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QSPR Analysis On Octane Isomers Using Degree-Based Topological Indices*

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Abstract

Octane isomers are structures with the chemical formula C8H18. Despite having the same formula, they have variations in the way their atoms are arranged, leading to differences in their chemical and physical properties. In this paper, we conduct a QSPR analysis on various isomers of octane, focusing on specific degree-based topological indices. In QSPR studies, these measures, known as topological indices, are helpful in understanding and quantifying the biological effects of chemical compounds. We specifically look at how certain properties of octane, such as complexity, acentric factor, standard enthalpy of vaporization, entropy, and enthalpy of vaporization, are connected to these topological indices. Our research provides valuable insights into how these indices can predict the behavior of octane isomers, contributing to a better overall understanding of their properties.

1 Introduction

Mathematical chemistry [1] is a field that uses mathematics and computational techniques to study chemical phenomena and solve chemical problems. Its goal is to develop mathematical models, algorithms, and methods to improve our understanding and prediction of chemical behavior, properties, and reactions. Chemical graph theory [2], a branch of mathematical chemistry, focuses on analyzing chemical structures using principles from graph theory. In simple terms, it represents chemical compounds as graphs, where atoms are vertices and chemical bonds are edges connecting them. This approach helps explore and understand the structural and topological features of chemical systems.

QSPR analysis [3] is a computational method used in chemistry and materials science to predict the characteristics or behaviors of molecules using their structural properties. It includes the development of a mathematical correlation between the structural descriptors and the physico-chemical properties of molecules. Utilizing QSPR analysis on topological indices offers researchers a valuable tool to simplify complex structural information, and promote efficient computational modeling. By using these benefits, researchers can improve how they make decisions, speed up their research, and do suitable development in various scientific areas.

Our study focusses on the investigation of five specific physico-chemical properties: Complexity (C), Acentric factor (AF), Standard enthalpy of vaporization (DHVAP), Entropy (S), and Enthalpy of vaporization (HVAP). In the world of mathematical chemistry, understanding the physical and chemical properties of substances (known as physico-chemical properties) [4, 5] is really important. These properties help us predict and picture how substances will act, build connections between a substance's structure and its properties, serve as descriptors, facilitate computational chemistry methods, and make it easier to analyze data. Using these properties helps us better understand chemical systems and contributes to creating new materials and compounds.

Our study includes the analysis of octane isomers. Octane isomers are really important in the world of mathematical chemistry. They act as examples for studying how different structures can exist, helping us understand concepts in graph theory and how a molecule's structure relates to its properties. By looking

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at these octane isomers, researchers can create mathematical models and computational techniques that find applications across various chemical systems, like designing better fuels, making new materials, and discovering new drugs etc. These are just a few examples of the various fields where QSPR analysis of octane isomers is applied.

Topological indices (TI's) [6] are numbers we get by looking at how atoms in a chemical compound are arranged. They give us useful information about how the atoms are connected, how the compound looks, and other important features. Researchers use these numbers a lot in mathematical chemistry and in the study of chemical graphs. TI's help us understand how the structure of a molecule is related to its physical and chemical properties, as well as its biological properties. The TI's used in our study are given as follows:

Ranjini et al. introduced the redefined third Zagreb index in [7] and is given by

$$ReZG_3(G) = \sum_{xy \in E(G)} (d(x)d(y))(d(x) + d(y)).$$

Ashrafi et al. introduced the first, second Zagreb coindex in [8, 9] and is given by

$$\overline{M}_1(G) = \sum_{xy \notin E(G)} (d(x) + d(y)) \quad \text{and} \quad \overline{M}_2(G) = \sum_{xy \notin E(G)} d(x)d(y),$$

respectively.

Shirdel et al. introduced the hyper-Zagreb index in [10] as

$$HM(G) = \sum_{xy \in E(G)} (d(x) + d(y))^2.$$

Milićević et al. introduced the reformulated first Zagreb index, reformulated second Zagreb index and modified reformulated second Zagreb index in [11] as

$$EM_1(G) = \sum_{f \in E(G)} d(f)^2, \quad EM_2(G) = \sum_{f \sim g} d(f)d(g) \quad \text{and} \quad {}^{m}EM_2(G) = \sum_{f \sim g} \frac{1}{d(f)d(g)},$$

respectively.

