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Inverse and Hyper Zagreb Indices: Application to Quantitative Structure Properties Relationship

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ABSTRACT

The topology index can be derived from molecular connectivity, which can be related to the chemical or physical properties of molecules. The topology indices of alkanes are calculated using the modified-Zagreb index, direct and reciprocal degree distance indices, and the modified-Zagreb index. These indices are tested as the structural descriptor for thermodynamic properties such as boiling point (bp), heat vaporization at 25ºC (hv), critical temperature (ct), critical pressure (PC) and magnetooptical properties. Multiple linear regression analyses were done to find the best fitting between these indices and the thermodynamic properties. The results indicate that the boiling point, critical temperature, and heat vapor are reasonably well accounted for by the presence of more than two parameters. The regression equation for the four thermodynamic properties and magnetooptical properties shows a good relation property.

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1. Introduction

Graph theory is not limited to, mathematics only, but it has grown into a significant area of mathematical research, with applications in chemistry, operations research, social sciences, and computer science. In chemistry, application graph theory is used to analyze various chemical phenomena such as chemical compound composition and classification[1]. Chemical graph theory uses the set points connected by lines to determine structure-property relationships. This structure can be derived from molecular connectivity or orientation, which can be related to chemical or physical properties of molecules. To obtain the chemical or physical correlation, it is crucial that appropriate descriptors like theoretical, empirical or readily available experimental feature derivation of the molecular structures are employed[2].

In 1972, the molecular graph depending on the connection number (degree of vertices at distance two) known as the Zagreb connection topological indices was introduced[3]. These indices compute the total electron energy of the alternant hydrocarbons. Then, a few other studies were conducted and changed the model of Zagreb indices to get better correlation coefficients for different isomer, alkanes and cycloalkanes. Ali and Trinajstić restudied these topological indices and renamed them as the modified first Zagreb connection index (ZCI)[4]. Shirdel et al. defined the new hyper-Zagreb index that was generalized from the first and second Zagreb[5]. The construction and

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investigation of topological indices which could uniquely characterize the molecular topology is one of the main directions of chemical graph theory. The structures that differ in the mathematical invariant properties are reflected in their physical, chemical, and biological properties.

Critical temperature and pressure are one of the important parameters to analyze the hydrocarbon phase. The critical temperature is the highest temperature at which a substance's vapor cannot be liquefied. The minimum pressure at this temperature to liquefy the substance is called critical pressure. Every hydrocarbon has its own, critical temperature and pressure. Beyond the critical temperature, the molecules have enough kinetic energy to overcome the van der Waals forces. Kamal reported that the critical pressure and temperature are related to the molecular weight and carbon atomic fraction of the hydrocarbon structure[6]. They also reported that these parameters relate to the Wiener index. In this paper, we report the relationship between the thermodynamic properties of alkanes such as the boiling point, heat vaporization at 25^{o}C (hv), critical temperature, and critical pressure using inverse and hyper-Zagreb. This study is useful to theoretical chemists for analyzing molecular topology relationships with the experimental results. Section 2 provides the literature review of the molecular descriptors. The following section explains the calculation of the topology index using the inverse and hyper-Zagreb indexes. Finally, section 4 discusses the mathematical modelling of physical parameters using multiple linear regression.

2. Literature Review

2.1 Molecular Descriptor using Degree Indexes

The Quantitative Structure Properties Relationship (QSPR) is an important tool for chemical and biological fields. It helps to analyze the physical and chemical properties of molecular structures. QSPR relates physical, biological, and chemical activities using molecular descriptors. The Topology index is one of the molecular descriptors using the application of graph theory. The atoms in the molecular structure are represented by vertexes. While the chemical bonding is described by the edge[7]. The degree based on the vertex is most commonly used in QSPR [8, 9]. The early approach has been introduced by Randic, which is known as the branching or connectivity index [10]. If *G*(*V, E*) represented as the molecular graph with vertex (*V*) and edge set (*E*). The Randic index is given by equation (1)

$$\chi(G) = \sum_{v,u \in V(G)} \frac{1}{\sqrt{d_v d_u}} \tag{1}$$

where d_v and d_u are the degree of vertex *u* and *v* respectively. Zhou and Trinajstić modified Randic connectivity index by replace the multiplication product by summation product [11]. This index also known as the sum connectivity index. The sum connectivity index is given by equation (2).

$$\chi^{+}(G) = \sum_{v,u \in V(G)} \frac{1}{\sqrt{d_v + d_u}} \tag{2}$$

Estrada also has modified the connectivity index by consideration of degree of vertex and edge. This index named as the atom–bond connectivity (ABC) is given by equation (3)[12].

$$\chi^{+}(G) = \sum_{v,u \in V(G)} \sqrt{\frac{d_v + d_u - 2}{d_v d_u}} \tag{3}$$

Another vertex degree-based topology index is called the geometry-arithmetic index (GA) index and is defined as[13]

$$\mathrm{GA}(G) = \sum_{v,u \in V(G)} \frac{\sqrt{d_v d_u}}{(d_v + d_u)/2} \tag{4}$$

where $\sqrt{d_v d_u}$ represent the geometry means and the denominator $(d_v + d_u)/2$ represent arithmetic mean of end-vertex degrees of the edge.

