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Kulli-Basava Indices of Graphs

B. Basavanagoud *[1], **Praveen Jakkannavar**[2]

[1,2]*Department of Mathematics, Karnatak University, Dharwad - 580 003, Karnataka, India*

ABSTRACT:
The mean isomer degeneracy d of a topological index decide its isomer discriminating power, the isomer discriminating power is high if $d = 1$ and the larger the d, the smaller is the isomer discriminating power. Bearing this in mind, we introduce new degree-based topological indices called Kulli-Basava indices and study their mathematical and chemical properties which have good response with the mean isomer degeneracy (i.e., the mean isomer degeneracy of modified first Kulli-Basava index is 1). Further, We obtain closed formulae for Kulli-Basava indices of some graph families and establish the relations connecting these new indices with other degree-based topological indices which are already in the literature. In addition, the Kulli-Basava indices of some graph operations are obtained.

AMS subject classification: 05C07, 05C76, 92E10.
Keywords: Kulli-Basava indices; graph operations; topological indices.

1. PRELIMINARIES

Let $G = (V, E)$ be a finite undirected graph with no loops and no multiple edges having V as its vertex set and E as its edge set. Let $|V| = n$ and $|E| = m$. A graph G is said to be r-regular if degree of each vertex in G is equal to r ($r \in Z^+$). The neighbourhood of a vertex $v \in V(G)$ is defined as the set $N_G(v)$ consisting of all vertices u which are adjacent to v in G. The degree of a vertex $v \in V(G)$, denoted by $d_G(v)$ and is defined as $|N_G(v)|$. The neighbourhood degree sum of a vertex $v \in V(G)$ is denoted by $S_G(v)$ and is defined as $S_G(v) = \sum_{u \in N_G(v)} d_G(u)$. The *degree* $d_G(e)$ *of an edge* $e = uv$ of G is given by $d_G(e) = d_G(u) + d_G(v) - 2$. We now define, an *edge neighbourhood of a vertex* $v \in V(G)$ as the set $N_e(v)$ consisting of all edges e which are incident with v and the *edge neighbourhood degree sum of a vertex* $v \in V(G)$ is denoted by $S_e(v)$ (If the graph is not specified then it can be denoted as $S_e(v/G)$) and is defined as $S_e(v) = \sum_{e \in N_e(v)} d_G(e)$.

Topological indices are numerical values associated with the molecular graphs. In mathematical chemistry, these graph invariants are known as molecular descriptors. Topological indices play a vital role in mathematical chemistry specially, in chemical documentation, isomer discrimination, quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) analysis. *Wiener index* is the first topological index used by Wiener [30] in the year 1947, to calculate boiling point of paraffins. There after Gutman and Trinajstić defined *Zagreb indices* in 1972, which now are most popular and have many applications in chemistry. The following indices are useful for proving our results. The *first and second Zagreb indices* of a graph G are defined as follows [12]:

$$M_1(G) = \sum_{v \in V(G)} d_G(v)^2 and M_2(G) = \sum_{uv \in E(G)} d_G(u) \cdot d_G(v),$$

respectively. The *first Zagreb index* [23] can also be expressed as

$$M_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)].$$

In [9], Fath-Tabar defined the *third Zagreb index* as

$$M_3(G) = \sum_{uv \in E(G)} |d_G(u) - d_G(v)|.$$

Another degree-based graph invariant,

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

was encountered in [12]. This index is called "forgotten topological index"[10].
Later, it was Randić [27] who gave most chemically efficient topological index called *Randić index*, which is defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u) \cdot d_G(v)}}.$$

In [26], Shirdel et al. introduced a new version of Zagreb index named *hyper-Zagreb index* which is defined as

$$HM_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]^2.$$

Further, in [31] Gao et al. defined the *second hyper Zagreb index* as

$$HM_2(G) = \sum_{uv \in E(G)} [d_G(u) \cdot d_G(v)]^2.$$

In [21], Li defined the *first general Zagreb index* as

$$M_1^\alpha(G) = \sum_{v \in V(G)} d_G(v)^\alpha,$$

*Corresponding Author: B. Basavanagoud

where $\alpha \in Z^+$.

In [11], Graovac et al. defined *fifth M -Zagreb indices* as

$$M_1G_5(G) = \sum_{uv\in E(G)} [S_G(u) + S_G(v)]$$
$$\text{and } M_2G_5(G) = \sum_{uv\in E(G)} S_G(u) \cdot S_G(v). \quad (1.1)$$

In [18], Kulli defined the *fifth M_3-Zagreb index* as

$$M_3G_5(G) = \sum_{uv\in E(G)} |S_G(u) - S_G(v)|.$$

The *minus F-index* of a graph G is introduced by Kulli in [20], defined as

$$M_iF(G) = \sum_{uv\in E(G)} \left|d_G(u)^2 - d_G(v)^2\right|$$

In [19], Kulli introduced the concept of *Gourava indices* and *coindices* of graphs. The *first* and *second Gourava indices* of a molecular graph G are defined as

$$GO_1(G) = \sum_{uv\in E(G)} [(d_G(u) + d_G(v)) + d_G(u) \cdot d_G(v)]$$

and

$$GO_2(G) = \sum_{uv\in E(G)} (d_G(u) + d_G(v))(d_G(u) \cdot d_G(v)),$$

respectively. Recently in [5], Basavanagoud et al. defined a new topological index called the *first neighbourhood Zagreb index* as

$$NM_1(G) = \sum_{v\in V(G)} S_G(v)^2.$$

Since then the theory of topological indices has been developed into two broad categories namely, distance-based and degree-based topological indices. However, there are numerous degree-based topological indices which are found applicable and employed in QSPR/QSAR analysis. With this point of view, we now proceed to introduce new degree-based topological indices and would name them as *Kulli-Basava indices* which are defined as

$$\text{first Kulli-Basava index:} \quad KB_1(G) = \sum_{uv\in E(G)} \big(S_e(u) + S_e(v)\big), \quad (1.2)$$

$$\text{modified first Kulli-Basava index:} \quad KB_1^*(G) = \sum_{v\in V(G)} S_e(v)^2, \quad (1.3)$$

$$\text{second Kulli-Basava index:} \quad KB_2(G) = \sum_{uv\in E(G)} S_e(u) \cdot S_e(v), \quad (1.4)$$

$$\text{third Kulli-Basava index:} \quad KB_3(G) = \sum_{uv\in E(G)} \big(|S_e(u) - S_e(v)|\big). \quad (1.5)$$

The rest of the paper is organized as follows. In section 2, we obtain explicit formulae for Kulli-Basava indices of some graph families. In section 3, we study the chemical applicability of first Kulli-Basava index and modified first Kulli-Basava index. In section 4, we derive first Kulli-Basava and modified first Kulli-Basava indices of some graph operations.

2. KULLI-BASAVA INDICES OF SOME GRAPH FAMILIES

In this section, we obtain explicit formulae for *Kulli-Basava indices* of various graph families. We denote P_n, C_n, K_n, $K_{a,b}$, $K_{1,b}$ and W_n for a path, a cycle, a complete graph, a complete bipartite graph, a star and a wheel graph, respectively.

Lemma 2.1. *If G is any graph of order n and size m, then*

(i) $S_G(v) \geq d_G(v)$, *equality holds if and only if* $G = nK_1$ *or* $G = nK_2$.

(ii) $\sum_{v\in V(G)} S_G(v) \geq 2m$, *equality holds if and only if* $G = nK_1$ *or* $G = nK_2$.

(iii) $\sum_{v\in V(G)} S_G(v) = M_1(G)$.

(iv) $S_G(v) \leq \Delta(G) \cdot d_G(v)$, *equality holds if and only if G is regular.*

(v) $\sum_{v\in V(G)} S_G(v) \leq 2m\Delta(G)$, *equality holds if and only if G is regular.*

Lemma 2.2. *If G is any graph of order n and size m, then*

(i) $S_e(v) \geq 2d_G(v) - 2$, *equality holds if and only if G is regular.*

(ii) $\sum_{v\in V(G)} S_e(v) \geq 2(2m - n)$, *equality holds if and only if G is regular.*

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(iii) $\sum_{v\in V(G)} S_e(v) = 2(M_1(G) - 2m)$.

