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Research Article

QSPR Analysis of Novel Topological Index Based on Proximity Degree

Deepasree S. Kumar*[1], P. S. Ranjini[2], Md. Samiul Haque[3] and V. Lokesha[4]

[1] *Department of Mathematics, Acharya Institute of Technology* (*affiliated to Visvesvaraya Technological University*), *Bangalore 560107, Karnataka, India*
[2] *Department of Mathematics, Don Bosco Institute of Technology* (*affiliated to Visvesvaraya Technological University*), *Kumbalagudu, Bangaluru 560074, Karnataka, India*
[3] *Department of Mathematics, Acharya Institute of Technology, Bangalore 560107, Karnataka, India*
[4] *Department of Studies in Mathematics, Vijyanagara Sri Krishnadevaraya University, Ballari 583105, Karnataka, India*
***Corresponding author:** deepasreebiju84@gmail.com

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Abstract. In this article, we define a k-proximity degree and based on this distance degree, we introduce a novel topological index named *Proximity Index* (PI_k). By considering octane and heptane isomers, we have studied QSPR regression analysis to predict the physio-chemical properties and chemical applicability of the index.

Keywords. Proximity degree, QSPR analysis, Octane isomers, Heptane isomers

Mathematics Subject Classification (2020). 05C09, 05C07, 05C92

1. Introduction

In chemical graph theory, topological descriptors have a prominent role especially in QSAR and QSPR modelling. Recent research on mathematical properties and chemical applications of degree based topological indices are as active as ever, see, Aouchiche and Ganesan [2], Bonchev

et al. [5], Carballosa *et al.* [7], Cruz *et al.* [8], Li *et al.* [16], Lin *et al.* [17], and Wang *et al.* [21]. A topological index is a numerical value, that calculates based on molecular graph of a chemical compound. It is a graph invariant which characterize its topology (Agustin *et al.* [1]). Famous chemist, Harold Wiener introduced first topological index known as Wiener index in 1947 [22], which is effective for the prediction of boiling points for alkanes. This starts the research on topological indices. After that many topological indices are introduced and used in QSPR and QSAR analysis. In 1972, Gutman and Trinajstić [9] proposed the Zagreb indices, which measure the degree of branching in the molecular carbon atom skeleton and characterize the molecular structures. The first and second Zagreb indices are defined as follows:

$$M_1(G) = \sum_{uw \in E(G)} (d_u + d_v), \qquad M_2(G) = \sum_{uw \in E(G)} (d_u d_v).$$

In this article, we introduce proximity index based on k-proximity degree of a vertex, where k is the minimum degree of a vertex in the graph.

Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. d_u denotes degree of the vertex u and $\delta(u,v)$ be the distance between the vertices u and v. Let n be the number of vertices with degree k and consider $v \in G$ with $d_v = k$. The proximity degree of a vertex u is defined as follows:

$$P_u^k = \begin{cases} \frac{1}{n^2} \sum\limits_{u \in V(G)} \delta(u,v), & \text{if } d_v \neq k, \\ \frac{1}{(n-1)^2} \sum\limits_{u \in V(G)} \delta(u,v), & \text{if } d_v = k. \end{cases}$$

1.1 Properties

(i) $p_u^k = 0$ means only the vertex u has degree k in G.

(ii) Lower the value of p_u^k indicates the vertex u is very close to the vertices of degree k and vice versa.

(iii) Symmetry in molecular structure gives same proximity to the corresponding vertices on either side of the symmetric plane.

1.2 Method of Estimation of k Proximity Degree

Consider a typical alkaline compound 2,2,4-trymethyl pentane. From the structure shown in Figure 1, it is seen that $P_{u_1}^k = P_{u_6}^k = P_{u_7}^k$ and $P_{u_5}^k = P_{u_8}^k$.

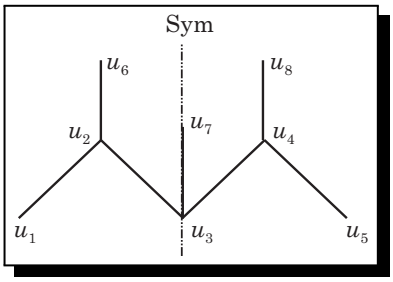


Figure 1

Table 1 gives the evaluation of proximity degree of alkaline compound trimethyl pentane for different values of k such that degree of the vertex v is k, i.e., $d_v = k$.

We consider octane and heptane isomers to check the chemical applicability of topological index, which can be evaluated by regression analysis.

The octane isomers data of Table 2 is collected from URL: https://www.moleculardiscriptors.eu/dataset/dataset.htm.

The proximity index helps to predict the chemical properties such as acentric factor and entropy with powerful accuracy. Also, we tested the degeneracy and gives the correlation of novel index with properties of octane and heptane isomers.

