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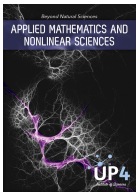

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Correlation of domination parameters with physicochemical properties of octane isomers

Sunilkumar M. Hosamani[†].

Department of Mathematics, Rani Channamma University, Belgaum
INDIA

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Abstract

In this paper, we find the values of three important domination parameters namely, connected domination number, total domination number and total edge domination number of molecular graph of octane isomers. Further, we show that these parameters are highly correlated with physical properties of octane isomers. Finally we carry out QSPR (Quantitative Structure-Property Relationship) analysis using several physicochemical properties of octane isomers.

Keywords: Dominating set; Octane isomers; QSPR analysis
AMS 2010 codes: 05C90, 05C69, 05C35, 05C12.

1 Introduction

Let $G = (V,E)$ be a graph. The number of vertices of G we denote by n and the number of edges we denote by m, thus $|V(G)| = n$ and $|E(G)| = m$. For undefined terminologies, we refer the reader to [7].

Chemical graph theory is the branch of mathematical chemistry. It is concerned with handling chemical graphs that represent chemical system. Hence chemical graph theory deals with analysis of all consequences of connectivity in a chemical system. It has found to be a useful tool in QSAR (Quantitative Structure-Activity Relationships) and QSPR (Quantitative Structure-Property Relationship) [4,10,16]. Numerous studies have been made relating to the above mentioned fields by using what are called topological indices.In 1975, Randić [13] proposed a topological index that has become one of the most widely used in both QSAR and QSPR studies.

One of the fastest growing areas in graph theory is the study of domination and related subset problems such as independence, irredundance, covering and matching. An excellent treatment of fundamentals of domination

[†]Corresponding author.
Email address: sunilkumar.rcu@gmail.com

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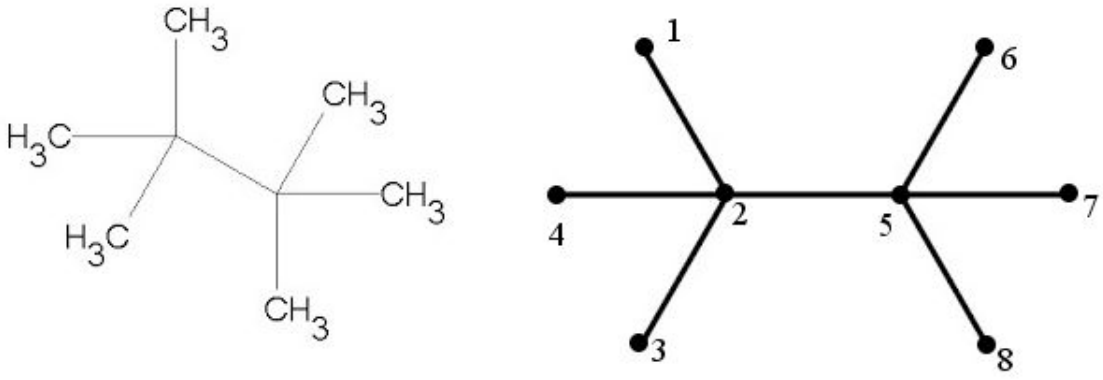

Fig. 1 $2,2,3,3-$tetramethylbutane and its molecular graph.

in graphs is given by the book by Haynes et. al [5]. Surveys of several advances topics in domination are given in the book edited by Haynes et. al [6].

Let $G=(V,E)$ be a graph. A subset S of V is called a dominating set of G if every vertex in $V-S$ is adjacent to at least one vertex in S. The domination number $\gamma(G)$ of a graph G is the minimum cardinality of a dominating set of G.

Sampathkumar and Walikar [15] have introduced an important domination invariant called connected domination number, which is defined as follows. Let $G=(V,E)$ be a graph. A subset S of V is called a connected dominating set of G if every vertex in $V-S$ is adjacent to at least one vertex in S and the subgraph induced by the set S is connected. The connected domination number $\gamma_c(G)$ of a graph G is the minimum cardinality of a connected dominating set of G.

