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MOLECULAR DESCRIPTORS OF A GENERALIZED KNESER-TYPE BIPARTITE GRAPH

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Abstract. This research paper focuses on the computation and analysis of molecular descriptors or topological indices for a generalised Kneser-type bipartite graph called bipartite Kneser B type-k graph denoted by $H_B(n, k)$. Topological indices are formulae that are obtained from graph connectivity patterns and are used to summarise and compress the data that is included in those patterns. In this study, we systematically compute several well-known degree based topological indices of $H_B(n, k)$. We employ combinatorial methods and graph-theoretic techniques to derive explicit formulas and recursive relations for these indices. These results provide insights into the structural properties of this graph.

1. Introduction

While graph theory produces conclusions with applications in many scientific domains, discrete mathematics provides an engaging environment for understanding proving procedures. Graphs are used in a specialist branch of mathematics called "chemical graph theory" to represent and analyse the properties and structure of chemical substances. The mathematical features of networks, referred to as topological indices or molecular descriptors, are crucial to chemistry. They provide a unique way to connect chemical compound molecular graphs to their associated structural attributes. A molecular graph is a particular type of connected, undirected graph that can be associated with a chemical substance's structural formula. The nodes in this graph stand in for the individual atoms that make up the molecule, and the edges represent the chemical bonds that hold the atoms together. Topological indices are extensively used in QSPR and QSAR studies. Topological indices are crucial for understanding the complex structural laws that govern the properties and behaviours of molecules and networks. Researchers may classify, compare, and predict a wide range of qualities and occurrences with the use of these numerical descriptors, which provide helpful quantitative information about the underlying topology. Topological indices are extensively used in a wide range of domains, such as network analysis, chemistry, materials science, and computational biology. Most of the topological indices are of different types, such as degree-based topological indices, distance-based topological indices, and spectrum-based topological indices.

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Kneser bipartite graphs are significant in the domains of combinatorics and graph theory because they provide deep insights and allow for complex applications in coding theory, optimisation, and algorithm design. They are useful tools for theoretical research and practical issue resolution due to their rich structures and attributes. The connection between classical Kneser graphs and other bipartite graph theories is established through the study of Kneser bipartite graphs.

The vertices of the bipartite Kneser graph and the Kneser graph were introduced as non-empty subsets of a n-element set. When the respective sets in the Kneser graph $K(n,k)$ are disjoint, then two vertices in the graph are adjacent. Different types of bipartite Kneser graphs were built and their algebraic structures were analysed [1], [16]. These graphs are important because they enable the application of graph theory to a large class of combinatorial problems involving sets.

Let $\mathscr{B}_n = \{1, 2, \cdots, n\}$ where $n \in \mathbb{Z}$ and $n > 1$. For any two integers $k \geq 1$ and $n \geq 2k+1$, the vertex set of the bipartite Kneser graph $H(n,k)$, [16], constitutes the k-element subsets and $(n-k)$ element subsets of $\mathscr{B}_n$. Two vertices are adjacent if and only if one of them is a subset of the other. Sreekumar K. G. et al., [19], introduced a modified version of the bipartite Kneser graph, $H_T(n,1)$. Here, for a fixed integer $n > 1$, let $\mathscr{A}_n = \{1, 2, 3, \ldots, n\}$. Let $\varphi(\mathscr{A}_n)$ be the set of all non-empty subsets of $\mathscr{A}_n$. Let V_1 be the set of 1-element subsets of $\mathscr{A}_n$, and $V_2 = \phi(\mathscr{A}_n) - V_1$. Let $X \in V_1$ and $Y \in V_2$. The adjacency of vertices in the bipartite graph is given by: $X \sim Y$ if and only if $X \subset Y$. This graph is called a bipartite Kneser type-1 graph, [19], and is denoted by $H_T(n,1)$. Sreekumar K. G. et al., [20], introduced a bipartite Kneser B type-k graph $G = H_B(n,k)$ which are more general bipartite graphs.

In Section 4, some degree-based topological indices of $G = H_B(n,k)$ such as the Narumi-Katayama index, the first Zagreb index, the forgotten index or F-index, the second Zagreb index, the second Hyper-Zagreb index, the Randic index, the reciprocal Randic index, the atom-bond connectivity index, the geometric-arithmetic index, the harmonic index, the Albertson index, and the sigma index are determined.

2. Fundamentals of $H_B(n,k)$

Definition 2.1. Let $\gamma_n = \{\pm x_1, \pm x_2, \pm x_3, \cdots, \pm x_{n-1}, x_n\}$ where $n > 1$ is fixed, $x_i \in \mathbb{R}^+$, $i = 1, 2, 3, \cdots, n$, and $x_1 < x_2 < x_3 < \cdots < x_n$. Let $\phi(\gamma_n)$ be the set of all non-empty subsets $S = \{u_1, u_2, \cdots, u_t\}$ of γ_n such that $|u_1| < |u_2| < \cdots < |u_{t-1}| < u_t$ where $u_t \in \mathbb{R}^+$. Let $\gamma_n^+ = \{x_1, x_2, x_3, \cdots, x_{n-1}, x_n\}$. For a fixed k, let V_1 be the set of k-element subsets of γ_n^+, $1 \leq k < n$. $V_2 = \phi(\gamma_n) - V_1$. For any $A \in V_2$, let $A^\dagger = \{|x| : x \in A\}$. A bipartite graph with parts V_1 and V_2 and having adjacency as $X \in V_1$ is adjacent to $Y \in V_2$ if and only if $X \subset Y^\dagger$ or $Y^\dagger \subset X$. A graph of this type is called the bipartite Kneser B type-k graph, [20], and is denoted by $H_B(n,k)$.

Definition 2.2. An r**-vertex** in $H_B(n,k)$ is an element in $\phi(\gamma_n) = V_1 \cup V_2$ containing r elements, where $1 \leq r \leq n$. Members of $\phi(\gamma_n)$ are called r**-vertices**.