Table 1. Estimation of P_u^k for 2,2,4-trymethyl pentane

Vertices	u_1	u_2	u_3	u_4	u_5	u_6	u_7	u_8
$\sum_{i=1}^{n} \delta(u_i, v)$	12	9	10	11	14	12	12	14
n	4	5	5	5	4	4	4	4
$P_{u_i}^1$	$\frac{12}{6}$	$\frac{9}{25}$	$\frac{10}{25}$	$\frac{11}{25}$	$\frac{14}{16}$	$\frac{12}{16}$	$\frac{12}{16}$	$\frac{14}{16}$
$\sum_{i=1}^{n} \delta(u_i, v)$	2	1	0	1	2	2	2	2
n	1	1	1	1	1	1	1	1
$P_{u_i}^2$	2	1	0	1	2	2	2	2
$P_{u_i}^3$	3	2	1	0	1	3	3	1
$P_{u_i}^4$	1	0	1	2	3	1	1	3

Here we introduce the novel topological index named Proximity Index PI_k based on k proximity degree. It is defined as

$$PI_k = \sum_{u \in V} \frac{1}{P_u^k - 1}.$$

Also, we define the proximity polynomial,

$$P(G,x) = \sum_{u \in V(G)} x^{p_u^k},$$

then PI_k is defined as

$$PI_k = \int_0^1 P(G,x)dx.$$

2. QSPR Analysis

Regression analysis can be used for evaluating toplogical index, which is the application of chemical graph theory (Balaban *et al.* [3], Hawkins *et al.* [11], Hawkins *et al.* [12], Huang *et al.* [13], and Randić and Trinajstić [20]). Here we consider isomers of octane and heptane compounds to study the QSPR analysis.

In this analysis of new index, we consider $k = 1$, least degree, for estimation of PI_k for molecular structures of octane isomers. Properties such as entropy (S), acentric factor (Acen Fac), enthalpy of vaporization (HVAP), standard enthalpy of vaporization (DHVAP) are used in this analysis.

From Table 2, we can correlate each property with the novel topological index.

From the regression analysis, we observe that proximity index at $k = 1$, that is proximity with pendant vertices gives better result in predicting properties.

The octane isomers data Table 2 is collected from URL: www.moleculardiscriptors.eu/dataset/dataset.htm.

Table 2. Proximity index of octane isomers

Alkaline	Entropy	Acen Fac	DHVAP	HVAP	$PI_{k=1}$
n-octane	111.67	0.397898	9.915	73.19	2.43
2-methyl heptane	109.84	0.377916	9.484	70.30	3.43
3-methyl heptane	111.26	0.371002	9.521	71.30	3.50
4-methyl heptane	109.32	0.371504	9.483	70.91	3.53
2,3-dimethyl hexane	108.02	0.348247	9.272	70.20	4.33
2,4-dimethyl hexane	106.98	0.344223	9.029	68.50	4.27
2,5-dimethyl hexane	105.72	0.356830	9.051	68.60	4.18
3,4-dimethyl hexane	106.59	0.340345	9.316	70.20	4.37
2,2-dimethyl hexane	103.42	0.339426	8.915	67.70	4.35
3,3-dimethyl hexane	104.74	0.322596	8.973	68.50	4.43
3-ethyl hexane	109.43	0.362472	9.476	71.7	3.55
2,2,3-trimethyl pentane	101.31	0.300816	8.826	67.30	5.03
2,2,4-trimethyl pentane	104.09	0.305370	8.402	64.87	4.92
2,3,3-trimethyl pentane	102.60	0.293177	8.897	68.10	5.05
2,3,4-trimethyl pentane	102.39	0.317422	9.014	68.37	4.94
2-methyl 3-ethyl pentane	106.03	0.332433	9.209	69.70	4.37
3-methyl 3-ethyl pentane	101.48	0.306899	9.081	69.30	4.47
2,2,3,3-tetra methyl butane	93.060	0.255294	8.410	66.20	5.55

2.1 Isomer Degeneracy

A major drawback of the topological indices are their degeneracy, that is two or more isomers possess the same topological index (Konstantinova [14]).