2.2 Molecular Descriptor using Distance Indexes

Molecular descriptors are closely related to the molecular structure. The aim of the development of molecular descriptors is to obtain strong correlations for the prediction of physicochemical properties and biological activities of chemical substances. Another approach is to use a distance-based molecular topology index. The Wiener index is the earliest distance index that

has been introduced. The Wiener index has been improved by Randic, which is known as the hyper-Wiener index[10]. Zhou et al. have introduced the reciprocal of the distance between vertex u and v, which is known as the Harary index [14]. While Ren combined the relations of distance and degree of the molecular graph to form a new index known as the Xu index [15]. The concept of the weighted distance graph index has also been implied according to the heteroatom molecule for QSPR application [16].

3. Method of Calculation

3.1 Topology Index Calculation

Let $G(V, E)$ represented as the chemical molecular graph with vertex (V) and edge set (E). For example if the chemical molecular G having vertex (V)set {c_1, c_2, c_3, c_4, c_5} and edge (E) set {{c_1, c_2}, {c_2, c_3}, {c_3,c_4}, {c_4, c_5}}. The first and second Zagreb indices are defined as[17]:

$$M1(G) = \sum_{v \in V(G)} d_v + d_v \tag{5a}$$

$$M2(G) = \sum_{uv \in V(G)} d_u d_v \tag{5b}$$

where d_v and d_u are the degree of vertex u and v respectively. The degree of vertex is the number of edges with it. While the hyper-Zagreb index is given by equation (6)[5]:

$$HM\ (G) = \sum_{uv \in V(G)} (d_u + d_v)^2 \tag{6}$$

In this calculation, we have also defined a new inversed hyper-Zagreb index, shown as follows:

$$^{*}HM\ (G) = \sum_{uv \in V(G)} \frac{1}{(d_u + d_v)^2} \tag{7}$$

To describe the method of calculation, it is illustrated with a specific example, molecules of 2,3-dimethylbutane. Figure 1(a) shows the structural graph for 2,3-dimethylbutane, whereas figure 1(b) shows the vertex degree for 2,3-dimethylbutane. Therefore, the HM index for 2,3-dimethylbutane = 4 $(3+1)^2$ + $(3+3)^2$ = 100. At the same time, the *HM = 4 / $(3+1)^2$ + 1 / $(3+3)^2$ = 0.27777. The inversed and hyper-Zagreb indices for the alkanes are tabulated in table A.

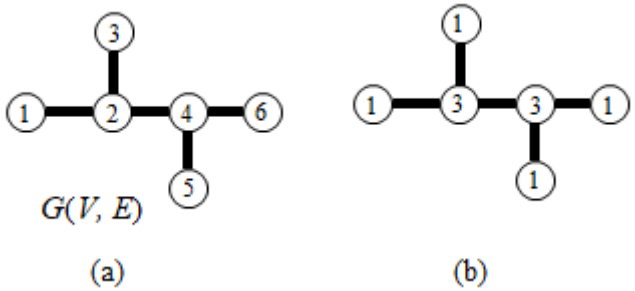

Figure 1(a) illustrative molecular graph $G(V, E)$ (b) vertex-degree for 2,3-dimethylbutane.

3.2 Data and Analysis

Four thermodynamic properties were selected based on the availability of suitable data. The thermodynamic properties were boiling points (bp), heats of vaporization at 25^{o}C (hv), critical temperature (ct) and critical pressure (PC). All data were retrieved from the reference [18, 19]. For the individual thermodynamic properties, the multiple linear regression (MLR) used the inversed and hyper-Zagreb indices. MLR is a quantitative statistical technique that is applied for the purpose of investigating the contribution of more than one topology index towards dependent thermodynamic properties. We perform regression using Excel's statistical data analysis tools.

4. Results and Discussion

The thermodynamic properties such as boiling points (bp), heats of vaporization at 25^{o}C (hv), critical temperature (ct), and critical pressure (PC) were the important parameters to relate with the molecular structure. Before we further analyse the regression equation, we examine the correlation

among the physical properties. Table 1 shows the correlations among the physical properties. As shown in this table, boiling point, molecular mass (MR) and heat of vaporization are strongly correlated. While critical pressure and temperature are not well correlated with other physical parameters.

