Relationship between Topological Indices and Thermodynamic Properties and of the Monocarboxylic Acids Applications in QSPR

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ABSTRACT Topological indices are the numerical value associated with chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. Graph theory is a delightful playground for the exploration of proof techniques in Discrete Mathematics and its results have applications in many areas of sciences. One of the useful indices for examination of structure- property relationship is Randic' index. In this study is represented the relationship between the Randic', Balaban and Szeged indices and Harary numbers to the enthalpies of combustion (ΔH_C° liquid), enthalpies of vaporization (ΔH_{vap}° gas), enthalpies of formation (ΔH_f° liquid) and enthalpies of sublimation (ΔH_{sub}°) of monocarboxylic acids (C_2–C_{20}) are established, and then, some useful topological indices for examination of the structure- property relationship are presented.

KEYWORDS Topological index · graph theory · monocarboxylic acid · QSPR.

1. INTRODUCTION

The fact that the properties of a molecule are tightly connected to its characteristics is one of the fundamental concepts in chemistry. In this connection, graph theory has been successfully applied and some thermodynamic properties [1–5].

Chemical graph theory is a branch of mathematical 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 graphs theory is concerned with all aspects of the application of graph theory to chemistry area.

A graph is a topological concept rather than a geometrical concept of fixed geometry. Therefore, Euclidean metric lengths, angles and three–dimensional spatial configurations have no significance in topological concept.

Chemists employ various types of designations and formulas when they want to communicate information about chemical compounds and their structures. In spite of this

fact, most of the names and formulas have no direct, immediate or explicit mathematical meaning.

It has been found to be a useful tool in QSAR (Quantitative Structure- Activity Relationship) and QSPR (Quantitative Structure- Property Relationship) [6-11]. Numerous studies have been made relating to the above mentioned fields by using what are called topological indices (TI). In 1975, Randic' proposed a topological index that has become one of the most widely used in both QSAR and QSPR studies [12].

Quantitative structure- activity relationship (QSAR) are mathematical models designed for the correlation of various types of biological activity, chemical reactivity, equilibrium, physical and physicochemical properties with electronic, steric, hydrophobic and other factors of a molecular structure of a given series of compounds such as substitution constants, topological indices (TI) as well as with solvent and other physicochemical parameters.

In this paper, a variant of QSAR studies, the so- called Quantitative structure- activity relationship (QSAR), using topological indices as molecular descriptors [10], 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 [13]. The classical topological approach [5] 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 indices.

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 of covalently linked atoms situated at a topological distance equal to unit.

In this study, the interesting results of structure- property relationship between the Randic'(^1X), Balaban (J) and Szeged (Sz) indices and Harary numbers (H) to the enthalpies of combustion (ΔH_C° liquid), enthalpies of vaporization (ΔH_{vap}° gas) , enthalpies of formation (ΔH_f° liquid) and enthalpies of sublimation (ΔH_{sub}°) of monocarboxylic acids ($C_2H_4O_2 - C_{20}H_{40}O_2$) and their the Quantitative structure- property relationship are presented.

At first, a brief review on the classical topological indices is presented. After wards, the molecular descriptors that include the necessary structural information for properly 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.

2. DATA SOURCES

Enthalpies of vaporization (ΔH°_{vap} kJ/mol) and enthalpies of sublimation (ΔH°_{sub} kJ/mol) of monocarboxylic acids ($C_2H_4O_2 - C_{20}H_{40}O_2$) are taken from book [19]. Enthalpies of combustion (ΔH°_{C} kJ/mol) and enthalpies of formation (ΔH°_{f} kJ/mol) liquid at standard conditions (nominally 298.15 K, 1 atm) of monocarboxylic acids ($C_2H_4O_2 - C_{20}H_{40}O_2$) are taken from National Institute of Standards and Technology (NIST) Chemistry Web Book [20].

3. TOPOLOGICAL INDICES

All the used topological indices were calculated using all hydrogen suppressed graph by deleting all the carbon hydrogen as well as heteroatomic hydrogen bonds from the structure of the monocarboxylic acids. The calculations of these indices are well documented in the literature and therefore, their detailed calculations are not given here. However, blow we have given the final expression for the calculation of these indices.