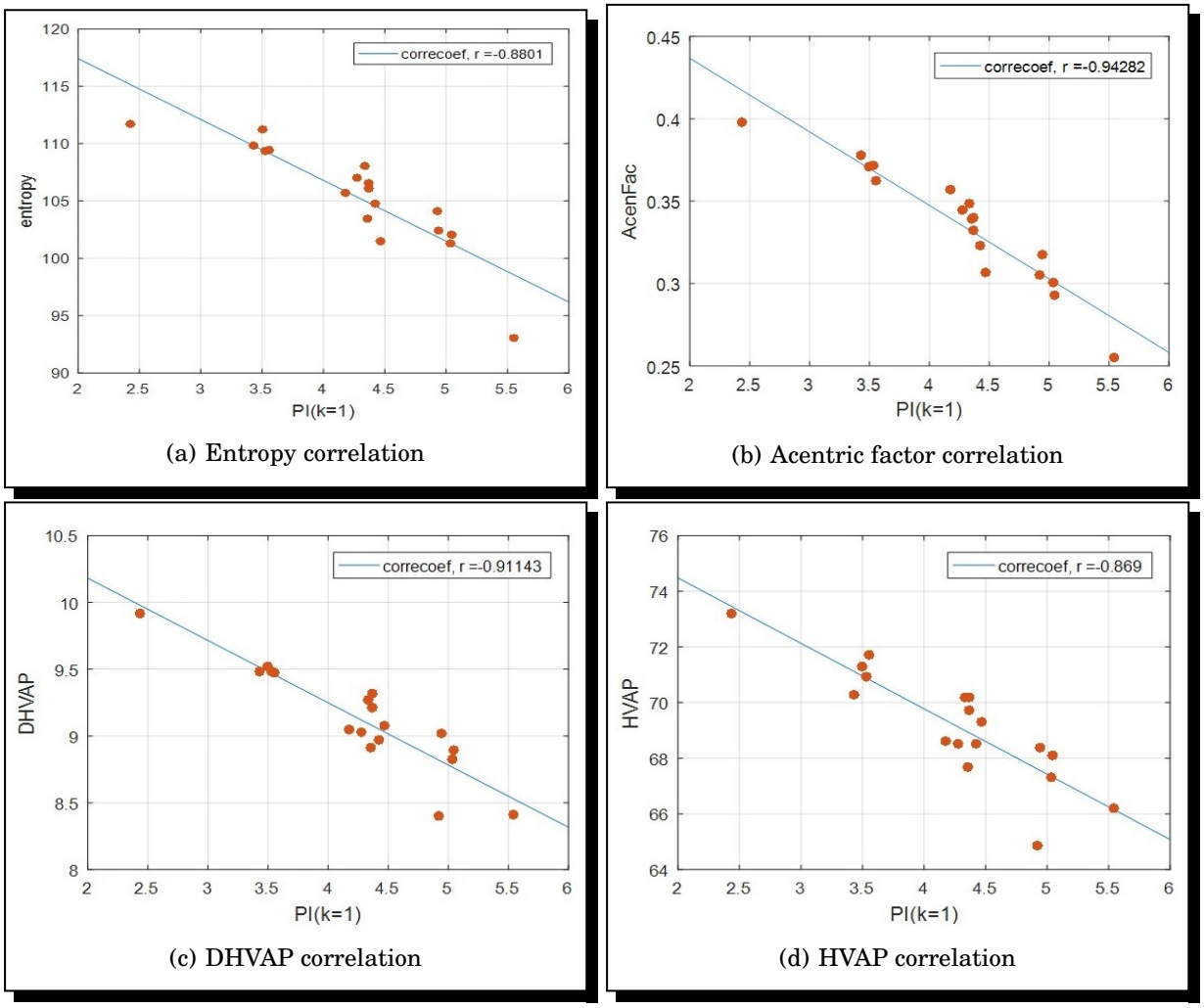
Basavanagoud and Jakkannavar [4], and Bonchev *et al.* [5] defined the mean isomers degeneracy as $\partial = \frac{N}{t}$, where N is the number of isomers considered and t is the number of distinct values that the index assumes for these isomers.

2.1.1 Properties

(i) Minimum value of ∂ is 1.

(ii) As the value of ∂ increases, the isomer discriminate the power of the topological index decrease. Thus, ∂ can decide the discriminating power of an index.

(iii) For octane isomers, PI_k exhibits good response as $\partial = 1$.



(a) Entropy correlation

(b) Acentric factor correlation

(c) DHVAP correlation

(d) HVAP correlation

Figure 2. Correlation of proximity index with properties of octane isomers

2.2 Correlation of Proximity Index With Properties of Heptane Isomers

Linear regression analysis of new index, PI_k for $k = 1$ estimated for molecular structures of heptane isomers with its corresponding properties as given in the Table 3 (Mondal *et al.* [19]).

Table 3. Proximity index of heptane isomers

Alkaline	BP (°C)	MV (cm^3)	MR (cm^3)	HVAP (kJ)	CT (°C)	CP (atm)	ST (dyne/cm)	MP (°C)	PI ($k = 1$)
Heptane	98.427	146.540	34.5504	36.55	267.55	27.01	20.26	−90.61	2.29
2-methyl hexane	90.052	147.656	34.5908	34.80	257.9	27.2	19.29	−118.2	3.20
3-methyl hexane	91.850	145.821	34.4597	35.08	262.4	28.1	19.79	−119.4	3.26
2,2-Dimethyl pentane	79.197	148.695	34.6166	32.43	247.7	28.4	18.02	−123.8	4.03
3,3-Dimethyl pentane	86.064	144.530	34.3323	33.02	263.0	30.0	19.59	−134.4	4.07
2,3-Dimethyl pentane	89.784	144.153	34.3237	34.24	264.6	29.2	19.96	−119.1	3.98
2,4-Dimethyl pentane	80.500	148.949	34.6192	32.88	247.1	27.4	18.15	−119.2	3.89
3-Ethyl pentane	93.475	143.517	34.2827	35.22	267.6	28.6	20.44	−118.6	3.29