(iv) $S_e(v) \leq 2\Delta(G)(d_G(v) - 1)$, *equality holds if and only if G is regular.*

(v) $\sum_{v\in V(G)} S_e(v) \leq 2\Delta(G)(2m - n)$, *equality holds if and only if G is regular.*

Lemma 2.3. *If G is any graph of order n and size m, then*

$$S_e(v) = d_G(v)^2 - 2d_G(v) + S_G(v).$$

Proof. From the definition of $S_e(v)$ of a vertex $v \in V(G)$, we have

$$\begin{aligned} S_e(v) &= \sum_{e\in N_e(v)} d_G(e) \\ &= \sum_{u\in N_G(v)} (d_G(v) + d_G(u) - 2) \\ &= d_G(v)^2 + \sum_{u\in N_G(v)} d_G(u) - 2d_G(v) \\ &= d_G(v)^2 - 2d_G(v) + S_G(v). \end{aligned}$$

□

Theorem 2.4. *If G is an r-regular graph with n vertices, then*

$$\begin{aligned} KB_1(G) &= 4mr(r-1) = \frac{4m(r-1)M_1(G)}{nr}, \\ KB_1^*(G) &= 4nr^2(r-1)^2 = 4(r-1)^2M_1(G), \\ KB_2(G) &= 4mr^2(r-1)^2 = 4(r-1)^2M_2(G), \\ KB_3(G) &= 0 = M_3(G). \end{aligned}$$

Proof. If G is an r-regular graph with n vertices, then for any vertex $v \in V(G)$,

$$S_e(v) = 2r(r-1).$$

Therefore,

$$\begin{aligned} KB_1(G) &= \sum_{uv\in E(G)} \big(S_e(u) + S_e(v)\big) \\ &= \sum_{uv\in E(G)} 4r(r-1) \\ &= 4mr(r-1). \\ KB_1^*(G) &= \sum_{v\in V(G)} S_e(v)^2 \\ &= \sum_{v\in V(G)} (2r(r-1))^2 \\ &= 4nr^2(r-1)^2 \\ &= 4(r-1)^2M_1(G), \text{ as } M_1(G) = nr^2 \text{ for an } r\text{-regular graph.} \\ KB_2(G) &= \sum_{uv\in E(G)} S_e(u)\cdot S_e(v) \\ &= \sum_{uv\in E(G)} 4r^2(r-1)^2 \\ &= 4mr^2(r-1)^2 = 4(r-1)^2M_2(G), \text{ as } M_2(G) = mr^2 \text{ for an } r\text{-regular graph.} \\ KB_3(G) &= \sum_{uv\in E(G)} \big(|S_e(u) - S_e(v)|\big) \\ &= \sum_{uv\in E(G)} (0) \\ &= 0 = M_3(G), \text{ as } M_3(G) = 0, \text{ for an } r\text{-regular graph.} \end{aligned}$$

□

Corollary 2.5. *If C_n is a cycle of order n, then*

$$\begin{aligned} KB_1(C_n) &= 8n = 2M_1(C_n), \\ KB_1^*(C_n) &= 16n = 4M_1(C_n), \\ KB_2(C_n) &= 16n = 4M_2(C_n), \\ KB_3(C_n) &= 0 = M_3(C_n). \end{aligned}$$

Corollary 2.6. *If K_n is a complete graph of order n, then*

$$\begin{aligned} KB_1(K_n) &= 2n(n-1)^2(n-2) = 2(n-2)M_1(K_n), \\ KB_1^*(K_n) &= 4n(n-1)^2(n-2)^2 = 4(n-2)^2M_1(K_n), \\ KB_2(K_n) &= 2n(n-1)^3(n-2)^2 = 4(n-2)^2M_2(K_n), \\ KB_3(K_n) &= 0 = M_3(K_n). \end{aligned}$$

Theorem 2.7. *If P_n is a path with n vertices, then*

$$\begin{aligned} KB_1(P_n) &= \begin{cases} 0 & \textit{if } n = 2, \\ 2(4n-9) & \textit{otherwise.} \end{cases} \\ KB_1^*(P_n) &= 4(4n-11) = M_1(P_n) + 12n - 38, \ \textit{for} \ \ n \geq 4, \\ KB_2(P_n) &= \begin{cases} 0 & \textit{if } n = 2, \\ 4 & \textit{if } n = 3, \\ 15 & \textit{if } n = 4, \\ 2(8n-25) & \textit{otherwise.} \end{cases} \\ KB_3(P_n) &= \begin{cases} 0 & \textit{if } n = 2, \\ 2 & \textit{if } n = 3, \\ 4 & \textit{if } n = 4, \\ 6 & \textit{otherwise.} \end{cases} \end{aligned}$$

Proof. If P_n is a path with $n \geq 2$ vertices, then there are two pendant vertices with $S_e(v) = \begin{cases} 0 & \text{if } n = 2, \\ 1 & \text{if otherwise,} \end{cases}$ and two vertices are with $S_e(v) = 3$, if $n \geq 4$ and the remaining $n - 4$ vertices are with $S_e(v) = 4$. Therefore, by substituting these values in Eqs. (1.2), (1.3), (1.4) and (1.5), we get the desired results. □

Theorem 2.8. *If $K_{a,b}$ is a complete bipartite graph with $a + b$ vertices and ab edges for $1 \leq a \leq b$ where $a, b \in Z^+$, then*

$$\begin{aligned} KB_1(K_{a,b}) &= ab(a+b)(a+b-2) = (a+b-2)M_1(K_{a,b}), \\ KB_1^*(K_{a,b}) &= ab(a+b)(a+b-2)^2 = (a+b-2)^2M_1(K_{a,b}), \\ KB_2(K_{a,b}) &= a^2b^2(a+b-2)^2 = (a+b-2)^2M_2(K_{a,b}), \\ KB_3(K_{a,b}) &= ab(|a-b|)(a+b-2) = (a+b-2)M_3(K_{a,b}). \end{aligned}$$

Proof. Let $K_{a,b}$ be a complete bipartite graph with $a + b$ vertices. let $V(K_{a,b}) = V_1 \cup V_2$ where $|V_1| = a$ and $|V_2| = b$. For every vertex $v \in V(K_{a,b})$, $S_e(v) = \begin{cases} b(a+b-2) & \text{if } v \in V_1(K_{a,b}), \\ a(a+b-2) & \text{if } v \in V_2(K_{a,b}). \end{cases}$ If $uv \in E(K_{a,b})$, then either $u \in V_1$ and $v \in V_2$ or $v \in V_1$ and $u \in V_2$.

Therefore,

$$\begin{aligned} KB_1(K_{a,b}) &= \sum_{uv \in E(K_{a,b})} \big(S_e(u) + S_e(v)\big) \\ &= \sum_{uv \in E(K_{a,b})} \big(b(a+b-2) + a(a+b-2)\big) \\ &= ab(a+b)(a+b-2). \end{aligned}$$

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$$\begin{aligned}
KB_1^*(K_{a,b}) &= \sum_{v\in V(K_{a,b})} S_e(v)^2 \\
&= \sum_{v\in V_1(K_{a,b})} (b(a+b-2))^2 + \sum_{v\in V_2(K_{a,b})} (a(a+b-2))^2 \\
&= ab(a+b)(a+b-2)^2 \\
&= (a+b-2)^2 M_1(K_{a,b}),\ \text{as } M_1(K_{a,b}) = ab(a+b). \\
KB_2(K_{a,b}) &= \sum_{uv\in E(K_{a,b})} S_e(u)\cdot S_e(v) \\
&= \sum_{uv\in E(K_{a,b})} (b(a+b-2))(a(a+b-2)) \\
&= a^2b^2(a+b-2)^2 = (a+b-2)^2 M_2(G),\ \text{as } M_2(K_{a,b}) = a^2b^2. \\
KB_3(K_{a,b}) &= \sum_{uv\in E(K_{a,b})} \big(|S_e(u) - S_e(v)|\big) \\
&= \sum_{uv\in E(K_{a,b})} |b(a+b-2) - a(a+b-2)| \\
&= ab(|a-b|)(a+b-2) = (a+b-2)M_3(K_{a,b}) \text{ as } M_3(K_{a,b}) = ab(|a-b|).
\end{aligned}$$

□

Corollary 2.9. *If $K_{1,b}$ is a star graph with $b \geq 2$, then*

$$\begin{aligned}
KB_1(K_{1,b}) &= b(b^2-1), \\
KB_1^*(K_{1,b}) &= b(b+1)(b-1)^2, \\
KB_2(K_{1,b}) &= b^2(b-1)^2, \\
KB_3(K_{1,b}) &= b(b-1)^2.
\end{aligned}$$

Corollary 2.10. *If $K_{a,a}$ is a complete bipartite graph, then*

$$\begin{aligned}
KB_1(K_{a,a}) &= 4a^3(a-1), \\
KB_1^*(K_{a,a}) &= 8a^3(a-1)^2, \\
KB_2(K_{a,a}) &= 4a^4(a-1)^2, \\
KB_3(K_{a,a}) &= 0.
\end{aligned}$$

Theorem 2.11. *If W_n is a wheel graph with $n+1$ vertices and $2n$ edges, then*

$$\begin{aligned}
KB_1(W_n) &= n(n^2+4n+27), \\
KB_1^*(W_n) &= n(n+9)^2 + n^2(n+1)^2, \\
KB_2(W_n) &= n(n+9)(n^2+2n+9), \\
KB_3(W_n) &= n(|n^2-9|).
\end{aligned}$$

Proof. Let W_n be a wheel graph with $n+1$ vertices and $2n$ edges. For every vertex $v \in V(W_n)$, $S_e(v) = \begin{cases} n(n+1) & \text{if } v \text{ is a central vertex,} \\ n+9 & \text{otherwise.} \end{cases}$
Therefore, by substituting these values in Eqs. (1.2), (1.3), (1.4) and (1.5), we get the desired results. □

In the following theorem, Kulli-Basava indices are expressed in terms of other topological indices which are already in the literature.

