Proceedings of the Jangjeon Mathematical Society
28 (2025), No. 2, pp. 165 - 180

www.jangjeon.or.kr
http://dx.doi.org/10.17777/pjms2025.28.2.165

TOPOLOGICAL INDICES OF BIPARTITE KNESER B TYPE-K GRAPHS

JAYAKUMAR. C., SREEKUMAR K. G., AND MANILAL. K.

Abstract. Let $\mathscr{B}_n = \{\pm x_1, \pm x_2, \pm x_3, \ldots, \pm x_{n-1}, x_n\}$, where $n > 1$ is fixed, $x_i \in \mathbb{R}^+$, $i = 1, 2, 3, \ldots, n$, and $x_1 < x_2 < x_3 < \cdots < x_n$. Let $\phi(\mathscr{B}_n)$ be the set of all non-empty subsets $S = \{u_1, u_2, \ldots, u_t\}$ of $\mathscr{B}_n$ such that $|u_1| < |u_2| < \ldots < |u_{t-1}| < u_t$, where $u_t \in \mathbb{R}^+$. Let $\mathscr{B}_n^+ = \{x_1, x_2, x_3, \ldots, x_{n-1}, x_n\}$. For a fixed k, let V_1 be the set of k-element subsets of $\mathscr{B}_n^+$, $1 \leq k < n$. $V_2 = \phi(\mathscr{B}_n) - V_1$. For any $A \in V_2$, $A^\dagger = \{|x| : x \in A\}$. Define 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 a bipartite Kneser B type-k graph and denoted by $H_B(n, k)$. In this paper, we calculated some topological indices of $H_B(n, k)$.

2010 Mathematics Subject Classification. 05C07,05C10,05C12

Keywords and phrases. Bipartite Kneser graphs, bipartite Kneser B type-k graph, degree sequence, topological indices.

submission Date: 15 July 2023

1. Introduction

Numerous studies have been conducted on the structural characteristics of Kneser graphs, which are used in a wide range of applications. Coding theory makes use of Kneser graph automorphism to its benefit. Error correction using low-density parity check (LDPC) codes becomes highly efficient. It is present in nearly all contemporary communication systems. Writing an LDPC code is challenging. T. Chowdhury and A. Pramanik[4] created LDPC codes from bipartite Kneser graphs. A bipartite Kneser graph $H(n, k)$ is a mathematical object that arises in the field of combinatorics and graph theory. It is a type of graph that is defined in terms of sets and partitions of sets. It is a bipartite graph, one part consisting of all k-element subsets of the set of n elements, and the other part consisting of all $(n-k)$-element subsets. Here n and k are positive integers. An edge exists between a vertex in the first part and a vertex in the second part if and only if the corresponding subsets are disjoint. The class of graphs that bear Martin Kneser's name are those studied by him for the first time in 1956. Then, several types of bipartite Kneser graphs are constructed, and their algebraic structures are examined.

Bipartite Kneser graphs have important applications in coding theory, computational geometry, network theory and quantum mechanics. They are also interesting objects to study in their own right, and many of their properties have been investigated. These graphs are important because they allow a large number of set-related combinatorial problems to be translated into graph theory.

SM balancing graph[12]was established using the combinatorial structure of the balanced ternary number system, which is used in the 'Setun computer' built in Russia (Moscow State University-1958). Consider the set $\mathbb{T}_n = \{3^m : m \textit{ is an integer}, 0 \leq m \leq n-1\}$ for a fixed positive integer $n \geq 2$. Let $I = \{-1, 0, 1\}$ and $x \leq \frac{1}{2}(3^n - 1)$ be any positive integer which is not a power of 3. Then x can be expressed as

$$x = \sum_{j=1}^{n} \alpha_j y_j \tag{1.1}$$

where $\alpha_j \in I$, $y_j \in \mathbb{T}_n$, and $y_j's$ are all distinct. Each y_j such that $\alpha_j \neq 0$ is called a balancing component of x.

