Journal of Mines, Metals and Fuels, *71(12C) : 435-439; 2023. DOI: 10.18311/jmmf/2023/47302*

Print ISSN : 0022-2755

Journal of Mines, Metals and Fuels

Contents available at: *www.informaticsjournals.com/index.php/jmmf*

Different Variants of the Nirmala Index and their Applications

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Abstract

Applications of graph theory include everything from arranging tournament games to analysing the structure of proteins. The Quantitative Structure-Property Relationship (QSPR) and the Quantitative Structure-Activity Relationship are current trends in graph theory (QSAR). The use of degree-based topological indices for QSPR and QSAR has been the subject of numerous publications. This study generalises a newly introduced distance-based topological index and uses the topological index to determine the boiling points of a particular family of aromatic compounds. This work also presents a unique way to determine the critical temperature of alkanes.

Keywords: Aromatic, Boiling Points, Nirmala Index, Status

1.0 Introduction

Several metals, non-metals, hydrocarbons and paraffins are exposed in nature. Experiments must be conducted to ascertain the physical and chemical properties of naturally occurring substances. Those properties can be mathematically ascertained through the utilisation of regression analysis.

The term 'topological index' has been established from the word 'topological space', and the two important methods describing this task are the Merrifield-Simmons method based on open set topology and the Polansky method based on neighbourhood topology. The important aspect is that it is theoretically possible to estimate the physio-chemical property of a given chemical compound using the topological index hence called a molecular descriptor. The entire study is a part of the Quantitative Structure-Property Relationship (QSPR).

The topological indices are classified based on the graph parameter used in it, i.e., either degree, distance or eccentricity. For a graph G, with V(G) and E(G) as its vertex and edge set, the distance between two vertices is the length of the shortest path joining them and the number of vertices incident with a given vertex is the degree of that vertex.

The first ever determined topological index was a distance-based one known as the Weiner Index[1], which found enormous application in analysing the boiling points of paraffin. The Randic index was the first to identify degree-based topological index[2]. Later many topological indices like the forgotten topological index[3], Zagreb index, Sum-status connectivity index[4] and Revan index were established.

The Sombor index was introduced by Gutman[5] and is given by

$$SO(G) = \sum_{u,v \in V(G)} \sqrt{d_G^2(u) + d_G^2(v)}.$$

With a similar idea, Kulli developed the Nirmala index of a graph, by taking the degree of vertices to power unity from the Sombor index.

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The status of a vertex $v \in V(G)$ is the sum of the distance of all vertices in the graph excluding itself. Considering the status and Nirmala index, the status-Nirmala index came into existence and is given by

$$SN(G) = \sum_{u,v \in V(G)} \sqrt{\sigma(u) + \sigma(v)}\,.$$

where σ(u) is the status of the vertex $u \in V(G)$.

The first and second inverse Nirmala index of a graph are given by

$$IN_1(G) = \left[\frac{1}{d_G(u)} + \frac{1}{d_G(v)}\right]^{\frac{1}{2}}$$

and

$$IN_2(G) = \left[\frac{1}{d_G(u)} + \frac{1}{d_G(v)}\right]^{-\frac{1}{2}}.$$

2.0 Generalisation of Status Nirmala Index for Certain Family of Standard Graphs

Theorem 2.1: For a complete bipartite graph

$$SN(K_{m,n}) = mn\sqrt{3m + 3n - 4}\,.$$

Proof: A complete bipartite graph is a graph in which the vertex set *V(G)* can be partitioned into two sets V_1 & V_2 such that there are no two vertices in V_1 (or V_2) are adjacent but every edge has one vertex in V_1 another in V_2.

Let $|V_1| = m$ and $|V_2| = n$.

The status of the vertices is as follows:

$$\sigma(v_i) = n + 2(m-1),\ 1 \le i \le m \text{ and}$$

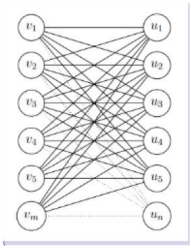


Figure 1. Complete bipartite graph.

$$\sigma(u_j) = m + 2(n-1),\ 1 \le j \le n\,.$$

The edge partition is as follows:

$$E_\alpha = \left\{\begin{matrix}\sigma(u) = n + 2(m-1)\,,\\ \sigma(v) = m + 2(n-1)\end{matrix}\right\},\ |E_\alpha| = mn.$$

Thus, $SN(K_{m,n}) = mn\sqrt{3m + 3n - 4}$.