Table 1: Correlation among the physical properties.

	bp	**MR**	**hv**	**cr**	**CP**
bp	1				
MR	0.977223	1			
hv	0.991595	0.965425	1		
ct	0.356223	0.375618	0.344035	1	
CP	-0.43116	-0.44091	-0.42146	-0.04858	1

Table A shows the experimental, inversed, hyper-Zagreb and Zagreb index. As shown in Table 1, inversed and hyper-Zagreb indices are not unique to the molecular structure. For example, 2,2-Dimethylpropane, 2,3-Dimethylbutane and 3-Methylhexane have the same HM index of 100. However, for the inversed hyper-Zagreb index (*HM), it has only 2 molecules with the same number of indices.

The data is instructive for examining the relationship between topological indices and the thermodynamic properties of alkanes. The best fitting of multiple-regression with the topological index was attempted. Multiple-regression is able to have a prediction model between the Zagreb topological indices and the experimental result. Table 3 shows R, R square (R^2), adjusted R square (R^2_{adj}), and also the number of observations, *n*. Most of the topology index is reasonably well accounted for in the present topology index. For boiling point, critical temperature, and heat vapor, they are reasonably well-accounted for by the presence of the two parameters. The multiple linear regression equation for the boiling point, critical temperature, and heat vapor are given in equation (8 – 10).

$$bp = - 82.530774 + 0.54414103\ HM + 279.631081\ {}^*HM \quad (8)$$

$$ct = 0.882794\ HM + 391.2915\ {}^*HM \quad (9)$$

$$hv = 0.098746566\ HM + 58.15906284\ {}^*HM \quad (10)$$

Table 3: Multiple Regression Equation (MRE) for physical properties using inversed, hyper and Zagreb indices of alkanes.

Properties	**MRE**
bp	bp (^{o}C) = -82.530774 +0.54414103 HM+279.631081 *HM R = 0.9853; R^2 = 0.9709; R^2_{adj} = 0.9595; *n* = 44
ct	ct (^{o}C) = 0.882794 HM + 391.2915 *HM R = 0.9987; R^2 = 0.9974; R^2_{adj} = 0.9735; *n* = 44
hv	hv (kJ/mol) = 0.098746566 HM + 58.15906284 *HM R = 0.9991; R^2 = 0.9982; R^2_{adj} = 0.9725; *n* = 41
PC	PC (atm) = 0.489243 M1 – 0.20653 M2 + 0.044112 HM + 26.14328 *HM R = 0.9524; R^2 = 0.9071; R^2_{adj} = 0.875; *n* = 44

The critical pressure is the pressure by which the vapor of a compound liquefies at a critical pressure. For estimating the critical pressure, the regression involves four topology indices of Zagreb indices (M1 and M2), inversed hyper-Zagreb index (*HM), and the hyper-Zagreb index (HM). The relationship is given by equation (11). Therefore, the critical pressure might be not dependent upon the molecular structure, but also other factors that are not well-defined using inversed and hyper-Zagreb indices.

$$PC\ (atm) = 0.489243\ M1 - 0.20653\ M2 + 0.044112\ HM + 26.14328\ *HM \quad (11)$$

The regression equation for four thermodynamic properties shows a good relation property. These results show that the molecule structure has a significant impact on the properties that rely on intermolecular forces. The intermolecular forces strongly depend on the branching of the molecule. The branching can be calculated using inversed, hyper-Zagreb and Zagreb index. The final model uses an alternative expression

$$\text{property} = a + \sum_{i=1} \left[b_i \ \text{index}_i \right] \quad (12)$$

where *a* and *b* are coefficients that has been calculated in equation (8-11). The topology index can be used to relate the relationship of physical properties with molecule branching. The concept of a chemical graph that is connected by an edge is closely related to the concept of valence in chemistry. This means that a simple graph of suppress-hydrogen with the carbon atom skeleton represents the covalent bond between the carbon-carbon atom. The thermodynamic properties of molecules (boiling points, heats of vaporization, critical temperature, and critical pressure) depend on the valence electrons that form the molecule. Although the covalent bond involves the sharing of electrons, the molecular forces which contribute to the thermodynamic properties differ based on the molecular structure. Since the interactions between the alkane molecules are very weak due to temporary polarization of molecules, the isomer of alkanes reflects the thermodynamic properties. For the prediction of thermodynamic properties of isomer alkanes, the inversed and hyper-Zagreb indexes are alternative approaches to representing the molecule with a numerical value that has a relationship with molecular bonding. The good relationship has been proven through the good values of R, R^2 and R^2_{adj}. There are two main reasons why there is a need to use the molecular descriptor based on degree. (i) The perception of branching influences molecular force, and (ii) different thermodynamic properties necessitate different orderings of the sets of isomers. The molecular descriptors are still improving due to the fact that the environmental conditions are not fully covered using the graph theory approach.

