

TG Index and Its Application on Alkanes and Alkenes

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Abstract

Topological indices have an important role in chemical graph theory. Description of chemical structure with a number provides being able to guess unmeasured properties of known and unknown compounds. (Turker-Gumus Index) TG Index has been described and its application on some physical properties of alkanes and alkenes have been reported. The TG Index is a novel index based on connectivity and distances in the graph of a molecular structure. The authors have tried to use TG index to model some important properties in alkanes and alkenes. The index is very well correlated with the applied properties with only a few exceptions.

Keywords

TG Index, Topological Indices, T(A) Graphs, Alkanes, Alkenes

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1. Introduction

Topological indices are numbers associated with constitutional formulas by mathematical operations on the graphs representing these formulas. The necessity of having to use such tools as topological indices originates in the fact that physico-chemical properties are expressed as numbers and thus have a metric enabling scientists to make comparisons and correlations. In order to evaluate quantitatively the degree of similarity or dissimilarity of chemical structures or to find correlations between structures and properties (QSAR or QSPR) one needs to translate structures into numbers. For electronic factors, quantum chemistry or linear free energy relationships provide such numerical data. For steric factors or hydrophobicity/hydrophilicity there are well-established numerical data. For shape, however, topological indices provided a simple solution [1-3].

Ever since structure theory became able to explain the isomerism phenomenon and to predict what substances with

a given molecular formula can exist, chemists have tried to predict the properties of these substances before they were synthesized. After some of these substances were prepared, the predictions could be checked and the prediction methods could be validated or improved [1-3].

Probably the first chemist who attempted such predictions was Kopp who published his results in 1844 [4]. His methods were primitive because the structure theory was just emerging. With the advent of quantum theory and more recently with the help of computer-assisted semiempirical or *ab initio* calculations, the theoretical background of molecular chemistry reached a satisfactory level for understanding chemical reactivity and for describing transition states. It was Erich Hückel who for the first time thought about applying to molecules the π -electron approximation and invented the equivalence between the eigenvalues of the adjacency matrix of a graph symbolizing the σ -electron framework and the energy levels of π -electrons in conjugated systems [5]. Thus, topological or graph theoretical data are deeply associated with the core of

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quantum chemistry [6].

Most of the proposed topological indices are related to either vertex adjacency relationship (connectivity) in the molecular graph or to graph theoretical (topological) distances. Therefore, the origin of topological indices can be traced either to the adjacency matrix of a molecular graph or to the distance matrix of a molecular graph. Furthermore, since the distance matrix can be generated from adjacency matrix [7], most of the topological indices are really related to the latter matrix [8].

Alkanes

Alkanes represent an attractive class of compounds as a starting point for the application of graph theoretical approaches because of their non-polar characteristics and presence of just two kinds of atoms. The use of more polar compounds is avoided due to some complexities. Moreover, many properties of alkanes change in a regular manner with their mass and the extent of branching.

The aim of this study is to investigate the possible structure-property relationships (QSPR) for the various physicochemical and electronic properties of the alkanes and alkenes. Such relationships can be employed to predict yet unmeasured values for the considered properties of compounds, in addition to that, it can be extended for design of non-existent structures possessing some desirable properties.

Since the alkanes are non-polar, a number of complexities due to polarity, polarizability, and hydrogen bonding that arise with more polar compounds are avoided. Thus, the physicochemical properties of alkanes are dominated by their inherent structural features, such as molecular dimension or shape. The molecular size has an impact and influence on most properties (activities), although other factors such as branching and steric factors also have smaller influences. In the present study, the authors are mainly concerned with the size and branching effects on some physical, physiological and electronic properties.

2. Method of Calculation

The physical properties considered in this part are boiling points (bp), molar volumes at 20 °C (MV), molar refractions at 20 °C (MR), heats of vaporization at 25 °C (HV), critical temperatures (TC), critical pressures (PC), surface tensions at 20 °C (ST), melting point (mp), molar susceptibility (χ_m), polarizability (α), density (d) and parachore (PR). Values for the properties were excerpted from the literature [9]. The molar volumes were calculated as MW/d where MW is the

molecular weight and d is the density (g/mL). The molar refractions were calculated by using Lorentz-Lorenz expression [10] where n_o is the index of refraction.

$$MR = \frac{n_o^2 - 1}{n_o^2 + 2} \frac{MW}{d} \quad (1)$$

In the present study, MR is considered due to its relationship to molecular polarizability [11-16]. Only liquid-phase values for MV, MR, HV and ST were used. Among the branched alkanes, the TG index of 2,2-dimethyl propane cannot be calculated since the distance-degree matrix of the unstarred set has only one element which leads TG index to be zero.

For the compounds considered, additional data have been gathered from the literature [17,18] for the aqueous solubilities (S_w , expressed as $\log S_w$), as well as the partition coefficient in octanol-water solvent system (P_{oct} , expressed as $\log P_{oct}$).

3. Results and Discussion

Consequent to above, unbranched alkanes were discussed, and the study was then extended to a large number of alkanes consisting of branched and unbranched structures. First, QSPR models based on boiling points (bp) were developed and then, several other properties of alkanes were considered [18].

3.1. Linear Alkanes

The correlation analyses have been performed between the natural logarithm of the TG Index and the physical properties (bp, mp, χ_m , α , d, PR, $\log P_{oct}$, $\log P_{16}$ and $-\log S_w$) of the linear alkanes. The properties of the linear alkanes together with the calculated TG Index data, and the results of the regression analyses have been given in Tables 1 and 2, respectively.

The boiling point (bp) of a compound is related directly to the chemical structure of the molecules. Pioneering work in applying QSPR to the boiling points of alkanes was done by Wiener [19]. Since then, there have been very extensive efforts to apply structural information to fit experimental boiling points. Most of this work was centered at homologous and congeneric series of compounds. Here the boiling points of 17 linear alkanes (butane to eicosane) have been considered for correlation with the TG index. As can be seen from Table 2 a very good fit is obtained for these class of compounds with a coefficient of determination of 0.9919.

Table 1. Calculated TG Index values and some physical properties of the linear alkanes. (Units: bp, °C; mp, °C; χ_m , m³/mol; d, g/cm³; α , C·m²·V⁻¹)

# of C atoms	Alkane	TG	bp	mp	χ_m	logP _{oct}
4	n-Butane	9	-0.5	-138	50.3	3.14
5	n-Pentane	40	36.1	-130	61.5	3.67
6	n-Hexane	169	68.7	-95	74.1	4.21
7	n-Heptane	448	98.4	-91	85.2	4.74
8	n-Octane	1156	125.7	-57	96.6	5.28
9	n-Nonane	2400	150.77	-54	108.1	5.82
10	n-Decane	4900	174.12	-30	119.5	6.35
11	n-Undecane	8800	196.8	-26	131.8	6.89
12	n-Dodecane	14641	216.3	-10		7.42
13	n-Tridecane	25480	235.4	-5.5		7.96
14	n-Tetradecane	41209	263.7	6		8.5
15	n-Pentadecane	62720	270.1	10		9.03
16	n-Hexadecane	97344	280	18	187.6	9.57
17	n-Heptadecane	137088	292	22		10.1
18	n-Octadecane	197136	308	28		10.64
19	n-Nonadecane	273600	320	32		11.18
20	n-Eicosane	378225	342.7	36.8		
		TG	-logS _w	d	PR	α
4	n-Butane	9	2.57		231	9.99
5	n-Pentane	40	3.18	0.626	270.8	11.83
6	n-Hexane	169	3.84	0.659	310.6	13.66
7	n-Heptane	448	4.53	0.684	350.4	15.5
8	n-Octane	1156	5.24	0.703	390.2	17.34
9	n-Nonane	2400	5.88	0.718	430	19.17
10	n-Decane	4900	6.98	0.73	469.7	21.01
11	n-Undecane	8800	7.59	0.74	509.5	22.85
12	n-Dodecane	14641	7.67	0.749	549.3	24.28
13	n-Tridecane	25480		0.756	589.1	26.52
14	n-Tetradecane	41209	7.96	0.763	628.9	28.36
15	n-Pentadecane	62720		0.769	668.7	30.19
16	n-Hexadecane	97344	8.4	0.773	708.4	32.03
17	n-Heptadecane	137088		0.778	748.2	33.87
18	n-Octadecane	197136		0.777	788	35.7
19	n-Nonadecane	273600		0.777	825.8	37.4
20	n-Eicosane	378225		0.789	1225.6	55.91

