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QSPR Techniques Using Different Variants of the Nirmala Index

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Abstract

A subfield of graph theory called chemical graph theory ties mathematics to chemistry and biology. By visualizing each chemical as a graph, it has been possible to determine the structural stability and physical characteristics of distinct compounds. A topological index is referred to as a molecular descriptor in this manner. The goal of this work is to generalize a recently developed degree-based topological index for a common family of graphs and use it to identify the various physical parameters of some alkanes using a linear regression model. We find a strong correlation between the topological index and a compound's physical attribute using elementary statistics.

Keywords: *Alkanes, Molecular Descriptor, Regression*

1.0 Introduction

Minerals and mines found in the earth's crust contain several naturally occurring aliphatic and aromatic hydrocarbons. Extracting and determining their physical and chemical properties is a time-consuming and hard operation. Chemical graph theory helps show scientific truths mathematically.

A well-known subfield of graph theory called chemical graph theory uses mathematical understanding to analyse specific chemical substances. All facets of applying graph theory to chemistry are addressed by chemical graph theory. For every actual or abstract chemical system molecule or reaction scheme in a chemical transformation, it offers a useful model. In other words, it is focused on investigations into every impact of connectedness inside a chemical system. A non-empty set and a topological structure built upon the set define a topological space. If it can be demonstrated that a topological structure can be defined upon a simple connected graph's vertex set, then the graph can be said to belong to a topological space. In the domains of chemical graph theory, molecular topology, and mathematical chemistry, a topological index, also known as a connectedness index, is a form of molecular descriptor that is derived based on the molecular graph of a chemical compound. Topological indices[1] are quantifiable characteristics of a graph's topology[2] that are often graph invariant. One use of topological indices is the finding of Quantitative Structure-Activity Relationships (QSAR), in which the biological activity or other characteristics of molecules are related to their chemical structure.

This work mainly focuses on the applicability of Nirmala index[4] and HDR Nirmala index[5] in analysing the properties of certain alkanes. We primarily look into eccentricity based HDR Nirmala index and degree based Nirmala index[3]

$$HDRN(G) = \sum_{u,v \in E(G)} \sqrt{\left(d_{hr}(u) + d_{hr}(v)\right)}$$

and

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$$N(G) = \sum_{u,v \in E(G)} \sqrt{(d_G(u) + d_G(v))}.$$

2.0 Generalization of the Nirmala Index for a Family of Standard Graphs

Theorem 2.1: For a path graph

$P_n (n \geq 4), \mathrm{N}(P_n) = 2\sqrt{3} + 2(n-3).$



Figure 1. Path graph.

Proof: A path graph P_n is a connected acyclic graph with order n and size n – 1. The degree of the end vertices is one and the degree of all other vertices are two.

Hence, the edge partition is as follows:

$E_a = \{uv \in E(G): d_G(u) = 1, d_G(v) = 2\}, |E_b| = 2.$
$E_b = \{uv \in E(G): d_G(u) = 2, d_G(v) = 2\}, |E_b| = n - 3.$

Thus, $N(P_n) = 2\sqrt{3} + 2(n-3)$.

Theorem 2.2: For a complete graph

$K_n, N(K_n) = \frac{n(n-1)}{2} \sqrt{2n-2}.$

Proof: A complete graph K_n is a connected $(n-1)$ regular graph with 'n'vertices and ${}^nC_2$ edges. Each vertex is a complete graph is of full degree, i.e., $d(v_i) = n-1$, $1 \leq i \leq n$.

Hence, the edge partition is as follows:

$E_a = \{d_G(u) = n-1, d_G(v) = n-1\},$
$|E_a| = \frac{n(n-1)}{2}.$
Thus, $\mathrm{N}(K_n) = \frac{n(n-1)}{2} \sqrt{2n-2}.$

