Application of Graph Theory to Some Thermodynamic Properties and Topological Indices

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ABSTRACT

The relationship between the Randic$^{/}$, Wiener, Hosoya , Balaban, Schultz indices, Harary numbers and Distance matrix to enthalpies of formation $\left(\Delta H^{o}{}_{f}\right)$, heat capacity, (Cp) , enthalpies of combustion $\left(\Delta H^{o}{}_{c}\right)$, enthalpy of vaporization $\left(\Delta H^{o}vap\right)$ and normal boiling points $\left(bpK\right)$ of $C_{2} - C_{10}$ normal alkanes is represented.

Keywords : QSAR ; QSPR; Topological indices; Alkanes; Graph Theory; Molecular structure.

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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 is, 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.

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. Hereinafter, Hammett also 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, 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 in considering that chemical structure contains information about activities. Assuming this very first premise, QSAR models quantify 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 studied. 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 with in 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 descriptor associated, 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 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 one.

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

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

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

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 one are presented below:

Wiener index: In 1947, Wiener introduced the Wiener Path Number [30], which can be defined as the total number of bonds among all the Paris of atoms in a graph. The number of path can be calculated from the topological distance matrix as the half – sum of the elements of this matrix:

$$W = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} D_{ij} \tag{1}$$

Hosoya index: The Hosoya index, Z = Z(G) , Was defined in 1971[31], for non – directed graphs , as follows :

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

where $P^{(G,i)}$ is the number of selections of i mutually non – adjacent edges in G.

By definition, $P^{(G,0)} = 1$, and $P^{(G,1)}$ is the number of edges in G.

The Hosoya index was firsty used to correlate with several of the thermodynamic quantities of saturated hydrocarbons, such as the boiling point.

Randic index: The Randic$^{/}$ index was introduced by Randic$^{/}$ in 1975, as the connectivity index [32]. Based in the Classification of bonds in molecular graphs, is one of the most widely used topological indices in quantitative structure – reactivity relationship (QSAR) analysis. Randic$^{/}$ classified the kind of bond between atoms, depending on the number of atoms bonded to each terminal vertex.

The Randic$^{/}$ index is defined as:

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

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

Balaban index: Balaban index, J = J(G) of G was introduced in 1982 [33] as one of the less degenerated indices. It calculates the average distance sum connectivity index, according to the equation:

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

where M is the number of edges in G ; μ is the cyclomatic number of G ; and $(D)_i$ is the distance sum where i = 1,2,...,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, $\mu = o$; 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.

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

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

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

Schultz index: The Schultz index (MTI) was introduced by Schultz in 1989 , as the molecular topological index [34]. It takes into account the effect of adjacency and distance matrices and the valence vector, and it is computed as:

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

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

$$V[A+D] = [e_1 e_2 ... e_N]$$

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 , [35] in honor of professor Frank Harary , due to his influence in 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:

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

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

Mathematical methods
The value 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 cocern with the above matrixes solved by using MAPLE – 9.01 package implemented to a PC – computer.

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

The boiling Points (K) of the alkanes are taken from the CRC Hand book of Chemistry and Physics [36] and Beilstein [37].
The thermodynamic values in Table 2 are from The NBS Tables of Chemical Thermodynamic Properties (1982), and NIST Chemistry Web Book.

The QSPR model is built using a multilineal regression technique. (7)

Discussion and Designing QSPR Models

A graph –theoretical approach to QSPR is based on the use of topological indices for encoding the structure information. The term

topological index 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 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 the alkanes

$(C_2 - C_{10})$ in Crease with the number of carbon. According to the data of Table 2&3 the logarithmic values of Distance matrixes and six topological indices increase by increasing values of Cp , ΔH^o_{vap} and bp (k) while the values ΔH^o_f

and ΔH^o_c decrease by increasing the above topological indices.

In Figs. 1-6, it is attempted to show two dimensional diagrams of the relationship between the Randic$^/$ index (X), Harary number (H), and the values of ΔH^o_c , $\Delta H^o vap$, ΔH^o_f, Cp, bP(K) for the $(C_2 - C_{10})$ alkanes. In those curves, there are high correlation between the values, but the curves Distance matrix (D), Wiener index (W), Hosoya index (Z), Balaban index (J), and the values of ΔH^o_c , $\Delta H^o vap$, ΔH^o_f, Cp, bP(K) for the $(C_2 - C_{10})$ alkanes are nonlinear correlation. Those nonlineary curves are not show and considered in this paper.