In the above mentioned equations, the degree of vertices x and y is denoted as $d(x)$ and $d(y)$ respectively. The degree of the edge f is represented by $d(f)$. The notation $f \sim g$ indicates that the edges f and g are adjacent. Motivated by previous studies [12, 13, 14, 15, 16, 17, 18, 19, 20, 21], our research focused on investigating the relationship between octane isomers and a set of specific physico-chemical properties. By identifying significant statistical properties, we were able to make accurate decisions based on our findings. Additionally, we used a linear regression model to calculate the values of the physico-chemical properties, thereby eliminating the need for experimental methods.

2 Materials and Methods

In this section, we provide a detailed account of the materials, procedures, experimental design, and data analysis used in our study. By presenting a clear understanding of the materials and methods used, we enable fellow researchers to reproduce our study and verify the results obtained, thereby promoting the advancement of scientific knowledge in this field. The octane isomers selected from [22] served as the materials for this study. The tools used for result computation in this study included graph theoretical tools, degree counting methods, and analytic techniques, all of which were dependent on the vertices and edges present in chemical structures. The topological indices of 18 octane isomers are obtained by treating each molecule as a graph. The connections between atoms are represented as edges, while the vertices consist of the hydrogen and carbon atoms involved in these connections. By analyzing the degrees of the vertices and the characteristics of the edges, a numerical measure known as a topological index is computed. These indices follow a specific