Table 2. The regression equations and the coefficients of determination of the regression analyses between the TG index and the experimental properties of linear alkanes.

Property	regression equation	R ²
bp (n = 17)	y = 32.602x + 92.423	0.9919
mp (n = 17)	y = 17.663x + 186.19	0.9901
χ_m (n = 9)	y = 14.194x + 186.19	0.9411
logP _{oct} (n = 16)	y = 0.793x + 0.2688	0.9466
-logS _w (n = 11)	y = 0.7015x + 0.6224	0.9693
d (n = 16)	y = 0.0169x + 0.5787	0.9735
PR (n = 16)	y = 58.809x + 18.486	0.9471
α (n = 16)	y = 2.7112x + 0.1828	0.9461

The boiling points of alkanes are determined by the forces of attraction between the molecules in the liquid form. Since the molecules in the solid state have a rigid three-dimensional structures, melting point unlike boiling point, is a solid state property and hence is influenced by properties of solids such as amorphous or crystalline nature, allotropy, polymorphism, molecular symmetry, as additional and more important

factors than intermolecular forces. Hence, the melting points of alkanes are more difficult to model. The data in Table 2 for the regression of TG index with the melting point indicate that in spite of the complexities of solid state properties included in melting points, the TG index is very successful in this correlation.

In physics, the susceptibility (χ) of a material or substance describes its response to an applied field. Molar susceptibility (χ_m) is measured as m³/mol. Magnetic susceptibility is measured by the force change felt upon the application of a magnetic field gradient [20]. Today, high-end measurement systems use a superconductive magnet. An alternative is to measure the force change on a strong compact magnet upon insertion of the sample. This system, widely used today, is called the Evans balance. For liquid samples, the susceptibility can be measured from the dependence of the NMR frequency of the sample on its shape or orientation [21]. This important property requires expensive apparatus to

be measured. Thus, being able to guess it by a simple mathematical formula is quite acceptable. As can be seen from Table 2 χ_m has a reasonable high coefficient of determination value of 0.9411. Therefore, the regression equation can be used to predict the χ_m data for the missing members of the series and the rest of linear alkanes which are not considered here.

For developing a QSPR model for the unbranched alkanes the authors have considered $\log P_{\text{oct}}$ (logarithm of octanol-water partition coefficient P_{oct}) and aqueous solubility (S_w) to represent their physiological activity. The solubility of liquids and solids in water (S_w) as well as partition coefficient of solutes in different solvents viz. partition coefficient in octanol-water (P_{oct}) are very important molecular properties that influence the release, transport, and the extent of absorption of drugs in the body. These properties are the key determinants of the environmental fate of agrochemicals and pollutants in the environment. The hydrophobic constant ($\log P$) is used to rationalize interactions of small ligands with various macromolecules in the fields of biochemistry, medicinal chemistry, and environmental sciences. Considerable experience in the use of $\log P$ in the study of QSPR by regression analysis clearly indicated that measured $\log P$ should be used whenever possible. Nevertheless, when the number of compounds is great and the structural variations limited, experimentally simple economics makes it desirable to measure $\log P_s$ for the key structures only and to calculate the remainder.

A number of methods are also reported for estimating the aforementioned parameters (P_{oct} and S_w) using molecular descriptors other than topological indices. However, very little work has been done for the estimation of aforementioned parameters using topological indices. This has prompted us to undertake the present investigation in that the novel TG index has been used for modeling, monitoring, and estimating P_{oct} and S_w . In doing so n-alkanes have been chosen (Table 1) since all these parameters for this set of compounds are easily available in the literature which can be adopted [17].

A perusal of Table 1 shows that both of the properties viz. $\log P_{\text{oct}}$ and $\log S_w$ increase with the size of the alkanes. It means that these properties are the function of size, shape, and branching of the molecules. Hence, it appears that TG index might be appropriate for modeling, monitoring, and estimating these properties. The data presented in Table 4 show that like the presently considered properties, the magnitude of TG index also increases with the size of the alkanes under present study. This means that, TG index would be quite suitable for modeling the two properties mentioned above.

To understand the performance of the TG index, the results of regression calculations can be seen in Table 2. The TG index shows very good correlation ($R^2 = 0.9466, 0.9693$ for $\log P_{\text{oct}}$ and $\log S_w$, respectively) with the properties mentioned. Therefore, TG index can serve as a potential parameter for predicting the physical and physiological properties of linear alkanes.

Density is another very important physical property and easily available for the small-sized members of the series. The density of the alkanes usually increases with increasing number of carbon atoms. The R^2 value for the linear regression of $\ln(\text{TG})$ versus density exceeds 0.97. Therefore, it can be concluded that the TG index is again capable of modeling this size dependent property, useful especially for nonexistent structures.

In this study parachor is also considered for regression analysis since it is a well known property leading to calculation of a very essential property of liquids; the surface tension. A well correlated equation will give us the ability to obtain the surface tensions of liquids.

Parachor is a quantity defined by the molecular weight of a liquid times the fourth root of its surface tension, divided by the difference between the density of the liquid and the density of the vapor in equilibrium with it; essentially constant over wide ranges of temperature. Parachor has been used in solving various structural problems [22, 23].

A small structural change in a molecular scale gives a big effect on the surface tension. The estimation of the surface tension by a rather simple empirical approach using the quantity parachor has been successful for a wide variety of molecular liquids. The accuracy of the parachor approach is quite good.

It has been known that the parachor obeys an additivity rule, i.e., parachor of a molecule is always the sum of the parachor value assigned to each part of the molecule or to the atoms existing in that molecule, regardless of the type of compound. Although corrections by assigning a small value for branching, ring formation, etc., are often made in the summation of atomic parachors, additivity rule of the atomic parachor means that the isomers essentially have similar values of the molecular parachor. Also, the success of the parachor additivity rule means that the anisotropic or structure-dependent part of the molecular interaction must give only minor effects on the surface tension of molecular liquids [24]. Considerable effort has been paid to explain the empirical relation. However, there seems to be no convincing explanation of the additivity rule of the parachor, which is the essential point for the success of parachor as a method of surface tension estimation.

The coefficient of determination for the regression analysis of parachor of linear alkanes versus the TG index is 0.9471, which is a satisfactorily good result (see Table 2).