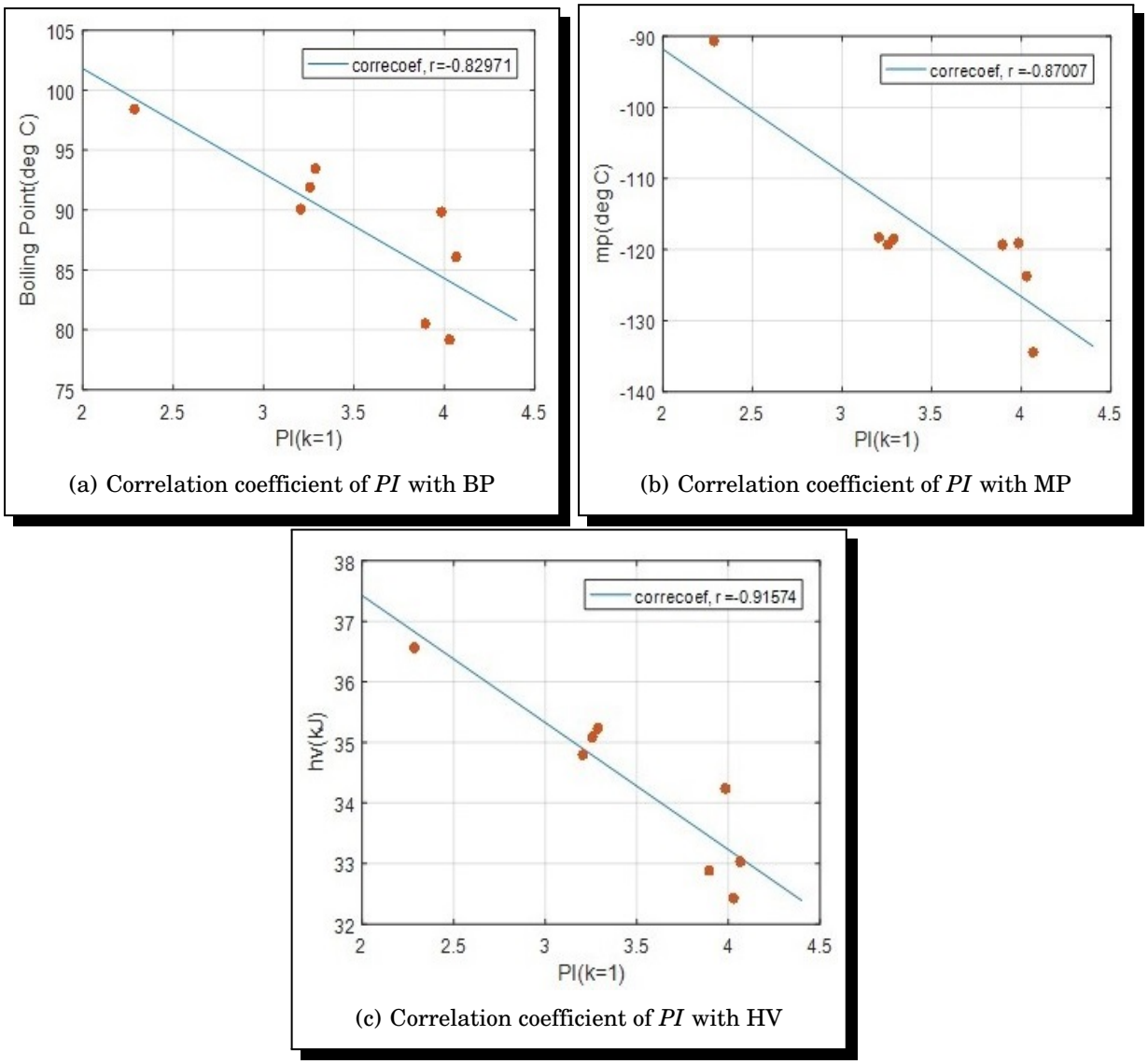
Abbreviations:
BP – Boiling Point, MV – Molar Volume, MR – Molar Refraction, HVAP – Heat of Vaporization, CT – Critical Temperature, CP – Critical Pressure, ST – Surface Tension, MP – Melting Point

Table 4 shows the correlation coefficient between the proximity index and the properties of heptane isomers.