Theorem 2.12. *If G is a graph with n vertices and m edges, then*

$$\begin{aligned}
KB_1(G) &= F(G) - 2M_1(G) + M_1G_5(G), \\
KB_1^*(G) &= M_1^4(G) + 4M_1(G) - 4F(G) + NM_1(G) - 8M_2(G) + 2GO_2(G), \\
KB_2(G) &= HM_2(G) + 4M_2(G) + M_2G_5(G) + M_1^4(G) - 2NM_1(G) - 2F(G) + 4GO_2(G), \\
KB_3(G) &\leq M_3G_5(G) - 2M_3(G) + M_iF(G).
\end{aligned}$$

Proof. By definition of first Kulli-Basava index, we have

$$\begin{aligned}
KB_1(G) &= \sum_{uv\in E(G)} (S_e(u) + S_e(v)) \\
&= \sum_{uv\in E(G)} (d_G(u)^2 - 2d_G(u) + S_G(u) + d_G(v)^2 - 2d_G(v) + S_G(v)) \\
&= \sum_{uv\in E(G)} (d_G(u)^2 + d_G(v)^2) - 2\sum_{uv\in E(G)} (d_G(u) + d_G(v)) + \sum_{uv\in E(G)} (S_G(u) + S_G(v)) \\
&= F(G) - 2M_1(G) + M_1G_5(G).
\end{aligned}$$

By definition of modified first Kulli-Basava index, we have

$$\begin{aligned}
KB_1^*(G) &= \sum_{v\in V(G)} S_e(v)^2 \\
&= \sum_{v\in V(G)} (d_G(v)^2 - 2d_G(v) + S_G(v))^2 \\
&= \sum_{v\in V(G)} d_G(v)^4 + 4\sum_{v\in V(G)} d_G(v)^2 - 4\sum_{v\in V(G)} d_G(v)^4 + 4\sum_{v\in V(G)} d_G(v)^3 + \sum_{v\in V(G)} S_G(v)^2 \\
&\quad +2\sum_{v\in V(G)} d_G(v)^2 S_G(v) - 4\sum_{v\in V(G)} d_G(v)S_G(v) \\
&= M_1^4(G) + 4M_1(G) - 4F(G) + NM_1(G) - 8M_2(G) + 2GO_2(G).
\end{aligned}$$

By definition of second Kulli-Basava index, we have

$$\begin{aligned}
KB_2(G) &= \sum_{uv\in E(G)} (S_e(u)S_e(v)) \\
&= \sum_{uv\in E(G)} (d_G(u)^2 - 2d_G(u) + S_G(u))(d_G(v)^2 - 2d_G(v) + S_G(v)) \\
&= \sum_{uv\in E(G)} (d_G(u)d_G(v))^2 + 4\sum_{uv\in E(G)} d_G(u)d_G(v) + \sum_{uv\in E(G)} S_G(v)S_G(u) \\
&\quad -2\sum_{uv\in E(G)} (d_G(u)S_G(v) + d_G(v)S_G(u)) - 2\sum_{uv\in E(G)} (d_G(u)^2 d_G(v) + d_G(v)^2 d_G(u)) \\
&\quad + \sum_{uv\in E(G)} (d_G(u)^2 S_G(v) + d_G(v)^2 S_G(u)) \\
&= HM_2(G) + 4M_2(G) + M_2G_5(G) + M_1^4(G) - 2NM_1(G) - 2F(G) + 4GO_2(G).
\end{aligned}$$

By definition of third Kulli-Basava index, we have

$$\begin{aligned}
KB_3(G) &= \sum_{uv\in E(G)} |S_e(u) - S_e(v)| \\
&= \sum_{uv\in E(G)} |d_G(u)^2 - 2d_G(u) + S_G(u) - d_G(v)^2 + 2d_G(v) - S_G(v)| \\
&\leq \sum_{uv\in E(G)} |d_G(u)^2 - d_G(v)^2| - 2\sum_{uv\in E(G)} |d_G(u) - d_G(v)| + \sum_{uv\in E(G)} |S_G(u) - S_G(v)| \\
&= M_iF(G) - 2M_3(G) + M_3G_5(G).
\end{aligned}$$

□

3. ON CHEMICAL APPLICABILITY OF THE FIRST AND MODIFIED FIRST KULLI-BASAVA INDICES

The topological indices with the higher correlation factor are of foremost important in quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) analysis. In this section, we discuss the linear regression analysis of first and modified first Kulli-Basava indices with entropy(S), acentric factor(AcentFac), enthalpy of vaporization (HVAP) and

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standard enthalpy of vaporization (DHVAP) of octane isomers on the degree-based topological indices of the corresponding molecular graph. The first and modified first Kulli-Basava indices were tested using a dataset of octane isomers found at http://www.moleculardiscriptors.eu/dataset.htm. The dataset of octane isomers(columns 1-5 of Table 2) are taken from above web link whereas last two column of Table 2 are computed by definition of first and modified first Kulli-Basava indices, respectively. Here, the correlation between acentric factor(AcentFac) and first Kulli-Basava index is **-0.97738** (See Fig. 1), between entropy and first Kulli-Basava index is **-0.95621** (See Fig. 2). Also, the correlation between acentric factor(AcentFac) and modified first Kulli-Basava index is **-0.96462** (See Fig. 5), between entropy and modified first Kulli-Basava index is **-0.94764** (See Fig. 6).

A major drawback of most of the topological indices is their degeneracy, i.e., two or more isomers posses the same topological index. But modified first Kulli-Basava index exceptional for octane isomers. Bonchev et al. [6] defined the mean isomer degeneracy as:

$$d = \frac{n}{t} \ ,$$

where n and t are the number of isomers considered and the number of distinct values that the index assumes for these isomers, respectively. Here, minimum value of d is 1. As the value of $'d'$ increases the isomer-discrimination power of the topological indices decreases. Thus, d can decide the discriminating power of an index. For octane isomers modified first Kulli-Basava index exhibits good response ($d = 1$).

Table 1: Mean isomer degeneracy (d) of different indices for octane isomers.

Index	**Mean isomer degeneracy (d)**
First Zagreb index (M_1)	3.000
Second Zagreb index (M_2)	1.286
Forgotten topological index (F)	2.571
Hosoya index (Z)	1.286
Connectivity index (χ)	1.125
Harary index (η)	1.059
First Kulli-Basava index (KB_1)	**1.125**
Modified first Kulli-Basava index (KB_1^*)	**1.000**

Table 2: Experimental values of the entropy, acentric factor, HVAP, DHVAP and the corresponding value of first and modified first Kulli-Basava indices of octane isomers.

