

New block-labelled topological indices and physicochemical properties of heptane isomers

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Abstract: *In this work, four new block-labelled topological indices, namely the block labelled product index, block labelled sum index, cluster block labelled product index, and cluster block labelled sum index, based on block label of the molecular structure, are defined. The new topological indices are investigated for Path and Star graphs in connection with AUM block mean labeling. In order to predict the physicochemical properties of heptane isomers, a comparative analysis is done, and the chemical applicability of these indices is determined for boiling point, vapour pressure, and enthalpy of vaporization. Through this work, we bridge the concept of AUM block mean labeling to the block-labelled topological indices. Also, these newly introduced indices are compared with other degree-based indices.*

Key words: AUM block mean labeling, Block-labelled topological indices, Heptane isomers, Topological index, Correlation.

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1. Introduction

A topological index is a numerical quantity and can be applied to the analysis of physicochemical properties of any graph that represents the molecule structure [17]. Topological indices and graph labeling are vast research areas in graph theory. It plays an essential part in QSPR (Quantitative structure-property relationship) and QSAR (Quantitative structure-activity relationship). A number of topological indices, including vertex-degree indices, neighbourhood degree-based indices, labelled topological indices and so on, have been examined in relation to the parameters of the graph. Wiener [19], Randic [9], and Zagreb [14] are the topological indices that have been used most out of all of them.

A graph that represents chemical structure is known as chemical graph. Chemical graphs are referred to molecular graphs if the chemical structures being considered as molecules. They are created by substituting vertices and edges for atoms and bonds, respectively. In order to investigate chemical processes, a branch of mathematics called chemical graph theory merges graph theory and mathematical design [18]. We recalled few concepts of chemical graph theory from [1], [2],[4], [5], [7] and [10].

Harold Wiener came up with the concept of the first topological index, known as the Wiener index, in 1947 [19]. The Wiener index of a connected graph G was defined as $W(G) = \frac{1}{2} \sum_{u,v \in V(G)} d(u,v)$. $d(u,v)$ - indicates the smallest number of edges between u and v . The first genuine degree-based topological index was found in 1975 by Milan Randić [9] and named as the connectivity index.

$$R(G) = \frac{1}{\sqrt{\deg_G(u)\deg_G(v)}}$$

$\deg_G(u)$ is the number of edges connected to u . Another topological index introduced in the initial stage is by Gutman and Trinajstić namely Zagreb index [14]. A molecular graph G 's first $M_1(G)$ and second $M_2(G)$ Zagreb indices are defined as follows:

$$M_1(G) = \sum_{v \in V(G)} \deg_G(v)^2$$

$$M_2(G) = \sum_{uv \in E(G)} \deg_G(u) \deg_G(v)$$

Furtula [3] introduced the forgotten topological index

$$F(G) = \sum_{v \in V(G)} \deg_G(v)^3 = \sum_{uv \in E(G)} \deg_G(u)^2 + \deg_G(v)^2$$

For octane isomers, Furtula [3] showed that $M_1(G)$ and $F(G)$ provided correlation coefficients higher than 0.95 for the physicochemical properties acentric factor and entropy. In order to predict certain specific physicochemical properties of octane isomers, such as entropy, acentric factor, enthalpy of vaporisation, and standard enthalpy of vaporisation, Süleyman Ediz [13] introduced the ev-degree Zagreb index, ve-degree Zagreb indices, and ve-degree Randić index.

These indices are compared with the other well-known and most commonly used topological indices such as the Wiener, Zagreb, and Randić indices. Density of a vertex has been defined by Princess Rathinabai, G. et al. [8] and density-based topological indices were presented for graphs that admit graceful, odd harmonious, and cordial labeling. In [18], Vinutha S.V. et al. established labelled topological indices, discussed the molecular graphs that allow cordial labeling, and analysed the molecular structure using regression models. Sourav Mondala [12] conducted a comparative investigation to ascertain the chemical applicability of neighbourhood degree-based indices for entropy and acentric factor to octane isomers. V. Shigehalli [11] computed the ABC index, GA index, and AG index of heptane isomers.

Motivation: Inspired by the above application of graph labeling in chemical graph theory, we introduced new block- labelled topological indices based on block labeling. The main aim of this work is to identify the chemical applicability of these newly introduced vertices to the chemical graphs.