Figs. 7-12 show the relation of log Z, log (D) and ΔH^o_c , ΔH^o_f, ΔH^0_{vap}, Cp, bP(K). In those curves, there are good correlation between the values.

Topological indices (TIS) such as X, H, Log (D), Log (Z) with ΔH^o_f, ΔH^o_c, ΔH^o_{vap}, bP(K) and Cp , respectively.

The QSPR model is built using a multilineal regression technique.

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

Step 1. Get a reliable source of experimental data for a given set of molecules. This initial set of molecules is sometimes called the training set[38]. 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[39]. 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° 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 alkanes. As the

initial set we will consider alkanes with up to 5 carbon atoms (8 molecules). The thermodynamic properties of these alkanes 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 table4).

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:

$$\Delta H_{vap}^{o} = 0.1214X^{3} - 1.6506X^{2} + 12.266X + 4.1897 \qquad R^{2}=0.9998 \qquad (9)$$

$$Cp = 0.0208X^{3} - 0.2257X^{2} + 0.8138X - 0.5852 \qquad R^{2}=0.9786 \qquad (10)$$

$$\Delta H_{f}^{o} = -0.2895X^{3} + 1.8424X^{2} + 39.796X + 44.09 \qquad R^{2}=0.9990 \qquad (11)$$

$$\Delta H_{c}^{o} = 1.0793X^{3} - 10.848X^{2} + 157.11X - 2.5201 \qquad R^{2}=0.9999 \qquad (12)$$

$$bp = 1.6968X^{3} - 22.507X^{2} + 149.01X + 57.896 \qquad R^{2}=0.9999 \qquad (13)$$

$$\Delta H_{vap}^{o} = 0.0049H^{3} - 0.1754H^{2} + 3.6265H + 11.397 \qquad R^{2}=0.9999 \qquad (14)$$

$$Cp = 0.0147H^{3} - 0.4315H^{2} + 18.965H + 33.848 \qquad R^{2}=0.9999 \qquad (15)$$

$$\Delta H_{f}^{o} = -0.0127H^{3} + 0.1014H^{2} + 15.025H + 69.893 \qquad R^{2}=0.9999 \qquad (16)$$

$$\Delta H_{c}^{o} = 0.0377H^{3} - 1.1226H^{2} + 51.267H + 93.353 \qquad R^{2}=1 \qquad (17)$$

$$bp = 0.0689H^{3} - 2.3643H^{2} + 42.951H + 144.61 \qquad R^{2}=0.9794 \qquad (18)$$

$$\Delta H_{vap}^{o} = -0.1785(\log D)^{3} + 0.805(\log D)^{2} + 6.494 \log D + 14.75 \qquad R^{2}=0.9999 \qquad (19)$$

$$Cp = -1.0745(\log D)^{3} + 9.935(\log D)^{2} + 32.449 \log D + 52.181 \qquad R^{2}=0.9999 \qquad (20)$$

$$\Delta H_{f}^{o} = -1.9472(\log D)^{3} + 13.781(\log D)^{2} + 24.695 \log D + 84.791 \qquad R^{2}=0.9999 \qquad (21)$$

$$\Delta H_{c}^{o} = -2.7455(\log D)^{3} + 26.147(\log D)^{2} + 89.376 \log D + 142.54 \qquad R^{2}=1 \qquad (22)$$

$$bp = -1.745(\log D)^{3} + 6.0289(\log D)^{2} + 77.554 \log D + 183.99 \qquad R^{2}=0.9999 \qquad (23)$$

$$\Delta H_{vap}^{o} = 1.3369(\log Z)^3 - 7.5926(\log Z)^2 + 25.698 \log Z + 7.851 \qquad R^2 = 0.9998 \qquad (24)$$

$$Cp = 3.9687(\log Z)^3 - 15.025(\log Z)^2 + 125.47 \log Z + 16.393 \qquad R^2 = 1 \qquad (25)$$

$$\Delta H_{f}^{o} = -5.4193(\log Z)^3 + 15.3(\log Z)^2 + 89.478 \log Z + 57.328 \qquad R^2 = 0.9990 \qquad (26)$$

$$\Delta H_{c}^{o} = 9.9035(\log Z)^3 - 37.437(\log Z)^2 + 337.45 \log Z + 46.562 \qquad R^2 = 0.9999 \qquad (27)$$

$$bp = 19.423(\log Z)^3 - 105.91(\log Z)^2 + 310.11 \log Z + 101.9 \qquad R^2 = 0.9999 \qquad (28)$$

We used eqs 9-28 to predict ΔH_{c}^{o}, ΔH_{f}^{o}, ΔH_{vap}^{0}, Cp, $bP(K)$ of the said alkanes for which the results of boiling points based on eqs 13, 18, 23 and 28 are shown in table 5.