Molecular polarizability is another important property related to electron movements. Many papers have investigated the effective polarizability effects on the properties of organic compound in gas phase (such as protonic acidities and basicities) [25-27]. Previous works showed that the molecular polarizability is an important factor affecting properties of organic compounds related to positive or negative charge. The regression equation and the coefficient of determination of the analysis of polarizability of linear alkanes have been given in Table 2.

In conclusion, the TG index is a very useful tool for the estimation of the considered properties for alkanes whose data are missing and sometimes difficult (expensive and time consuming) to measure within only a few percents of error. The molecular size of the unbranched alkanes increase steadily, so does the TG index. Therefore, the TG index can be considered as successful for the correlation of size dependent physical properties. The effect of branching on the success of TG index will be investigated in the following part of the paper.

3.2. Branched Alkanes

The calculated indices and the experimental values for the eight physical properties (bp, MV, MR, HV, TC, PC, ST, mp)

and coefficients of determination between the eight physical properties of the alkanes under consideration can be seen in Tables 3 and 4, respectively. A representative illustration for the calculation of the TG index for branched alkanes can be seen in Figure 1.

Before starting the correlation analyses between the novel topological index and each physical property, it is instructive to examine the correlations among the properties themselves. The results of these correlation studies are given in Table 4. As can be seen from the table, it is readily apparent that most of the properties show strong internal correlation (colinearity). Melting points are exceptional, which are very weakly correlated with the other properties. In addition to melting points, surface tensions and the critical temperatures do not correlate well with the critical pressures. For the remaining properties, all the coefficients of determination are greater than 0.807, and even exceed 0.942 for the subset (bp, MV, MR, and HV). It can be anticipated that if a given set of structural parameters successfully models a given property, this parameter set should also be reasonably successful in modeling other, strongly correlated properties. The converse can also be anticipated; i.e., lack of success should be transferred to the correlated properties.

The results of the regression analysis for branched alkanes have been given in Table 5. The properties are correlated with the logarithm of the index to obtain a linear plot.

Table 3. Calculated TG indices and experimental values for the physical properties of the 70 alkanes (Units: bp, °C; MV, cm³/mol; MR, cm³/mol; HV, kJ/mol; TC, °C; PC, atm; ST, dyn/cm; mp, °C).

Entry	Name	TG	bp	MV	MR	HV	TC	PC	ST	mp
1	n-Butane	9	-0.5	-	-	-	152.01	37.47	-	-138.35
2	n-Pentane	40	36.074	115.205	25.2656	26.42	196.62	33.31	16	-129.72
3	2-Methylbutane	32	27.852	116.426	25.2923	24.59	187.8	32.9	15	-159.9
4	n-Hexane	169	68.74	130.688	29.9066	31.55	234.7	29.92	18.42	-95.35
5	2-Methylpentane	110	60.271	131.933	29.9459	29.86	224.9	29.95	17.38	-153.67
6	3-Methylpentane	120	63.282	129.717	29.8016	30.27	231.2	30.83	18.12	-118
7	2,3-Dimethylbutane	100	57.988	132.744	29.9347	29.12	216.2	30.67	16.3	-99.87
8	2,2-Dimethylbutane	75	49.741	130.24	29.8104	29.12	227.1	30.99	17.37	-128.54
9	n-Heptane	448	98.427	146.54	34.5504	36.55	267.01	27.01	20.26	-90.61
10	2-Methylhexane	304	90.052	147.656	34.5908	34.8	257.9	27.2	19.29	-118.28
11	3-Methylhexane	285	91.85	145.821	34.4597	35.08	262.4	28.1	19.79	-119.4
12	3-Ethylpentane	288	93.475	143.517	34.2827	35.22	267.6	28.6	20.44	-118.6
13	2,2-Dimethylpentane	150	79.197	148.695	34.6166	32.43	247.7	28.4	18.02	-123.81
14	2,3-Dimethylpentane	264	89.784	144.153	34.3237	34.24	264.6	29.2	19.96	-119.1
15	2,4-Dimethylpentane	192	80.5	148.949	34.6192	32.88	247.1	27.4	18.15	-119.24
16	3,3-Dimethylpentane	252	86.064	144.53	34.3323	33.02	263	30	19.59	-134.46
17	2,2,3-Trimethylbutane	216	80.882	145.191	34.3736	32.04	258.3	24.64	18.76	-24.91
18	n-Octane	1156	125.655	162.592	39.1922	41.48	296.2	24.8	21.76	-56.79
19	2-Methylheptane	855	117.647	163.663	39.2316	39.68	288	25.6	20.6	-109.04
20	3-Methylheptane	896	118.925	161.832	39.1001	39.83	292	25.6	21.17	-120.5
21	4-Methylheptane	756	117.709	162.105	39.1174	39.67	290	25.74	21	-120.95
22	2,2-Dimethylhexane	703	106.84	160.072	38.9441	37.29	292	25.6	21.51	-
23	2,3-Dimethylhexane	729	115.607	164.285	39.2525	38.79	279	26.6	19.6	-121.18
24	2,4-Dimethylhexane	684	109.429	160.395	38.9808	37.76	293	25.8	20.99	-
25	2,5-Dimethylhexane	841	109.103	163.093	39.13	37.86	282	25	20.05	-137.5
26	3,3-Dimethylhexane	595	111.969	164.697	39.2596	37.93	279	27.2	19.73	-91.2
27	3,4-Dimethylhexane	676	117.725	160.879	39.0087	39.02	290.84	27.4	20.63	-126.1

Entry	Name	TG	bp	MV	MR	HV	TC	PC	ST	mp
28	3-Ethylhexane	783	118.534	158.814	38.8453	39.4	298	27.4	21.64	-
29	2,2,3-Trimethylpentane	476	109.84	158.794	38.8362	36.91	295	28.9	21.52	-114.96
30	2,2,4-Trimethylpentane	329	99.238	157.026	38.7171	35.13	305	28.2	21.99	-90.87
31	2,3,3-Trimethylpentane	525	114.76	159.526	38.9249	37.22	294	25.5	20.67	-112.27
32	2,3,4-Trimethylpentane	504	113.467	165.083	39.2617	37.68	271.15	29	18.77	-107.38
33	3-Ethyl-2-methylpentane	532	115.65	157.292	38.7617	38.84	303	27.6	21.56	-100.7
34	3-Ethyl-3-methylpentane	567	118.259	158.852	38.8681	38.48	295	24.5	21.14	-109.21
35	2,2,3,3-Tetramethylbutane	441	106.47	-	-	-	270.8	22.74	-	-
36	n-Nonane	2400	150.798	178.713	43.8423	46.49	322	23.6	22.92	-53.52
37	2-Methyloctane	2160	114.76	157.292	38.7617	37.22	303	29	21.56	-100.7
38	3-Methyloctane	1976	113.467	158.852	38.8681	37.61	295	27.6	21.14	-109.21
39	4-Methyloctane	1900	142.48	178.15	43.7687	45.09	318.3	23.98	22.34	-113.2
40	3-Ethylheptane	1664	143	176.41	43.642	44.96	318	23.98	22.81	-114.9
41	4-Ethylheptane	1572	141.2	175.685	43.4907	45	318.3	22.8	22.81	-
42	2,2-Dimethylheptane	1408	132.69	180.507	43.9138	41.82	302	23.79	20.8	-113

Table 3. (Continued)