Alkane	**S**	**AcentFac**	**DHVAP**	**HVAP**	KB_1	KB_1^*
n-octane	111.67	0.397898	9.915	73.19	46	84
2-methyl-heptane	109.84	0.377916	9.484	70.3	58	124
3-methyl-heptane	111.26	0.371002	9.521	71.3	60	136
4-methyl-heptane	109.32	0.371504	9.483	70.91	60	138
3-ethyl-hexane	109.43	0.362472	9.476	71.7	62	150
2,2-dimethyl-hexane	103.42	0.339426	8.915	67.7	88	258
2,3-dimethyl-hexane	108.02	0.348247	9.272	70.2	74	192
2,4-dimethyl-hexane	106.98	0.344223	9.029	68.5	72	178
2,5-dimethyl-hexane	105.72	0.35683	9.051	68.6	70	164
3,3-dimethyl-hexane	104.74	0.322596	8.973	68.5	92	286
3,4-dimethyl-hexane	106.59	0.340345	9.316	70.2	76	204
2-methyl-3-ethyl-pentane	106.06	0.332433	9.209	69.7	76	206
3-methyl-3-ethyl-pentane	101.48	0.306899	9.081	69.3	96	312
2,2,3-trimethyl-pentane	101.31	0.300816	8.826	67.3	106	344
2,2,4-trimethyl-pentane	104.09	0.30537	8.402	64.87	100	302
2,3,3-trimethyl-pentane	102.06	0.293177	8.897	68.1	105	341
2,3,4-trimethyl-pentane	102.39	0.317422	9.014	68.37	82	212
2,2,3,3-tetramethylbutane	93.06	0.255294	8.41	66.2	138	504

The linear regression models for the entropy, acentric factor, HVAP, and DHVAP using the data of Table 2 are obtained using the least squares fitting procedure as implemented in R software [28]. The fitted models for KB_1 are:

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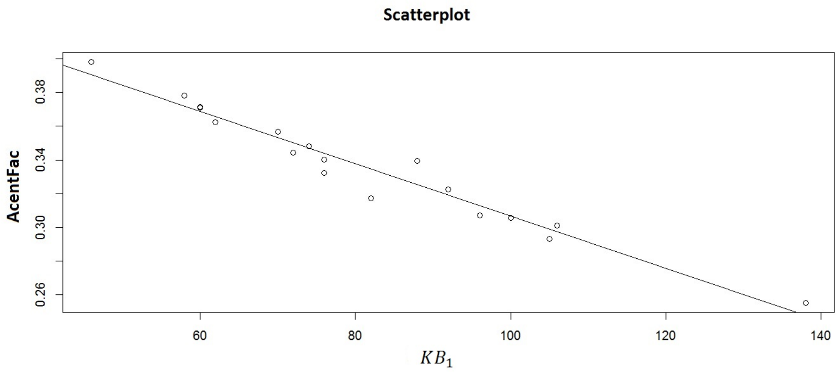


Figure 1: Scatter diagram of $AcentFac$ on KB_1 super imposed by the fitted regression line.

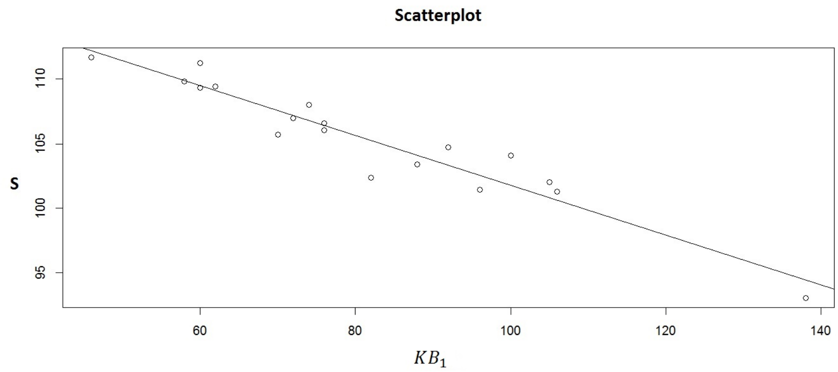


Figure 2: Scatter diagram of S on KB_1 super imposed by the fitted regression line.

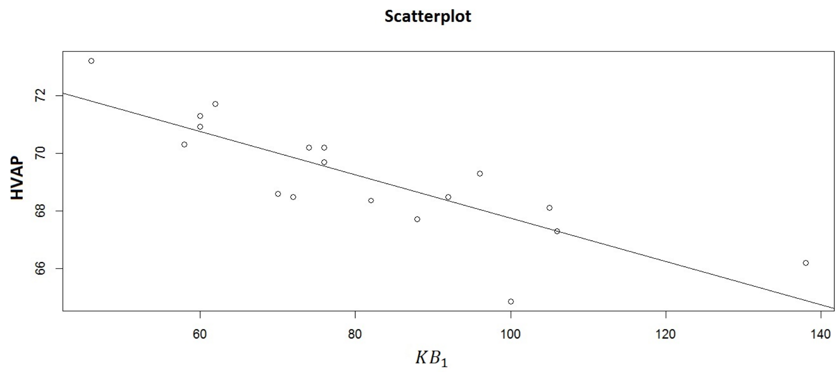


Figure 3: Scatter diagram of $HVAP$ on KB_1 super imposed by the fitted regression line.

$$\hat{AcentFac} = 0.4615054(\pm 0.0070412) - 0.0015491(\pm 0.0000838)KB_1 \quad (3.1)$$
$$\hat{S} = 121.08930(\pm 1.24186) - 0.19313(\pm 0.01478)KB_1 \quad (3.2)$$
$$\hat{HVAP} = 75.25859(\pm 1.06449) - 0.07510(\pm 0.01267)KB_1 \quad (3.3)$$
$$\hat{DHVAP} = 10.371745(\pm 0.160347) - 0.015344(\pm 0.001908)KB_1. \quad (3.4)$$

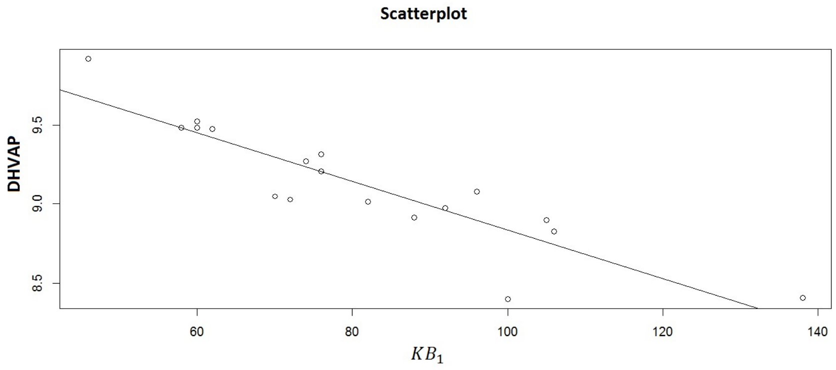


Figure 4: Scatter diagram of $DHVAP$ on KB_1 super imposed by the fitted regression line.

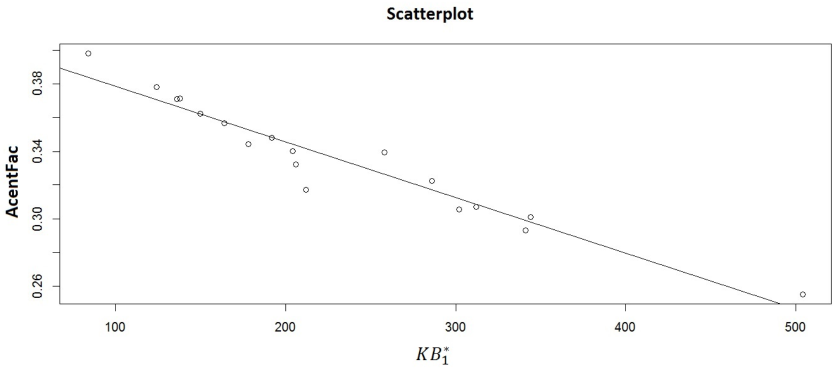


Figure 5: Scatter diagram of $AcentFac$ on KB_1^* super imposed by the fitted regression line.

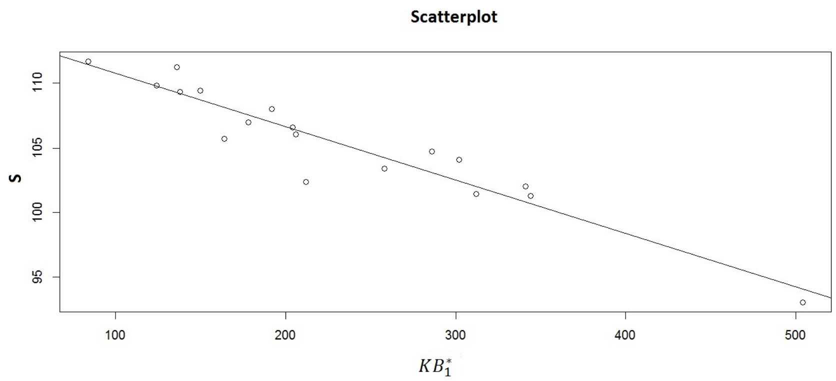


Figure 6: Scatter diagram of S on KB_1^* super imposed by the fitted regression line.