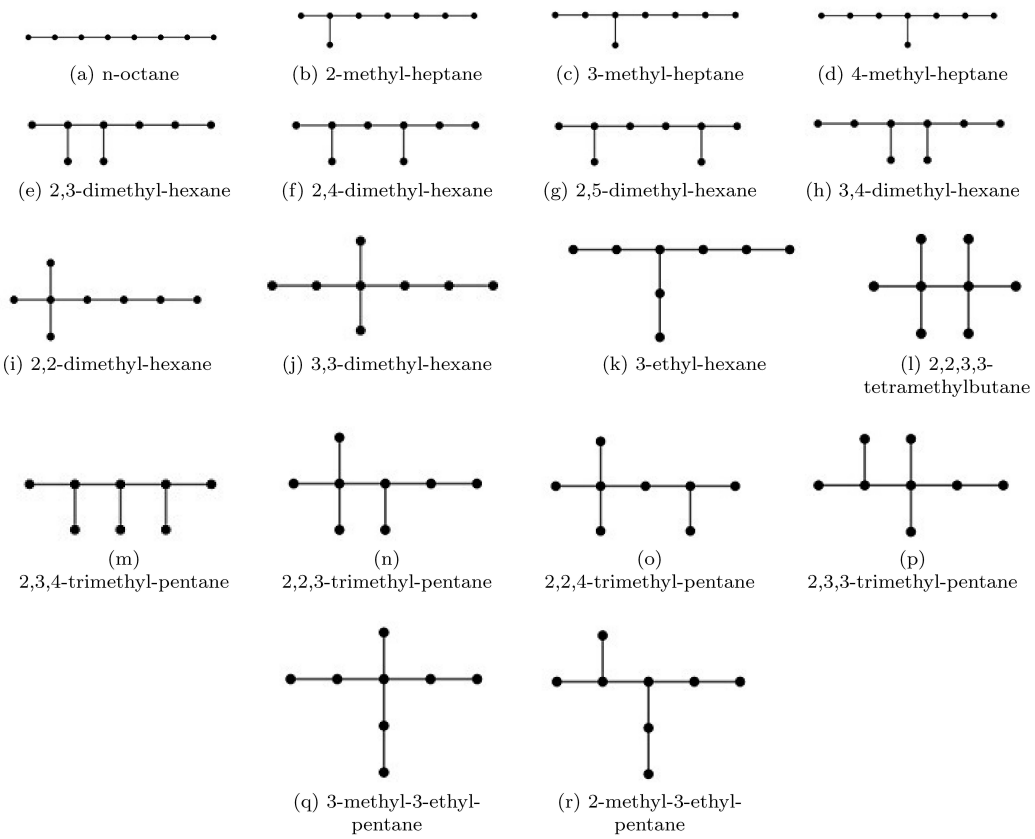


Figure 1: Structures of Octane isomers

set of rules. This proposed study aims to explore 7 degree-based topological indices, specifically focusing on the redefined third Zagreb index $[ReZG_3(G)]$, first Zagreb coindex $[\overline{M}_1(G)]$, second Zagreb coindex $[\overline{M}_2(G)]$, hyper Zagreb index $[HM(G)]$, reformulated first Zagreb index $[EM_1(G)]$, reformulated second Zagreb index $[EM_2(G)]$, and modified reformulated second Zagreb index $[^mEM_2(G)]$. These indices will be used to model and analyze the Complexity (C), Acentric factor (AF), Standard enthalpy of vaporization (DHVAP), Entropy (S), and Enthalpy of vaporization (HVAP) properties of 18 octane isomers. The information regarding the physico-chemical properties given below in Table 1 is gathered from [23] and PubChem databases. By using the graphs illustrated in Figure 1 and referring to the various topological indices definitions given above, the outcomes displayed in Table 2 are obtained. By using the SPSS software, we calculate different statistical parameters, and these are presented in Table 3-10.

3 Results

3.1 Calculation of Topological Indices and Comparing them with Correlation Coefficients of Specific Physico-Chemical Properties

Table 1 presents the measurements of five physico-chemical properties of 18 molecules. Table 2 provides the computation of 7 topological indices based on the molecular structures of the octane isomers. The correlation coefficients between five physico-chemical properties and each topological index are calculated and presented in Table 3. Figure 2 shows the graphical representation of the correlation coefficients between various physico-chemical properties, including complexity, acentric factor, standard enthalpy of vaporization,

Molecules	C	AF	$DHVAP$	S	$HVAP$
n-octane	25	0.3978	9.915	111.67	73.19
2M	37.3	0.3779	9.484	109.84	70.3
3M	39.3	0.371	9.521	111.26	71.3
4M	33.3	0.3715	9.483	109.32	70.91
23MM	46	0.3482	9.272	108.02	70.2
24MM	46	0.3442	9.029	106.98	68.5
25MM	36	0.3568	9.051	105.72	68.6
34MM	40	0.3403	9.316	106.59	70.2
22MM	47.5	0.3394	8.915	103.42	67.7
33MM	53.1	0.3225	8.973	104.74	68.5
3E	35.3	0.3624	9.476	109.43	71.7
2233MMMM	55	0.2552	8.41	93.06	66.2
234MMM	45.1	0.3174	9.014	102.39	68.37
223MMM	56.9	0.3008	8.826	101.31	67.3
224MMM	54.9	0.3053	8.402	104.09	67.87
233MMM	60.4	0.2931	8.897	102.06	68.1
3M3E	42.8	0.3068	9.081	101.48	69.3
2M3E	42	0.3324	9.209	106.06	69.7

Table 1: Physico-chemical properties of Octane isomers.

entropy, and enthalpy of vaporization, across different topological indices.

3.2 Linear Regression Models

By using SPSS software, a linear regression model was created to examine the relationship between the physico-chemical property (P) and a topological index (TI). The model is expressed as:

$$P = u + v(TI)$$

where u and v are constants. Based on this model we have computed several linear regression models for $ReZG_3$, $\overline{M}_1$, $\overline{M}_2$, HM,EM_1, EM_2 and ${}^mEM_2$ and are as follows:

3.2.1 Redefined Third Zagreb Index $ReZG_3(G)$:

$$C = 14.041 + 0.2[ReZG_3(G)]$$
$$AF = 0.473 - 0.001[ReZG_3(G)]$$
$$DHVAP = 10.344 - 0.008[ReZG_3(G)]$$
$$S = 122.348 - 0.112[ReZG_3(G)]$$
$$HVAP = 74.881 - 0.037[ReZG_3(G)]$$