Theorem 2.2: For a complete graph

$K_n (n \ge 2)$ $SN(K_n) = \dfrac{n(n-1)^{3/2}}{\sqrt{2}}$.

Proof: A complete graph with n vertices is a graph with vertices in which every vertex is adjacent to every other vertex in the graph and has $\dfrac{n(n-1)}{2}$ edges.

Hence,

$\sigma(v_i) = n - 1\,, \forall 1 \le i \le n\,.$

The edge partition is as follows:

$$E_\alpha = \{\sigma(u) = \sigma(v) = n - 1\}$$

and $|E_\alpha| = \dfrac{n(n-1)}{2}$.

Hence, $SN(K_n) = \dfrac{n(n-1)^{3/2}}{\sqrt{2}}$.

3.0 Computation of Second Inverse Nirmala Index for Certain Alkanes

Table 1. The topological indices of alkanes with their critical temperature

Sl.No.	Alkane	ct(°C)	IN 2
1	Butane	152.01	2.633
2	2-methylpropane	134.98	2.5981
3	Pentane	196.62	3.633
4	2-methyl butane	187.7	3.644
5	2,2dimethylpropane	160.6	3.266
6	Hexane	234.7	4.633

Table 1. continued...

7	2-methylpentane	224.9	4.644
8	3-methyalpentane	231.2	4.6243
9	2,2-methyl butane	216.2	4.6545
10	2,3-dimethylbutane	227.1	4.688
11	Heptanes	267.55	5.633
12	2-methyl hexane	257.9	5.643993
13	3-methyl hexane	262.4	5.6899
14	3-ethylpentane	267.6	4.873412
15	2,2-dimethyl pentane	247.7	5.65448
16	2,3-dimethyl pentane	264.6	5.7348
17	2,4-dimethyl pentane	247.1	5.65499
18	3,3-dimethyl pentane	263	5.73125
19	Octane	296.2	6.63299
20	2-methyl heptane	288	6.64399
21	3-methyl heptane	292	6.6899
22	4-methyl heptane	290	6.689
23	3-ethyl hexane	292	6.7358
24	2,3-dimethyl hexane	293	6.6545
25	2,2-dimethyl hexane	279	6.7348
26	2,4-dimethyl hexane	282	6.7009
27	2,5-dimethyl hexane	279	6.655
28	3,3-dimethyl hexane	290.84	6.7312
29	3,4-dimethyl hexane	298	6.7807
30	3-ethyl-2-methyl pentane	295	6.780679
31	3-ethyl-3-methyl pentane	305	6.78067
32	2,2,3-trimethylpentane	294	6.77055
33	2,2,4-trimethylpentane	271.15	6.66547
34	2,3,3-trimethylpentane	303	6.801409
35	2,3,4-trimethylpentane	295	6.77961
36	Nonane	322	7.63299
37	2-methyl octane	315	7.64399
38	3-methyl octane	318	7.6899
39	4-methyl octane	318.3	7.6899
40	3-methyl heptane	318	7.735825
41	4-methyl heptane	318.3	7.7358
42	2,2-dimethyl heptane	302	7.6545
43	2,3-dimethyl heptane	315	7.7348
44	2,4-dimethyl heptane	306	7.7009
45	2,5-dimethyl heptane	307.8	7.7009
46	2,6-dimethyl heptane	306	7.5894
47	3,3-dimethyl heptane	314	7.7312

Table 1. continued...

48	3,4-dimethyl heptane	322.7	7.7807
49	3,5-dimethyl heptane	312.3	7.7468
50	4,4-dimethyl heptane	317.8	7.731248
51	3-ethyl-2-methyl hexane	322.7	8.78067
52	4-ethyl-2-methyl hexane	330.3	7.746824
53	3-ethyl-3-methyl hexane	327.2	7.808019
54	2,2,4-trimethylhexane	301	7.711394
55	2,2,5-trimethylhexane	296.6	7.665478
56	2,3,3-trimethylhexane	326.1	7.80141
57	2,3,4-trimethylhexane	324.2	7.825533
58	2,3,5-trimethylhexane	309.4	7.745762
59	3,3,4-trimethylhexane	330.6	7.847325
60	3,3-diethylpentane	342.8	7.884788
61	2,2-dimethyl-3-ethyl pentane	322.6	7.816472
62	2,3-dimethyl-3-ethyl pentane	338.6	7.878179
63	2,4-dimethyl-3-ethyl pentane	324.2	7.82553
64	2,2,3,3-tetramethylpentane	334.5	7.857546
65	2,2,3,4-tetramethylpentane	319.6	7.8154
66	2,2,4,4-tetramethylpentane	301.6	7.675964
67	2,3,3,4-tetramethylpentane	334.5	7.871571