The fitted models for KB_1^* are:

$$\widehat{AcentFac} = 4.116e-01(\pm 5.655e-03) - 3.300e-04(\pm 2.255e-05)KB_1^* \quad (3.5)$$
$$\hat{S} = 114.90369(\pm 0.87298) - 0.04131(\pm 0.00348)KB_1^* \quad (3.6)$$
$$H\hat{V}AP = 72.667417(\pm 0.767163) - 0.015254(\pm 0.003059)KB_1^* \quad (3.7)$$
$$DH\hat{V}AP = 9.8532852(\pm 0.1201055) - 0.0031645(\pm 0.0004788)KB_1^* \quad (3.8)$$

Note: The values in brackets of the Eqs. (3.1) to (3.8) are the corresponding standard errors of the regression coefficients. The index is better as $|r|$ approaches 1. From Table 3, we can observe that KB_1 correlates highly with Acentric Factor and the correlation coefficient $|r| = 0.9773818$. Also KB_1 has good correlation ($|r| > 0.9$) with entropy, acentric factor and ($|r| > 0.8$) with HVAP, DHVAP. From Table 4, we can observe that KB_1^* correlates highly with Acentric Factor and the correlation coefficient

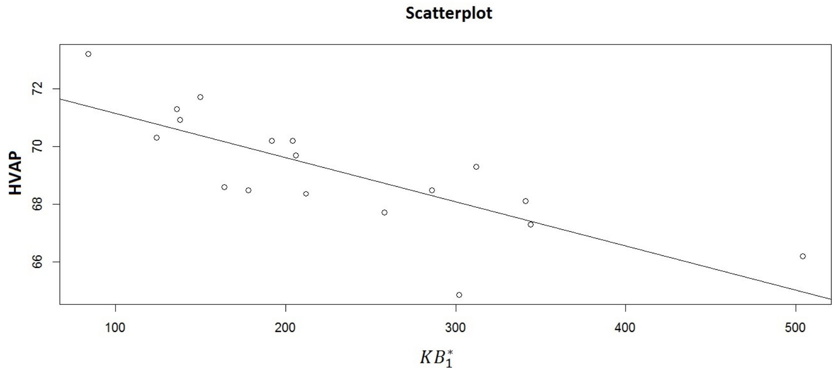


Figure 7: Scatter diagram of $HVAP$ on KB_1^* super imposed by the fitted regression line.

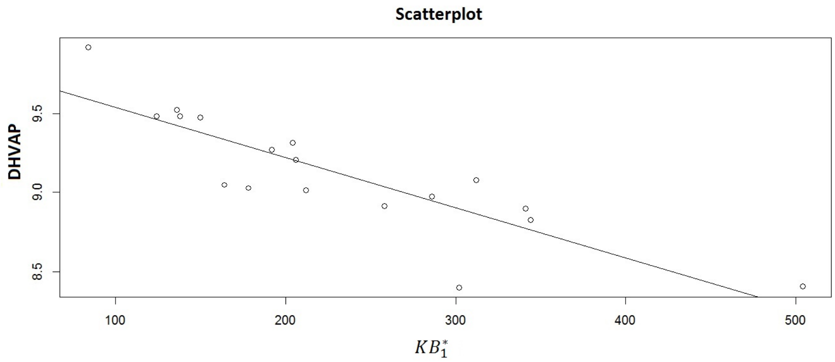


Figure 8: Scatter diagram of $DHVAP$ on KB_1^* super imposed by the fitted regression line.

Table 3: Correlation coefficient and residual standard error of regression models for KB_1

Physical Property	Absolute value of the correlation coefficient ($\|r\|$)	Residual standard error
Acentric Factor	0.9773818	0.007728
Entropy	0.956207	1.363
HVAP	0.8289296	1.168
DHVAP	0.8953306	0.176

Table 4: Correlation coefficient and residual standard error of regression models for KB_1^*

Physical Property	Absolute value of the correlation coefficient ($\|r\|$)	Residual standard error
Acentric Factor	0.9646228	0.009633
Entropy	0.9476403	1.487
HVAP	0.7800876	1.307
DHVAP	0.8554989	0.2046

$|r| = 0.9646228$. Also KB_1^* has good correlation ($|r| > 0.9$) with entropy, acentric factor and ($|r| > 0.75$) with HVAP, DHVAP.

In the following section, we study the *first Kulli-Basava and modified first Kulli-Basava indices* of some graph operations such as cartesian product, composition, tensor product and corona of graphs, since the mean isomer degeneracy of these indices have good response.

4. FIRST KULLI-BASAVA AND MODIFIED FIRST KULLI-BASAVA INDICES OF SOME GRAPH OPERATIONS

Graph operations play an important role as some important graphs can be obtained by simple graph operations. For example, C_4-nanotorus, C_4-nanotube, planar grids, n-prism and Rook's graph are obtained by cartesian product of $C_m \times C_n$, $P_m \times C_n$, $P_n \times P_m$, $K_2 \times C_m$ and $K_n \times K_m$, respectively. Fence graph, closed fence graph and Catlin graph are obtained by composition of graphs. For more on graph operations we refer Imrich and Klavažar [15].

There are several papers devoted to topological indices of graph operations. To mention few, Khalifeh et al., obtained first and second Zagreb index of graph operations in [17], Aktaret al., obtained F-index in [1], Basavanagoud et al., obtained hyper-Zagreb index in [4, 3], N. De et al., obtained F-coindex in [7], Fath-Tabar derived GA_2 index in [8], Nadjafi-Arani et al., obtained degree distance based topological indices of tensor product of graphs in [22], Paulraj et al., computed degree distance of product graphs in [25], Yarahmadi et al., computed Szeged, vertex PI, first and second Zagreb indices of corona product of graphs in [32]. For some other topological indices of graph operations on can refer [16, 32] and references cited there in. At this stage, we evaluate *first Kulli-Basava and modified first Kulli-Basava indices* of some graph operations.

Definition 1. *The product [14] $G \times H$ of graphs G and H has the vertex set $V(G \times H) = V(G) \times V(H)$ and $(a, x)(b, y)$ is an edge of $G \times H$ if and only if [$a = b$ and $xy \in E(H)$] or [$x = y$ and $ab \in E(G)$].*

Lemma 4.1. *If G_1 and G_2 are two graphs of order n_1 and n_2 and size m_1 and m_2, respectively, then we have*

$$S_e((u,v)/G_1 \times G_2) = S_e(u/G_1) + S_e(v/G_2) + 4d_{G_1}(u)d_{G_2}(v)$$

Proof. By Lemma 2.3, we have

$$\begin{aligned} S_e((u,v)/G_1 \times G_2) &= d_{G_1\times G_2}(u,v)^2 - 2d_{G_1\times G_2}(u,v) + S_{G_1\times G_2}(u,v) \\ &= (d_{G_1}(u) + d_{G_2}(v))^2 - 2(d_{G_1}(u) + d_{G_2}(v)) + S_{G_1}(u) + S_{G_2}(v) + 2d_{G_1}(u)d_{G_2}(v) \\ &= S_e(u/G_1) + S_e(v/G_2) + 4d_{G_1}(u)d_{G_2}(v). \end{aligned}$$

□

Theorem 4.2. *If G_1 and G_2 are two graphs of order n_1, n_2 and size m_1, m_2 respectively, then the first Kulli-Basava index of $G_1 \times G_2$ is given by*

$$KB_1(G_1 \times G_2) = (n_2 + 8m_2)KB_1(G_1) + (n_1 + 8m_1)KB_1(G_2) + 4(m_2M_1(G_1) + m_1M_1(G_2)) - 16m_1m_2.$$

Proof. By definition,

$$KB_1(G_1 \times G_2) = \sum_{(a,x)(b,y)\in E(G_1\times G_2)} (S_e((a,x)/G_1 \times G_2) + S_e((b,y)/G_1 \times G_2))$$

Using Lemma 4.1 we get,

$$\begin{aligned} &= \sum_{a\in V(G_1)} \sum_{xy\in E(G_2)} \big(S_e(a/G_1) + S_e(x/G_2) + 4d_{G_1}(a)d_{G_2}(x) + S_e(a/G_1) + S_e(y/G_2) + 4d_{G_1}(a)d_{G_2}(y)\big) \\ &\quad + \sum_{x\in V(G_2)} \sum_{ab\in E(G_1)} \big(S_e(x/G_2) + S_e(a/G_1) + 4d_{G_1}(a)d_{G_2}(x) + S_e(x/G_2) + S_e(b/G_1) + 4d_{G_1}(b)d_{G_2}(x)\big) \\ &= 4m_2(M_1(G_1) - 2m_1) + n_1KB_1(G_2) + 8m_1KB_1(G_2) + 4m_1(M_1(G_2) - 2m_2) + n_2KB_1(G_1) \\ &\quad +8m_2KB_1(G_1). \end{aligned}$$