We present four new block-labelled topological indices with respect to block labeling. The physicochemical properties of chemical compounds can be predicted using topological indices, so it's important to examine the relationship between the physicochemical characteristics and the topological indices introduced.

We compare the block- labelled topological indices with respect to AUM block mean labeling to the physicochemical properties of heptane isomers and other well-known and most used topological indices. AUM block mean labeling is introduced by the authors and established for Path and Star families of graphs [15].

We use the following heptane isomers physicochemical characteristics, since they provide comparatively strong relationships.

- Boiling point (the temperature at which any liquid starts to boil)
- Enthalpy of Vaporization (the quantity of heat needed at a constant temperature and pressure to convert a unit mass of a substance from a liquid to a vapour)
- Vapour Pressure (the pressure exerted by a vapour in a closed space)

For convenience, the topological index is denoted as TI.

2. Preliminaries

Basic definitions required for further investigations are listed below:

2.1. Definition: AUM block mean labeling [15]

Let G be a graph with p vertices, with a vertex set $V(G)$, q edges, with an edge set $E(G)$, and r blocks, with a block set $B(G)$, $p, q, r \geq 1$.

We say that graph G admits **AUM block mean labeling** if there exists a bijection $\phi: V(G) \rightarrow \{1, 3, 5, \dots, 2p - 1\}$ and an injective function $\phi^*: E(G) \rightarrow \{2, 3, 4, \dots, 2p - 2\}$

induced from ϕ by $\phi^*(uv) = \frac{\phi(u) + \phi(v)}{2}$ and $\phi^{**}: B(G) \rightarrow Z^+$ defined as follows:

Let B_k be incident with the vertices $v_{k_1}, v_{k_2}, \dots, v_{k_m}$, $1 \leq k_m \leq p$ and edges $e_{k_1}, e_{k_2}, \dots, e_{k_n}$, $1 \leq k_n \leq q$.

Define $\phi^{**}(B_k) = \frac{\sum_{i=1}^m \phi(v_{k_i}) + \sum_{i=1}^n \phi^*(e_{k_i})}{\text{No. of vertices incident with } B_k + \text{No. of edges incident with } B_k}$ and

$\phi^{**}(B_k) \neq \phi^{**}(B_j)$ for $1 \leq k, j \leq r$ and $k \neq j$.

A graph G is known as an **AUM block mean labelled graph** if it admits AUM block mean labeling.

2.2. Definition: Neighbourhood of a block [16]

Let G be any (nontrivial, finite) graph. The neighbourhood of a block B of G is the set of all blocks that have a common vertex with B , and it is denoted by $N(B)$.

2.3. Definition: Star graph [7]

A Star graph S_n is the complete bipartite graph $K_{1,n}$.

2.4. Definition: Density of a vertex [8]

The density of a vertex u , with respect to a labeling L , of a labelled graph G , is defined as $\eta_L(u) = \sum f(uv)$ where the sum ranges over all $v \in N(u)$, and $f(uv)$ is the label assigned to the edge uv .

Based on the above definition, the following TI's were introduced:

1. Square Index of $(G)_L, SQI(G)_L = \sum_{v \in V(G)} \eta_L(v)^2$
2. Product Index of $(G)_L, PI(G)_L = \sum_{uv \in E(G)} \eta_L(u)\eta_L(v)$
3. Sum Index of $(G)_L, SI(G)_L = \sum_{uv \in E(G)} \eta_L(u) + \eta_L(v)$
4. Cluster Square Index of $(G)_L, CSQI(G)_L = \frac{SQI(G)_L}{\sum_{v \in V(G)} \eta_L(v)}$
5. Cluster Product Index of $(G)_L, CPI(G)_L = \frac{PI(G)_L}{\sum_{v \in V(G)} \eta_L(v)}$
6. Cluster Sum Index of $(G)_L, CSI(G)_L = \frac{SI(G)_L}{\sum_{v \in V(G)} \eta_L(v)}$

The topological indices defined above are called the density-based TI's of the labelled graph G .

3. Main results

In this section, TI's based on blocks of the molecular structure in connection with block labeling are defined. Establishing the mathematical application of these recently developed indices to the physicochemical features of chemical graphs are the objective of this work. The following physicochemical characteristics of the heptane isomers are considered to determine the correlation coefficients:

- Boiling point
- Enthalpy of Vaporization
- Vapour Pressure

3.1. Block-labelled Topological Indices

Based on the block label of the graph G , the following Topological Indices are introduced:

Here, $L_{\mathcal{B}}^G(B_i)$ denotes the block label of the graph G with respect to the block labeling \mathcal{B} .