43	2,3-Dimethylheptane	1600	140.5	176.653	43.6269	43.51	315	22.7	22.34	-116
44	2,4-Dimethylheptane	1323	133.5	179.12	43.7393	43.31	306	22.7	21.3	-
45	2,5-Dimethylheptane	1683	136	179.371	43.8484	42.91	307.8	23.7	21.3	-
46	2,6-Dimethylheptane	1496	135.21	180.914	43.9258	42.3	306	24.19	20.83	-102.9
47	3,3-Dimethylheptane	1512	137.3	176.897	43.687	42.78	314	24.77	22.01	-
48	3,4-Dimethylheptane	1457	140.6	175.349	43.5473	43.44	322.7	23.59	22.8	-
49	3,5-Dimethylheptane	1586	136	177.386	43.6378	43.49	312.3	24.18	21.77	-
50	4,4-Dimethylheptane	1140	135.2	176.897	43.6022	43.09	317.8	24.77	22.01	-
51	3-Ethyl-2-methylhexane	1395	138	175.445	43.655	43.65	322.7	25.56	22.8	-
52	4-Ethyl-2-methylhexane	1496	133.8	177.386	43.6472	43.26	330.3	25.66	21.77	-
53	3-Methyl-3-ethylhexane	1280	140.6	173.077	43.268	43.11	327.2	23.59	23.22	-
54	3-Ethyl-4-methylhexane	1320	140.4	172.844	43.3746	43.79	312.3	25.07	23.27	-
55	2,2,3-Trimethylhexane	1271	133.6	175.878	43.6226	41.5	318.1	23.39	21.86	-
56	2,2,4-Trimethylhexane	1155	126.54	179.22	43.7638	40.83	301	22.41	20.51	-120
57	2,2,5-Trimethylhexane	1496	124.084	181.346	43.9356	40.03	296.6	25.56	20.04	-105.78
58	2,3,3-Trimethylhexane	1120	137.68	173.78	43.4347	41.91	326.1	25.46	22.41	-116.8
59	2,3,4-Tri methylhexane	1260	139	173.498	43.3917	42.45	324.2	23.49	22.8	-
60	2,3,5-Trimethylhexane	1408	131.34	177.656	43.6474	41.8	309.4	23.79	21.27	-127.8
61	2,4,4-Trimethylhexane	1080	130.648	177.187	43.6598	41.25	309.1	26.45	21.17	-113.38
62	3,3,4-Trimethylhexane	1131	140.46	172.055	43.3407	41.99	330.6	26.94	23.27	-101.2
63	3,3-Diethylpentane	1584	146.168	170.185	43.1134	43.1	342.8	25.96	23.75	-33.11
64	2,2-Dimethyl-3-ethylpentane	864	133.83	174.537	43.4571	41.63	322.6	26.94	22.38	-99.2
65	2,3-Dimethyl-3-ethylpentane	1008	142	170.093	42.9542	42.01	338.6	25.46	23.87	-
66	2,4-Dimethyl-3-ethylpentane	896	136.73	173.804	43.4037	42.38	324.2	27.04	22.8	-122.2
67	2,2,3,3-Tetramethylpentane	988	140.274	169.495	43.2147	40.07	334.5	25.66	23.38	-9.9
68	2,2,3,4-Tetramethylpentane	832	133.016	173.557	43.4359	40.25	319.6	24.58	21.98	-121.09
69	2,2,4,4-Tetramethylpentane	528	122.284	178.256	43.8747	38.41	301.6	26.85	20.37	-66.54
70	2,3,3,4-Tetramethylpentane	960	141.551	169.928	43.2016	40.81	334.5	29.75	23.31	-102.12

According to the results of the regression analyses, the novel TG index is successful for modeling most of the properties considered. In the previous section, the success of the index had been proved over the linear alkane series. The results obtained in this part of the article indicate that the novel TG index is also capable of reflecting the effect of branching in molecules. Small variations in between the values of the coefficients of determination are not due to the failure of the index but the improper correlations between the properties themselves. The index correlated best with boiling point ($R^2 = 0.9595$) and heat of vaporization ($R^2 = 0.9639$).

The failure of the present index to model the melting points of the presently considered 70 alkane molecules is not surprising; a similar result was obtained by Seybold et al. [28]. A melting transition maintains a condensed phase and

involves a partial disruption of intermolecular orientations. Therefore, melting might depend on some geometrical and other crystalline factors, which are not well defined with any topological descriptors, yet.

3.3. Cycloalkanes

Cycloalkanes (also called naphthenes, especially if from petroleum sources) are types of alkanes which have one or more rings of carbon atoms in the chemical structure of their molecules. Cycloalkanes consist of only carbon (C) and hydrogen (H) atoms and are saturated because there are no multiple C-C bonds to hydrogenate. A general chemical formula for cycloalkanes would be $C_nH_{2(n+g)}$ where n = number of C atoms and g = number of rings in the molecule. Cycloalkanes with a single ring are named analogously to

their normal alkane counterpart of the same carbon count: cyclopropane, cyclobutane, cyclopentane, cyclohexane, etc. The larger cycloalkanes, with greater than 20 carbon atoms are typically called cycloparaffins.

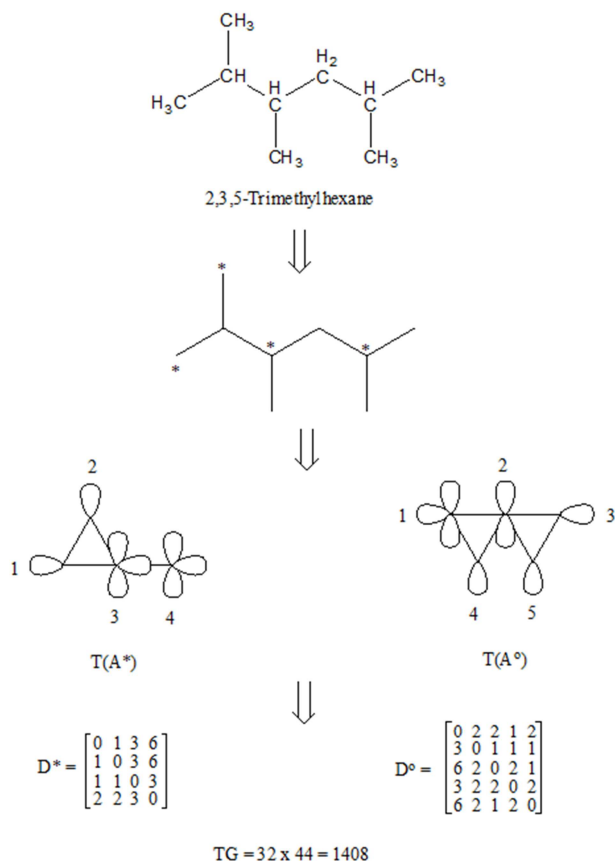


Figure 1. Calculation of the TG index for 2,3,5-trimethyl hexane (Entry 60).

Table 4. Coefficients of determination (R^2) among the properties examined, for branched alkanes considered presently.

	bp	MV	MR	HV	TC	PC	ST	mp
bp	1.000							
MV	0.956	1.000						
MR	0.975	0.992	1.000					
HV	0.981	0.946	0.952	1.000				
TC	0.975	0.909	0.951	0.930	1.000			
PC	-	-	-	-	-	1.000		
ST	0.923	0.807	0.865	0.892	0.965	-	1.000	
mp	0.397	0.293	0.329	0.319	0.432	-	0.421	1.000

Table 5. The regression equation and the coefficient of determination between the natural logarithm of the TG index and branched alkanes.