□

Theorem 4.3. *If G_1 and G_2 are two graphs of order n_1, n_2 and size m_1, m_2 respectively, then modified first Kulli-Basava index of $G_1 \times G_2$ is given by*

$$\begin{aligned} KB_1^*(G_1 \times G_2) &= n_2KB_1^*(G_1) + n_1KB_1^*(G_2) + 8(M_1(G_1) - 2m_1)(M_1(G_2) - 2m_2) + 16M_1(G_1)M_1(G_2) \\ &\quad +16m_2F(G_1) + 16m_1F(G_2) - 32m_2M_1(G_1) - 32m_1M_1(G_2) + 32m_2M_2(G_1) \\ &\quad +32m_1M_2(G_2). \end{aligned}$$

Proof. By definition, $KB_1^*(G_1 \times G_2) = \sum_{(u,v)\in V(G_1\times G_2)} S_e((u,v)/G_1 \times G_2)^2$

Using Lemma 4.1 we get,

$$\begin{aligned} &= \sum_{(u,v)\in V(G_1\times G_2)} \big(S_e(u/G_1) + S_e(v/G_2) + 4d_{G_1}(u)d_{G_2}(v)\big)^2 \\ &+ \sum_{u\in V(G_1)} \sum_{v\in V(G_2)} \big(S_e(u/G_1)^2 + S_e(v/G_2)^2 + 2S_e(u/G_1)S_e(v/G_2) + 16d_{G_1}(u)^2 d_{G_2}(v)^2 \\ &+8(S_e(u/G_1) + S_e(v/G_2))d_{G_1}(u)d_{G_2}(v)\big) \\ &= n_2KB_1^*(G_1) + n_1KB_1^*(G_2) + 8(M_1(G_1) - 2m_1)(M_1(G_2) - 2m_2) + 16M_1(G_1)M_1(G_2) \\ &+16m_2F(G_1) + 16m_1F(G_2) - 32m_2M_1(G_1) - 32m_1M_1(G_2) + 32m_2M_2(G_1) \\ &+32m_1M_2(G_2). \end{aligned}$$

□

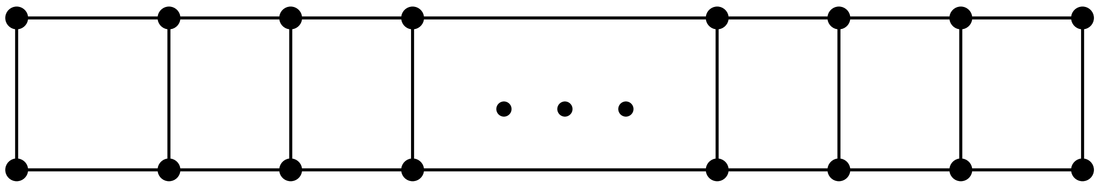


Figure 9: The Ladder graph L_n.

Corollary 4.4. *The ladder graph L_n is defined as the cartesian product of P_2 and P_n. From Theorem 4.3, we derive the following results.*

$$KB_1(L_n) = 4(22n - 49),$$
$$KB_1^*(L_n) = 8(36n - 71).$$

Corollary 4.5. *For a C_4-nanotorus, $TC_4(m, n) = C_m \times C_n$, the first Kulli-Basava and modified first Kulli-Basava indices are given by*

$$KB_1(TC_4(m, n)) = 160mn,$$
$$KB_1^*(TC_4(m, n)) = 576mn.$$

Corollary 4.6. *The cartesian product of P_n and C_m yields a C_4-nanotube, $TUC_4(m, n) = P_n \times C_m$. Its first Kulli-Basava and modified first Kulli-Basava indices are given by*

$$KB_1(TUC_4(m, n)) = 10m(16n - 25),$$
$$KB_1^*(TUC_4(m, n)) = 4m(144n - 227).$$

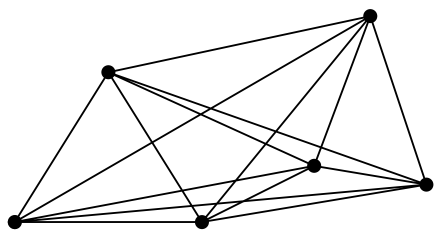
Corollary 4.7. *The first Kulli-Basava and modified first Kulli-Basava indices of planar grid $P_n \times P_m$ are given by*

$$KB_1(P_n \times P_m) = 2(88mn - 125m - 125n + 160),$$
$$KB_1^*(P_n \times P_m) = 4(144mn - 227m - 227n + 320).$$

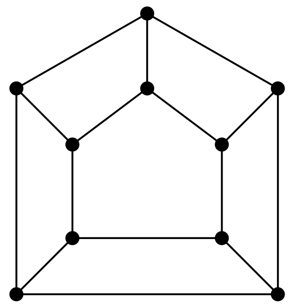
Corollary 4.8. *For a n-prism, $K_2 \times C_n$, the first Kulli-Basava and modified first Kulli-Basava indices are given by*

$$KB_1(K_2 \times C_n) = 18n^2(n - 1)^2(n - 2) + 88n.$$
$$KB_1^*(K_2 \times C_n) = 288n.$$

Corollary 4.9. *The cartesian product of K_n and K_m yields the Rook's graph. Its first Kulli-Basava and modified first Kulli-Basava indices are given by*
$KB_1(K_n \times K_m) = 2mn((n-1)^2(n-2)(4m-3) + (m-1)^2(m-2)(4n-3))$
$+2mn(m-1)(n-1)(n+m-4)$.
$KB_1^*(K_n \times K_m) = 4mn((n-1)^2(n-2)^2 + (m-1)^2(m-2)^2)$
$+8mn(m-1)(n-1)(2m^2+2n^2+3mn-10m-10n+14)$.



$K_3 \times K_2$



$K_2 \times C_5$

Figure 10: The example of Rook's graph ($K_3 \times K_2$) and $n-$Prism graph ($n = 5$)

Definition 2. *The composition [14] $G[H]$ of graphs G and H with disjoint vertex sets $V(G)$ and $V(H)$ and edge sets $E(G)$ and $E(H)$ is the graph with vertex set $V(G[H]) = V(G) \times V(H)$ and $(a, x)(b, y)$ is an edge of $G[H]$ if and only if [a is adjacent to b] or [$a = b$ and x is adjacent to y].*

Lemma 4.10. *If G_1 and G_2 are two graphs of order n_1 and n_2 and size m_1 and m_2, respectively, then we have*

$$\begin{aligned} S_e((u,v)/G_1[G_2]) &= n_2 S_e(u/G_1) + S_e(v/G_2) + (n_2^2 - n_2)(d_{G_1}(u)^2 + S_{G_1}(u)) + 2(m_2 - n_2)d_{G_1}(u) \\ &\quad +3n_2 d_{G_1}(u) d_{G_2}(v). \end{aligned}$$

Proof. By Lemma 2.3, we have

$$\begin{aligned} S_e((u,v)/G_1[G_2]) &= d_{G_1[G_2]}(u,v)^2 - 2d_{G_1[G_2]}(u,v) + S_{G_1[G_2]}(u,v) \\ &= (n_2 d_{G_1}(u) + d_{G_2}(v))^2 - 2(d_{G_1}(u) + d_{G_2}(v)) + n_2^2 S_{G_1}(u) + S_{G_2}(v) + 2m_2 d_{G_1}(u) \\ &\quad +n_2 d_{G_1}(u) d_{G_2}(v) \\ &= n_2 S_e(u/G_1) + S_e(v/G_2) + (n_2^2 - n_2)(d_{G_1}(u)^2 + S_{G_1}(u)) + 2(m_2 - n_2)d_{G_1}(u) \\ &\quad +3n_2 d_{G_1}(u) d_{G_2}(v). \end{aligned}$$

□

Theorem 4.11. *If G_1 and G_2 are two graphs of order n_1, n_2 and size m_1, m_2 respectively, then the first Kulli-Basava index of $G_1[G_2]$ is given by*

$$\begin{aligned} KB_1(G_1[G_2]) &= n_2^3 KB_1(G_1) + (n_1 + 6m_1n_2)KB_1(G_2) + n_2^3(n_2 - n_1)F(G_1) + n_2^3(n_2 - n_1)M_1G_5(G_1) \\ &\quad +2n_2(5m_2n_2 - n_2^2 + m_2)M_1(G_1) + 4m_1n_2M_1(G_2) + 4m_1m_2(n_2^2 - 7n_2 + 2m_2). \end{aligned}$$

Proof. By definition, $KB_1(G_1[G_2]) = \sum_{(a,x)(b,y)\in E(G_1[G_2])} (S_e((a,x)/G_1[G_2]) + S_e((a,x)/G_1[G_2]))$