Table 4. Correlation of property of heptane isomers with PI_k

BP	MV	MR	HV	CT	CP	ST	MP
−0.83	0.03	−0.17	−0.92	−0.52	0.66	−0.55	−0.87

The scatter diagram of these properties with proximity index are shown in Figure 3. If the coefficient of correlation is close to 1 or −1, then it has a strong relation with the index. We can see that proximity index is the best model to predict acentric factor, DHVAP and HV of the the isomers.



(a) Correlation coefficient of PI with BP

(b) Correlation coefficient of PI with MP

(c) Correlation coefficient of PI with HV

Figure 3. Correlation of proximity index with properties of heptane isomers

Isomer degeneracy of heptane, $\partial = \frac{N}{t} = 1.0$, which shows good response to discriminate the isomers.

3. Linear Regression Model for Proximity Index With Isomers

The linear regression model is

$$p = c(\pm 2e) + m(\pm 2e)TI,$$

where p, c, e, m and TI represent property, intercept, standard error of coefficient, slope and topological index, respectively.

The equation yields the linear regression model of entropy, acentric factor (Acen Fac), DHVAP and HVAP of octane isomers and BP, MP and HV of heptane isomers for the proximity index.

- Entropy $= 128.03(\pm 5.533) - 5.3068\ PI$
- Acen Fac $= 0.5258(\pm 0.023) - 0.04467\ PI$
- DHVAP $= 11.114(\pm 0.4154) - 0.46631\ PI$
- HVAP $= 79.179(\pm 2.7338) + 2.3503\ PI$
- BP $= 119.3(\pm 5.317) - 8.7508\ PI$
- MP $= -57.024(\pm 6.71) - 17.4\ PI$
- HV $= 41.624(\pm 0.97) - 2.0985\ PI$

The scatter diagram of these properties with proximity index are shown in Figure 2 and Figure 3. If the coefficient of correlation is close to 1 or -1, then it has a strong relation with the index. We can see that proximity index is the best model to predict acentric factor, DHVAP and HV of the the isomers.

4. Maximum and Minimum Value of *PI*

Motivated from (Božović *et al.* [6], and Manjunath *et al.* [18]), we estimated maximum and minimum value of PI.

We have estimated proximity index of octane and heptane isomers in previous sections. We can see that the molecular structures of isomers are obtained by relocating edges from the end to non-pendent vertex locations in the structure of primary compound. Variation of proximity index with relocation of multiple edges are studied in this section.

Equation for proximity index for a path graph with one edge connected to different vertices in the path is derived and studied. Then, a generalised equation for graphs with multiple branches also derived and it is applied for isomers with two branches. Single edge branches are considered in both cases.

Consider a path graph with n vertices and one of the vertices is connected to vertex u_{m_1} which is located at m_1th vertex from one end and serves as a branch to the structure. m_1 can vary from position 2 to $(n-2)$. $PI_{k=1}$ of this structure depends on the location of the branch and it can be written as equation (4.1),

$$PI_{(k=1)} = \frac{(2)^2}{(n+2)+m_1} + \frac{(2)^2}{(2n-m_1+2)} + \sum_{p=2}^{(n-2)} \frac{(3)^2}{n+8+|m_1-p|} + \frac{4}{n+4}. \tag{4.1}$$

Equation (4.1) contains four terms and variation of each term for a typical case of $n = 14$ is plotted in Figure 4.

Let *eqn*-1(1) and *eqn*-1(2) represent the first and second terms in the equation corresponds to first and last vertices (end vertices), respectively. Third term represents *eqn*-1(3), is the contribution from all vertices except the pendant vertices. Fourth term denotes *eqn*-1(4), is the contribution from the branch vertex which is a constant for a particular value of n, irrespective of location of the branch. Major contribution is from third term and it reaches the maximum value when m_1 is at the centre of the path.

When $(n-1)$ is odd, then peak value of this term happens at $m_1 = \frac{n}{2}$ and when $(n-1)$ is an even number, peak value will be same for two vertices located at the centre, $m = \frac{n-1}{2}$ and $\frac{n-1}{2}+1$. For the end vertices, proximity index reduces as the added edge moves away from the corresponding vertex.

Values of *eqn*-1(1) and *eqn*-1(2) are very less compared to *eqn*-1(3), hence the variation of proximity index, the sum of four terms follows the trend of the third term as seen in Figure 4, with peak when branch is at the centre.