3.1. The connectivity index (^{1}X)

The connectivity index $^{1}X = {}^{1}X(G)$ of G is defined by Randic' [12] as:

$$^{1}x = {}^{1}x(G) = \sum_{alledges}\left[d_{(i)}d_{(j)}\right]^{-0.5},$$

where $d_{(i)}$ and $d_{(j)}$ are the valences of the vertices and j that define the edge ij.

3.2. Szeged index (Sz)

The Szeged index, $Sz = Sz(G)$, is calculated [16,17] according to the following expression:

$$Sz = Sz(G) = \sum_{alledges} n_u \cdot n_v .$$

Edges where n_u is the number of vertices lying closer to one end of the edge e = uv; the meaning of n_v is analogous. Edges equidistance from both the ends of an edges, e = uv are not taken into account.

3.3. Balaban index (J)

The Balaban index, $J = J(G)$ of G, was introduced by Balaban [1,5,18] as the average distance sum connectivity. It is defined as:

$$J = \frac{M}{\mu + 1} \sum_{alledges}\left[d_{(i)}d_{(j)}\right]^{-0.5},$$

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 $M = M(G)$ 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, M = 0; for monocycles M = 1.

3.4. Harary number (H)

The Harary number (H) was introduced in 1991 by Harary [14, 15]. This index is defined from the inverse of the squared elements of the distance matrix according to the expression:

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

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

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

4. Discussion and Designing The QSPR Models

A graph – theoretical approach to QSPR is based on the use of topological indices for encoding the structural information. The topological indices 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 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, molecular topological indices are calculated. The values of topological indices of Randic' (^1X), Harary (H), Balaban (J) and Szeged (Sz) for the 19 compounds of training set are also described in Table 1.

After words, the molecular descriptors, which include the structural information necessary to property describe the system, are employed to derive numerical correlation with property. The Thermodynamic values of Tables 2 are taken from book [19] for the compounds of training set.

The Figures 1–8 were shown, respectively, the plots of ΔH_{vap}°, ΔH_{sub}°, ΔH_C°, ΔH_f° and their logarithmic values for the compounds of training set against the ^1X, $\log^1 X$, J, log J, H, logH, Sz and logSz. Linear dependence is obtained in each plot of Figures 1 to 8.

The coefficient of determination (R^2) for the linear regression is shown in respective figures. The resultant curves, show highly correlation between the respect values. It is noticeable that some relationship such as Balaban index (J), against the values of ΔH_C° (liquid), ΔH_{sub}°, ΔH_{vap}° (gas) and ΔH_f° (liquid) for the (C_2–C_{20}) monocarboxylic acids are not linear. Now these nonlinear curves are not included.

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

Step 1. We get a reliable source of experimental data for a given set of molecules. This initial set of molecules is sometimes called the training set. 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 quality of the QSPR models can be conveniently measured by the correlation coefficient (R^2). A good QSPR model must have $R^2 > 0.99$. 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 thermodynamic properties of monocarboxylic acids. As the initial set we will consider monocarboxylic acids with up to 5 carbon atoms (4 molecules). The thermodynamic properties of these monocarboxylic acids are taken from [19,20], and the molecular topological indices such as the Randic' index (^1X), Harary number (H), Balaban index (J) and Szeged index (Sz) of the above mentioned are calculated (see table 1).

The following structure – property models are the most successful for the Randic' index (^1X), Harary number (H), logarithmic values of Randic' index (^1X), Harary number (H), Szeged index (Sz) considered:

$$\log \Delta H_{vap}^{\circ} = 0.4302(\log X) + 1.5799 \qquad R^2 = 0.9924 \tag{1}$$

$$\log \Delta H_{vap}^{\circ} = 6.7314(\log Sz) + 10.393 \qquad R^2 = 0.9940 \tag{2}$$