1. Block labelled product index = $BLPI(G)_{\mathcal{B}} = \sum_{B_i \in \mathcal{B}(G)} \{L_{\mathcal{B}}^G(B_i) \sum_{B_j \in N(B_i)} L_{\mathcal{B}}^G(B_j)\}$
2. Block labelled sum index = $BLSI(G)_{\mathcal{B}} = \sum_{B_i \in \mathcal{B}(G)} \{L_{\mathcal{B}}^G(B_i) + \sum_{B_j \in N(B_i)} L_{\mathcal{B}}^G(B_j)\}$
3. Cluster block labelled product index = $CBLPI(G)_{\mathcal{B}} = \frac{BLPI(G)_{\mathcal{B}}}{\sum_{B_i \in \mathcal{B}(G)} L_{\mathcal{B}}^G(B_i)}$
4. Cluster block labelled sum index = $CBLSI(G)_{\mathcal{B}} = \frac{BLSI(G)_{\mathcal{B}}}{\sum_{B_i \in \mathcal{B}(G)} L_{\mathcal{B}}^G(B_i)}$

3.2. Block-labelled Topological Indices of Path graph $P_n (n \geq 2)$:

Let G denote the Path graph $P_n, n \geq 2$ with AUM block mean labeling [15].

Sum of the block labels of $G = \sum_{B_i \in \mathcal{B}(G)} L_{\mathcal{B}}^G(B_i) = n(n-1)$

Here, \mathcal{B} indicates AUM block mean labeling.

$$BLPI(G)_{\mathcal{B}} = \frac{4(n-2)(n-1)(2n-3)}{3} + 4(n-1)(n-2)$$

$$BLSI(G)_{\mathcal{B}} = 3(n-3)(n-2) + 4n - 6 + 6(n-2)$$

$$CBLPI(G)_{\mathcal{B}} = \frac{4(n-2)(2n-3) + 12(n-2)}{3n}$$

$$CBLSI(G)_{\mathcal{B}} = \frac{3(n-3)(n-2) + 4n - 6 + 6(n-2)}{n(n-1)}$$

Example: Consider the Path graph $P_5 = G$

Sum of the block labels of $G = \sum_{B_i \in \mathcal{B}(G)} L_{\mathcal{B}}^G(B_i) = 2 + 4 + 6 + 8 = 20$

$$BLPI(G)_B = 2(4) + 4(2 + 6) + 6(4 + 8) + 8(6) = 160$$

$$BLSI(G)_B = [2 + (4)] + [4 + (2 + 6)] + [6 + (4 + 8)] + [8 + (6)] = 50$$

$$CBLPI(G)_B = \frac{160}{20} = 8$$

$$CBLSI(G)_B = \frac{50}{20} = 2.5$$

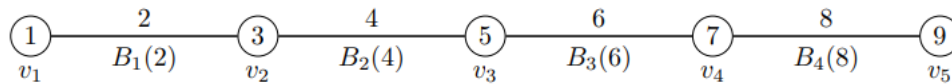


Figure 1: Path graph P_5

3.3. Block-labelled Topological Indices of Star graph S_n ($n \geq 3$):

Let G denote the Star graph S_n , $n \geq 3$ with AUM block mean labeling (B) [15].

$$\text{Sum of the block labels of } G = \sum_{B_i \in B(G)} L_B^G(B_i) = \frac{n^2 + 3n}{2}$$

$$BLPI(G)_B = \frac{6n^4 + 28n^3 + 18n^2 - 52n}{24}$$

$$BLSI(G)_B = \frac{n^3 + 3n^2}{2}$$

$$CBLPI(G)_B = \frac{6n^4 + 28n^3 + 18n^2 - 52n}{12(n^2 + 3n)}$$

$$CBLSI(G)_B = n$$

Example: Consider the Star graph $S_8 = G$

$$\text{Sum of the block labels of } G = \sum_{B_i \in B(G)} L_B^G(B_i) = 2 + 3 + 4 + 5 + 6 + 7 + 8 + 9 = 44$$