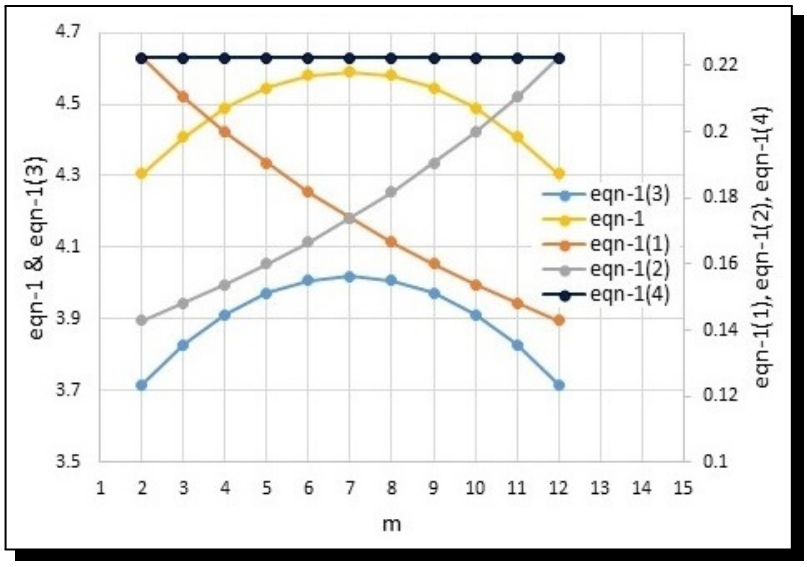


Figure 4. Terms in equation (4.1)

The above cases can be compared with the edge added to the pendent vertex of the path graph. Drastic reduction in value of index is seen with additional edge at the end. This is because of the reduction in number of pendent vertices compared to the branch structure variation. Proximity index of the graph with relocation of single branch, including the end locations for different values of n is shown in Figure 5.

Proximity index of a path graph with an additional edge becomes maximum when it is attached at the middle of the molecular structure and it is minimum when it is attached to the ends. Same can be observed in the case of octane isomers and heptane isomers.

Bounds of $PI_{(k=1)}$ are given in following expressions:

$PI_{(k=1)}$ is maximum when $(n-1)$ is odd $\left(m_1 = \frac{n}{2}\right)$, then

$$PI_{(k=1)} = \sum_{p=2}^{(n-2)} \frac{(3)^2}{n+8+|\frac{n}{2}-p|} + \frac{16}{3n+4} + \frac{4}{n+4}.$$

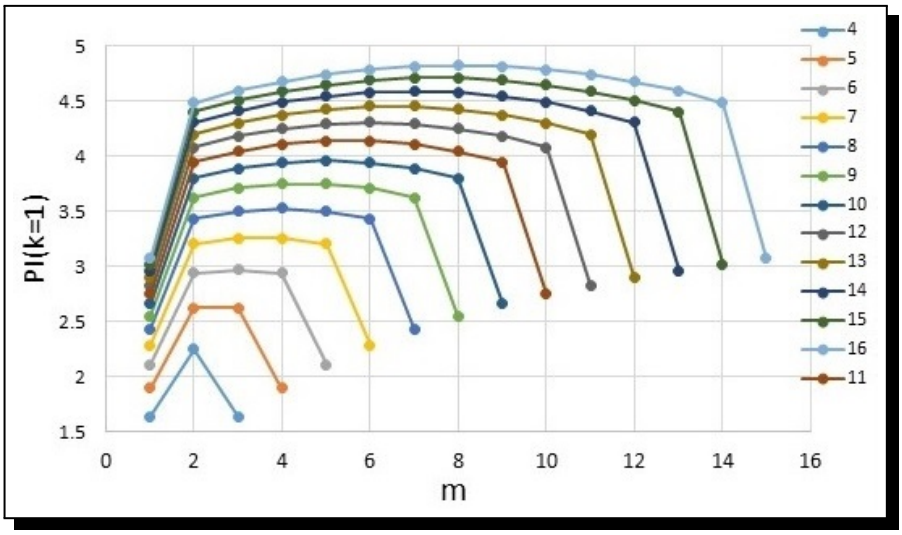


Figure 5. Proximity for path graph

$PI_{(k=1)}$ is maximum when $(n-1)$ is even $\left(m_1 = \frac{n-1}{2} \text{ or } \frac{n+1}{2}\right)$, then

$$PI_{(k=1)} = \sum_{p=2}^{(n-2)} \frac{(3)^2}{n+8+|\frac{n-1}{2}-p|} + \frac{8}{3n+5} + \frac{8}{3n+3} + \frac{4}{n+4}.$$

$PI_{(k=1)}$ is minimum when n is odd or even $(m_1 = 1 or (n-1))$, then

$$PI_{(k=1)} = \frac{2}{n} + \frac{4(n-2)}{(n+3)}.$$

4.1 Generalised Form

In continuation to the previous case of single branch isomers, generalised form of proximity index is derived here for path graphs with multiple single edge branches. Let the total number of vertices be n and total number of branches attached to the primary path is b such that l^{th} branch is attached to the to the vertex u_{m_l}. u_p is the identification of any vertex on the primary path except that of end vertices. Graphical representation of this arrangement is shown in Figure 6 and equation for $PI_{(k=1)}$ for this structure is given as equation (4.2).