3.0 Computation of Nirmala Index, HDR Nirmala Index for Certain Alkanes

Table 1. The topological indices of alkanes with its physiochemical properties

Alkane	bp(°C)	ct(°C)	HDR Nirmala Index	Nirmala Index
Butane	-0.5	152.01	4.2426	5.4641
2,methylpropane	-11.73	134.98	6	6
Pentane	36.074	196.62	6.2925	7.4641
2,methylbutane	27.852	187.7	6.9282	7.9681
2,2dimethylpropane	9.503	160.6	8.9443	8.9442
Hexane	68.74	234.7	7.071	9.4641
2,methylpentane	60.271	224.9	8.8783	9.9681
3,methyalpentane	63.282	231.2	8.8783	7.9681
2,2,methylbutane	49.741	216.2	10	10.8897
2,3,dimethylbutane	57.988	227.1	10	10.4495

Heptane	98.427	267.55	9.1209	11.4641
2,methylhexane	90.052	257.9	9.1209	11.9681
3methylhexane	91.85	262.4	8.0246	11.9362
3,ethylpentane	93.475	267.6	11.9043	11.9043
2,2,dimethyl pentane	79.197	247.7	11.8863	12.8897
2,3-dimethylpentane	89.784	264.6	12.4402	12.4176
2,4-dimethylpentan	80.5	247.1	11.4003	12.4721
3,3-dimethylpentane	86.064	263	12.9442	13.3711
Octane	125.665	296.2	9.8995	13.4641
2methylheptane	117.647	288	10.5352	13.9681
3-methylheptane	118.925	292	11.1708	13.9362
4-methylheptane	117.709	290	12.3923	13.9362
3-ethylhexane	118.53	292	13.4322	13.9043
2,3-dimethylhexane	115.607	293	12.3424	14.4176
2,2-dimethylhexane	10.84	279	11.071	14.8897
2,4-dimethylhexane	109.42	282	12.3923	14.4402
2,5-dimethylhexane	109.1	279	11.1209	14.4721
3,3-dimethylhexane	111.96	290.84	10.2925	14.8352
3,4-dimethylhexane	117.72	298	13.8863	14.3857
3-ethyl-2-methylpentane	115.65	295	14.8121	14.3857
3-ethyl-3-methylpentane	118.25	305	15.7979	9.8817
2,2,3-trimethylpentane	109.84	294	15.7887	15.322
2,2,4-trimethylpentane	99.23	271.15	14.363	15.3937
2,3,3-trimethylpentane	114.76	303	16.27	15.2994
2,3,4-trimethylpentane	113.46	295	15.3484	14.899
Nonane	150.79	322	11.9494	15.6411
2-methyloctane	143.26	315	11.9494	15.9681
3-methyloctane	144.18	318	11.9494	15.9362
4-methyloctane	142.48	318.3	12.585	15.936
3-ethylheptane	143	318	10.8783	15.9043
4-ethylheptane	141.2	318.3	12.8284	15.9043
2,2-dimethylheptane	132.69	302	12.4859	16.8897
2,3-dimethylheptane	140.5	315	14.2672	14.1815
2,4-dimethylheptane	133.5	306	14.8963	16.4402
2,5-dimethylheptane	136	307.8	13.1209	16.4402

3,3-dimethylheptane	137.3	314	13.1708	16.8352
3,4-dimethylheptane	140.6	322.7	15.4322	16.3857
3,5-dimethylheptane	136	312.3	14.9282	16.4083
4,4-dimethylheptane	135.2	317.8	15.4641	16.8352
3-ethyl-2-methylhexane	138	322.7	15.9362	16.3857
4-ethyl-2-methylhexane	133.8	330.3	15.4641	14.4083
3-ethyl-3-methylhexane	140.6	327.2	16.4402	14.3312
2,2,4-trimethylhexane	126.54	301	16.4402	13.1258
2,2,5-trimethylhexane	124.084	296.6	13.0392	15.1577
2,3,3-trimethylhexane	137.68	326.1	15.3823	12.8499
2,3,4-trimethylhexane	139	324.2	15.9362	16.8671
2,3,5-trimethylhexane	131.34	309.4	14.8962	16.9216
3,3,4-trimethylhexane	140.46	330.6	15.8545	12.3854
3,3-diethylpentane	146.168	342.8	18.583	16.7261
2,2-dimethyl-3-ethylpentane	133.83	322.6	16.8805	17.2901
2,3-dimethyl-3-ethylpentane	142	338.6	19.0551	14.7954
2,4-dimethyl-3-ethylpentane	136.73	324.2	17.6693	16.8671
2,2,3,3-tetramethylpentane	140.274	334.5	19.9315	18.1903
2,2,3,4-tetramethylpentane	133.016	319.6	18.6454	17.8034
2,2,4,4-tetramethylpentane	122.284	301.6	17.2915	18.3154
2,3,3,4-tetramethylpentane	141.551	334.5	19.2812	17.7636