E. J. Cockayne et. al [3] have introduced the concept of total domination as follows. Let $G=(V,E)$ be a graph. A subset S of V is called a total dominating set of G if every vertex G is adjacent some vertex in S. The total domination number $\gamma_t(G)$ of a graph G is the minimum cardinality of a total dominating set of G.

The total edge domination is an analogues concept total domination, which is introduced and studied in [9]. For more details on domination see [1,2].

2 Octane isomers

Octane isomers have become an important set of organic molecules to test the applicability of various topological parameters in quantitative structure-property/activity relationships (QSPR/QSAR). These compounds are structurally diverse enough to yield considerable variation in shape, branching and non polarity [14]. In a comprehensive study of numerous properties of octane isomers, Randić et. al [10,12,14] have used single molecular descriptors and concluded that different physicochemical properties depend on different descriptors.

So far in the literature of chemical graph theory, domination parameters have not been used to predict the physical properties of chemical compounds. Therefore, in the present study an attempt has been made to study physical properties of octane isomers by using domination parameters.

The values of γ_c, γ_t and γ_t' of molecular graph of $2,2,3,3-$tetramethyl butane are illustrated below.

From Fig. 1, it is clear that the minimal connected dominating set $D_c=\{2,5\}$, the total dominating set $D_t=\{2,5\}$, and the total edge dominating set $D_t'=\{2,5,7\}$. Hence, $\gamma_c(G)=|D_c|=2$, $\gamma_t(G)=|D_t|=2$, and $\gamma_t'(G)=|D_t'|=3$.

3 Data based and analytical method

Eight physicochemical properties of octane isomers have been selected on the availability [8] of a suitable body of data: boiling point (BP), critical temperature (CT), critical pressure (CP), entropy (S), density (D), mean radius (R_m^2), and heat of vaporization (H_v), heat of formation (H_f). The values are compiled in Table 1.

Table 1 Domination parameters and physicochemical properties of octane isomers.

Alkane	γ_c	γ_t	γ_t'	BP	TC	PC	S	D	R_m^2	$-\Delta H_f$	$-\Delta H_v$
$n-$octane	6	5	4	125.70	296.20	24.64	111.67	0.7025	2.0449	208.6	41.49
2M	5	4	4	117.6	288.0	24.80	109.84	0.6980	1.8913	215.4	39.67
3M	5	4	4	118.9	292.0	25.60	111.26	0.7058	1.7984	212.5	39.83
4M	5	5	4	117.7	290.0	25.60	109.32	0.7046	1.7673	210.7	39.64
3E	5	5	4	118.5	292.0	25.74	109.43	0.7136	1.7673	210.7	39.64
22MM	4	4	3	106.8	279.0	25.60	103.42	0.6953	1.6744	224.6	37.28
23MM	4	4	3	115.6	293.0	26.60	108.02	0.7121	1.6464	213.8	38.78
24MM	4	4	3	109.4	282.0	25.80	106.98	0.7004	1.6142	219.2	37.76
25MM	4	4	3	109.1	279.0	25.00	105.72	0.6935	1.6449	222.5	37.85
33MM	4	4	3	112.0	290.8	27.20	104.74	0.7100	1.7377	220.0	37.53
34MM	4	4	3	117.7	298.0	27.40	106.59	0.7200	1.5230	212.8	38.97
2M3E	4	4	3	115.6	295.0	27.40	106.06	0.7193	1.5525	211.0	38.52
3M3E	4	4	3	118.3	305.0	28.90	101.48	0.7274	1.5212	214.8	37.99
223MMM	3	3	2	109.8	294.0	28.20	101.31	0.7161	1.4306	220.0	36.91
224MMM	3	3	2	99.24	271.1	25.50	104.09	0.6919	1.4010	224.0	35.14
233MM	3	3	2	114.8	303.0	29.00	102.06	0.7262	1.4931	216.3	37.27
234MMM	3	3	2	113.5	295.0	27.60	102.39	0.7191	1.3698	217.3	37.75
2233MMMM	2	2	2	106.5	270.8	24.50	93.06	0.8242	1.4612	225.6	42.90

Next, we obtain a cross-correlation matrix of domination parameters, which is shown in Table 2.