Example 2.3. $H_B(n,k)$ for $n = 3,\ k = 2$ is illustrated in FIGURE 1.

The 2-vertex $\{1,3\} \in V_1$ is adjacent to the 1-vertex $\{3\}$ because $\{3\} \subset \{1,3\}^\dagger = \{|1|,|3|\} = \{1,3\}$. Simiarly $\{1,3\}$ is adjacent to the 1-vertex $\{1\}$. Additionally, $\{1,3\}$ is adjacent to $\{-1,3\}$ as $\{1,3\} \subset \{-1,3\}^\dagger = \{|-1|,|3|\} = \{1,3\}$. The adjacency relationships shown in FIGURE 1 can be illustrated by similar arguments.

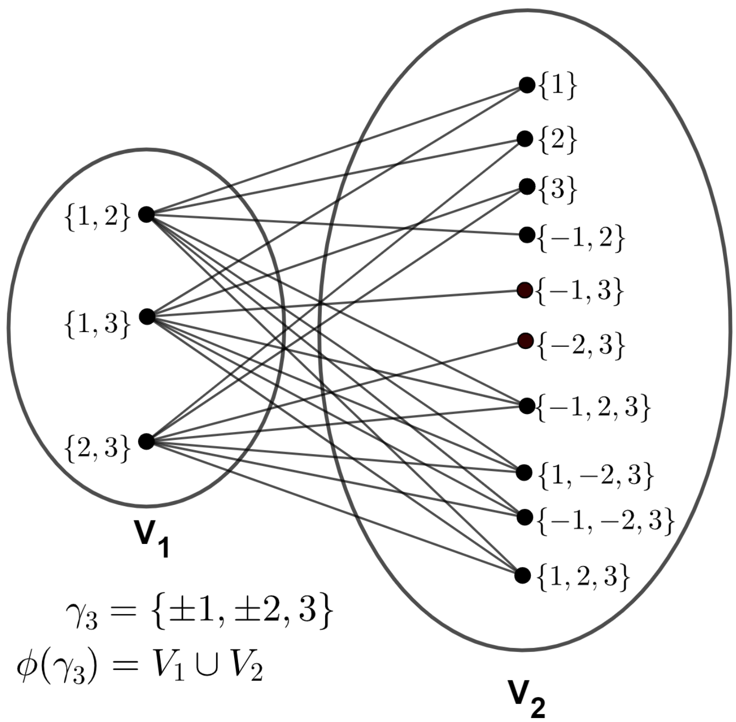

FIGURE 1. $H_B(3,2)$

Example 2.4. As the size of $H_B(4,3)$ is large , we give its bipartition here. By the definition of $H_B(n,k)$, the vertex $A \in V_1$ is adjacent to the vertex $B \in V_2$ if and only if $A \subset B^\dagger$ or $B^\dagger \subset A$.

$$\gamma_4 = \{\pm 1,\ \pm 2,\ \pm 3,\ 4\},$$
$$V_1 = \big\{\{1,2,3\},\{1,2,4\},\{1,3,4\},\{2,3,4\}\big\},$$

$$\begin{aligned}V_2 = \big\{&\{1\},\{2\},\{3\},\{4\},\{1,2\},\{1,3\},\{1,4\},\{2,3\},\{2,4\},\{3,4\},\\&\{-1,2\},\{-1,3\},\{-1,4\},\{-2,3\},\{-2,4\},\{-3,4\},\\&\{-1,2,3\},\{1,-2,3\},\{-1,-2,3\},\{-1,2,4\},\{1,-2,4\},\{-1,-2,4\},\\&\{-2,3,4\},\{2,-3,4\},\{-2,-3,4\},,\{-1,3,4\},\{1,-3,4\},\{-1,-3,4\},\\&\{1,2,3,4\},\{-1,2,3,4\},\{1,-2,3,4\},\{1,2,-3,4\},\{-1,-2,3,4\},\\&\{1,-2,-3,4\},\{-1,2,-3,4\},\{-1,-2,-3,4\}\big\}.\end{aligned}$$

While V_1 contains four 3-vertices, V_2 contains four 1-vertices, twelve 2-vertices, twelve 3-vertices, and eight 4-vertices.

3. Preliminary results

The following results proved in [14] are used in the computation of topological indices.

Result 1. *The order of* $G = H_B(n,k)$, $|V(G)| = \dfrac{3^n-1}{2}$.

Result 2. *The size of* $G = H_B(n,k)$, $|E(G)| = \binom{n}{k}\left(\dfrac{3^k-3}{2} + 2^{k-1}(3^{n-k}-1)\right)$.

Result 3. *The degree of a vertex in* $G = H_B(n,k)$ *and the number of vertices having a specific degree are determined. The degree sequence is obtained by arranging the sequence* $\Big\{d_{V_2}(1)^{N_{V_2}(1)}, d_{V_2}(2)^{N_{V_2}(2)} \ldots, d_{V_2}(k-1)^{N_{V_2}(k-1)}, d_{V_1}(k)^{N_{V_1}(k)},$ $d_{V_2}(k)^{N_{V_2}(k)}, d_{V_2}(k+1)^{N_{V_2}(k+1)}, \ldots, d_{V_2}(n)^{N_{V_2}(n)}\Big\}$ *of degrees with corresponding multiplicities as a monotonic nonincreasing sequence.*

Here $d_{V_2}(r)$ *where* $r = 1,2,3,\ldots,k-1,k+1,\ldots n$ *denotes the degrees of r-vertices in* V_2 *and* $d_{V_1}(k)$ *denotes the degree of any k-vertex in* V_1 *. Degrees of vertices are:* $d_{V_2}(r) = \binom{n-r}{k-r}$ *for* $1 \le r \le k-1$, $d_{V_1}(k) = \left(\dfrac{3^k-3}{2} + 2^{k-1}(3^{n-k}-1)\right)$, $d_{V_2}(k) = 1$, *and* $d_{V_2}(r) = \binom{r}{k}$ *for* $k+1 \le r \le n$. *The number of r-vertices in* V_2, *where* $r = 1,2,3,\ldots,k-1,k+1,\ldots n$, *is* $N_{V_2}(r) = 2^{r-1}\binom{n}{r}$. *The number of k-vertices in* V_1 *is* $N_{V_1}(k) = \binom{n}{k}$, *and the number of k-vertices in* V_2 *is* $N_{V_2}(k) = (2^{k-1}-1)\binom{n}{k}$.