$$\log \Delta H_{vap}^{\circ} = 6.4079(X) + 41.033 \qquad R^2 = 0.9972 \tag{3}$$

$$\Delta H_f^{\circ} = 59.684(^1X) + 367.28 \qquad R^2 = 0.9981 \tag{4}$$

$$\Delta H_f^{\circ} = 9.6661(H) + 450.32 \qquad R^2 = 0.9971 \tag{5}$$

$$\log \Delta H_f^{\circ} = 0.0361(^1X) + 2.6313 \qquad R^2 = 0.9934 \tag{6}$$

$$\Delta H_C^{\circ} = 209.72(H) + 417.07 \qquad R^2 = 0.9934 \tag{7}$$

$$\log \Delta H_C^{\circ} = 0.9878(\log H) + 2.3724 \qquad R^2 = 0.9932 \tag{8}$$

$$\Delta H_C^{\circ} = 1297(^1X) - 1397.5 \qquad\qquad R^2 = 1 \qquad\qquad (9)$$

$$\Delta H_{sub}^{\circ} = 13.614(^1X) + 31.47 \qquad\qquad R^2 = 0.9972 \qquad\qquad (10)$$

$$\Delta H_{sub}^{\circ} = 2.2052(H) + 50.403 \qquad\qquad R^2 = 0.9964 \qquad\qquad (11)$$

Eqs. 1 to 11 exhibit the applicability of topological and thermodynamics properties for QSPR study of mentioned monocarboxylic acids.

Table 3 shows the variance and highest (positive and negative) differences between experimental values of (ΔH_C° liquid), $\log \Delta H_C^{\circ}$ and the values obtained using H, ^1X and log H for the 4 compounds of training set (Table 1). The coefficient of determination (R^2) for applying Eq. (9) to the experimental data (Table 2) is 1 and it is higher than the respective parameter obtained for the others predictors. Thus, according to this result, the topological ^1X can be used for predicting the enthalpies of combustion (ΔH_C°) and logH can be used for predicting the $\log \Delta H_C^{\circ}$ of monocarboxylic acids.

Table 4 shows the variance and highest (positive and negative) differences between experimental values of ΔH_{sub}° and the values obtained using ^1X and H for the 4 compounds of training set. Comparison of the predicted ΔH_{sub}° with the experimental values, revealed that Eqs 10 and 11 are shown that the topological H is quite suitable for predicting the ΔH_{sub}° of these carboxylic acids.

Table 5 shows comparison of the predicted ΔH_{vap}° with the experimental values through the use of topological indices such as ^1X and log ^1X and log Sz (Eq 1 to 3) for the compounds listed in Table 5. The Eq (3) establish a relationship between the topological ^1X and ΔH_{vap}° by a high squared regression coefficient (0.9972), which explains the Randic' index for predicting the ΔH_{vap}° have better results than the other indices.

Table 6 shows comparison of the predicted ΔH_f° (liquid) with the experimental values through the use of topological indices such as H and ^1X (Eq 4 to 6) for the compounds listed in Table6. The resultant ΔH_f° (liquid) and log ΔH_f° are shown the Randic' index (^1X) for predicting this property have better results that the Harary number.

5. 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 structure – property relationship based on topological indices. The instructive example was directed to the design of the structure – property model for predicting the enthalpies of combustion, ((ΔH_c° liquid), enthalpies of vaporization (ΔH_{vap}° gas), enthalpies of formation (ΔH_f° liquid) and enthalpies of sublimation ((ΔH_{sub}°) of monocarboxylic acids ($C_2H_4O_2 - C_{20}H_{40}O_2$. Four selected topological indices were tested. The

correlation of the Randic index (^1X) with (ΔH°_f liquid), (ΔH°_{vap} gas) and (ΔH°_c liquid), appeared to have better results than the other indices. The Harary number (H) is suitable for predicting the (ΔH°_{sub}) of these carboxylic acids. Meanwhile, the discussion of relationship areas becomes straightforward.

Table 1. The values of Randic' (^1X), Balaban (J) and Szeged indices (Sz) and Harary numbers (H) of monocarboxylic acids ($C_2H_4O_2$-$C_{20}H_{40}O_2$).