Using Lemma 4.10 we get,

$$\begin{aligned}
&= \sum_{x\in V(G_2)}\sum_{y\in V(G_2)}\sum_{ab\in E(G_1)} \big((n_2^2-n_2)(d_{G_1}(a)^2+S_{G_1}(a))+n_2S_e(a/G_1)+S_e(x/G_2)+2(m_2-n_2)d_{G_1}(a)\\
&\quad +3n_2d_{G_1}(a)d_{G_2}(x)+(n_2^2-n_2)(d_{G_1}(b)^2+S_{G_1}(b))+n_2S_e(b/G_1)+S_e(y/G_2)+2(m_2-n_2)d_{G_1}(b)\\
&\quad +3n_2d_{G_1}(b)d_{G_2}(y)\big)\\
&\quad + \sum_{a\in V(G_1)}\sum_{xy\in E(G_2)} \big((n_2^2-n_2)(d_{G_1}(a)^2+S_{G_1}(a))+n_2S_e(a/G_1)+S_e(x/G_2)+2(m_2-n_2)d_{G_1}(a)\\
&\quad +3n_2d_{G_1}(a)d_{G_2}(x)+(n_2^2-n_2)(d_{G_1}(a)^2+S_{G_1}(a))+n_2S_e(a/G_1)+S_e(y/G_2)+2(m_2-n_2)d_{G_1}(a)\\
&\quad +3n_2d_{G_1}(a)d_{G_2}(y)\big).
\end{aligned}$$

Solving these summations one can get the desired result. □

Theorem 4.12. *If G_1 and G_2 are two graphs of order n_1, n_2 and size m_1, m_2 respectively, then modified first Kulli-Basava index of $G_1[G_2]$ is given by*

$$\begin{aligned}
KB_1^*(G_1[G_2]) &= n_2^2KB_1^*(G_1)+KB_1^*(G_2)+(n_2^4+n_2^3-2n_2^2)M_1^4(G_1)+(n_2^4+n_2^3-2n_2^2)NM_1(G_1)\\
&\quad +2n_2^2(n_2^2-1)GO_2(G_1)+(28m_2^2n_2-64m_2n_2^2-16m_2n_2+4n_2^3+8n_2^2)M_1(G_1)\\
&\quad +16m_1(m_2-2n_2)M_1(G_2)+(12m_2n_2^3+20m_2n_2^2-16n_2^3+8n_2^2)M_2(G_1)\\
&\quad +24m_1n_2M_2(G_2)+n_2(13n_2+4)M_1(G_1)M_1(G_2)\\
&\quad +(16m_2n_2^3-4m_2n_2^2+4m_2n_2-4n_2^4)F(G_1)+64m_1m_2n_2-32m_1m_2^2.
\end{aligned}$$

Proof. By definition, $KB_1^*(G_1[G_2]) = \sum_{(u,v)\in V(G_1[G_2])} S_e((u,v)/G_1[G_2])^2$

Using Lemma 4.10 we get,

$$\begin{aligned}
&= \sum_{(u,v)\in V(G_1[G_2])} \big(n_2S_e(u/G_1)+S_e(v/G_2)+(n_2^2-n_2)(d_{G_1}(u)^2+S_{G_1}(u))+2(m_2-n_2)d_{G_1}(u)\\
&\quad +3n_2d_{G_1}(u)d_{G_2}(v)\big)^2.
\end{aligned}$$

Solving this summation one can get the desired result. □

Definition 3. *The corona [14] $G_1\circ G_2$ of two graphs G_1 and G_2 of order n_1 and n_2 respectively, is defined as the graph obtained by taking one copy of G_1 and n_1 copies of G_2 and then joining the i^{th} vertex of G_1 to every vertex in the i^{th} copy of G_2.*

Lemma 4.13. *If G_1 and G_2 are two graphs of order n_1 and n_2 and size m_1 and m_2, respectively, then we have*

$$S_e(v/G_1\circ G_2)=\begin{cases} S_e(v/G_1)+n_2^2+2n_2d_{G_1}(v)+2m_2 & \text{if } v\in V(G_1),\\ S_e(v/G_2)+3d_{G_2}(v)+d_{G_1}(v_i)+n_2-1 & \text{if } v\in V(G_2), v_i\in V(G_1).\end{cases}$$

Proof. By Lemma 2.3, we have $S_e(v/G_1\circ G_2)=d_{G_1\circ G_2}(v)^2-2d_{G_1\circ G_2}(v)+S_{G_1\circ G_2}(v)$

$$\begin{aligned}
&= \begin{cases} (d_{G_1}(v)+n_2)^2-2(d_{G_1}(v)+n_2)+S_{G_1}(v)+2(n_2+m_2) & \text{if } v\in V(G_1)\\ (d_{G_2}(v)+1)^2-2(d_{G_1}(v)+1)+S_{G_2}(v)+d_{G_2}(v)+d_{G_1}(v_i)+n_2 & \text{if } v\in V(G_2), v_i\in V(G_1)\end{cases}\\
&= \begin{cases} S_e(v/G_1)+n_2^2+2n_2d_{G_1}(v)+2m_2 & \text{if } v\in V(G_1)\\ S_e(v/G_2)+3d_{G_2}(v)+d_{G_1}(v_i)+n_2-1 & \text{if } v\in V(G_2), v_i\in V(G_1).\end{cases}
\end{aligned}$$

□

Theorem 4.14. *If G_1 and G_2 are two graphs of order n_1, n_2 and size m_1, m_2 respectively, then the first Kulli-Basava index of $G_1\circ G_2$ is given by*

$$\begin{aligned}
KB_1(G_1\circ G_2) &= KB_1(G_1)+n_1KB_1(G_2)+4n_2M_1(G_1)+5n_1M_1(G_2)\\
&\quad +8m_1m_2+2m_1n_2(3n_2-1)+2n_1m_2(3n_2-1)+n_1n_2(n_2^2+n_2-1).
\end{aligned}$$

Proof. By definition, $KB_1(G_1 \circ G_2) = \sum_{uv \in E(G_1 \circ G_2)} (S_e(u/G_1 \circ G_2) + S_e(v/G_1 \circ G_2))$

Using Lemma 4.13 we get,

$$\begin{aligned} &= \sum_{uv \in E(G_1)} \big(S_e(u/G_1) + n_2^2 + 2n_2 d_{G_1}(u) + 2m_2 + S_e(v/G_1) + n_2^2 + 2n_2 d_{G_1}(v) + 2m_2\big) \\ &\quad + \sum_{uv \in E(G_1)} \sum_{v_i \in V(G_1)} \big(S_e(u/G_2) + 3d_{G_2}(u) + d_{G_1(v_i)} + n_2 - 1 + S_e(v/G_2) + 3d_{G_2}(v) + d_{G_1(v_i)} + n_2 - 1\big) \\ &\quad + \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} \big(S_e(u/G_1) + n_2^2 + 2n_2 d_{G_1}(u) + 2m_2 + S_e(v/G_2) + 3d_{G_2}(v) + d_{G_1}(u) + n_2 - 1\big). \end{aligned}$$

Solving these summations one can get the desired result. □

Theorem 4.15. *If G_1 and G_2 are two graphs of order n_1, n_2 and size m_1, m_2 respectively, then modified first Kulli-Basava index of $G_1 \circ G_2$ is given by*

$$\begin{aligned} KB_1^*(G_1 \circ G_2) &= KB_1^*(G_1) + n_1 KB_1^*(G_2) + (8n_2^2 - 7n_2 + 8m_2)M_1(G_1) + (9n_1 + 4n_2 + 8m_1 - 16)M_1(G_2) \\ &\quad + 4n_2 F(G_1) + 6F(G_2) + 8n_2 M_2(G_1) + 12M_2(G_2) + (n_1 + 8m_1 n_2)(n_2^2 + 2m_2)^2 \\ &\quad - 8m_1 n_2^2 + 8(3n_2 - 4)m_1 m_2 + n_1 n_2 (n_2 - 1)^2 + 8m_2(n_2 - 1). \end{aligned}$$

Proof. By definition, $KB_1^*(G_1 \circ G_2) = \sum_{v \in V(G_1 \circ G_2)} S_e(v/G_1 \circ G_2)^2$

Using Lemma 4.13 we get,

$$\begin{aligned} &= \sum_{v \in V(G_1 \circ G_2)} \big(S_e(u/G_1) + S_e(v/G_2) + 4d_{G_1}(u) d_{G_2}(v)\big)^2 \\ &= \sum_{v \in V(G_1)} \big(S_e(v/G_1) + n_2^2 + 2n_2 d_{G_1}(v) + 2m_2\big)^2 \\ &\quad + \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} \big(S_e(v/G_2) + 3d_{G_2}(v) + d_{G_1}(u) + n_2 - 1\big)^2 \\ &= KB_1^*(G_1) + n_1 KB_1^*(G_2) + (8n_2^2 - 7n_2 + 8m_2)M_1(G_1) + (9n_1 + 4n_2 + 8m_1 - 16)M_1(G_2) \\ &\quad + 4n_2 F(G_1) + 6F(G_2) + 8n_2 M_2(G_1) + 12M_2(G_2) + (n_1 + 8m_1 n_2)(n_2^2 + 2m_2)^2 \\ &\quad - 8m_1 n_2^2 + 8(3n_2 - 4)m_1 m_2 + n_1 n_2 (n_2 - 1)^2 + 8m_2(n_2 - 1). \end{aligned}$$

□

As an application of Theorem 4.14 and Theorem 4.15, we obtain explicit formulae for *first Kulli-Basava and modified first Kulli-Basava indices* of $k-$ thorny cycle $C_n \circ \overline{K_k}$.