Result 4. $H_B(n,k)$ *has the maximum vertex degree* $\Delta = d_{V_1}(k)$ *and the minimum vertex degree* $\delta = d_{V_2}(k) = 1$.

Example 3.1. The degree sequence for $H_B(4,3)$ given in Example 2.4 is obtained by arranging the sequence,
$\{d_{V_2}(1)^{N_{V_2}(1)}, d_{V_2}(2)^{N_{V_2}(2)}, d_{V_1}(3)^{N_{V_1}(3)}, d_{V_2}(3)^{N_{V_2}(3)}, d_{V_2}(4)^{N_{V_2}(4)}\} =$
$\{3^4, 2^{12}, 20^4, 1^{12}, 4^8\}$ of degrees with corresponding multiplicities as a monotonic, non-increasing sequence. Thus, the degree sequence is $\Big\{20^4, 4^8, 3^4, 2^{12}, 1^{12}\Big\}$.

4. Some degree-based topological indices of $H_B(n,k)$

Numerous vertex-degree-based graph invariants—also known as "topological indices"—have been presented and thoroughly examined in the literature on mathematics and chemistry, [18, 21]. Their general formula is :

$$TI = TI(G) = \sum_{e_{ij} \in E(G)} F(deg(v_i), deg(v_j)).$$

Here $F(x,y)$ is some function with the property $F(x,y) = F(y,x)$, [10].

For the simple graph $G = H_B(n,k)$ with vertex set $V(G)$ and edge set $E(G)$, we compute the following well-known degree-based topological indices: Here, $deg(v_i)$ denotes the degree of vertex v_i, and e_{ij} denotes the edge joining vertices v_i and v_j.

Narumi-Katayama index[8], $NK(G) = \prod_{i=1}^{n} deg(v_i)$.

The first Zagreb index[9], $M_1(G) = \sum_{v_i \in V(G)} deg(v_i)^2$.

The forgotten index, or F-index [2, 13, 11], $\mathrm{F}(G) = \sum_{v_i \in V(G)} deg(v_i)^3$.

The second Zagreb index[7], $M_2(G) = \sum_{e_{ij} \in E(G)} deg(v_i)deg(v_j)$.

The second Hyper-Zagreb index[4], $M_2(G) = \sum_{e_{ij} \in E(G)} (deg(v_i)deg(v_j))^2$.

The Randic index[17], $R(G) = \sum_{e_{ij} \in E(G)} \frac{1}{\sqrt{deg(v_i)deg(v_j)}}$.

The reciprocal Randic index[15], $RR(G) = \sum_{e_{ij} \in E(G)} \sqrt{deg(v_i)deg(v_j)}$.

Atom-bond-connectivity index[5], $ABC(G) = \sum_{v_iv_j \in E(G)} \sqrt{\frac{deg(v_i)+deg(v_j)-2}{deg(v_i)deg(v_j)}}$.

The geometric-arithmetic index[22], $GA(G) = \sum_{v_iv_j \in E(G)} \frac{\sqrt{deg(v_i)deg(v_j)}}{\frac{1}{2}[deg(v_i)+deg(v_j)]}$.

The harmonic index[6], $H(G) = \sum_{v_iv_j \in E(G)} \frac{2}{deg(v_i)+deg(v_j)}$.

The Albertson index[3], $Alb(G) = \sum_{v_iv_j \in E(G)} |deg(v_i) - deg(v_j)|$.

The sigma index, or irregularity index[12],
$\sigma(G) = \sum_{v_iv_j \in E(G)} (deg(v_i) - deg(v_j))^2$.

In chemical graph theory, the Narumi-Katayama index is used to model physicochemical, pharmacologic, toxicologic and biological properties of chemical compounds.

Theorem 4.1. *For $G = H_B(n,k)$ with vertex set $V(G)$, the Narumi-Katayama index is* $NK(G) = (d_{V_1}(k))^{\binom{n}{k}} (d_{V_2}(1))^{N_{V_2}(1)} (d_{V_2}(2))^{N_{V_2}(2)} \cdots d_{V_2}(n)^{N_{V_2}(n)}$.

Proof. Let $V(H_B(n,k)) = \{v_1, v_2, \ldots, v_{\frac{(3^n-1)}{2}}\}$. The degrees of vertices with corresponding multiplicities are given in Result 3.

$$\begin{aligned} NK(G) &= \prod_{i=1}^{\frac{3^n-1}{2}} deg(v_i) \\ &= (d_{V_1}(k))^{\binom{n}{k}} (d_{V_2}(1))^{N_{V_2}(1)} (d_{V_2}(2))^{N_{V_2}(2)} \cdots d_{V_2}(n)^{N_{V_2}(n)}. \end{aligned}$$ □

The First Zagreb index has been used to predict the π-electronic energy of benzenoid hydrocarbons. It has been shown to be crucial in real-world situations including corporate networking and road traffic management.