3.2.2 First Zagreb Coindex $\overline{M}_1(G)$:

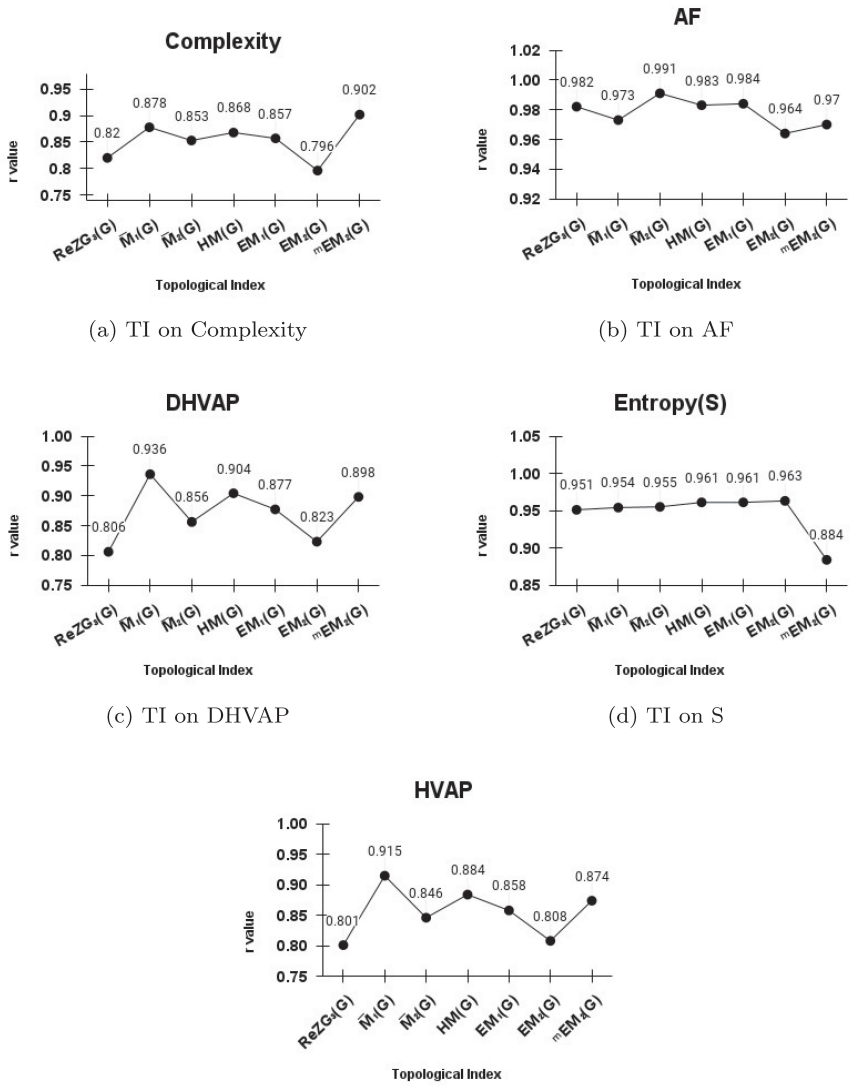
$$C = 232.015 - 2.798[\overline{M}_1(G)]$$
$$AF = -0.455 + 0.012[\overline{M}_1(G)]$$
$$DHVAP = 0.903 + 0.123[\overline{M}_1(G)]$$
$$S = 6.613 + 1.472[\overline{M}_1(G)]$$
$$HVAP = 32.482 + 0.549[\overline{M}_1(G)]$$

Molecules	$ReZG_3(G)$	$\overline{M}_1(G)$	$\overline{M}_2(G)$	$HM(G)$	$EM_1(G)$	$EM_2(G)$	${}^mEM_2(G)$
n-octane	92	72	61	98	22	20	2
2M	108	70	58	114	30	32	1.75
3M	116	70	57	116	32	36	1.6944
4M	116	70	57	116	32	37	1.7777
23MM	142	68	53	134	42	54	1.5416
24MM	132	68	54	132	40	49	1.4722
25MM	124	68	55	130	38	38	1.5
34MM	150	68	52	136	44	58	1.4166
22MM	146	66	52	152	52	77	1.4583
33MM	164	66	50	156	56	78	1.2708
3E	124	70	56	118	34	41	1.6666
2233MMMM	248	60	39	214	90	162	1
234MMM	168	66	49	152	52	72	1.3125
223MMM	192	64	46	174	66	97	1.0888
224MMM	162	64	49	168	60	82	1.1388
233MMM	202	64	45	176	68	102	1.05
3M3E	182	66	48	160	60	96	1.1875
2M3E	150	68	53	136	44	59	1.4444

Table 2: Topological indices values of Octane isomers.

