-1}\text{K}^{-1}}$	$\frac{\Delta H^\circ_{\text{vap}}}{\text{kJ.mol}^{-1}}$	T(K)	$\frac{\Delta H^\circ_c}{\text{kJ mol}^{-1}}$
Ethanol	1	1	1	2	1	4	1	-235.3	-277	112.4	42	351.5	-1367.6
Propanol	1.4142	4	4	3	1.6330	16	2.2500	-255.6	-302.54	143.96	47.5	370.3	-2021.31
Butanol	1.9142	12	10	5	1.9747	38	3.6111	-275.28	-328	176.67	51	390.6	-2670
Pentanol	2.4142	32	20	8	2.1906	74	5.0347	-295.63	-351.62	207.45	56	411	-3330.91
Hexanol	2.9142	80	35	13	2.3391	128	6.4983	-314.7	-337.5	243.2	61.61	430	-3984.37
Heptanol	3.4142	192	56	21	2.4475	204	7.9897	-339.7	-403.4	270.8	66.81	448	-4637.8
Octanol	3.9142	448	84	34	2.5301	306	9.5015	-356.9	-426.6	304	70.98	468	-5294
Nonanol	4.4142	1024	120	55	2.5951	438	11.0289	-375.6	-453.6	337	76.86	485	-5946
Decanol	4.9142	2304	165	89	2.6476	604	12.5687	-395.2	-478.1	372.98	81.5	505	-6619

Table 3. Logarithm values of Randic' indices (X), Distance matrixs (D), Wiener numbers (W), Hosoya indices (Z), Balaban indices (J), Schultz indices (MTI), Harary numbers (H)

Alcohol	log X	log D	log W	log Z	log J	log MTI	log H
Ethanol	0	0	0	0.3010	0	0.6020	0
Propanol	0.1505	0.6020	0.6020	0.4771	0.2130	1.2041	0.3522
Butanol	0.2820	1.0792	1	0.6990	0.2955	1.5798	0.5576
Pentanol	0.3828	1.5051	1.3010	0.9031	0.3406	1.8692	0.7020
Hexanol	0.4645	1.9031	1.5441	1.1139	0.3690	2.1072	0.8128
Heptanol	0.5333	2.2833	1.7482	1.3222	0.3887	2.3096	0.9025
Octanol	0.5926	2.6513	1.9243	1.5315	0.4031	2.4857	0.9778
Nonanol	0.6448	3.0103	2.0792	1.7404	0.4141	2.6415	1.0425
Decanol	0.6914	3.3625	2.2175	1.9494	0.4228	2.7810	1.0993

Table 4. The values of Randic indices (X) and Harary numbers (H), logarithmic values of Hosoya indices (Z), Distance matrixes of respect alcohols

Alcohol	X	H	Z	log (Z)	D	log (D)
2,2,4-trimethylpentanol	3.4165	10.4306	19	1.2787	320	2.5051
2,2-dimethyloctanol	4.5607	13.2751	60	1.7782	8448	3.9267
2,2-dimethylheptanol	4.0607	11.7225	37	1.5682	1024	3.0103
2-methyl propanol	1.7321	3.7500	4	0.6021	12	1.0792
3,3- dimethylpentanol	3.1213	8.7292	16	1.2041	208	2.3181
2,3- dimethylbutanol	2.6427	6.9444	10	1	80	1.9031
3-ethylheptanol	4.3461	11.4794	52	1.7160	1024	3.0103
3-methylhexanol	3.3081	8.2831	19	1.2787	192	2.2833
2-methylbutanol	2.2701	5.2222	7	0.8451	32	1.5051
2-methylnonanol	4.7701	12.8064	76	1.8808	2304	3.3625
4-methylheptanol	3.8081	9.8369	30	1.4771	448	2.6513

**Table 5.** Comparison between predicted (four model) and experimental values of normal boiling point (K) of respect alcohols

Alcohol	bp(exp)/K	bp(cal)/K				$\Delta[(bp_{exp} - bp_{calc})]$			
		model (13)	model (19)	model (25)	model (31)	model (13)	model (19)	model (25)	model (31)
2,2,4-trimethylpentanol	438.15	448.64	478.48	444.62	413.95	-10.49	-40.33	-6.47	24.2
2,2-dimethyloctanol	481.15	491.23	513.48	489.18	532.15	-10.08	-32.33	-8.03	-51
2,2-dimethylheptanol	464.92	472.47	494.24	470.38	486.23	-7.55	-29.32	-5.46	-21.31
2-methyl propanol	380.80	383.46	392.80	382.07	393.30	-2.66	-12	-1.27	-12.5
3,3- dimethylpentanol	440.15	437.67	457.71	437.95	450.41	2.48	-17.56	2.2	-10.26
2,3- dimethylbutanol	415.00	419.62	435.46	419.51	429.41	-4.62	-20.46	-4.51	-14.41
3-ethylheptanol	479.65	483.13	491.26	483.58	486.23	-3.48	-11.61	-3.93	-6.58
3-methylhexanol	445.35	444.62	452.22	444.62	448.63	0.73	-6.87	0.73	-3.28
2-methylbutanol	402.00	405.19	413.04	405.22	410.10	-3.19	-11.04	-3.22	-8.1
2-methylnonanol	495.15	499.20	507.62	498.48	504.29	-4.05	-12.47	-3.33	-9.14
4-methylheptanol	455.85	463.09	471.25	462.27	467.62	-7.24	-15.4	-6.42	-11.77

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