Name of compounds	Formula	X	J	H	Sz
ethanoic acid	$C_2H_4O_2$	1.73	2.32	4.50	9
propanoic acid	$C_3H_6O_2$	2.27	2.54	6.67	18
butanoic acid	$C_4H_8O_2$	2.77	2.36	9.00	32
pentanoic acid	$C_5H_{10}O_2$	3.27	2.68	11.48	52
hexanoic acid	$C_6H_{12}O_2$	3.77	2.72	14.10	79
heptanoic acid	$C_7H_{14}O_2$	4.27	2.75	16.84	114
octanoic acid	$C_8H_{16}O_2$	4.77	2.77	19.68	158
nonanoic acid	$C_9H_{18}O_2$	5.27	2.80	22.62	212
decanoic acid	$C_{10}H_{20}O_2$	5.77	2.82	25.65	277
undecanoic acid	$C_{11}H_{22}O_2$	6.27	2.84	28.76	354
dodecanoic acid	$C_{12}H_{24}O_2$	6.77	2.85	31.94	444
tridecanoic acid	$C_{13}H_{26}O_2$	7.27	2.87	35.20	548
tetradecanoic acid	$C_{14}H_{28}O_2$	7.77	2.88	38.52	667
pentadecanoic acid	$C_{15}H_{30}O_2$	8.27	2.89	41.91	802
hexadecanoic acid	$C_{16}H_{32}O_2$	8.77	2.90	45.35	954
heptadecanoic acid	$C_{17}H_{34}O_2$	9.27	2.91	48.85	1124
octadecanoic acid	$C_{18}H_{36}O_2$	9.77	2.92	52.40	1313
nonadecanoic acid	$C_{19}H_{38}O_2$	10.27	2.93	56.00	15.22
eicosanoic acid	$C_{20}H_{40}O_2$	10.77	2.94	59.65	1752

Table 2. The values of enthalpies of combustion of liquid (ΔH_C° kJ/mol), enthalpies of formation of liquid (ΔH_f° kJ/mol), enthalpies of sublimation (ΔH_{sub}° kJ/mol) and enthalpies of vaporization (ΔH_{vap}° kJ/mol gas) of monocarboxylic acids ($C_2H_4O_2-C_{20}H_{40}O_2$) at conditions (nominally 298.15 K, 1 atm).

| Compounds	$\Delta H_{C_{liquid}}^{\circ}$ kJ/mol	$\Delta H_{f_{liquid}}^{\circ}$ kJ/mol	ΔH_{vap}° kJ/mol	ΔH_{sub}° kJ/mol
$C_2H_4O_2$	875.16	483.5	46.3	49.7
$C_3H_6O_2$	1527.3	510.8	50.0	56.1
$C_4H_8O_2$	2183.5	533.9	54.9	62.9
$C_5H_{10}O_2$	2837.8	558.9	58.2	69.0
$C_6H_{12}O_2$	3494.3	581.8	63.0	75.0
$C_7H_{14}O_2$	4146.9	608.5	64.8	81.7
$C_8H_{16}O_2$	4799.9	634.8	69.4	86.9
$C_9H_{18}O_2$	5456.1	658.0	72.3	93.6
$C_{10}H_{20}O_2$	6079.3	713.7	76.3	100.8
$C_{11}H_{22}O_2$	6736.5	736.2	78.9	106.7
$C_{12}H_{24}O_2$	73.77.0	775.1	82.2	115.9
$C_{13}H_{26}O_2$	8024.2	807.2	84.9	121.2
$C_{14}H_{28}O_2$	8676.7	834.1	87.7	130.2
$C_{15}H_{30}O_2$	9327.7	862.4	91.4	136.5
$C_{16}H_{32}O_2$	9977.2	892.2	94.5	144.3
$C_{17}H_{34}O_2$	10624.4	924.4	100.7	159.6
$C_{18}H_{36}O_2$	11280.1	947.2	102.8	164.7
$C_{19}H_{38}O_2$	11923.4	984.1	105.0	172.9
$C_{20}H_{40}O_2$	12574.2	1012.6	109.9	179.2

Table 3. Comparison between predicted (three model) and experimental values of enthalpies of combustion and their logarithmic of respect monocarboxylic acids (T= 298.15 K in kJ/mol).