Index	C	AF	$DHVAP$	S	$HVAP$
$ReZG_3(G)$	0.82	0.982	0.806	0.951	0.801
$\overline{M}_1(G)$	0.878	0.973	**0.936**	0.954	**0.915**
$\overline{M}_2(G)$	0.853	**0.991**	0.856	0.955	0.846
$HM(G)$	0.868	0.983	0.904	0.961	0.884
$EM_1(G)$	0.857	0.984	0.877	0.961	0.858
$EM_2(G)$	0.796	0.964	0.823	**0.963**	0.808
${}^mEM_2(G)$	**0.902**	0.97	0.898	0.884	0.874

Table 3: Correlation coefficient values between topological indices and physico-chemical properties of Octane isomers.



(a) TI on Complexity

(b) TI on AF

(c) TI on DHVAP

(d) TI on S

Figure 2: Physico-chemical properties of Octane isomers with topological indices

3.2.3 Second Zagreb Coindex $\overline{M}_2(G)$:

$$C = 121.255 - 1.485[\overline{M}_2(G)]$$
$$AF = -0.004 + 0.007[\overline{M}_2(G)]$$
$$DHVAP = 5.956 + 0.061[\overline{M}_2(G)]$$
$$S = 63.691 + 0.804[\overline{M}_2(G)]$$
$$HVAP = 54.953 + 0.277[\overline{M}_2(G)]$$

3.2.4 Hyper Zagreb Index $HM(G)$:

$$C = 3.315 + 0.285[HM(G)]$$
$$AF = 0.512 - 0.001[HM(G)]$$
$$DHVAP = 10.875 - 0.012[HM(G)]$$
$$S = 127.32 - 0.153[HM(G)]$$
$$HVAP = 77.172 - 0.055[HM(G)]$$

3.2.5 Reformulated First Zagreb Index $EM_1(G)$:

$$C = 21.435 + 0.476[EM_1(G)]$$
$$AF = 0.435 - 0.002[EM_1(G)]$$
$$DHVAP = 10.083 - 0.02[EM_1(G)]$$
$$S = 117.769 - 0.258[EM_1(G)]$$
$$HVAP = 73.625 - 0.09[EM_1(G)]$$

3.2.6 Reformulated Second Zagreb Index $EM_2(G)$:

$$C = 29.859 + 0.217[EM_2(G)]$$
$$AF = 0.402 - 0.001[EM_2(G)]$$
$$DHVAP = 9.736 - 0.009[EM_2(G)]$$
$$S = 113.816 - 0.127[EM_2(G)]$$
$$HVAP = 72.074 - 0.041[EM_2(G)]$$

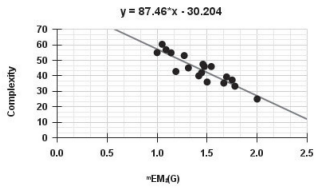
3.2.7 Modified Reformulated Second Zagreb Index ${}^mEM_2(G)$:

$$C = 87.46 - 30.204[{}^mEM_2(G)]$$
$$AF = 0.159 + 0.123[{}^mEM_2(G)]$$
$$DHVAP = 7.36 + 1.234[{}^mEM_2(G)]$$
$$S = 84.914 + 14.318[{}^mEM_2(G)]$$
$$HVAP = 61.447 + 5.506[{}^mEM_2(G)]$$

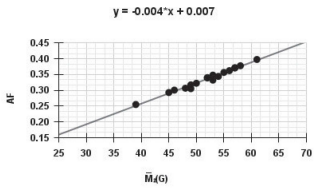
Figure 3 shows the relationships between specific TI and various physico-chemical properties. The position of each data point indicates the strength and direction of the correlation. Clustered data points suggest a significant correlation, while scattered points indicate a weak or negligible correlation.