We have compared the predicted and experimental values of the alkanes boiling points (see table 5). This comparison showed that the eqs 18 and 23 are not suitable for predicting the bp (K) of these alkanes. In this connection, though the models 13 and 28 having problems with some members of the alkanes series, but model 13 proved to have less problems. However, when Step 3 is repeated using the boiling points of all alkanes with up to 9 carbon atoms, we see that the QSPR models based on log (Z) and X did not improve. The slight improvement happened only when a biparametric model with X and N (N is the number of carbon atoms in alkanes) was used.

Conclusions

Graph theory has provided the chemist with a variety of very useful tools. In this report we 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 capacity, enthalpies of combustion, enthalpy of vaporization and the boiling points of alkanes. Six selected topological indices and distance matrix were tested. The correlation of the

Randic[1] index (X) , Harary number (H) , logarithmic values Distance matrix (D) and Hosoya index (Z) with ΔH_{f}^{o}, ΔH_{vap}^{o}, ΔH_{c}^{o}, Cp and $bP(K)$ can show better results , in the comparison of using other indices for prediction the same of the properties of alkanes. A characteristic polynomial is constructed for the reference structure with the graphs for the given molecule taken into account.
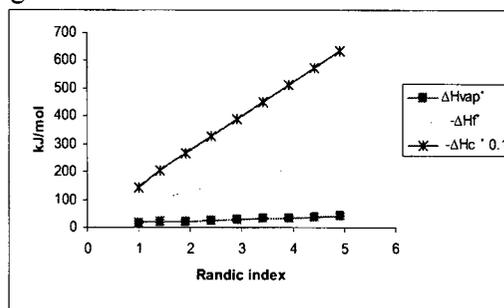
Fig.1.The curve of the Randic indices(X) versus ΔH_{vap}^{o} ΔH_{f}^{o}, ΔH_{c}^{o} for the $C_2 - C_{10}$ normal alkanes
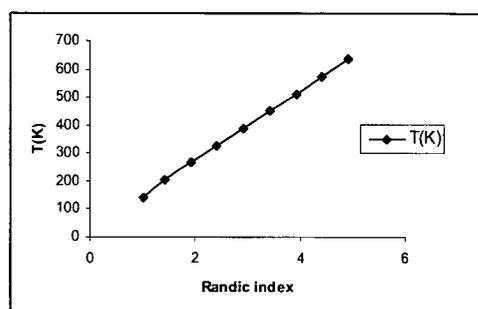
Fig.2.The curve of the Randic indices(X) versus normal boiling point(K0 for the $C_2 - C_{10}$ normal alkanes
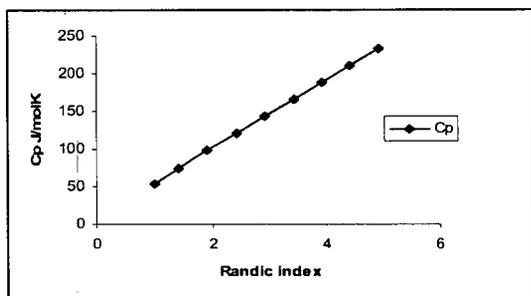
Fig.3.The curve of the Randic indices(X) versus Cp for the $C_2 - C_{10}$ normal alkanes.

Fig.7. The curve of the log (D) versus ΔH_{vap}^o, ΔH_f^o, ΔH_c^o for the $C_2 - C_{10}$ normal alkanes.

Fig.4. The curve of the Harary number (H) versus ΔH_{vap}^o, ΔH_f^o, ΔH_c^o for the $C_2 - C_{10}$ normal alkanes.
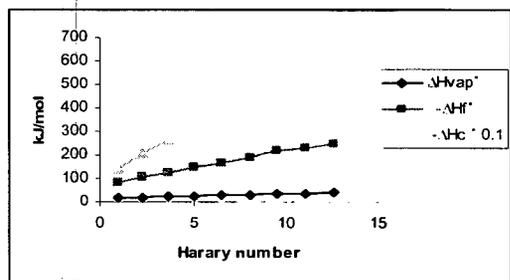
Fig.8. The curve of the log (D) versus normal boiling point for the $C_2 - C_{10}$ normal alkanes
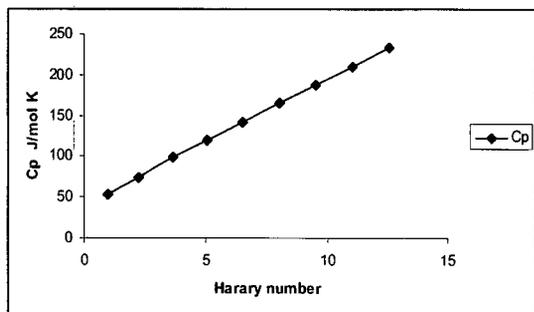
Fig.5. The curve of the Harary number (H) versus Cp for the $C_2 - C_{10}$ normal alkanes.