	$\Delta H^{\circ}_{C_{liquid}}$ kJ/mol	ΔH°_{C} Predicted		Deleted Residuals		$\log \Delta H^{\circ}_{C}$	$\log \Delta H^{\circ}_{C}$	Deleted residuals
Compounds	Experimental	Model (7)	Model (9)	Model (7)	Model (9)	Experimental	Predicted	Model (8)
$C_6H_{12}O_2$	3494.29	3374.12	3492.19	120.17	2.10	3.5434	3.5074	3.6×10^{-2}
$C_9H_{18}O_2$	5456.10	5160.94	5437.69	295.16	18.41	3.7369	3.7099	2.7×10^{-2}
$C_{12}H_{24}O_2$	7377.0	7115.52	7383.19	261.48	-6.19	3.8679	3.8580	9.8×10^{-3}
$C_{17}H_{34}O_2$	10624.40	10661.89	10625.69	-37.49	-1.29	4.0263	4.0408	-1.4×10^{-2}

Table4. Comparison between predicted (two model) and experimental values of sublimation of respect monocarboxylic acids (T= 298.15 K in kJ/mol).

|	ΔH°_{Sub} kJ/mol	ΔH°_{Sub} Predicted		Deleted Residuals	
Compounds	Experimental	Model 10	Model 11	Model 10	Model 11
$C_6H_{12}O_2$	75.00	82.79	81.50	-7.79	-6.50
$C_9H_{18}O_2$	100.80	103.20	100.3	-2.40	0.50
$C_{12}H_{24}O_2$	121.25	123.64	120.84	-2.39	0.41
$C_{17}H_{34}O_2$	159.60	157.68	158.10	1.92	1.50
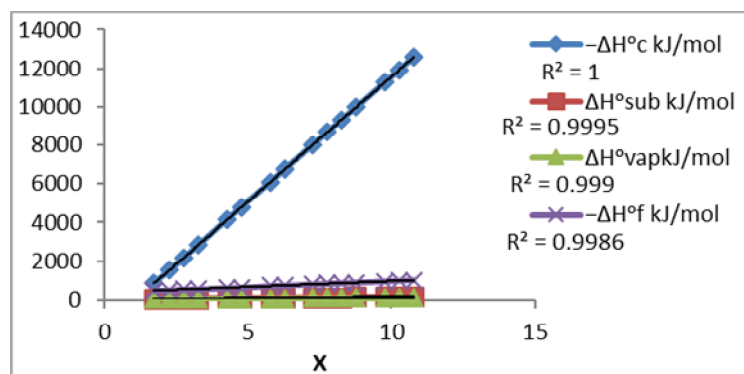
Figure 1. Plots of the Randic' index (^{1}X) versus ΔH°_{C} (liquid), ΔH°_{sub}, ΔH°_{vap}, ΔH°_{f} (liquid) for (C_2- C_{20}) monocarboxylic acids (without C_6, C_9, C_{12}, C_{17}).

Table 5. Comparison between predicted (three model) and experimental values of enthalpies of vaporization and their logarithmic of respect monocarboxylic acids (T= 298.15 K in kJ/mol).

Compounds	$\log \Delta H^{\circ}_{Vap}$	$\log \Delta H^{\circ}_{Vap}$ predicted		Deleted residuals		$\Delta H^{\circ}_{Vap} \; kJ/mol$	ΔH°_{Vap}	Deleted Residuals
	Experimental	Model 1	Model 2	Model 1	Model 2	Experimental	Predicted Model 3	
$C_6H_{12}O_2$	1.8117	1.8278	2.3832	1.6×10^{-2}	0.57	64.82	65.19	-0.37
$C_9H_{18}O_2$	1.8823	1.8904	5.2642	8.1×10^{-3}	3.30	76.26	74.80	1.46
$C_{12}H_{24}O_2$	1.9292	1.9372	7.4250	8×10^{-3}	5.50	84.95	84.41	0.54
$C_{17}H_{34}O_2$	2.0031	1.9959	10.1445	7.2×10^{-3}	8.10	100.72	100.43	0.29