Table 2 Cross correlation matrix of domination parameters.

	γ_c	γ_t	γ_t'
γ_c	1.000		
γ_t	0.926	1.000	
γ_t'	0.949	0.878	1.000

Table 3 contains the correlation of domination parameters with physicochemical properties of octane isomers.

4 Results and Discussion

From Table 2, it is found that the cross correlation coefficient of domination parameters are found to be high $(0.878 - 0.949)$. Also from Table 3, the correlation coefficient of domination parameters with physicochemical properties of isomers are found to be good except critical pressure (CP) and density (D). For these two

Table 3 Correlation of Domination parameters with physicochemical properties of octane isomers.

	BP	TC	PC	S	D	R_m^2	ΔH_f	ΔH_v
γ_c	0.730	0.316	-0.349	0.902	-0.579	0.903	0.716	0.305
γ_t	0.644	0.334	-0.216	0.840	-0.599	0.766	0.682	0.159
γ_t	0.683	0.196	-0.449	0.825	-0.415	0.895	0.653	0.446

physicochemical properties of octane isomers the domination parameters are not well-correlated.

A generalized linear regression model has been proposed for the relationship of physicochemical properties of octane isomers with the domination parameters γ_c, γ_t, and γ_t', respectively.

$$P = a + \sum_{i=1}^{3} b_i \gamma_i, \tag{1}$$

where P refers to a physicochemical property, a is constant, and b_i is the sensitivity of γ_i towards P. For our convince, we assume that $\gamma_1 = \gamma_c$, $\gamma_2 = \gamma_t$, and $\gamma_3 = \gamma_t'$.

We first consider the regression model containing single descriptors connected domination number γ_c, total domination number γ_t and total edge domination γ_t' separately.

$$P = a + b\gamma_c. \tag{2}$$
$$P = a + b\gamma_t. \tag{3}$$
$$P = a + b\gamma_t'. \tag{4}$$

In Tables 4, 5, and 6, statistical parameters for the linear QSPR models in Eqs. (2)-(4) are given.

Table 4 Statistical parameters for the linear QSPR model (2).

Physical property	R	S	F
BP	0.730	4.3097	18.307
TC	0.316	9.6182	1.778
PC	0.349	1.3882	2.223
S	0.902	2.008	70.017
D	0.579	0.0247	8.063
R_m^2	0.903	0.0800	70.944
$-\Delta H_f$	0.716	3.7360	16.826
ΔH_v	0.305	1.7463	1.638

Next, we consider the multiple regression model containing two descriptors of the combination of connected domination number γ_c, total domination number γ_t, and total edge domination γ_t', separately.

$$P = a + \sum_{i=1}^{2} b_i \gamma_i. \tag{5}$$

In Table 7, statistical parameters for the regression model containing two descriptors γ_c and γ_t are provided. Table 8 collects the statistical parameters for the regression model containing two descriptors γ_c and γ_t'.
In Table 9, statistical parameters for the regression model containing two descriptors γ_t and γ_t' appear.

Table 5 Statistical parameters for the linear QSPR model (3).

Physical property	R	S	F
BP	0.644	4.8274	11.343
TC	0.334	9.5547	2.015
PC	0.216	1.4467	0.780
S	0.840	2.5277	38.299
D	0.599	0.0242	8.973
R_m^2	0.766	0.1200	22.696
$-\Delta H_f$	0.682	3.9151	13.891
ΔH_v	0.159	1.1802	0.415

Table 6 Statistical parameters for the linear QSPR model (4).

Physical property	R	S	F
BP	0.683	4.6065	14.028
TC	0.196	9.9424	0.637
PC	0.449	1.3236	4.046
S	0.825	2.6297	34.168
D	0.415	0.0275	3.320
R_m^2	0.895	0.0831	64.657
$-\Delta H_f$	0.653	4.0529	11.893
ΔH_v	0.446	1.6408	3.979

Table 7 Statistical parameters for the QSPR model (5).