Theorem 4.2. *For $G = H_B(n,k))$ with vertex set $V(G)$, the first Zagreb index is*

$$M_1(G) = \sum_{i=1}^{k-1} 2^{i-1} \binom{n}{i} \binom{n-i}{k-i}^2 + \binom{n}{k} (2^{k-1} - 1 + d_{V_1}(k)^2) + \sum_{i=k+1}^{n} 2^{i-1} \binom{n}{i} \binom{i}{k}^2.$$

Proof. Let $V(H_B(n,k)) = \{v_1, v_2, \ldots, v_{\frac{(3^n-1)}{2}}\}$. The degrees of vertices with corresponding multiplicities are given in Result 3. First Zagreb index is:

$$\begin{aligned} M_1(G) = &\sum_{v_i \in V(G)} deg(v_i)^2 \\ &= deg(v_1)^2 + deg(v_2)^2 + \cdots + deg\left(v_{\frac{(3^n-1)}{2}}\right)^2 \\ &= N_{V_2}(1) d_{V_2}(1)^2 + N_{V_2}(2) d_{V_2}(2)^2 + \cdots + N_{V_2}(k-1) d_{V_2}(k-1)^2 + \\ &\quad N_{V_1}(k) d_{V_1}(k)^2 + N_{V_2}(k) d_{V_2}(k)^2 + N_{V_2}(k+1) d_{V_2}(k+1)^2 + \cdots + \\ &\quad N_{V_2}(n) d_{V_2}(n)^2 \\ &= 2^0 \binom{n}{1} \binom{n-1}{k-1}^2 + 2^1 \binom{n}{2} \binom{n-2}{k-2}^2 + \cdots + \\ &\quad 2^{k-2} \binom{n}{k-1} \binom{n-(k-1)}{k-(k-1)}^2 + (2^{k-1} - 1) \binom{n}{k} 1^2 + \binom{n}{k} d_{V_1}(k)^2 + \\ &\quad 2^k \binom{n}{k+1} \binom{k+1}{k}^2 + \cdots + 2^{n-1} \binom{n}{n} \binom{n}{k}^2 \\ &= \sum_{i=1}^{k-1} 2^{i-1} \binom{n}{i} \binom{n-i}{k-i}^2 + \binom{n}{k} (2^{k-1} - 1 + \\ &\quad d_{V_1}(k)^2) + \sum_{i=k+1}^{n} 2^{i-1} \binom{n}{i} \binom{i}{k}^2. \end{aligned}$$ □

The forgotten index provides insight into the branching of the carbon-atom skeleton within the molecular structure. In molecular graph theory, the forgotten index plays a fundamental role in analyzing quantitative structure–activity or property relationships.

Theorem 4.3. *For $G = H_B(n,k))$ with vertex set $V(G)$, the forgotten index or F-index is*

$$F(G) = \sum_{i=1}^{k-1} 2^{i-1}\binom{n}{i}\binom{n-i}{k-i}^3 + \binom{n}{k}(2^{k-1} - 1 + d_{V_1}(k)^3) + \sum_{i=k+1}^{n} 2^{i-1}\binom{n}{i}\binom{i}{k}^3.$$

Proof. The forgotten index or F-index is

$$\begin{aligned}
\mathrm{F}(G) = &\sum_{v_i \in V(G)} deg(v_i)^3 \\
=&deg(v_1)^3 + deg(v_2)^3 + \cdots + deg\left(v_{\frac{(3^n-1)}{2}}\right)^3 \\
=&N_{V_2}(1)d_{V_2}(1)^3 + N_{V_2}(2)d_{V_2}(2)^3 + \cdots + N_{V_2}(k-1)d_{V_2}(k-1)^3 + \\
&N_{V_1}(k)d_{V_1}(k)^3 + N_{V_2}(k)d_{V_2}(k)^3 + N_{V_2}(k+1)d_{V_2}(k+1)^3 + \cdots \\
&N_{V_2}(n)d_{V_2}(n)^3 \\
=&2^0\binom{n}{1}\binom{n-1}{k-1}^3 + 2^1\binom{n}{2}\binom{n-2}{k-2}^3 + \cdots + 2^{k-2}\binom{n}{k-1}\binom{n-(k-1)}{k-(k-1)}^3 \\
&+ (2^{k-1} - 1)\binom{n}{k}1^3 + \binom{n}{k}d_{V_1}(k)^3 + 2^k\binom{n}{k+1}\binom{k+1}{k}^3 + \cdots \\
&+ 2^{n-1}\binom{n}{n}\binom{n}{k}^3 \\
=&\sum_{i=1}^{k-1} 2^{i-1}\binom{n}{i}\binom{n-i}{k-i}^3 + \binom{n}{k}(2^{k-1} - 1 + d_{V_1}(k)^3) + \\
&\sum_{i=k+1}^{n} 2^{i-1}\binom{n}{i}\binom{i}{k}^3.
\end{aligned}$$

□

The second Zagreb index contributes to our knowledge of the stability and electronic structure of molecular systems. It is used in modeling the boiling points of benzenoid hydrocarbons.

Theorem 4.4. *For $G = H_B(n,k))$ with vertex set $V(G)$, the second Zagreb index is*

$$\begin{aligned}
M_2(G) = \binom{n}{k}(d_{V_1}(k))\Big[&\sum_{i=1}^{k-1} 2^{i-1}\binom{k}{i}\binom{n-i}{k-i} + 2^{k-1} - 1 + \\
&\sum_{i=1}^{n-k} 2^{k-1+i}\binom{n-k}{i}\binom{k+i}{k}\Big].
\end{aligned}$$

Proof. We know that the degree of any k-vertex u in V_1 is $deg(u) = d_{V_1}(k)$. Also, the degree of any r-vertex where $1 \leq r \leq n$ in V_2 is $d_{V_2}(r)$.

Let $n_{V_2}(r)$ be the number of r-vertices,$1 \leq r \leq n$ adjacent to $u \in V_1$.The values of $n_{V_2}(r)$ as given in [14] are

$$n_{V_2}(r) = \begin{cases} 2^{r-1}\binom{k}{r} & \text{for } 1 \leq r \leq k-1 \\ 2^{k-1} - 1 & \text{for } r = k \\ 2^{r-1}\binom{n-k}{r-k} & \text{for } k+1 \leq r \leq n. \end{cases}$$

It is also clear that $d_{V_1}(k) = \sum\limits_{r=1}^{n} n_{V_2}(r)$.