Property	regression equation	R^2
bp (n = 70)	$y = 28.446x - 68.686$	0.9595
MV (n = 68)	$y = 16.385x + 56.678$	0.9116
MR (n = 68)	$y = 4.9354x + 7.593$	0.9125
HV (n = 68)	$y = 4.6939x + 6.7157$	0.9639
TC (n = 70)	$y = 32.959x + 78.730$	0.8772
PC (n = 70)	$y = -2.3142x + 41.249$	0.7718
ST (n = 68)	$y = 1.7268x + 9.7065$	0.7541
mp (n = 52)	$y = 9.0646x - 163.16$	0.1348

Cycloalkanes are classified into small, common, medium, and large cycloalkanes, where cyclopropane and cyclobutane are the small ones, cyclopentane, cyclohexane, cycloheptane are the common ones, cyclooctane through cyclotridecane are the medium ones, and the rest are the larger ones. Cycloalkanes are similar to alkanes in their general physical properties, but they have higher boiling points, melting points, and densities than alkanes.

Table 6. The TG index and experimental boiling points ($^{\circ}C$) of cyclohexane systems with 6-10 carbon atoms.

	Name	TG	bp
1	c6	144	80.7
2	1mc6	336	101
3	1ec6	840	131.8
4	14mc6	784	121.8
5	13mc6	640	122.3
6	12mc6	729	126.6
7	11mc6	640	119.5
8	1pc6	1820	156.7
9	1ipc6	1536	154.8
10	1m4ec6	1700	150.8
11	1m3ec6	1564	150
12	1m2ec6	1457	154.3
13	135mc6	1080	139.5
14	124mc6	1395	144.8
15	123mc6	1320	149.4
16	1m1ec6	1485	152
17	113mc6	1062	136.6
18	112mc6	1350	145.1
19	1bc6	3840	180.9
20	1ibc6	3078	171.3
21	1m4pc6	3481	173.4
22	1m3pc6	2964	169
23	1sbc6	3078	179.3
24	14ec6	3249	175.5
25	13ec6	3016	172
26	1m2pc6	3078	174.5
27	1m4ipc6	2664	170
28	12ec6	2809	176
29	1m3ipc6	2808	167
30	1e35mc6	2584	168.5
31	1m2ipc6	2415	171
32	1m1pc6	2774	174.3
33	1tbc6	2268	171.5
34	11ec6	2592	179.5
35	14m1ec6	2695	168
36	1245mc6	2500	167
37	13m1ec6	2516	166.6
38	1235mc6	2244	166.5
39	1234mc6	2401	172.5
40	1135mc6	1640	153

Although, boiling points of alkanes are traditionally used for testing and/or demonstrating the correlating abilities of topological indices. Boiling points of cycloalkanes have been examined to a much lesser extent [29,30]. Moreover, Rücker and Rücker [31] produced a critical compilation of

experimental boiling points of cycloalkanes and reported their correlations with numerous topological indices and (linear) combinations. In this part of the text, novel QSPR models have been extended over the boiling points of cycloalkanes.

The calculated TG indices and the experimental boiling point data of the cyclohexanes with 6-10 carbon atoms, and the plot of bp (°C) versus ln(TG) have been given in Table 6 and Figure 2, respectively. As in the case of linear and branched alkanes, the TG index and the boiling point increases with the number of carbon atoms present in the structure. The regression analysis yielded 0.9721 for the coefficient of determination. Consequently, the TG index has proved itself as a successful parameter for modeling the cyclic systems as well.

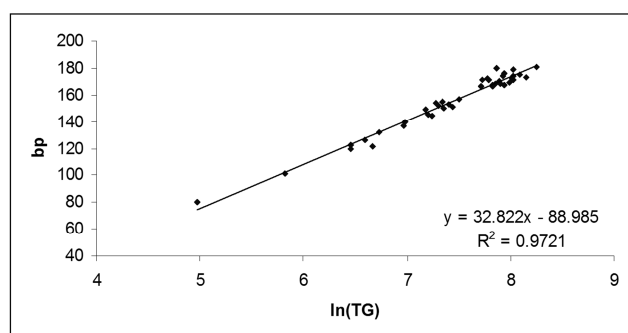


Figure 2. The plot of boiling points of cyclohexane derivatives versus ln(TG)

3.4. Alkenes

In the previous part, the topological descriptors have been applied to some physical and electronic properties of a set of normal and branched alkanes. In that part, it has been found that the TG index is successful in obtaining high-quality structure-property relationships. Good regression equations were obtained for most of the physical properties of the alkanes (the melting points (mp), traditionally a subtle and difficult property to handle, were an exception). In this part of the work, the TG index has been employed as a structural measure for the physical and chemical properties of a set of monoalkenes, where a new structural feature, the double bond, is introduced. Only a few previous QSPR studies have been devoted to the properties of this class of compounds [32-35], and these have generally been limited to single properties.

The properties examined in this point of the study are: boiling points (bp), molar refractions (MR), molar volumes (MV) at 20°C, heats of combustion (HC), molar heats of vaporization (HV) at 25°C, flashpoints (FLASH), second virial coefficients (VIRC) at 25°C, critical temperatures (TC), critical pressures (PC), and melting points (mp). The property values were excerpted from the reference source [36]. MV values were calculated as MW/d, where MW is the molecular weight, and d is the density (g/cm³) at 20°C.

The calculated indices, and the experimental values for the eleven properties, of the alkenes under consideration can be seen in Tables 7 and Table 8, respectively.

Table 7. The TG indices and the experimental values for the physical properties of the alkenes series considered (Units: bp, °C; mp, °C; MV, cm³/mol; MR, cm³/mol; HC, kJ/mol; FLASH, K; VIRC, cm³/mol; HV, kJ/mol; TC, °C; PC, MPa).

Name	TG	bp	mp	MR	MV	HC	HV	FLASH	VIRC	TC	PC
1-Butene	16	-6.3	-185.4	22.66	94.3	2716.8	20204	-	-650	146.5	4.02
Cis-2-butene	16	3.7	-138.9	20.59	90.3	2710.0	21963	-	-713	162.4	4.21
Trans-2-butene	16	0.9	-105.6	20.73	-	-	21483	-	-700	155.5	4.10
1-Pentene	65	30.0	-165.2	24.85	109.4	3375.4	25501	-	-1093	191.6	3.53
Cis-2-pentene	60	36.9	-151.4	24.95	107.0	3370.0	26885	-	-1150	201.8	3.70
Trans-2-pentene	60	37.0	-140.2	25.02	-	-	-	228.15	-1140	201.9	3.65
2-Methyl-1-butene	45	31.2	-137.6	24.85	107.8	3361.6	-	-	-1111	191.9	3.51
3-Methyl-1-butene	50	20.1	-168.5	24.94	111.8	3368.9	-	-	-974	191.9	3.44
2-Methyl-2-butene	50	38.6	-133.8	24.95	105.9	3355.7	27090	228.15	-1264	197.2	3.38
1-Hexene	256	63.5	-139.8	29.49	125.0	4034.1	30587	247.15	-1729	230.8	3.14
Cis-2-hexene	240	68.8	-141.1	29.53	122.5	4023.8	33744	-	-	-	-
Trans-2-hexene	240	67.9	-133.0	29.67	-	-	32136	253.15	-	-	-
Cis-3-hexene	225	66.4	-137.8	29.66	123.8	4028.5	31724	-	-	-	-
Trans-3-hexene	225	67.1	-113.4	29.75	-	-	32072	261.15	-	-	-
2-Methyl-1-pentene	138	60.7	-135.7	29.48	123.8	4016.8	31042	247.15	-	-	-
3-Methyl-1-pentene	180	54.1	-153.0	29.49	126.1	4026.1	29262	245.15	-	-	-
4-Methyl-1-pentene	144	53.9	-153.6	29.55	126.8	4024.9	29376	242.15	-	-	-
2-Methyl-2-pentene	132	67.3	-135.1	29.74	122.6	4007.3	32088	250.15	-	-	-
3-Methyl-cis-2-pentene	168	70.5	-138.4	29.55	122.2	4013.9	31812	-	-	-	-
3-Methyl-trans-2-pentene	168	67.6	-134.8	29.55	-	-	32536	-	-	-	-
4-Methyl-cis-2-pentene	132	56.3	-134.4	29.67	125.8	4018.7	30096	245.15	-	-	-
4-Methyl-trans-2-pentene	132	58.6	-140.8	29.75	-	-	30550	-	-	-	-
2-Ethyl-1-butene	168	64.7	-131.5	29.37	122.0	4020.2	31614	-	-	-	-
2,3-Dimethyl-1-butene	144	55.7	-157.3	29.43	124.1	4011.2	29800	255.15	-	-	-
3,3-Dimethyl-1-butene	108	41.2	-115.2	29.58	128.9	4015.4	27449	245.15	-	-	-