Equation (4.2) is used for deriving proximity index for the graph with two branches and the branches are located at anywhere between the pendent vertices on the primary path. Location of branches on the path are m_1 and m_2 respectively. Variation of proximity index with respect to these locations are given in Figure 7. Values of m_1 and m_2 at which PI reaches its upper and lower bounds is a scope for future work in this area,

$$PI = \frac{(b+1)^2}{(n-b-1)+\sum_{i=1}^{l}(m_i)+(b+1)^2} + \frac{(b+1)^2}{(n-1)+(n-b)b-\sum_{i=1}^{l}(m_i)+(b+1)^2}$$
$$+ \sum_{p=2}^{(n-b-1)} \frac{(b+2)^2}{(n-1)+\sum_{i=1}^{b}|m_i-p|+(b+2)^2} + \sum_{l=1}^{b} \frac{(b+1)^2}{(n-b)-1+2b+\sum_{i=1}^{b}|m_i-m_l|+(b+1)^2}. \quad (4.2)$$

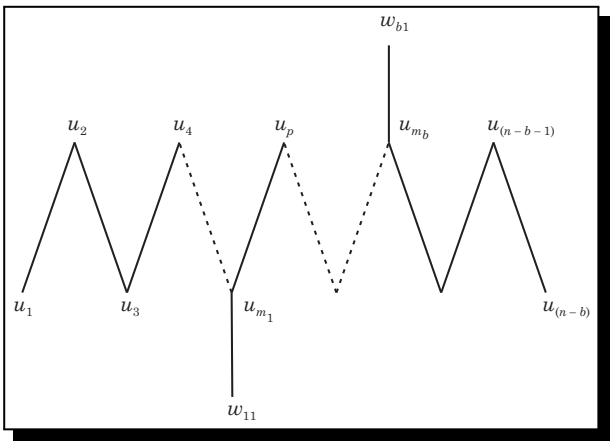


Figure 6. Branches

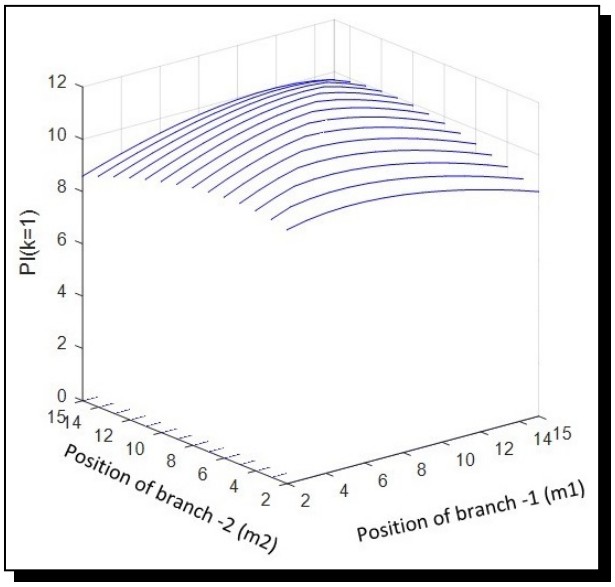


Figure 7. Variation of proximity index with respect to the location

5. Evaluation of Proximity Index

Here we evaluate the proximity index of triangular oxide network and generalized wheel graph via proximity polynomial.

5.1 Proximity Index of Triangular Oxide Network

A triangular oxide network typically refers to a structure in which oxide ions are arranged in a triangular lattice or pattern. The properties of materials with a triangular oxide network can vary depending on the specific compounds involved and the arrangement of the oxide ions. Material with triangular oxide networks have a range of practical applications across different industries like ceramics, electrical insulators, dielectric materials, optical material etc.

The specific application of materials with triangular oxide networks depends on their properties, which can be tailored through the choice of elements,doping and crystal structure. These materials play a crucial role in various technological advancements and industrial processes. Oxide network play a vital role in the study of silicate network (Kuang *et al.* [15], and Yang *et al.* [23]). If we delete the silicon vertices from a silicate network, we get an oxide network.

A triangular oxide network is denoted as TOX(n), where n is the length of the triangular network. An oxide network TOX(n) for $n = 1$, $n = 2$ and $n = 5$ are depicted in Figure 8.

Let τ_n be the graph of triangular oxide network, has $\frac{3n(n+1)}{2}$ edges and $\frac{n^2+3n+2}{2}$ vertices.

We can observe that all three corners have minimum degree which is $k = 2$. All the boundary vertices having degree 4 and inside vertices are of degree 6.

Therefore, we have 3 category of similar proximity degree vertices. Three corner vertices having proximity degree $\frac{n}{2}$ and $3(n-1)$ number of vertices having proximity degree $\frac{2n}{9}$. Also, $\frac{n(n-1)}{2}$ inside vertices having proximity degree $\frac{2n}{9}$.