Let $\{u_1, u_2, \cdots u_{d_{V_1}(k)}\}$ be the neighbourhood set of u. This set contains $n_{V_2}(r)$, r-vertices of degree $d_{V_2}(r)$ for $1 \leq r \leq n$.

$$\sum_{\substack{uu_i \in E(G) \\ 1 \leq i \leq d_{V_1}(k)}} deg(u)deg(u_i) = d_{V_1}(k) \sum_{r=1}^{n} n_{V_2}(r) d_{V_2}(r). \tag{4.1}$$

$$\begin{aligned} d_{V_1}(k) \sum_{r=1}^{n} n_{V_2}(r) d_{V_2}(r) =& d_{V_1}(k)\Big(n_{V_2}(1)d_{V_2}(1) + n_{V_2}(2)d_{V_2}(2) + \cdots + \\ & n_{V_2}(k-1)d_{V_2}(k-1) +) n_{V_2}(k)d_{V_2}(k) + \\ & n_{V_2}(k+1)d_{V_2}(k+1) + \cdots n_{V_2}(n)d_{V_2}(n)\Big) \\ =& d_{V_1}(k)\left(2^0\binom{k}{1}\binom{n-1}{k-1} + 2^1\binom{k}{2}\binom{n-2}{k-2} + \cdots + \right. \\ & 2^{k-2}\binom{k}{k-1}\binom{n-(k-1)}{k-(k-1)} + (2^{k-1} - 1) + \\ & \left. 2^k\binom{n-k}{1}\binom{k+1}{k} + \cdots + 2^{n-1}\binom{n-k}{n-k}\binom{n}{k}\right). \end{aligned}$$

As there are $\binom{n}{k}$, k-vertices in V_1, the second Zagreb index is:

$M_2(G) = \sum\limits_{e_{ij} \in E(G)} deg(v_i)deg(v_j) = \binom{n}{k} d_{V_1}(k) \sum\limits_{r=1}^{n} n_{V_2}(r) d_{V_2}(r)$. Therefore,

$$\begin{aligned} M_2(G) =& \binom{n}{k} d_{V_1}(k)\left[\sum_{i=1}^{k-1} 2^{i-1}\binom{k}{i}\binom{n-i}{k-i} + 2^{k-1} - 1 + \right. \\ & \left. \sum_{i=1}^{n-k} 2^{k-1+i}\binom{n-k}{i}\binom{k+i}{k}\right]. \end{aligned}$$

□

An extension of the Zagreb index that is used to forecast the physicochemical characteristics of organic molecules is the hyper-Zagreb index.

Theorem 4.5. *For $G = H_B(n,k))$ with vertex set $V(G)$, the second hyper-Zagreb index is*

$$HM_2(G) = \binom{n}{k} d^2_{V_1}(k)\left[\sum_{i=1}^{k-1} 2^{i-1}\binom{k}{i}\binom{n-i}{k-i}^2 + 2^{k-1} - 1 + \sum_{i=1}^{n-k} 2^{k-1+i}\binom{n-k}{i}\binom{k+i}{k}^2\right].$$

Proof. We choose $u, n_{V_2}(r), d_{V_1}(k)$ and $d_{V_2}(r)$ for $1 \leq r \leq n$ as in Theorem 4.4.

$$\sum_{\substack{uu_i \in E(G)\\ 1 \leq i \leq d_{V_1}(k)}} deg^2(u)deg^2(u_i) = d^2_{V_1}(k)\sum_{r=1}^{n} n_{V_2}(r)d^2_{V_2}(r) \tag{4.2}$$

$$\begin{aligned} d^2_{V_1}(k)\sum_{r=1}^{n} n_{V_2}(r)d^2_{V_2}(r) =& d^2_{V_1}(k)\Big(n_{V_2}(1)d^2_{V_2}(1) + n_{V_2}(2)d^2_{V_2}(2) + \cdots + \\ & n_{V_2}(k-1)d^2_{V_2}(k-1) + n_{V_2}(k)d^2_{V_2}(k) + \\ & n_{V_2}(k+1)d^2_{V_2}(k+1) + \cdots n_{V_2}(n)d^2_{V_2}(n)\Big) \\ =& d^2_{V_1}(k)\left(2^0\binom{k}{1}\binom{n-1}{k-1}^2 + 2^1\binom{k}{2}\binom{n-2}{k-2}^2 + \cdots + \right. \\ & 2^{k-2}\binom{k}{k-1}\binom{n-(k-1)}{k-(k-1)}^2 + (2^{k-1}-1) + \\ & \left. 2^k\binom{n-k}{1}\binom{k+1}{k}^2 + \cdots + 2^{n-1}\binom{n-k}{n-k}\binom{n}{k}^2\right). \end{aligned}$$

As there are $\binom{n}{k}$ k vertices in V_1, we have

$HM_2(G) = \sum_{e_{ij} \in E(G)} (deg(v_i)deg(v_j))^2 = \binom{n}{k} d^2_{V_1}(k)\sum_{r=1}^{n} n_{V_2}(r)d^2_{V_2}(r)$.

Therefore, the second hyper-Zagreb index is

$$HM_2(G) = \binom{n}{k} d^2_{V_1}(k)\left[\sum_{i=1}^{k-1} 2^{i-1}\binom{k}{i}\binom{n-i}{k-i}^2 + 2^{k-1} - 1 + \sum_{i=1}^{n-k} 2^{k-1+i}\binom{n-k}{i}\binom{k+i}{k}^2\right].$$

□

If each vertex in a graph has the same degree, the graph is said to be regular. Regular graphs are instances or counterexamples in many applications of graph theory, and regularity often makes calculations easier. If a graph has two or more uneven vertex degrees, it is considered irregular. A number of writers have defined irregularity and used various measurements for it. The most in-depth research has been done on the sigma and Albertson indices. For $H_B(n,k)$, they are computed using the next two theorems.