Physical property	R	S	F
BP	0.735	4.4162	8.836
TC	0.335	9.8663	0.947
PC	0.451	1.3657	1.914
S	0.902	2.0734	32.852
D	0.603	0.0249	4.280
R_m^2	0.922	0.0744	42.743
$-\Delta H_f$	0.718	3.8486	7.966
ΔH_v	0.446	1.6947	1.864

Finally, we consider the multiple regression model containing three descriptors, connected domination number γ_c, total domination number γ_t, and total edge domination γ_t'.

$$P = a + \sum_{i=1}^{3} b_i \gamma_i. \tag{6}$$

In Table 10, statistical parameters for the regression model containing three descriptors γ_c, γ_t, and γ_t' are shown.

The correlation coefficients of physicochemical properties with individual γ_i values show some significant results. The entropy and the mean radius values, which generally do not show good relationships with any single

Table 8 Statistical parameters for the QSPR model (5).

Physical property	R	S	F
BP	0.731	4.4467	8.613
TC	0.457	9.3140	1.979
PC	0.511	1.3153	2.650
S	0.907	2.0211	34.964
D	0.719	0.0217	8.007
R_m^2	0.911	0.0793	36.801
$-\Delta H_f$	0.721	3.8312	8.107
ΔH_v	0.583	1.5385	3.861

Table 9 Statistical parameters for the QSPR model (5).

Physical property	R	S	F
BP	0.690	4.7201	6.800
TC	0.392	9.6316	1.364
PC	0.585	1.2411	3.900
S	0.860	2.4573	21.228
D	0.644	0.0239	5.302
R_m^2	0.896	0.0854	30.663
$-\Delta H_f$	0.691	3.9946	6.856
ΔH_v	0.661	1.4213	5.812

Table 10 Statistical parameters for the QSPR model (6).

Physical property	R	S	F
BP	0.736	4.5666	5.518
TC	0.470	9.5666	1.323
PC	0.585	1.2844	2.430
S	0.907	2.0912	21.777
D	0.738	0.0218	5.580
R_m^2	0.930	0.0731	30.018
$-\Delta H_f$	0.722	3.9554	5.095
ΔH_v	0.668	1.4589	3.757

descriptor, are found to have a good correlation coefficient $(0.825-0.902)$ and $(0.766-0.903)$, respectively. The critical temperature,pressure, density, and enthalpy of vaporization values are found to have poor correlation coefficient $(-0.599-0.446)$.

The regression analysis of models (2)-(4) with single descriptors, reveals some interesting results for mean radius R_m^2 and entropy S.

From Table 4, we can see that for entropy S, $R=0.902$ (standard error of $2.008^{\circ}C$) and $F=70.017$, and for mean radius R_m^2, $R=0.903$ (standard error of $0.0800^{\circ}C$) and $F=70.944$.

From Table 5, we can see that for entropy S, $R=0.840$ (standard error of $2.5277^{\circ}C$) and $F=38.299$, and

for mean radius R_m^2, $R = 0.766$ (standard error of $0.1200°C$) and $F = 22.696$.

From Table 6, we can see that for entropy S, $R = 0.825$ (standard error of $2.6297°C$) and $F = 34.168$, and for mean radius R_m^2, $R = 0.895$ (standard error of $0.0831°C$) and $F = 64.657$.

The use of two descriptors, the combination of γ_c, γ_t, and γ_t' gave a good correlation coefficients for entropy ranging from $R = (0.860 - 0.907)$ having standard error ranging from $(2.0211 - 2.4573)$ and $F = (21.228 - -34.964)$. For mean radius R_m^2, $R = (0.896 - 0.922)$ having standard error ranging from $(0.0744 - 0.0854)$ and $F = (30.663 - 42.743)$.

However, the addition of third descriptor does not produce any significant improvement in the regression model. Hence, for other physical properties of the octane isomers, the relationship with domination parameters can be seen in Tables 4-10.

5 Conclusions

The results of QSPR studies reveals that the regression model (2) is the most significant model to predict the physicochemical properties like entropy and mean radius of isomers. Hence, domination parameters be used as candidate to represent the molecular structure for predicting physicochemical properties.

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