4.0 Computation of Status Nirmala Index for Certain Benzenoid Hydrocarbons

Table 2. The topological indices of benzenoid hydrocarbons with their boiling points

Sl No.	Name	Status Nirmala Index	Boiling Points
1	Naphthalene	71.7601	218
2	Phenapthalene	138.6272	338
3	Anthracene	140.8339	340
4	Chrysene	227.4901	431
5	Benz[a]anthracene	229.345	425
6	Triphenylene	220.109	429
7	Naphthacene	232.9495	440
8	Benzo[c]pyrene	275.484	496
9	Benzo[e]pyrene	269.3911	493
10	Perylene	269.9637	497
11	Dibenzo[def.mno] chrysene	328.5464	547

Table 2. Continued...

12	Benzo[ghi]perylene	233.510	542
13	Benzo[b]triphenylene	328.128	535
14	Dibenz[a,h]anthracene	340.4303	536
15	Dibenzo[a,j]anthracene	337.522	531
16	Picene	338.8309	519
17	Coronene	381.9917	590
18	Naphtho[1,2,3,4-def] chrysenre	382.6116	592
19	Dibenzo[b.def] chrysenre	393.5984	596
20	Benzo[rst]pentaphene	393.5984	594
21	Dibenzo[def.p]chrysene	379.06428	595

5.0 Results and Discussion

A variable's value can be predicted using linear regression analysis based on the value of another variable. The dependent variable is the one that we want to be able to forecast. The independent variable is the variable we are using to forecast the value of the other variable.

5.1 Critical Temperature Against Degree-based Topological Index

The regression analysis of the critical temperature of alkanes against the second Nirmala index shows the following results (Figure 2 and 3):

The equation of the linear line of regression is:

$$CT = 31.06501659\left(IN_2\right) + 79.15294068$$

5.2 Boiling Points Against Distance-based Topological Index

The status Nirmala index is considered the independent variable and the boiling point of benzenoid hydrocarbons is treated as the dependent variable for regression the results are as follows (Figure 4 and 5):

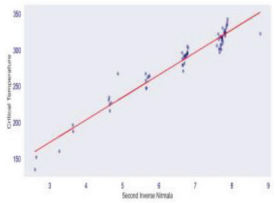


Figure 2. Plot of Second inverse Nirmala index against the critical temperature of alkanes.

SUMMARY OUTPUT	
Regression Statistics	
Multiple R	0.970191882
R Square	0.941272288
Adjusted R Square	0.940368785
Standard Error	11.15594345
Observations	67

Figure 3. Regression Summary of Status Nirmala index against the boiling points of benzenoid hydrocarbons.

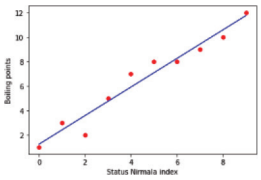


Figure 4. Plot of Status Nirmala index against the boiling points of benzenoid hydrocarbons.

SUMMARY OUTPUT	
Regression Statistics	
R Square	0.978088
Intercept	195.1772
X Variable 1	1.045795
Observations	21

Figure 5. Regression Summary of Status Nirmala index against the boiling points of benzenoid hydrocarbons.

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

$$BP = 1.045795\left(SN\right) + 195.1772$$

6.0 Conclusion

The regression analysis suggests that there is a positive correlation between the status Nirmala index and the boiling points of benzenoid hydrocarbons, the second inverse Nirmala index along with the critical temperature of alkanes. This forms a relationship between the physical parameter of a chemical compound and the topological index.

This technique is more beneficial when:

- Handling materials can be dangerous and determination is not always easy when compounds degrade quickly.
- Experimental determinations become very expensive and life-threatening.

7.0 References

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