Theorem 4.6. *For $G = H_B(n,k)$ with vertex set $V(G)$, the Albertson index (which is also called irregularity index, third Zagreb index or Kekule index) is*

$$Alb(G) = \binom{n}{k}\Bigg(d^2_{V_1}(k) - \Big[\sum_{i=1}^{k-1} 2^{i-1}\binom{k}{i}\binom{n-i}{k-i} + 2^{k-1} - 1 + \sum_{i=1}^{n-k} 2^{k-1+i}\binom{n-k}{i}\binom{k+i}{k}\Big]\Bigg).$$

Proof. We choose $u, n_{V_2}(r), d_{V_1}(k)$ and $d_{V_2}(r)$ for $1 \le r \le n$ as in theorem 4.4.

$$\begin{aligned}\sum_{\substack{uu_i\in E(G)\\1\le i\le d_{V_1}(k)}} |deg(u) - deg(u_i)| &= \sum_{\substack{uu_i\in E(G)\\1\le i\le d_{V_1}(k)}} (d_{V_1}(k) - deg(u_i))\\ &= d_{V_1}(k)\times d_{V_1}(k) - \sum_{\substack{uu_i\in E(G)\\1\le i\le d_{V_1}(k)}} deg(u_i)\\ &= d^2_{V_1}(k) - \sum_{r=1}^{n} n_{V_2}(r)d_{v_2}(r)\\ &= d^2_{V_1}(k) - \left[\sum_{i=1}^{k-1} 2^{i-1}\binom{k}{i}\binom{n-i}{k-i} + 2^{k-1} - 1 + \sum_{i=1}^{n-k} 2^{k-1+i}\binom{n-k}{i}\binom{k+i}{k}\right].\end{aligned}$$

As there are $\binom{n}{k}$ k vertices in V_1, the Albertson index is:
$Alb(G) = \sum\limits_{v_iv_j\in E(G)} |deg(v_i) - deg(v_j)| = \binom{n}{k} \sum\limits_{\substack{uu_i\in E(G)\\1\le i\le d_{V_1}(k)}} |deg(u) - deg(u_i)|.$ □

Theorem 4.7. *For $G = H_B(n,k)$, the sigma index of G,*
$\sigma(G) = \binom{n}{k}\Big(d^3_{V_1}(k) + \sum\limits_{r=1}^{n} n_{V_2}(r)d^2_{v_2}(r) - 2d_{V_1}(k)\sum\limits_{r=1}^{n} n_{V_2}(r)d_{v_2}(r)\Big).$

Proof. We choose $u, n_{V_2}(r), d_{V_1}(k)$ and $d_{V_2}(r)$ for $1 \le r \le n$ as in Theorem 4.4.

$$\begin{aligned}\sum_{\substack{uu_i\in E(G)\\1\le i\le d_{V_1}(k)}}(deg(u)-deg(u_i))^2 &= \sum_{\substack{uu_i\in E(G)\\1\le i\le d_{V_1}(k)}}(d_{V_1}^2(k)+deg^2(u_i)-2d_{V_1}(k)deg(u_i))\\ &= d_{V_1}^3(k)+\sum_{\substack{uu_i\in E(G)\\1\le i\le d_{V_1}(k)}}deg^2(u_i)-\\ &\quad 2d_{V_1}(k)\sum_{\substack{uu_i\in E(G)\\1\le i\le d_{V_1}(k)}}deg(u_i)\\ &= d_{V_1}^3(k)+\sum_{r=1}^{n}n_{V_2}(r)d_{v_2}^2(r)-\\ &\quad 2d_{V_1}(k)\sum_{r=1}^{n}n_{V_2}(r)d_{v_2}(r).\end{aligned}$$

As there are $\binom{n}{k}$ k vertices in V_1, the sigma index is $\sigma(G)=\binom{n}{k}\Big(d_{V_1}^3(k)+\sum_{r=1}^{n}n_{V_2}(r)d_{v_2}^2(r)-2d_{V_1}(k)\sum_{r=1}^{n}n_{V_2}(r)d_{v_2}(r)\Big)$.

From Eqn. (4.1), we get

$\sum_{r=1}^{n}n_{V_2}(r)d_{v_2}(r)=\sum_{i=1}^{k-1}2^{i-1}\binom{k}{i}\binom{n-i}{k-i}+2^{k-1}-1+\sum_{i=1}^{n-k}2^{k-1+i}\binom{n-k}{i}\binom{k+i}{k}$.

From Eqn. (4.2), we get

$\sum_{r=1}^{n}n_{V_2}(r)d_{v_2}^2(r)=\sum_{i=1}^{k-1}2^{i-1}\binom{k}{i}\binom{n-i}{k-i}^2+2^{k-1}-1+\sum_{i=1}^{n-k}2^{k-1+i}\binom{n-k}{i}\binom{k+i}{k}^2$. □

Theorem 4.8. *For $G=H_B(n,k))$ with vertex set $V(G)$, the Randic index is*

$$R(G)=\frac{\binom{n}{k}}{\sqrt{d_{V_1}(k)}}\left[\sum_{i=1}^{k-1}\frac{2^{i-1}\binom{k}{i}}{\sqrt{\binom{n-i}{k-i}}}+2^{k-1}-1+\sum_{i=1}^{n-k}\frac{2^{k-1+i}\binom{n-k}{i}}{\sqrt{\binom{k+i}{k}}}\right].$$