Name	TG	bp	mp	MR	MV	HC	HV	FLASH	VIRC	TC	PC
2,3-Dimethyl-2-butene	144	73.2	-74.3	29.59	118.8	4007.3	32476	257.15	-1929	-	-
1-Heptene	646	93.6	-119.0	34.13	140.9	4692.6	35484	272.15	-2810	264.1	-
Cis-2-heptene	608	98.5	-	34.17	138.9	4686.5	-	-	-	-	-
Trans-2-heptene	608	98.0	-109.5	34.28	-	-	-	272.15	-	-	-
Cis-3-heptene	576	95.8	-	34.31	139.7	4686.5	-	-	-	-	-
Trans-3-heptene	576	95.7	-136.6	34.43	-	-	-	-	-	-	-
2-Methyl-1-hexene	532	92.0	-102.8	34.12	139.7	4678.0	-	267.15	-	-	-
3-Methyl-1-hexene	486	84.0	-	34.16	142.0	4688.7	-	267.15	-	-	-
4-Methyl-1-hexene	504	86.7	-141.5	34.08	140.6	4688.7	-	-	-	-	-
5-Methyl-1-hexene	551	85.3	-	34.14	141.9	4686.0	-	-	-	-	-
2-Methyl-2-hexene	513	95.4	-130.4	34.40	138.7	4672.2	-	-	-	-	-
3-Methyl-cis-2-hexene	459	94.0	-	34.18	137.2	4674.9	-	-	-	-	-
3-Methyl-trans-2-hexene	459	94.0	-	34.19	137.5	4674.9	-	-	-	-	-
4-Methyl-cis-2-hexene	468	87.4	-	34.22	-	-	-	-	-	-	-
4-Methyl-trans-2-hexene	468	87.6	-126.5	34.35	-	-	-	-	-	-	-
5-Methyl-cis-2-hexene	522	91.0	-	34.20	139.9	4679.3	-	-	-	-	-
5-Methyl-trans-2-hexene	522	86.0	-	34.41	-	-	-	-	-	-	-

Table 7. (Continued)

2-Methyl-cis-3-hexene	486	86.0	-	34.37	141.5	4679.3	-	-	-	-	-
2-Methyl-trans-3-hexene	486	86.0	-	34.52	-	-	-	-	-	-	-
3-Methyl-cis-3-hexene	494	95.4	-	34.32	137.7	4674.9	-	-	-	-	-
3-Methyl-trans-3-hexene	494	93.6	-	34.34	-	-	-	-	-	-	-
2-Ethyl-1-pentene	459	94.0	-	33.99	138.7	4680.7	-	-	-	-	-
3-Ethyl-1-pentene	406	85.1	-127.4	34.06	141.1	4691.3	-	-	-	-	-
2,3-Dimethyl-1-pentene	364	84.3	-134.8	34.00	139.2	4673.8	-	-	-	-	-
2,4-Dimethyl-1-pentene	266	81.6	-123.8	34.18	141.5	4670.9	33344	-	-	-	-
3,3-Dimethyl-1-pentene	357	77.5	-134.3	34.01	140.8	4679.4	-	-	-	-	-
3,4-Dimethyl-1-pentene	378	81.0	-	34.05	140.7	4681.7	-	-	-	-	-
4,4-Dimethyl-1-pentene	259	72.5	-136.6	34.23	143.9	4674.7	31598	-	-	-	-
3-Ethyl-2-pentene	442	96.0	-	34.11	136.3	4677.5	-	-	-	-	-
2,3-Dimethyl-2-pentene	350	97.5	-118.3	34.22	134.9	4667.1	-	-	-	-	-
2,4-Dimethyl-2-pentene	252	83.4	-	34.53	141.3	4665.1	34418	-	-	-	-
3,4-Dimethyl-cis-2-pentene	350	87.0	-	34.12	137.6	4667.9	-	-	-	-	-
3,4-Dimethyl-trans-2-pentene	350	87.0	-	34.15	-	-	-	-	-	-	-
4,4-Dimethyl-cis-2-pentene	238	80.4	-135.5	34.23	140.4	4667.9	32973	-	-	-	-
4,4-Dimethyl-trans-2-pentene	238	76.8	-115.2	34.41	-	-	33187	-	-	-	-
2-Ethyl-3-methyl-1-butene	350	89.0	-	33.96	138.5	4673.7	34634	-	-	-	-
2,3,3-Trimethyl-1-butene	322	77.9	-119.9	33.99	139.3	4668.2	32485	256.15	-	-	-
1-Octene	1600	121.3	-101.7	38.78	157.0	5351.1	41224	-	-	-3948	-
Cis-2-octene	1520	125.6	-100.2	38.79	154.9	-	-	-	-	-	-
Trans-2-octene	1520	-	125.0	-87.7	38.88	-	-	-	-	-	-
Cis-3-octene	1444	-	122.9	-	38.85	155.8	-	-	-	-	-
Trans-3-octene	1444	-	123.3	-	39.09	-	-	-	-	-	-
Cis-4-octene	1444	-	122.5	-	38.94	155.6	-	-	-	-	-
Trans-4-octene	1444	-	122.3	-	39.08	-	-	-	-	-	-
2-Methyl-1-heptene	1144	-	119.3	-	38.78	155.7	-	-	-	-	-
3-Methyl-1-heptene	1216	-	111.0	-	38.76	157.8	-	-	-	-	-
4-Methyl-1-heptene	1050	-	112.8	-	38.77	156.5	-	-	-	-	-
5-Methyl-1-heptene	1254	-	113.3	-	38.76	156.6	-	-	-	-	-
6-Methyl-1-heptene	1188	-	113.2	-	38.79	157.6	-	-	-	-	-
2-Methyl-2-heptene	1100	-	122.6	-	38.97	155.0	-	-	-	-	-
3-Methyl-cis-2-heptene	1152	-	122.0	-	38.87	153.9	-	-	-	-	-
3-Methyl-trans-2-heptene	1152	-	122.0	-	38.87	-	-	-	-	-	-
4-Methyl-cis-2-heptene	987	-	114.0	-	38.83	156.7	-	-	-	-	-
4-Methyl-trans-2-heptene	987	-	114.0	-	38.83	-	-	-	-	-	-
5-Methyl-cis-2-heptene	1188	-	118.0	-	38.78	155.2	-	-	-	-	-
5-Methyl-trans-2-heptene	1188	-	118.0	-	38.78	-	-	-	-	-	-
6-Methyl-cis-2-heptene	1122	-	117.0	-	38.89	156.3	-	-	-	-	-
6-Methyl-trans-2-heptene	1122	-	117.0	-	38.89	-	-	-	-	-	-
2-Methyl-cis-3-heptene	1050	-	112.0	-	39.12	158.9	-	-	-	-	-
2-Methyl-trans-3-heptene	1050	-	112.0	-	39.12	-	-	-	-	-	-
3-Methyl-cis-3-heptene	1116	-	121.0	-	38.84	154.1	-	-	-	-	-