4.0 Results and Discussion

4.1 Boiling Points Against Eccentricity-based Topological Index

The linear regression is performed using least square method by treating the topological index as an independent variable and the physical property of the compound as a dependent variable.

Using the linear regression model, the correlation between the boiling point of alkanes and eccentricity based HDR Nirmala index has been estimated.

The equation of the linear line of regression is found to be

BP=8.360099806(HDRN)+0.537289956

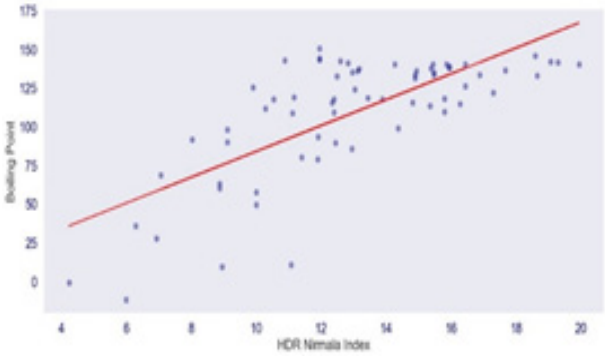


Figure 2. Plot of HDR Nirmala index against the boiling points of alkanes.

The value of the multiple R seems to slight less, hence estimating the boiling point using this eccentricity based index does not provide accurate results.

SUMMARY OUTPUT	
Regression Statistics	
Multiple R	0.899967
R Square	0.80994
Adjusted R Square	0.80939
Standard Error	27.00684
Observations	67

Figure 3. Regression Summary of HDR Nirmala index against the boiling points of alkanes.

4.2 Boiling Points Against Degree Based Topological index

The plot of degree based Nirmala index against boiling point of alkanes shows the following results:

The equation of the linear line of regression is found to be:

BP=10.8188040(N)-42.16704528

The value of multiple R suggests that it is a better tool for predicting the boiling points compared to the eccentricity based topological index but not the best one.

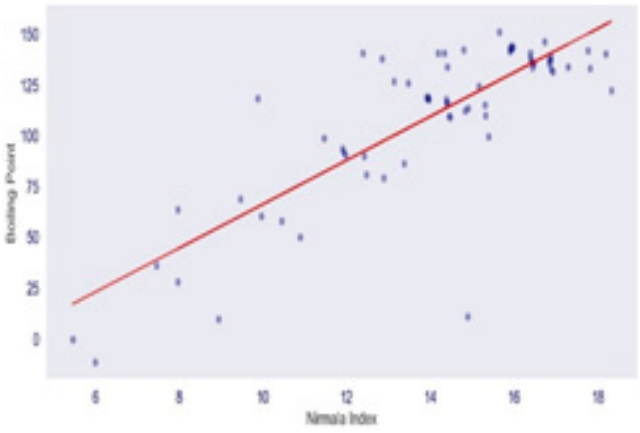


Figure 4. The plot of Nirmala index against the boiling points of alkanes.

5.0 Conclusion

The results can be summarized as follows:

It is clearly evident that the different variants of Nirmala index can be used as an efficient tool to determine the boiling points of alkanes. The degree based second Nirmala inverse index can be used to determinethe critical temperature of alkanes.

SUMMARY OUTPUT	
Regression Statistics	
Multiple R	0.919235032
R Square	0.844993044
Adjusted R Square	0.844893
Standard Error	22.70920462
Observations	67

Figure 5. Regression Summary of HDR Nirmala index against the boiling points of alkanes.

Topological Index	Physical property	Multiple R
HDR-Nirmala index	Boiling point	0.899967
Nirmala Index	Boiling point	0.919235

6.0 References

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