Corollary 4.16. $KB_1(C_n \circ \overline{K_k}) = nk(k^2 + 7k + 13) + 8n$ *and*
$KB_1^*(C_n \circ \overline{K_k}) = n(8k^5 + k^4 + k^3 + 22k^2 + 37k + 16)$.

Definition 4. *The tensor product [29] $G_1 \circledast G_2$ of two graphs G_1 and G_2 of order n_1 and n_2 respectively, is defined as the graph with vertex set $V_1 \times V_2$ and (u_1, v_1) is adjacent with (u_2, v_2) if and only if $u_1 u_2 \in E(G_1)$ and $v_1 v_2 \in E(G_2)$.*

Lemma 4.17. *If G_1 and G_2 are two graphs of order n_1 and n_2 and size m_1 and m_2, respectively, then we have*

$$S_e((u,v)/G_1 \circledast G_2) = S_{G_1}(u) S_{G_2}(v) + d_{G_1}(u)^2 d_{G_2}(v)^2 - 2d_{G_1}(u) d_{G_2}(v).$$

Proof. By Lemma 2.3, we have

$$\begin{aligned} S_e((u,v)/G_1 \circledast G_2) &= d_{G_1 \circledast G_2}(u,v)^2 - 2d_{G_1 \circledast G_2}(u,v) + S_{G_1 \circledast G_2}(u,v) \\ &= d_{G_1}(u)^2 d_{G_2}(v)^2 - 2d_{G_1}(u) d_{G_2}(v) + S_{G_1}(u) S_{G_2}(v). \end{aligned}$$

□

Theorem 4.18. *If G_1 and G_2 are two graphs of order n_1, n_2 and size m_1, m_2 respectively, then the first Kulli-Basava index of $G_1 \circledast G_2$ is given by*

$$KB_1(G_1 \circledast G_2) \quad = \quad F(G_1)F(G_2) - 2M_1(G_1)M_1(G_2) + NM_1(G_2)M_1G_5(G_1).$$

Proof. By definition,

$$KB_1(G_1 \circledast G_2) = \sum_{(a,x)(b,y)\in E(G_1\circledast G_2)} (S_e((a,x)/G_1 \circledast G_2) + S_e((b,y)/G_1 \circledast G_2))$$

Using Lemma 4.17 we get,

$$= \sum_{ab\in E(G_1)} \sum_{xy\in E(G_2)} \big(d_{G_1}(a)^2 d_{G_2}(x)^2 - 2d_{G_1}(a)d_{G_2}(x) + S_{G_1}(a)S_{G_2}(x)$$
$$+d_{G_1}(b)^2 d_{G_2}(y)^2 - 2d_{G_1}(b)d_{G_2}(y) + S_{G_1}(b)S_{G_2}(y)\big).$$

Solving these summations one can get the desired result. □

Theorem 4.19. *If G_1 and G_2 are two graphs of order n_1, n_2 and size m_1, m_2 respectively, then modified first Kulli-Basava index of $G_1 \circledast G_2$ is given by*

$$\begin{aligned} KB_1^*(G_1 \circledast G_2) &= M_1^4(G_1)M_1^4(G_2) + 4M_1(G_1)M_1(G_2) - 4F(G_1)F(G_2) + NM_1(G_1)NM_1(G_2) \\ &\quad +2GO_2(G_1)GO_2(G_2) - 16M_2(G_1)M_2(G_2). \end{aligned}$$

Proof. By definition, $KB_1^*(G_1 \circledast G_2) = \sum_{(u,v)\in V(G_1\circledast G_2)} S_e((u,v)/G_1 \circledast G_2)^2$
Using Lemma 4.17 we get,

$$\begin{aligned} &= \sum_{u\in V(G_1)} \sum_{v\in V(G_2)} \big(S_{G_1}(u)S_{G_2}(v) + d_{G_1}(u)^2 d_{G_2}(v)^2 - 2d_{G_1}(u)d_{G_2}(v)\big)^2 \\ &= \sum_{u\in V(G_1)} \sum_{v\in V(G_2)} \big(S_{G_1}(u)^2 S_{G_2}(v)^2 + (d_{G_1}(u)^2 d_{G_2}(v)^2 - 2d_{G_1}(u)d_{G_2}(v))^2 \\ &\quad +2S_{G_1}(u)S_{G_2}(v)(d_{G_1}(u)^2 d_{G_2}(v)^2 - 2d_{G_1}(u)d_{G_2}(v))\big) \\ &= M_1^4(G_1)M_1^4(G_2) + 4M_1(G_1)M_1(G_2) - 4F(G_1)F(G_2) + NM_1(G_1)NM_1(G_2) \\ &\quad +2GO_2(G_1)GO_2(G_2) - 16M_2(G_1)M_2(G_2). \end{aligned}$$

□

As an application of Theorem 4.18 and Theorem 4.19, we obtain following computations.

Corollary 4.20. *The first Kulli-Basava index of tensor product of different graphs is as follows:*
(i) $KB_1(P_n \circledast P_m) = 8(4n-7)(6m-13) - 8(2n-3)(2m-3), m,n \geq 3.$

(ii) $KB_1(P_n \circledast C_m) = 32m(5n-9), m,n \geq 3.$

(iii) $KB_1(P_n \circledast K_m) = 2m(m-1)^2(4m^2n - 7m^2 - 4mn + 7m - 4n + 6), m,n \geq 3.$

(iv) $KB_1(C_n \circledast C_m) = 160mn, m,n \geq 3.$

(v) $KB_1(C_n \circledast K_m) = 8mn(m-1)^2(m^2 - m - 1), m,n \geq 3.$

(vi) $KB_1(K_n \circledast K_m) = mn(m-1)^2(n-1)^2(2m^2 - 3m - n + mn + 1), m,n \geq 3.$

Corollary 4.21. *The modified first Kulli-Basava index of tensor product of different graphs is as follows:*
(i) $KB_1^*(P_n \circledast P_m) = 4(8m-15)(8n-15) + 16(2m-3)(2n-3) + 16(4m-7)(4n-7)$

$+ 4(8m - 19)(8n - 19) - 256(m - 2)(n - 2), m, n \geq 4.$

(ii) $KB_1^*(P_n \circledast C_m) = 32m(18n - 35), m \geq 3, n \geq 4.$

(iii) $KB_1^*(P_n \circledast K_m) = 4m(m - 1)^2(16m^2n - 31m^2 - 48mn + 92m + 36n - 67),$
$m \geq 3, n \geq 4.$

(iv) $KB_1^*(C_n \circledast C_m) = 576mn, m, n \geq 3.$

(v) $KB_1^*(C_n \circledast K_m) = 16mn(m - 1)^2(4m^2 - 12m + 9), m, n \geq 3.$

(vi) $KB_1^*(K_n \circledast K_m) = 4mn(m - 1)^4(n - 1)^4 + 4mn(m - 1)^2(n - 1)^2$
$- 8mn(m - 1)^3(n - 1)^3, m, n \geq 3.$

Similarly, one can find the expressions for the second and third Kulli-Basava indices of these graph operations.

5. CONCLUSION

In this paper, we proposed a set of new topological indices called Kulli-Basava indices. We have explicitly studied first Kulli-Basava and modified first Kulli-Basava indices of some graph families. Further, we have obtained first Kulli-Basava and modified first Kulli-Basava indices of some graph operations. In addition, we have studied the chemical applicability of these indices. In future, one can derive the results for some other graph operations.

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