Table 7. (Continued)

3-Methyl-trans-3-heptene	1116	121.0	-	38.84	-	-	-	-	-	-
4-Methyl-cis-3-heptene	980	122.0	-	38.92	154.8	-	-	-	-	-
4-Methyl-trans-3-heptene	980	122.0	-	38.92	-	-	-	-	-	-
5-Methyl-cis-3-heptene	1116	112.0	-	38.99	157.4	-	-	-	-	-
5-Methyl-trans-3-heptene	1116	112.0	-	38.99	-	-	-	-	-	-
6-Methyl-cis-3-heptene	1071	115.0	-	38.99	157.4	-	-	-	-	-
6-Methyl-trans-3-heptene	1071	115.0	-	38.99	-	-	-	-	-	-
2-Ethyl-1-hexene	1152	120.0	-	38.71	154.3	-	-	-	-	-
3-Ethyl-1-hexene	1054	110.3	-	38.63	156.9	-	-	-	-	-
4-Ethyl-1-hexene	1088	113.0	-	38.46	154.6	-	-	-	-	-
2,3-Dimethyl-1-hexene	961	110.5	-	38.70	155.5	-	-	-	-	-
2,4-Dimethyl-1-hexene	924	111.2	-	38.70	155.8	-	-	-	-	-
2,5-Dimethyl-1-hexene	1122	111.6	-	38.80	156.5	-	-	-	-	-
3,3-Dimethyl-1-hexene	800	104.0	-	38.69	157.2	-	-	-	-	-
3,4-Dimethyl-1-hexene	930	112.0	-	38.65	155.0	-	-	-	-	-
3,5-Dimethyl-1-hexene	924	104.0	-	38.76	158.5	-	-	-	-	-
4,4-Dimethyl-1-hexene	840	107.2	-	38.64	155.9	-	-	-	-	-
4,5-Dimethyl-1-hexene	1024	109.0	-	38.52	154.1	-	-	-	-	-
5,5-Dimethyl-1-hexene	968	102.5	-	38.78	158.3	-	-	-	-	-
3-Ethyl-cis-2-hexene	992	121.0	-	38.85	152.3	-	-	-	-	-
3-Ethyl-trans-2-hexene	992	121.0	-	38.85	-	-	-	-	-	-
4-Ethyl-cis-2-hexene	1020	113.0	-	38.51	154.8	-	-	-	-	-
4-Ethyl-trans-2-hexene	1020	113.0	-	38.51	-	-	-	-	-	-
2,3-Dimethyl-2-hexene	837	121.8	-115.1	38.87	151.5	-	-	-	-	-
2,4-Dimethyl-2-hexene	882	110.6	-	38.69	155.6	-	-	-	-	-
2,5-Dimethyl-2-hexene	1054	112.2	-	38.94	155.8	-	-	-	-	-
3,4-Dimethyl-cis-2-hexene	870	116.0	-	38.37	152.3	-	-	-	-	-
3,4-Dimethyl-trans-2-hexene	870	116.0	-	38.37	-	-	-	-	-	-
3,5-Dimethyl-cis-2-hexene	880	112.0	-	38.84	154.8	-	-	-	-	-
3,5-Dimethyl-trans-2-hexene	880	112.0	-	38.84	-	-	-	-	-	-
4,4-Dimethyl-cis-2-hexene	780	106.0	-	38.75	155.4	-	-	-	-	-
4,4-Dimethyl-trans-2-hexene	780	106.0	-	38.75	-	-	-	-	-	-
4,5-Dimethyl-cis-2-hexene	960	110.0	-	38.59	154.8	-	-	-	-	-
4,5-Dimethyl-trans-2-hexene	960	110.0	-	38.59	-	-	-	-	-	-
5,5-Dimethyl-cis-2-hexene	924	106.9	-	38.89	156.5	-	-	-	-	-
5,5-Dimethyl-trans-2-hexene	924	104.1	-	38.96	-	-	-	-	-	-
3-Ethyl-3-hexene	870	116.0	-	38.79	153.9	-	-	-	-	-
2,2-Dimethyl-cis-3-hexene	861	105.4	-137.4	38.99	157.4	-	-	-	-	-
2,2-Dimethyl-trans-3-hexene	861	100.9	-	39.18	-	-	-	-	-	-
2,3-Dimethyl-cis-3-hexene	900	114.0	-	38.68	154.1	-	-	-	-	-
2,3-Dimethyl-trans-3-hexene	900	114.0	-	38.68	-	-	-	-	-	-
2,4-Dimethyl-cis-3-hexene	840	109.0	-	39.06	156.3	-	-	-	-	-
2,4-Dimethyl-trans-3-hexene	840	107.6	-	39.13	-	-	-	-	-	-
2,5-Dimethyl-cis-3-hexene	1024	102.0	-	38.82	158.0	-	-	-	-	-

Table 7. (Continued)

2,5-Dimethyl-trans-3-hexene	1024	102.0	-	38.82	-	-	-	-	-	-
3,4-Dimethyl-cis-3-hexene	841	122.0	-	38.80	150.2	-	-	-	-	-
3,4-Dimethyl-trans-3-hexene	841	122.0	-	38.80	-	-	-	-	-	-
2-n-Propyl-1-pentene	960	117.7	-	38.70	155.0	-	-	-	-	-
2-Isopropyl-1-pentene	930	113.0	-	38.67	154.8	-	-	-	-	-
2-Ethyl-3-methyl-1-pentene	870	112.5	-	38.48	15.9	-	-	-	-	-
2-Ethyl-4-methyl-1-pentene	880	110.3	-	38.68	156.0	-	-	-	-	-
3-Ethyl-2-methyl-1-pentene	856	110.0	-	38.49	153.7	-	-	-	-	-
3-Ethyl-3-methyl-1-pentene	768	112.0	-	38.71	153.6	-	-	-	-	-
3-Ethyl-4-methyl-1-pentene	720	107.5	-	38.59	155.8	-	-	-	-	-
2,3,3-Trimethyl-1-pentene	696	108.3	-69.0	38.41	152.6	-	-	-	-	-
2,3,4-trimethyl-1-pentene	672	108.0	-	38.54	153.9	-	-	-	-	-
2,4,4-Trimethyl-1-pentene	440	101.4	-93.5	38.77	156.9	-	-	-	-	-
3,3,4-Trimethyl-1-pentene	720	105.0	-	38.50	153.9	-	-	-	-	-
3,4,4-Trimethyl-1-pentene	560	104.0	-	38.83	156.1	-	-	-	-	-
3-Ethyl-2-methyl-2-pentene	672	117.0	-	38.80	151.8	-	-	-	-	-
3-Ethyl-4-methyl-cis-2-pentene	672	116.0	-	38.74	151.8	-	-	-	-	-
3-Ethyl-4-methyl-trans-2-pentene	672	114.3	-	38.71	-	-	-	-	-	-
2,3,4-Trimethyl-2-pentene	640	116.3	-133.3	38.79	150.9	-	-	-	-	-
2,4,4-Trimethyl-2-pentene	364	104.9	-106.3	39.01	155.5	-	37224	-	-	-