$$\begin{aligned} BLPI(G)_B &= 2(3 + 4 + 5 + 6 + 7 + 8 + 9) + 3(2 + 4 + 5 + 6 + 7 + 8 + 9) \\ &\quad + 4(2 + 3 + 5 + 6 + 7 + 8 + 9) + 5(2 + 3 + 4 + 6 + 7 + 8 + 9) \\ &\quad + 6(2 + 3 + 4 + 5 + 7 + 8 + 9) + 7(2 + 3 + 4 + 5 + 6 + 8 + 9) \\ &\quad + 8(2 + 3 + 4 + 5 + 6 + 7 + 9) + 9(2 + 3 + 4 + 5 + 6 + 7 + 8) = 1652 \end{aligned}$$

$$\begin{aligned}
BLSI(G)_B &= [2 + (3 + 4 + 5 + 6 + 7 + 8 + 9)] + [3 + (2 + 4 + 5 + 6 + 7 + 8 + 9)] \\
&+ [4 + (2 + 3 + 5 + 6 + 7 + 8 + 9)] + [5 + (2 + 3 + 4 + 6 + 7 + 8 + 9)] \\
&+ [6 + (2 + 3 + 4 + 5 + 7 + 8 + 9)] + [7 + (2 + 3 + 4 + 5 + 6 + 8 + 9)] \\
&+ [8 + (2 + 3 + 4 + 5 + 6 + 7 + 9)] + [9 + (2 + 3 + 4 + 5 + 6 + 7 + 8)] = 352
\end{aligned}$$

$$CBLPI(G)_B = \frac{1652}{44} = 37.55$$

$$CBLSI(G)_B = \frac{352}{44} = 8$$

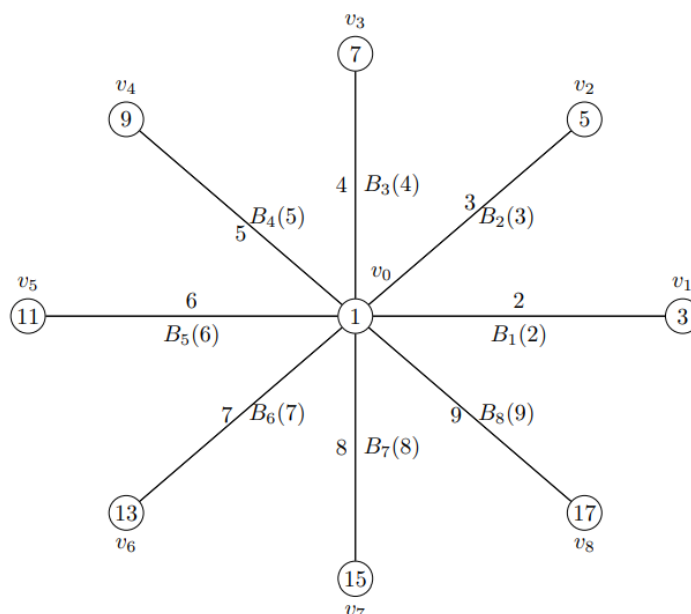


Figure 2: Star graph S_8

3.4. Significance of the new Topological Indices with respect to AUM block mean labeling:

In this section, the newly introduced block-labelled topological indices with respect to AUM block mean labeling (\mathcal{B}) are found for the chemical structures of heptane isomers. Therefore, $L_{\mathcal{B}}^G(B_i)$ is the mean of the labels of the vertices and the labels of the edges incident in that block B_i . Hereafter, G represents the chemical structure of the corresponding heptane isomer.

The topological indices $BLPI(G)_B$, $BLSI(G)_B$, $CBLPI(G)_B$, and $CBLSI(G)_B$ are calculated for the chemical structures of heptane isomers. Also, physicochemical properties of heptane isomers, namely boiling point, enthalpy of vaporization and vapour pressure, are considered for

the comparative study. The data of heptane isomers are collected from the source *ChemSpider* and given in Table 1 along with the value of block-based density topological indices.