Table 6. Comparison between predicted (three model) and experimental values of enthalpies of formation and their logarithmic of respect monocarboxylic acids (T= 298.15 K in kJ/mol).

| Compounds	$\Delta H^{\circ}_{f_{liquid}} \; kJ/mol$	$\Delta H^{\circ}_{f_{liquid}} \; kJ/mol$ predicted		Deleted residuals		$\log \Delta H^{\circ}_{f_{liquid}}$	$\log \Delta H^{\circ}_{f_{liquid}}$	Deleted Residuals
	Experimental	Model 4	Model 5	Model 4	Model 5	Experimental	Predicted Model 6	
$C_6H_{12}O_2$	581.8	592.3	586.6	-4.8	-10.5	2.7648	2.7674	2.6×10^{-3}
$C_9H_{18}O_2$	658.0	681.8	669.0	-23.8	-11	2.8182	2.8215	3.3×10^{-5}
$C_{12}H_{24}O_2$	775.1	771.3	759.1	3.8	16	2.8894	2.8757	1.4×10^{-2}
$C_{17}H_{34}O_2$	924.4	920.6	922.5	3.8	1.9	2.9658	2.9659	1×10^{-4}
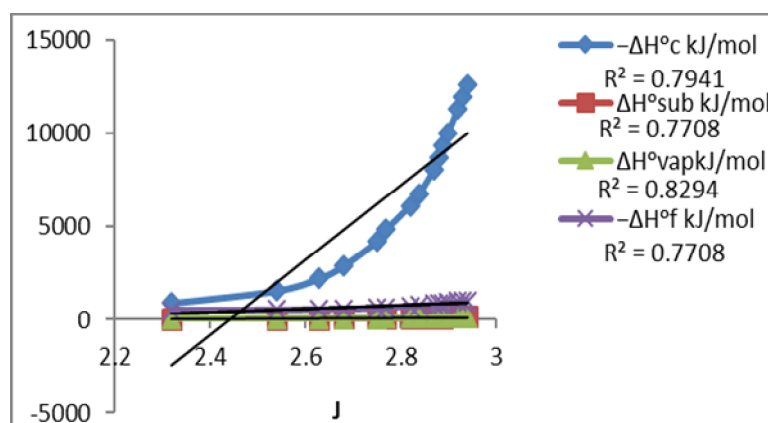
Figure 2. Plots of the Balaban index (J) versus ΔH_C° (liquid), ΔH_{sub}°, ΔH_{vap}°, ΔH_f° (liquid) for (C_2-C_{20}) monocarboxylic acids (without C_6, C_9, C_{12}, C_{17}).
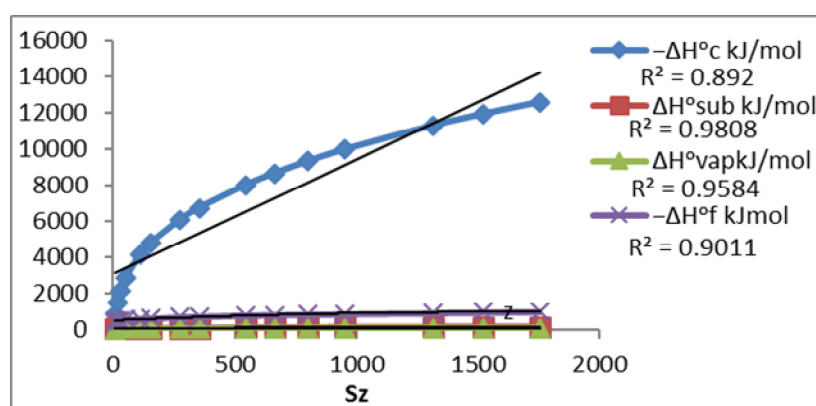