3,4,4-Trimethyl-cis-2-pentene	608	112.0	-	38.66	151.8	-	-	-	-	-	-
3,4,4-Trimethyl-trans-2-pentene	608	112.0	-	38.66		-	-	-	-	-	-
2-Isopropyl-3-methyl-1-butene	640	104.0	-	38.38	155.4	-	-	-	-	-	-
2-Ethyl-3,3-dimethyl-1-butene	608	110.0	-	38.67	154.1	-	-	-	-	-	-
1-Nonene	3220	146.9	-81.4	43.45	173.2	6010.1	-	-	-	320.1	2.33
Cis-2-nonene	3082	150.8	-	-	-	-	-	-	-	-	-
Trans-2-nonene	3082	150.1	-	-	-	-	-	-	-	-	-
Cis-3-nonene	2992	148.4	-	-	-	-	-	-	-	-	-
Trans-3-nonene	2992	148.2	-	-	-	-	-	-	-	-	-
Cis-4-nonene	2904	147.4	-	-	-	-	-	-	-	-	-
Trans-4-nonene	2904	147.8	-	-	-	-	-	-	-	-	-

Table 8. Coefficients of determination among the properties of the alkene series examined.

	bp	MR	MV	HC	HV	FLASH	VIRC	TC	PC	mp
bp	1.000									
MR	0.967	1.000								
MV	0.946	0.992	1.000							
HC	0.970	0.996	0.992	1.000						
HV	0.993	0.921	0.903	0.938	1.000					
FLASH	0.933	0.905	0.844	0.897	0.878	1.000				
VIRC	-0.960	-0.981	-0.969	-0.976	-0.974	-0.975	1.000			
TC	0.996	0.965	0.979	0.989	0.998	0.997	-0.942	1.000		
PC	-0.950	-0.940	-0.958	-0.958	-0.920	-0.825	0.903	-0.954	1.000	
mp	0.664	0.640	0.614	0.525	0.482	0.518	-0.543	0.607	-0.467	1.000

The correlations among the properties examined are shown in Table 8. As can be seen, most of the properties are highly correlated with one another, with the exception of mp, which is poorly correlated with the other properties. The remaining nine properties all have coefficients of determination greater than 0.82, and the subset of bp, MR, MV, and HV all have correlations greater than 0.90.

Table 9 gives the regression equations and the coefficients of determination (R^2) values obtained by examining the relation between each property of the alkenes and $\ln(\text{TG})$ separately. In Figure 3, the plot of boiling point values versus $\ln(\text{TG})$ for the 161 alkenes studied can be seen for the representation of the acceptable scattering of the data.

Table 9. The regression equations and the coefficients of determination (R^2) for the eleven properties of the alkene series obtained by the application of the index.

	regression equation	R^2
bp (n=117)	$y = 28.06x - 79.59$	0.949
MR (n=114)	$y = 4.47x + 7.82$	0.911
MV (n=114)	$y = 15.54x + 47.79$	0.909
HC (n=49)	$y = 590.14x + 1079.51$	0.940
HV (n=27)	$y = 4275.20x + 9208.43$	0.903
FLASH (n=14)	$y = 14.83x + 173.78$	0.806
VIRC (n=11)	$y = -663.95x + 1427.25$	0.921
TC (n=10)	$y = 29.99x + 73.25$	0.983
PC (n=9)	$y = -0.32x + 4.85$	0.921
mp (n=48)	$y = 13.52x - 202.85$	0.423

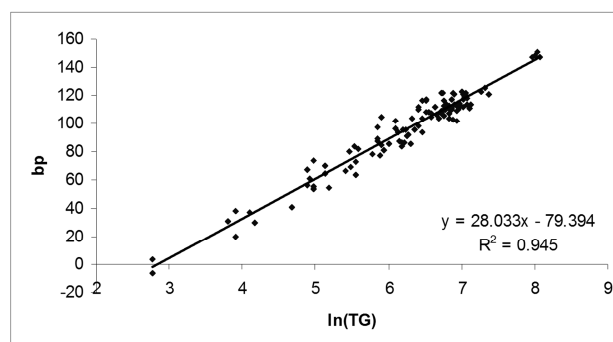


Figure 3. The plot of $\ln(\text{TG})$ versus the boiling points of alkene derivatives (n = 117)

The regression equations presented in Table 9 are generally of high-quality for properties other than the mp. Therefore, property values estimated on the basis of these equations, with the exception of mp, should be sufficiently accurate for many practical purposes.

As can be seen from the table, the molecular mass/bulk clearly exerts the dominant influence on the properties other than mp, suggesting that dispersion forces play a dominant role for those properties which depend on intermolecular forces. A similar conclusion was reached in the earlier alkane study (see the previous part). This is a reasonable conclusion in the present case for bp, HV, VIRC, TC, PC, and VISC. For MV the 'mass/bulk' dependence can be attributed directly to the larger volume of compounds with higher number of carbon atoms. Likewise, MR depends largely on the higher

number of electrons in larger compounds. For the two strictly “chemical” properties, the HC and the flashpoints (FLASH), the dependence on the mass/bulk dimension is more accurately attributed to the larger number of reacting bonds in the larger, higher number of carbon atoms containing compounds.

Branching, steric factors, and the double bond environment exert smaller influences on the properties, as demonstrated by the coefficients in the regression equations. Molecular branching sequesters interior parts of these compounds and reduces the extent of contact between neighboring molecules. The latter effect is reflected on the MVs. Because dispersion forces are strongly dependent on distance -the interaction energies fall as $1/r^6$, where r is the separation- a decrease in the amount of close contact decreases the cohesive forces experienced by the compounds. Therefore, bp and HV decrease as molecular branching increases.

The failure of the TG index to model the mp in this case is not surprising, either since this property was also not well modeled by these same topological parameters in the previous section, which deals with the alkanes. This illustrates the greater subtlety of the melting transition as compared to the boiling and critical transitions. The latter transitions involve a direct dependence on the operative intermolecular forces, and so directly reflect the strengths of these forces. The melting transition, in contrast, maintains a condensed phase and involves a partial disruption of intermolecular orientations. Melting, thus, depends on geometric factors, and other factors as well that are not well addressed by the present topological parameters (The TG index is directly influenced by the molecular shape and size.). This dependence on shape and entropic factors, in contrast to a simple intermolecular force dependence, is reflected in the melting point rather than the mass/bulk related factor. Dearden [37] has given a comprehensive review of mp predictions.

4. Conclusion

A novel topological index (TG Index) has been introduced and its application to some physical properties of alkanes and alkenes have been performed. TG Index is easy to calculate from the connectivity and distances of the chemical graph of a molecule. The correlation analysis of the index and the properties yielded quite reasonable data.

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