Proof. We choose $u, n_{V_2}(r), d_{V_1}(k)$ and $d_{V_2}(r)$ for $1 \le r \le n$ as in Theorem 4.4.
$\sum\limits_{\substack{uu_i \in E(G) \\ 1 \le i \le d_{V_1}(k)}} \frac{1}{\sqrt{deg(u)deg(u_i)}} = \frac{1}{\sqrt{d_{V_1}(k)}} \sum\limits_{\substack{uu_i \in E(G) \\ 1 \le i \le d_{V_1}(k)}} \frac{1}{\sqrt{deg(u_i)}} = \frac{1}{\sqrt{d_{V_1}(k)}} \sum\limits_{r=1}^{n} \frac{n_{V_2}(r)}{\sqrt{d_{V_2}(r)}}$

$$\begin{aligned}
\frac{1}{\sqrt{d_{V_1}(k)}} \sum_{r=1}^{n} \frac{n_{V_2}(r)}{\sqrt{d_{V_2}(r)}} =& \frac{1}{\sqrt{d_{V_1}(k)}} \left(\frac{n_{V_2}(1)}{\sqrt{d_{V_2}(1)}} + \frac{n_{V_2}(2)}{\sqrt{d_{V_2}(2)}} + \cdots + \frac{n_{V_2}(k-1)}{\sqrt{d_{V_2}(k-1)}} + \right. \\
& \left. \frac{n_{V_2}(k)}{\sqrt{d_{V_2}(k)}} + \frac{n_{V_2}(k+1)}{\sqrt{d_{V_2}(k+1)}} + \cdots + \frac{n_{V_2}(n)}{\sqrt{d_{V_2}(n)}} \right) \\
=& \frac{1}{\sqrt{d_{V_1}(k)}} \left(\frac{2^0\binom{k}{1}}{\sqrt{\binom{n-1}{k-1}}} + \frac{2^1\binom{k}{2}}{\sqrt{\binom{n-2}{k-2}}} + \cdots + \frac{2^{k-2}\binom{k}{k-1}}{\sqrt{\binom{n-(k-1)}{k-(k-1)}}} + \right. \\
& \left. (2^{k-1}-1) + \frac{2^k\binom{n-k}{1}}{\sqrt{\binom{k+1}{k}}} + \cdots + \frac{2^{n-1}\binom{n-k}{n-k}}{\sqrt{\binom{n}{k}}} \right) \\
=& \frac{1}{\sqrt{d_{V_1}(k)}} \left[\sum_{i=1}^{k-1} \frac{2^{i-1}\binom{k}{i}}{\sqrt{\binom{n-i}{k-i}}} + 2^{k-1} - 1 + \sum_{i=1}^{n-k} \frac{2^{k-1+i}\binom{n-k}{i}}{\sqrt{\binom{k+i}{k}}} \right].
\end{aligned}$$

As there are $\binom{n}{k}$ k-vertices in V_1, the Randic index of G,
$R(G) = \sum\limits_{e_{ij} \in E(G)} \frac{1}{\sqrt{deg(v_i)deg(v_j)}} = \frac{\binom{n}{k}}{\sqrt{d_{V_1}(k)}} \sum\limits_{r=1}^{n} \frac{n_{V_2}(r)}{\sqrt{d_{V_2}(r)}}$.
Therefore,

$$R(G) = \frac{\binom{n}{k}}{\sqrt{d_{V_1}(k)}} \left[\sum_{i=1}^{k-1} \frac{2^{i-1}\binom{k}{i}}{\sqrt{\binom{n-i}{k-i}}} + 2^{k-1} - 1 + \sum_{i=1}^{n-k} \frac{2^{k-1+i}\binom{n-k}{i}}{\sqrt{\binom{k+i}{k}}} \right]. \qquad \square$$

Theorem 4.9. *For $G = H_B(n,k)$ with vertex set $V(G)$, the reciprocal Randic index is*

$$\begin{aligned}
RR(G) = \binom{n}{k}\sqrt{d_{V_1}(k)} \Bigg[& \sum_{i=1}^{k-1} 2^{i-1}\binom{k}{i}\sqrt{\binom{n-i}{k-i}} + 2^{k-1} - 1 + \\
& \sum_{i=1}^{n-k} 2^{k-1+i}\binom{n-k}{i}\sqrt{\binom{k+i}{k}} \Bigg].
\end{aligned}$$

Proof. We choose $u, n_{V_2}(r), d_{V_1}(k)$ and $d_{V_2}(r)$ for $1 \le r \le n$ as in Theorem 4.4.

$$\begin{aligned}
\sum_{\substack{uu_i \in E(G) \\ 1 \le i \le d_{V_1}(k)}} \sqrt{deg(u)deg(u_i)} &= \sqrt{d_{V_1}(k)} \sum_{\substack{uu_i \in E(G) \\ 1 \le i \le d_{V_1}(k)}} \sqrt{deg(u_i)} \\
&= \sqrt{d_{V_1}(k)} \sum_{r=1}^{n} n_{V_2}(r)\sqrt{d_{V_2}(r)}.
\end{aligned}$$

.

$$\begin{aligned}\sqrt{d_{V_1}(k)}\sum_{r=1}^{n} n_{V_2}(r)\sqrt{d_{V_2}(r)} =& \sqrt{d_{V_1}(k)}\Big(n_{V_2}(1)\sqrt{d_{V_2}(1)} + n_{V_2}(2)\sqrt{d_{V_2}} + \cdots \\ & + n_{V_2}(k-1)\sqrt{d_{V_2}(k-1)} + n_{V_2}(k)\sqrt{d_{V_2}(k)} + \\ & n_{V_2}(k+1)\sqrt{d_{V_2}(k+1)} + \cdots + n_{V_2}(n)\sqrt{d_{V_2}(n)}\Big) \\ =& \sqrt{d_{V_1}(k)}\left(2^0\binom{k}{1}\sqrt{\binom{n-1}{k-1}} + 2^1\binom{k}{2}\sqrt{\binom{n-2}{k-2}} + \right. \\ & \cdots + 2^{k-2}\binom{k}{k-1}\sqrt{\binom{n-(k-1)}{k-(k-1)}} + (2^{k-1}-1) + \\ & \left. 2^k\binom{n-k}{1}\sqrt{\binom{k+1}{k}} + \cdots + 2^{n-1}\binom{n-k}{n-k}\sqrt{\binom{n}{k}}\right) \\ =& \sqrt{d_{V_1}(k)}\left[\sum_{i=1}^{k-1} 2^{i-1}\binom{k}{i}\sqrt{\binom{n-i}{k-i}} + 2^{k-1} - 1 + \right. \\ & \left. \sum_{i=1}^{n-k} 2^{k-1+i}\binom{n-k}{i}\sqrt{\binom{k+i}{k}}\right].\end{aligned}$$