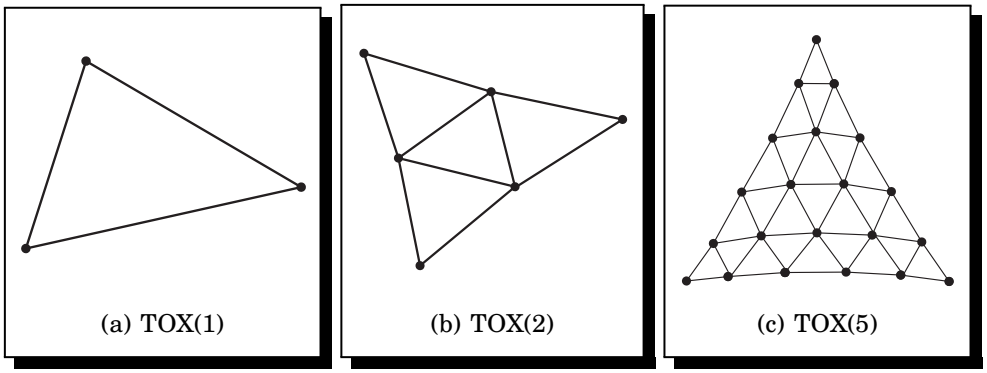


Figure 8. Triangular oxide networks

Proximity polynomial:

$$P(\tau_n, x) = 3x^{\frac{n}{2}} + 3(n-1)x^{\frac{2n}{9}} + \frac{n(n-1)}{2}x^{\frac{2n}{9}}.$$

Proximity index:

$$\begin{aligned} PI_k(\tau_n) &= \int_0^1 P(\tau_n, x)dx \\ &= \left[3\frac{x^{\frac{n}{2}+1}}{\frac{n}{2}+1} + 3(n-1)\frac{x^{\frac{2n}{9}+1}}{\frac{2n}{9}+1} + \frac{n(n-1)}{2}\frac{x^{\frac{2n}{9}+1}}{\frac{2n}{9}+1}\right]_0^1 \\ &= \frac{3n(3n^2+21n+10)}{2(n+2)(2n+9)}. \end{aligned}$$

5.2 Proximity Index of m-level Wheel Graph

The generalized wheel graph is known as m-level wheel network, denoted by W_{mn} (Hasan *et al.* [10]). It is obtained by m copies of cycle c_n connected with a common vertex such that all the vertices are adjacent in all copies of c_n (refer Figure 9 for W_{44}).

W_{mn} has $mn+1$ number of vertices and $2mn$ number of edges, $m \geq 2$ and $n \geq 3$.

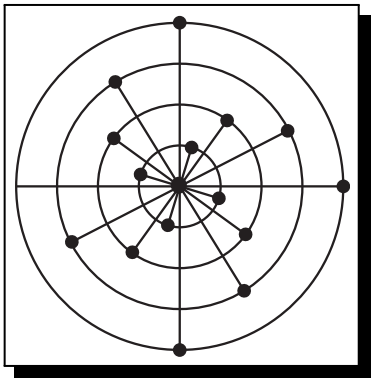


Figure 9. Wheel graph W_{44}

5.2.1 Properties

- All vertices except the center vertex have degree 3 and central vertex is of degree mn.
- All vertices in each cycle is connected to the center by a single edge

Here we find proximity degree for each vertex at $k=3$, which is the minimum degree in Wmn. Let u_0 be the central vertex with degree mn, proximity of u_0 is $P^3_{u_0} = \frac{1}{mn}$ and proximity degree of other vertices $P_{u^3_{mn}} = \frac{2(mn-2)}{(mn-1)^2}$.

Proximity polynomial:

$$P(W_{mn},x) = mnx^{\frac{2(mn-2)}{(mn-1)^2}} + x^{\frac{1}{mn}}.$$

Proximity index:

$$\begin{aligned} PI_3(W_{mn}) &= \int_0^1 P(W_{mn},x) \\ &= \left[mn\frac{x^{\frac{2(mn-2)}{(mn-1)^2}+1}}{(mn-1)^2+1} + \frac{x^{\frac{1}{mn}+1}}{\frac{1}{mn}+1} \right]_0^1 \\ &= \frac{(mn)^2}{mn+1}. \end{aligned}$$

6. Conclusion

We introduced a new term called k-proximity degree (P_k) of vertex, which indicates the proximity of a vertices to other vertices of degree k. Also, introduced a new topological index (PI) based on P_k and proximity polynomial are defined and applied for QSPR analysis of octane and heptane isomers. From QSPR studies, we observed that the novel topological index, PI shows a good correlation with properties like entropy and acentric factor of octane isomers and also with heat of vaporization of heptane isomers. Regression models are generated for the cases of good correlation. The value of degeneracy of PI is 1, that indicates it can discriminate the isomers. Also, we found the proximity index of triangular oxide network and generalized wheel graph.

Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

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