Molecular structure of heptane isomers along with AUM block mean labeling is given as follows:

1	Heptane	
2	2-Methylhexane	
3	3-Methylhexane	
4	2,3-Dimethylpentane	
5	2,4-Dimethylpentane	
6	2,2-Dimethylpentane	
7	3,3-Dimethylpentane	

8	3-Ethylpentane	
9	2,2,3-Trimethylbutane	

Table 1. Values of boiling point, vapour pressure and enthalpy of vaporization of heptane isomers and the corresponding values of $BLPI(G)_B$, $BLSI(G)_B$, $CBLPI(G)_B$ and $CBLPI(G)_B$

Molecular name	Boiling Point(°C)	Vapour Pressure (Pa)	Enthalpy of vaporization (kJ/mol)	$BLPI(G)_B$	$BLSI(G)_B$	$CBLPI(G)_B$	$CBLPI(G)_B$
Heptane	98.8	45.2	31.8	560	112	13.33	2.67
2- Methylhexane	90.0	64.7	30.6	716	129	17.46	3.15
3- Methylhexane	90.7	62.9	30.9	628	124	15.32	3.02
2, 3-Dimethylpentane	89.4	66.2	30.5	718	136	17.95	3.4
2, 4-Dimethylpentane	80.5	94.5	29.5	705	133	17.63	3.33
2,2-Dimethylpentane	77.9	104.7	29.2	968	162	23.61	3.95
3,3-Dimethylpentane	85.7	76.8	29.6	668	140	17.13	3.59
3-Ethylpentane	92.3	58.8	31.1	556	120	13.56	2.93
2,2,3-Trimethylbutane	81.7	90	28.9	803	152	21.13	4

Now, the correlation coefficients between boiling point, enthalpy of vaporization and vapour pressure with the new topological indices $BLPI(G)_B$, $BLSI(G)_B$, $CBLPI(G)_B$, and $CBLPI(G)_B$, some well-known degree-based topological indices, such as $M_1(G)$, $M_2(G)$ and $F(G)$ of heptane isomers are found.

Table2: Correlation coefficient of $BLPI(G)_B$, $BLSI(G)_B$, $CBLPI(G)_B$, and $CBLPI(G)_B$ with Boiling Point, Enthalpy of Vaporization and Vapour Pressure

Index Property of Molecular	$BLPI(G)_B$	$BLSI(G)_B$	$CBLPI(G)_B$	$CBLSI(G)_B$	$M_1(G)$	$M_2(G)$	$F(G)$
Boiling point	-0.8295	-0.8884	-0.8663	-0.8804	-0.8375	-0.6801	-0.8101
Enthalpy of Vaporization	-0.7832	-0.905	-0.8579	-0.9448	-0.857	-0.8213	-0.8197
Vapour Pressure	0.8495	0.8873	0.8761	0.8666	0.819	0.6339	0.7907

The block-labelled indices have correlation coefficients with absolute values greater than 0.9. Table 2 shows that the block-labelled indices are suitable for modelling the boiling point ($BLSI(G)_B$), enthalpy of vaporization ($CBLSI(G)_B$) and the vapour pressure ($BLSI(G)_B$). Here, the indices show the strong negative correlation for boiling point and enthalpy of vaporization and the strong positive correlation for vapour pressure.

Now, we investigate the relation between $BLPI(G)_B$, $BLSI(G)_B$, $CBLPI(G)_B$, $CBLPI(G)_B$ and $M_1(G)$, $M_2(G)$, $F(G)$.

Index	$M_1(G)$	$M_2(G)$	$F(G)$
$BPI(G)_B$	0.7155	0.5111	0.701
$BSI(G)_B$	0.9026	0.7638	0.8468
$CBPI(G)_B$	0.8129	0.6289	0.7361
$CBSI(G)_B$	0.9684	0.8605	0.8354

This leads us to the conclusion that the topological indices $BLPI(G)_B$, $BLSI(G)_B$, $CBLPI(G)_B$, and $CBLPI(G)_B$ presented now shows notable correlations with some well-known degree-based topological indices. As a result, we can conclude that the block-based density topological indices have chemical significance.

Conclusion:

We have introduced block-labelled topological indices namely, the block labelled product Index, block labelled sum index, cluster block labelled product index, cluster block labelled sum index, with respect to block labeling. These topological indices are connected with AUM block mean labeling and discussed for Path and Star graphs. Also, these topological indices are calculated for the chemical structure of heptane isomers and the results are correlated to the physicochemical properties of heptane isomers, such as boiling point, enthalpy of vaporization and vapour pressure. The significance of these topological indices is discussed and compared with the well-known topological indices $M_1(G)$, $M_2(G)$ and $F(G)$. Thus, these four indices can be considered as applicable topological indices and possible tools for QSAR/QSPR research. For further research, these indices can be computed for various molecular structures and the analysis between their physicochemical properties can be investigated.

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