As there are $\binom{n}{k}$ k-vertices in V_1, the reciprocal Randic index is

$$\begin{aligned}RR(G) =& \sum_{e_{ij}\in E(G)} \sqrt{deg(v_i)deg(v_j)} \\ =& \binom{n}{k}\sqrt{d_{V_1}(k)}\sum_{r=1}^{n} n_{V_2}(r)\sqrt{d_{V_2}(r)}.\end{aligned}$$

Therefore,

$$\begin{aligned}RR(G) =& \binom{n}{k}\sqrt{d_{V_1}(k)}\left[\sum_{i=1}^{k-1} 2^{i-1}\binom{k}{i}\sqrt{\binom{n-i}{k-i}} + 2^{k-1} - 1 + \right. \\ & \left. \sum_{i=1}^{n-k} 2^{k-1+i}\binom{n-k}{i}\sqrt{\binom{k+i}{k}}\right].\end{aligned}$$ □

Theorem 4.10. *The geometric-arithmetic index of* $G = H_B(n,k)$ *is* $GA(G) = 2\binom{n}{k}\sum_{r=1}^{n} n_{V_2}(r)\frac{\sqrt{d_{V_1}(k)}\sqrt{d_{V_2}(r)}}{d_{V_1}(k)+d_{V_2}(r)}$.

Proof. We choose $u, n_{V_2}(r), d_{V_1}(k)$ and $d_{V_2}(r)$ for $1 \le r \le n$ as in Theorem 4.4. Hence $\sum_{\substack{uu_i\in E(G)\\ 1\le i\le d_{V_1}(k)}} \frac{2\sqrt{deg(u)deg(u_i)}}{deg(u)+deg(u_i)} = \sum_{r=1}^{n} n_{V_2}(r)\frac{2\sqrt{d_{V_1}(k)}\sqrt{d_{V_2}(r)}}{d_{V_1}(k)+d_{V_2}(r)}$. As there are $\binom{n}{k}$, k-vertices in V_1, the geometric-arithmetic index is

$$GA(G) = \sum_{v_iv_j \in E(G)} \frac{\sqrt{deg(v_i)deg(v_j)}}{\frac{1}{2}[deg(v_i) + deg(v_j)]}$$
$$= 2\binom{n}{k} \sum_{r=1}^{n} n_{V_2}(r) \frac{\sqrt{d_{V_1}(k)}\sqrt{d_{V_2}(r)}}{d_{V_1}(k) + d_{V_2}(r)}. \quad \square$$

.

Theorem 4.11. *The harmonic index of $G = H_B(n,k)$,*
$H(G) = \binom{n}{k} \sum_{r=1}^{n} n_{V_2}(r) \frac{2}{d_{V_1}(k)+d_{V_2}(r)}$.

Proof. We choose $u, n_{V_2}(r), d_{V_1}(k)$ and $d_{V_2}(r)$ for $1 \leq r \leq n$ as in Theorem 4.4. Hence $\sum_{\substack{uu_i \in E(G) \\ 1 \leq i \leq d_{V_1}(k)}} \frac{2}{deg(u)+deg(u_i)} = \sum_{r=1}^{n} n_{V_2}(r) \frac{2}{d_{V_1}(k)+d_{V_2}(r)}$. As there are $\binom{n}{k}$, k-vertices in V_1, the harmonic index of G is $H(G) = \binom{n}{k} \sum_{r=1}^{n} n_{V_2}(r) \frac{2}{d_{V_1}(k)+d_{V_2}(r)}$. $\square$

Theorem 4.12. *Atom-bond-connectivity index of $G = H_B(n,k)$ is $ABC(G) = \frac{\binom{n}{k}}{\sqrt{d_{V_1}(k)}} \sum_{r=1}^{n} \frac{n_{V_2}(r)\sqrt{d_{V_1}(k)+d_{V_2}(r)-2}}{\sqrt{d_{V_2}(r)}}$.*

Proof. We choose $u, n_{V_2}(r), d_{V_1}(k)$ and $d_{V_2}(r)$ for $1 \leq r \leq n$ as in Theorem 4.4. Then $\sum_{\substack{uu_i \in E(G) \\ 1 \leq i \leq d_{V_1}(k)}} \frac{\sqrt{deg(u)+deg(u_i)-2}}{\sqrt{deg(u)deg(u_i)}} = \frac{1}{\sqrt{d_{V_1}(k)}} \sum_{r=1}^{n} \frac{n_{V_2}(r)\sqrt{d_{V_1}(k)+d_{V_2}(r)-2}}{\sqrt{d_{V_2}(r)}}$. As there are $\binom{n}{k}$ k-vertices in V_1, the ABC index of $H_B(n,k)$,
$ABC(G) = \sum_{v_iv_j \in E(G)} \sqrt{\frac{deg(v_i)+deg(v_j)-2}{deg(v_i)deg(v_j)}} = \frac{\binom{n}{k}}{\sqrt{d_{V_1}(k)}} \sum_{r=1}^{n} \frac{n_{V_2}(r)\sqrt{d_{V_1}(k)+d_{V_2}(r)-2}}{\sqrt{d_{V_2}(r)}}$.
$\square$

Conflict of interest. The authors hereby declare that there is no potential conflict of interest.

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