Fig.9.The curve of the log (D) versus Cp for the $C_2 - C_{10}$ normal alkanes
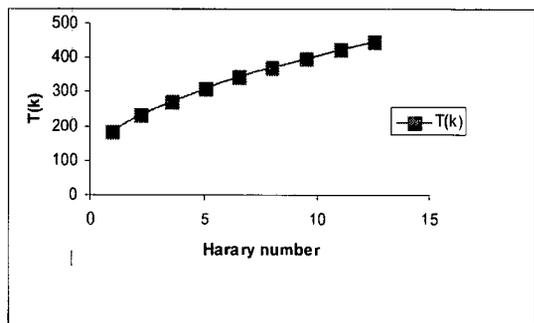
Fig.6. The curve of the Harary number (H) versus normal boiling point for the $C_2 - C_{10}$ normal alkanes
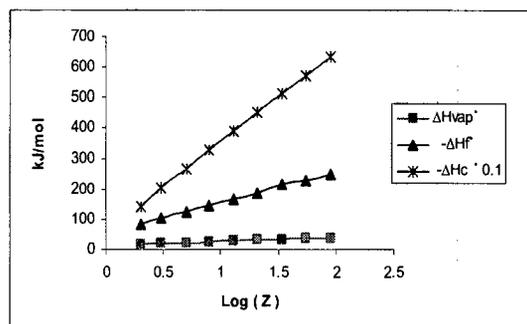
Fig.10. The curve of the log (Z) versus ΔH_{vap}^o, ΔH_f^o, ΔH_c^o for the $C_2 - C_{10}$ normal alkanes.
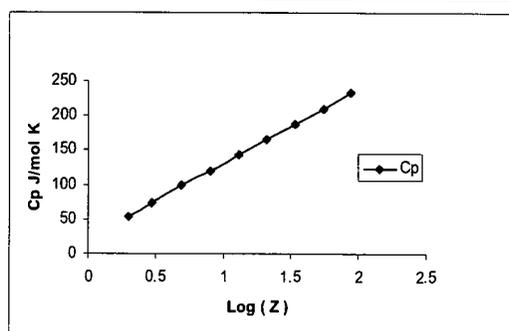
Fig.11.The curve of the log (Z) versus Cp for the $C_2 - C_{10}$ normal alkanes
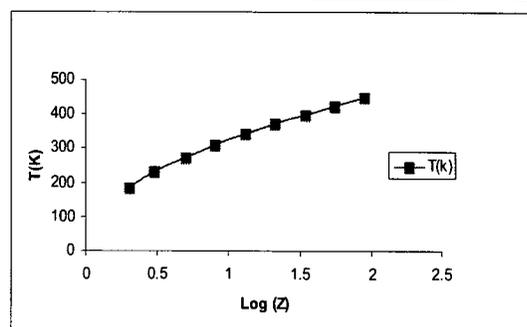
Fig.12. The curve of the log (Z) versus normal boiling point for the $C_2 - C_{10}$ normal alkanes

Table 2. The Randic indices (X), Distance matrixs (D), Wiener numbers (W) Hosoya indices(Z), Balaban indices(J), Schultz indices (MTI),

Harary numbers (H) and $\Delta H^{\circ}{}_f, \Delta H^{\circ}{}_c, Cp, \Delta H^{\circ}{}_{vap}$ and the normal Boiling points

(bp inK) of Alkanes $(C_2 - C_{10})$ (In Pressure 1 bar and 298 K)