3.3 Determination of Statistical Attributes

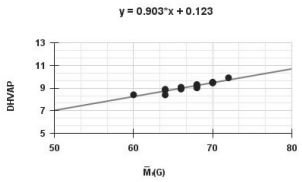
In this section, we present the calculated regression parameters. The sample size, denoted as N, represents the number of observations in the dataset. The constant or Y-intercept is denoted by u, while v represents the slope. The correlation coefficient is denoted as r, describing the strength and direction of the linear relationship. The r^2 indicates the proportion of the dependent variable's variation that is accounted for by the linear model. The p-value associated with each term examines the null hypothesis, assuming that the coefficient equals zero, signifying no effect. If the p-value is higher (insignificant), it indicates that modifications in the predictor variable do not have any impact on changes in the response variable. The computation of statistical parameters for linear QSPR models of distinct topological indices is showcased in



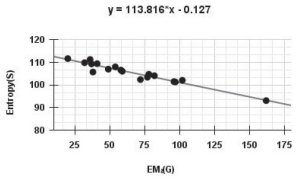
(a) Correlation of ${}^{m}EM_2(G)$ with C



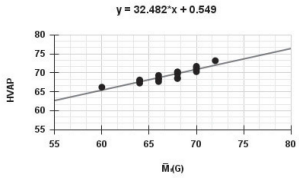
(b) Correlation of $\overline{M}_2(G)$ with AF



(c) Correlation of $\overline{M}_1(G)$ with DHVAP



(d) Correlation of $EM_2(G)$ with S



(e) Correlation of $\overline{M}_1(G)$ with HVAP

Figure 3: Correlation of topological indices with physico-chemical properties based on best-fit model.

Properties	N	u	v	r	r^2	p	**Indicator**
C	18	14.041	0.2	0.82	0.672	0.000	significant
AF	18	0.473	-0.001	**0.982**	0.964	0.000	significant
$DHVAP$	18	10.344	-0.008	0.806	0.65	0.000	significant
S	18	122.348	-0.112	0.951	0.904	0.000	significant
$HVAP$	18	74.881	-0.037	0.801	0.641	0.000	significant

Table 4: Statistical attributes employed in linear QSPR Modeling of $ReZG_3(G)$

Tables 4-10. It is worth noting that all of these analysis consistently yield a p-value of zero, signifying the significance of the outcomes.

3.4 Comparison

This section presents an analysis of the similarities and differences between actual and predicted values obtained from our regression models. Predicted values play an important role in making informed decisions, managing risks, allocating resources, and optimizing processes. Accurate predictions have the potential to save costs, time and yield favorable outcomes across various domains. In Table 1(as mentioned earlier), you can find the actual values for various physico-chemical properties used in our study. The predicted values for different physico-chemical properties used in our study are given below:

Properties	N	u	v	r	r^2	p	**Indicator**
C	18	232.015	-2.798	0.878	0.771	0.000	significant
AF	18	-0.455	0.012	**0.973**	0.947	0.000	significant
$DHVAP$	18	0.903	0.123	0.936	0.876	0.000	significant
S	18	6.613	1.472	0.954	0.91	0.000	significant
$HVAP$	18	32.482	0.549	0.915	0.837	0.000	significant

Table 5: Statistical properties used in linear QSPR Modeling of $\overline{M}_1(G)$

Properties	N	u	v	r	r^2	p	**Indicator**
C	18	121.255	-1.485	0.853	0.728	0.000	significant
AF	18	-0.004	0.007	**0.991**	0.982	0.000	significant
$DHVAP$	18	5.956	0.061	0.856	0.733	0.000	significant
S	18	63.691	0.804	0.955	0.912	0.000	significant
$HVAP$	18	54.953	0.277	0.846	0.716	0.000	significant

Table 6: Statistical properties used in linear QSPR Modeling of $\overline{M}_2(G)$

Properties	N	u	v	r	r^2	p	**Indicator**
C	18	3.315	0.285	0.868	0.753	0.000	significant
AF	18	0.512	-0.001	**0.983**	0.966	0.000	significant
$DHVAP$	18	10.875	-0.012	0.904	0.817	0.000	significant
S	18	127.32	-0.153	0.961	0.924	0.000	significant
$HVAP$	18	77.172	-0.055	0.884	0.781	0.000	significant

Table 7: Statistical properties used in linear QSPR Modeling of $HM(G)$

Properties	N	u	v	r	r^2	p	**Indicator**
C	18	21.435	0.476	0.857	0.734	0.000	significant
AF	18	0.435	-0.002	**0.984**	0.968	0.000	significant
$DHVAP$	18	10.083	-0.02	0.877	0.769	0.000	significant
S	18	117.769	-0.258	0.961	0.924	0.000	significant
$HVAP$	18	73.625	-0.09	0.858	0.736	0.000	significant