Figure 3. Plots of the Szeged index (Sz) versus ΔH_C° (liquid), ΔH_{sub}°, ΔH_{vap}°, ΔH_f° (liquid) for (C_2-C_{20}) monocarboxylic acids (without C_6, C_9, C_{12}, C_{17}).
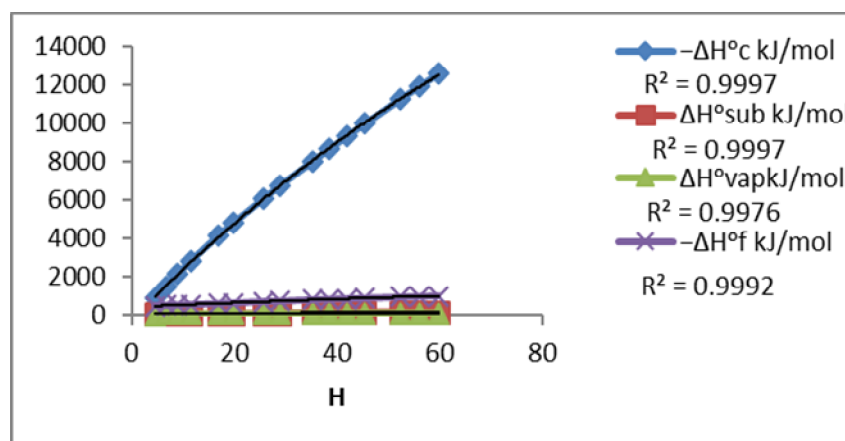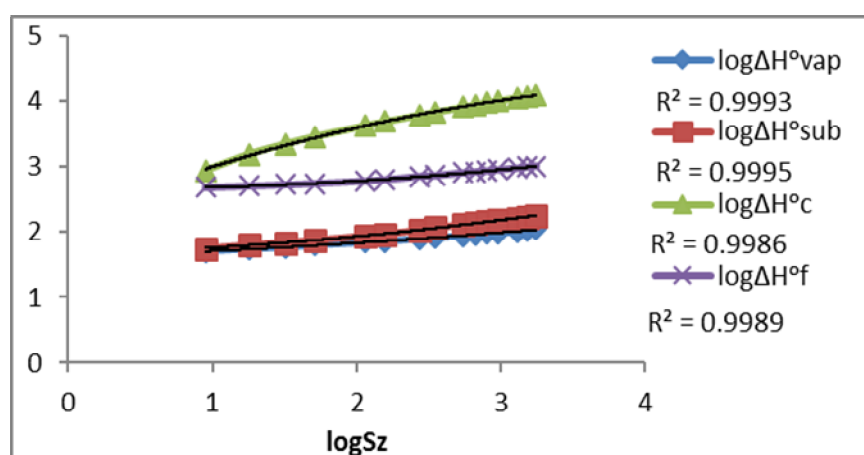