Alkane	X	D	W	Z	J	MTI	H	$\dfrac{\Delta H^{\circ}{}_f}{kJmol^{-1}}$	$\dfrac{Cp_{gas}}{Jmol^{-1}K^{-1}}$	$\dfrac{\Delta H^{\circ}{}_{vap}}{kJmol^{-1}}$	$bp(K)$	$\dfrac{\Delta H^{\circ}{}_c}{kJ\ mol^{-1}}$
Ethane	1	1	1	2	1	4	1	-84.738	52.63	14.79	184.55	-1428.51
Propane	1.4142	4	4	3	1.6330	16	2.2500	-103.890	73.60	18.80	231.05	-2044.97
Butane	1.9142	12	10	5	1.9747	38	3.6111	-126.190	98.49	22.49	272.65	-2659.60
Pentane	2.4142	32	20	8	2.1906	74	5.0347	-146.490	120.07	25.83	309.25	-3273.50
Hexane	2.9142	80	35	13	2.3391	128	6.4983	-167.290	142.60	28.82	342.15	-3888.50
Heptan	3.4142	192	56	21	2.4475	204	7.9897	-187.890	165.20	31.59	371.55	-4503.50
Octane	3.9142	448	84	34	2.5301	306	9.5015	-214.780	187.80	34.29	398.85	-5118.5
Nonane	4.4142	1024	120	55	2.5951	438	11.0289	-229.190	210.40	36.71	423.92	-5733.55
Decane	4.9142	2304	165	89	2.6476	604	12.5687	-249.790	233.10	38.93	447.27	-6348.60

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

Alkane	Log X	Log D	Log W	Log Z	Log J	Log MTI	Log H
Ethane	0	0	0	0.3010	0	0.6020	0
Propane	0.1505	0.6020	0.6020	0.4771	0.2130	1.2041	0.3522
Butane	0.2820	1. 0792	1	0.6990	0.2955	1.5798	0.5576
Pentane	0.3828	1.5051	1.3010	0.9031	0.3406	1.8692	0.7020
Hexane	0.4645	1.9031	1.5441	1.1139	0.3690	2.1072	0.8128
Heptan	0.5333	2.2833	1.7482	1.3222	0.3887	2.3096	0.9025
Octane	0.5926	2. 6513	1.9243	1.5315	0.4031	2.4857	0.9778
Nonane	0.6448	3.0103	2.0792	1.7404	0.4141	2.6415	1.0425
Decane	0.6914	3.3625	2.2175	1.9494	0.4228	2.7810	1.0993

Table 4. The Randic indices (X), Harary numbers (H), logarithmic values of Hosoya indices (Z), Distance matrixes of alkanes with up to 5 carbon atoms

Alkanes	X	H	Z	Log (Z)	D	Log (D)
2,2,4-trimethylhexane	3.9545	12.0853	33	1.5185	5120	3.7093
2,2,5-trimethylhexane	3.9165	11.9692	32	1.5051	5120	3.7093
2,4,4-trimethylhexane	3.9772	12.1564	34	1.5315	4608	3.6635
2-methyl propane	1.7321	3.7500	4	0.6021	12	1.0792
3,3- dimethylpentane	3.1213	8.7292	16	1.2041	208	2.3181
2,3- dimethylbutane	2.6427	6.9444	10	1	80	1.9031
3-ethylheptan	4.3461	11.4794	52	1.7160	1024	3.0103
4-ethyl-2-methyhexane	4.2019	11.7364	44	1.6434	5120	3.7093

Table 5. Comparison between predicted (four model) and experimental values of the normal boiling point (K) of alkanes with up to 5 carbon atoms

Alkanes	bp(exp)/K	bp(cal)/K				$\Delta[(bp_{exp} - bp_{calc})]$			
		model (13)	model (18)	model (23)	model (28)	model (13)	model (18)	model (23)	model (28)
2,2,4-tri methyl hexane	399.65	400.121	439.99	471.66	396.55	-1.61	-40.34	-72.01	3.10
2,2,5-tri methyl hexane	397.15	398.195	438.13	471.66	394.95	-1.045	-40.98	-74.51	2.20
2,4,4-tri methyl hexane	399.65	401.26	441.12	468.11	398.19	-1.62	-41.47	-68.46	1.46
2-methyl propane	261.45	257.288	276.06	272.51	254.46	4.162	-14.61	-11.06	6.99
3,3- di methyl pentane	359.25	355.324	385.21	363.77	355.66	3.926	-25.96	-4.52	3.59
2,3- di methyl butane	331.15	325.81	351.94	331.58	325.52	5.34	-20.79	-0.43	5.63
3-ethyl heptan	416.15	419.676	430.33	472.08	420.33	-3.526	-14.18	-55.93	-4.18
4-ethyl-2-methyl hexane	406.95	412.521	434.42	471.66	411.70	-5.570	-27.47	-64.71	-4.75

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