Table 8: Statistical properties used in linear QSPR Modeling of $EM_1(G)$

Properties	N	u	v	r	r^2	p	**Indicator**
C	18	29.859	0.217	0.796	0.634	0.000	significant
AF	18	0.402	-0.001	**0.964**	0.929	0.000	significant
$DHVAP$	18	9.736	-0.009	0.823	0.677	0.000	significant
S	18	113.816	-0.127	0.963	0.927	0.000	significant
$HVAP$	18	72.074	-0.041	0.808	0.653	0.000	significant

Table 9: Statistical properties used in linear QSPR Modeling of $EM_2(G)$

Properties	N	u	v	r	r^2	p	**Indicator**
C	18	87.46	-30.204	0.902	0.814	0.000	significant
AF	18	0.159	0.123	**0.97**	0.941	0.000	significant
$DHVAP$	18	7.360	1.234	0.898	0.806	0.000	significant
S	18	84.914	14.318	0.884	0.781	0.000	significant
$HVAP$	18	61.447	5.506	0.874	0.764	0.000	significant

Table 10: Statistical properties used in linear QSPR Modeling of ${}^mEM_2(G)$

Octane Isomers	**Predicted** C **for** ${}^{m}EM_2(G)$	**Predicted** AF **for** $\overline{M}_2(G)$	**Predicted** $DHVAP$ **for** $\overline{M}_1(G)$	**Predicted** S **for** $EM_2(G)$	**Predicted** $HVAP$ **for** $\overline{M}_1(G)$
Octane	27.052	0.423	9.759	111.276	72.01
2M	34.603	0.402	9.513	109.752	70.912
3M	36.282	0.395	9.513	109.244	70.912
4M	33.766	0.395	9.513	109.117	70.912
23MM	40.898	0.367	9.267	106.958	69.814
24MM	42.994	0.374	9.267	107.593	69.814
25MM	42.154	0.381	9.267	108.99	69.814
34MM	44.673	0.36	9.267	106.45	69.814
22MM	43.414	0.36	9.021	104.037	68.716
33MM	49.077	0.346	9.021	103.91	68.716
3E	37.122	0.388	9.513	108.609	70.912
2233MMMM	57.256	0.269	8.283	93.242	65.422
234MMM	47.817	0.339	9.021	104.672	68.716
223MMM	54.574	0.318	8.775	101.497	67.618
224MMM	53.064	0.339	8.775	103.402	67.618
233MMM	55.746	0.311	8.775	100.862	67.618
3E3M	51.593	0.332	9.021	101.624	68.716
3E2M	43.833	0.367	9.267	106.323	69.814

Table 11: Predicted values for physico-chemical properties based on best-fit model

4 Discussion

In Table 2, various topological indices of the eighteen Octane isomers are obtained by analyzing the molecular graphs of these isomers. In Table 3, the correlation values with respect to $ReZG_3(G)$ display a range of 0.801 to 0.982. The correlation values with respect to $\overline{M}_1(G)$ display a range of 0.878 to 0.973. The correlation values with respect to $\overline{M}_2(G)$ display a range of 0.846 to 0.991. The correlation values with respect to $HM(G)$ display a range of 0.868 to 0.983. The correlation values with respect to $EM_1(G)$ display a range of 0.857 to 0.984. The correlation values with respect to $EM_2(G)$ display a range of 0.796 to 0.964. The correlation values with respect to ${}^{m}EM_2(G)$ display a range of 0.874 to 0.97. AF shows the highest correlation coefficient having the values $r = 0.982$, 0.973, 0.991, 0.983, 0.984, 0.964, and 0.97 with the $ReZG_3(G)$, $\overline{M}_1(G)$, $\overline{M}_2(G)$, $HM(G)$, $EM_1(G)$, $EM_2(G)$ and ${}^{m}EM_2(G)$ respectively indicating a significant and noticeable relationship compared to other factors. Based on the findings from Table 3 and Figure 2(a), it is clear that the ${}^{m}EM_2(G)$ shows the highest correlation ($r = 0.902$) with complexity compared to other topological indices. Based on the findings from Table 3 and Figure 2(b), it is clear that the $\overline{M}_2(G)$ shows the highest correlation ($r = 0.991$) with AF compared to other topological indices. Based on the findings from Table 3 and Figure 2(c), it is clear that the $\overline{M}_1(G)$ shows the highest correlation ($r = 0.936$) with DHVAP compared to other topological indices. Based on the findings from Table 3 and Figure 2(d), it is clear that the $EM_2(G)$ shows the highest correlation ($r = 0.963$) with S compared to other topological indices. Based on the findings from Table 3 and Figure 2(e), it is clear that the $\overline{M}_1(G)$ shows the highest correlation ($r = 0.915$) with HVAP compared to other topological indices. By applying linear regression models, we are able to calculate the predicted values for the various physico-chemical properties considered in our study, as shown in Table 11. Also, note that the predicted values of only the best-fit model are shown in Table 11. Figures 3(a) and 3(d) show a strong negative correlation. Figure 3(b), Figure 3(c), and Figure 3(e) show a strong positive correlation. A strong negative correlation would suggest that as the topological index increases, the physico-chemical property of the molecules decreases. A strong positive correlation would suggest that as the topological index increases, the physico-chemical property of the molecules also