5. Conclusion

In this paper, the relationships between the thermodynamic properties of alkanes such as the boiling point, heat vaporization at 25^{o}C (hv), critical temperature, and critical pressure using inversed and hyper-Zagreb were investigated. The inversed and hyper-Zagreb indices were not unique to the molecular structure. The boiling point, critical temperature, and heat vapor were reasonably well accounted for by the presence of two parameters (HM and *HM). For the critical pressure, the regression equation involved four topology indices of Zagreb indices (M1 and M2), HM and *HM. The regression equation for the four thermodynamic properties showed a good relation property. The good relationship has been proven through the good value of R, R^2 and R^2_{adj}.

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Appendix

Table A: The Experimental values, inversed, hyper and Zagreb index of alkanes

	bp (ºC)	hv (kJ/mol)	ct (°C)	PC (atm)	M1	M2	HM	*HM
n-Butane	-0.5		152.01	37.47	10	8	34	0.284722
2-Methylpropane	-11.7		134.98	36	11	9	48	0.1875
n-Pentane	36	26.42	196.62	33.31	14	12	50	0.3472222
2-methylbutane	27.8	24.59	187.8	32.9	16	14	66	0.2761111
2,2-Dimethylpropane	9.5	21.78	160.6	31.57	20	16	100	0.16
n-Hexane	68.7	31.55	234.7	29.92	18	16	66	0.4097222
2-Methylpentane	60.3	29.86	224.9	29.95	20	17	82	0.33861111
3-Methylpentane	63.3	30.27	231.2	30.83	20	19	84	0.36472222
2,2-Dimethylbutane	49.7	27.69	216.2	30.67	24	22	120	0.258888
2,3-Dimethylbutane	58	29.12	227.1	30.99	22	21	100	0.27777
n-Heptane	98.5	36.55	267.01	27.01	22	20	82	0.4722222
2-Methylhexane	90	34.8	257.9	19.29	24	22	98	0.4011111
3-Methylhexane	92	35.08	262.4	19.79	24	23	100	0.427222
3-Ethylpentane	93.5	35.22	267.6	20.44	24	24	102	0.453333
2,2-Dimethylpentane	79.2	32.43	247.7	18.02	28	26	136	0.3213888
2,3-Dimethylpentane	89.8	34.24	264.6	19.96	26	29	118	0.3663889
2,4-Dimethylpentane	80.5	32.88	247.1	18.15	26	24	114	0.33
3,3-Dimethylpentane	86.1	33.02	263	19.59	28	28	140	0.377777
2,2,3-Trimethylbutane	80.9	32.04	258.3	18.76	30	30	156	0.26540816
n-Octane	125.7	41.48	296.2	21.76	26	24	98	0.53472222
2-Methylheptane	117.6	39.68	288	20.6	28	26	114	0.4636111
3-Methylheptane	118.9	39.83	292	25.6	28	27	116	0.4897222
4-Methylheptane	117.7	39.67	290	25.6	28	27	116	0.489722
3-Ethylhexane	118.5	39.4	292	25.74	28	28	118	0.5158333
2,2-Dimethylhexane	106.8	37.29	279	25.6	32	30	152	0.38388888
2,3-Dimethylhexane	115.6	38.79	293	26.6	30	30	134	0.4288889
2,4-Dimethylhexane	109.4	37.76	282	25.8	30	29	132	0.4186111
2,5-Dimethylhexane	109.1	37.86	279	25	30	28	130	0.3925
3,3-Dimethylhexane	112	37.93	290.83	27.2	32	2	156	0.4202777
3,4-Dimethylhexane	117.7	39.02	298	27.4	30	31	136	0.455
3-Ethyl-2-Methylhexane	115.6	38.52	295	27.4	30	31	136	0.455
3-Ethyl-3-Methylhexane	118.2	37.99	305	28.9	32	34	160	0.4566667
2,2,3-Trimethylpentane	109.8	36.91	294	28.2	34	35	174	0.354019
2,2,4-Trimethylpentane	99.2	35.13	271.15	25.5	34	32	168	0.312777
2,3,3-Trimethylpentane	114.8	37.22	303	29	34	36	176	0.364297
2,3,4-Trimethylpentane	113.5	37.61	295	27.6	32	33	152	0.36805555
2,2,3,3-tetrametylbutane	106.5		270.8	24.5	38	40	214	0.255625
n-nonane	46.44	322	22.74	46.44	30	28	114	0.597222
2-Methyloctane	44.65	315	23.6	44.65	32	30	130	0.5261111

3-Methyloctane	44.75	318	23.7	44.75	32	31	132	0.552222
4-Methyloctane	44.75	318.3	23.06	44.75	32	31	132	0.552222
3-ethylheptane	44.81	318	23.98	44.81	32	26	134	0.5783333