Figure 4. Plots of the Harary index (H) versus ΔH_C° (liquid), ΔH_{sub}°, ΔH_{vap}°, ΔH_f° (liquid) for (C_2-C_{20}) monocarboxylic acids (without C_6, C_9, C_{12}, C_{17}).
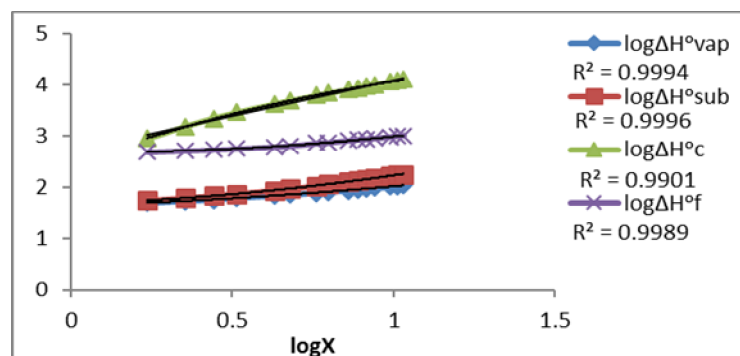
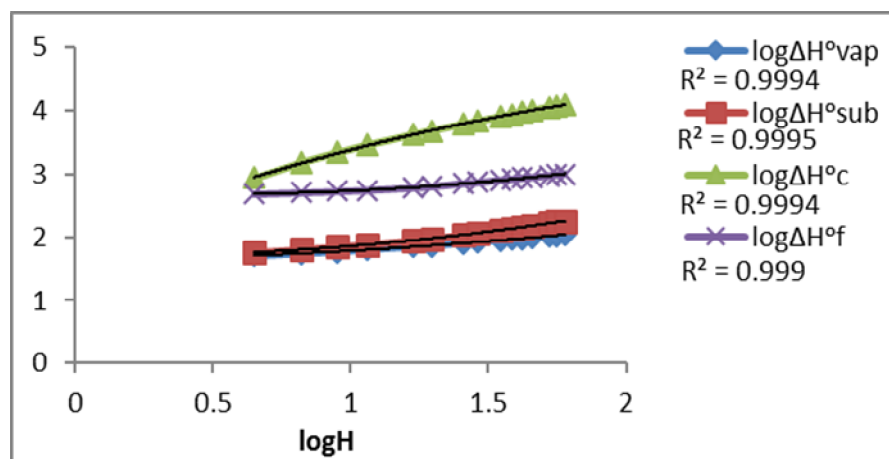**Figure 5.** Plots of the log X versus $\log \Delta H^{\circ}_{vap}$, $\log \Delta H^{\circ}_{sub}$, $\log \Delta H^{\circ}_{C}$ and $\log \Delta H^{\circ}_{f}$ for (C_2–C_{20}) monocarboxylic acids (without C_6, C_9, C_{12} , C_{17}).
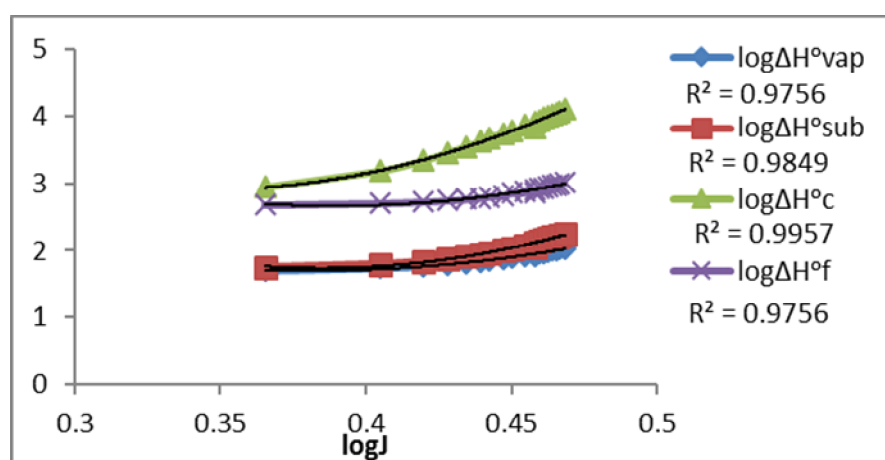
Figure 6. Plots of the log J versus $\log \Delta H^{\circ}_{vap}$, $\log \Delta H^{\circ}_{sub}$, $\log \Delta H^{\circ}_{C}$ and $\log \Delta H^{\circ}_{f}$ for (C_2–C_{20}) monocarboxylic acids (without C_6, C_9, C_{12} , C_{17}).

Figure7. Plots of the logSz versus $\log \Delta H^{\circ}_{vap}$, $\log \Delta H^{\circ}_{sub}$, $\log \Delta H^{\circ}_{C}$ and $\log \Delta H^{\circ}_{f}$ for (C_2- C_{20}) monocarboxylic acids (without C_6, C_9, C_{12} , C_{17}).

Figure 8. Plots of the logH versus $\log \Delta H^{\circ}_{vap}$, $\log \Delta H^{\circ}_{sub}$, $\log \Delta H^{\circ}_{C}$ and $\log \Delta H^{\circ}_{f}$ for(C_2–C_{20}) monocarboxylic acids (without C_6, C_9, C_{12}, C_{17}).

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