increases. To make sure the results are correct, it's important to analyze the correlation graph carefully using strong statistical methods. This helps us understand the findings more accurately. In Table 4-10, it is observed that the $ReZG_3(G)$ shows the highest coefficient of determination with both AF ($r^2 = 0.964$) and S ($r^2 = 0.904$) among the properties examined. The $\overline{M}_1(G)$ shows the highest coefficient of determination with AF ($r^2 = 0.947$), S ($r^2 = 0.91$), DHVAP ($r^2 = 0.876$) and HVAP ($r^2 = 0.837$). The $\overline{M}_2(G)$ shows the highest coefficient of determination with AF ($r^2 = 0.982$) and S ($r^2 = 0.912$). The $HM(G)$ shows the highest coefficient of determination with AF ($r^2 = 0.966$), S ($r^2 = 0.924$) and DHVAP ($r^2 = 0.817$). The $EM_1(G)$ shows the highest coefficient of determination with AF ($r^2 = 0.968$) and S ($r^2 = 0.924$). The $EM_2(G)$ shows the highest coefficient of determination with AF ($r^2 = 0.929$) and S ($r^2 = 0.927$). The ${}^mEM_2(G)$ shows the highest coefficient of determination with AF ($r^2 = 0.941$), C ($r^2 = 0.814$) and DHVAP ($r^2 = 0.806$). Based on the given data, it can be seen that the ${}^mEM_2(G)$ showcases the highest correlation ($r = 0.902$) and coefficient of determination ($r^2 = 0.814$) in relation to the Complexity property, the $\overline{M}_2(G)$ showcases the highest correlation ($r = 0.991$) and coefficient of determination ($r^2 = 0.982$) in relation to the acentric factor property, the $\overline{M}_1(G)$ showcases the highest correlation ($r = 0.936$) and coefficient of determination ($r^2 = 0.876$) in relation to the DHVAP property, the $EM_2(G)$ showcases the highest correlation ($r = 0.963$) and coefficient of determination ($r^2 = 0.927$) in relation to the entropy property and the $\overline{M}_1(G)$ showcases the highest correlation ($r = 0.915$) and coefficient of determination ($r^2 = 0.837$) in relation to the HVAP property. Given that all the calculated p-values are below the threshold of 0.05, we can tell that the results are statistically significant.

5 Conclusions

This paper focuses on the examination of topological indices for eighteen octane isomers. Additionally, a linear regression model was formulated to calculate the values of physico-chemical properties. Various statistical parameters were utilized to verify the precision of the obtained results. The plots included in the study were useful in identifying the strongest correlation and understanding the relationship between the variables. Our findings indicate a striking correlation: the predicted values closely resemble the physico-chemical values of octane isomers, or they maintain a proportional relationship. This observation presents an exciting opportunity to predict the physico-chemical values of unknown octane isomers based solely on their topological index obtained from their chemical graph. This discovery is a big deal in the chemical world of octane isomers. It gives us really useful information and practical uses. Also, we can explore more about different molecular structures, expanding the scope of our research.

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