Consider the simple digraph $G = (V, E)$ where $V = \{v_1, v_2, v_3, \ldots, v_{\frac{1}{2}(3^n-1)}\}$ and adjacency of vertices is defined as follows: for any two distinct vertices v_x and v_{y_j}, $(v_x, v_{y_j}) \in E$ if (1.1) holds and $\alpha_j = -1$, and $(v_{y_j}, v_x) \in E$ if (1.1) holds and $\alpha_j = 1$. This digraph G is called the $n^{th} SMD$ balancing graph, denoted by $SMD(B_n)$. Its underlying undirected graph is called the n^{th} SM balancing graph or SM balancing graph, denoted by $SM(B_n)$.

In [11], the authors constructed a bipartite Kneser B type-k graph $G = H_B(n, k)$, which are more general bipartite graphs analogous to SM balancing graphs, for integers $n > 1$ and $k \geq 1$.

Topological indices are mathematical descriptors that capture the structural and geometrical features of a molecule or material. They are commonly used in the field of chemoinformatics, where they help to predict properties of chemicals based on their structure. Recently, the research on this topic has evolved on general graphs, and there are more than 3000 topological indices based on degree, distance, eccentricity, and spectrum of graphs.

In this paper, we analysed the graph $G = H_B(n, k)$ and determined its topological indices, like the Sombor index, eccentricity indices, Zagreb indices, Padmakar-Ivan index, and terminal Wiener index. Also, the M-polynomial and Wiener polarity index of this graph were obtained. In Section 4, definitions of various topological indices and M-polynomials are given. Calculation of these indices and M polynomial for $G = H_B(n, k)$ are included in section 5.

2. Preliminaries

The greatest distance between any two vertices in a graph is known as its diameter. The eccentricity of a vertex, $e(v)$, is the largest possible distance between it and any other vertex.

Definition 2.1. Let $\mathscr{B}_n = \{\pm x_1, \pm x_2, \pm x_3, \dots, \pm x_{n-1}, x_n\}$, where $n > 1$ is fixed, $x_i \in \mathbb{R}^+$, $i = 1, 2, 3, \dots, n$ and $x_1 < x_2 < x_3 < \cdots < x_n$. Let $\phi(\mathscr{B}_n)$ be the set of all non-empty subsets $S = \{u_1, u_2, \dots, u_t\}$ of $\mathscr{B}_n$ such that $|u_1| < |u_2| < \dots < |u_{t-1}| < u_t$ where $u_t \in \mathbb{R}^+$. Let $\mathscr{B}_n^+ = \{x_1, x_2, x_3, \dots, x_{n-1}, x_n\}$. For a fixed k, let V_1 be the set of k-element subsets of $\mathscr{B}_n^+$, $1 \leq k < n$. $V_2 = \phi(\mathscr{B}_n) - V_1$. For any $A \in V_2$, let $A^\dagger = \{|x| : x \in A\}$. Define 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 [11, 13] and is denoted by $H_B(n, k)$.

Definition 2.2. An r-**vertex** in $H_B(n, k)$ is an element in $\phi(\mathscr{B}_n)$ containing r elements, where $1 \leq r \leq n$. Members of $\phi(\mathscr{B}_n)$ are called r-**vertices**.

$H_B(n, k)$ for $n = 2, k = 1$ and $n = 3, k = 2$ are illustrated in Fig. 1 and Fig. 2.

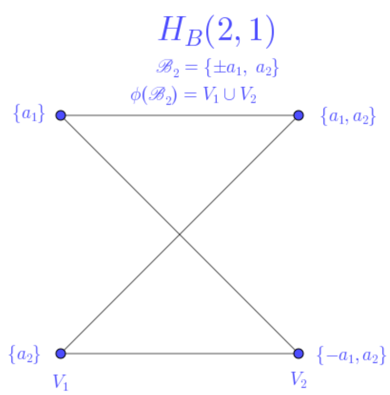

Figure 1. $H_B(2, 1)$

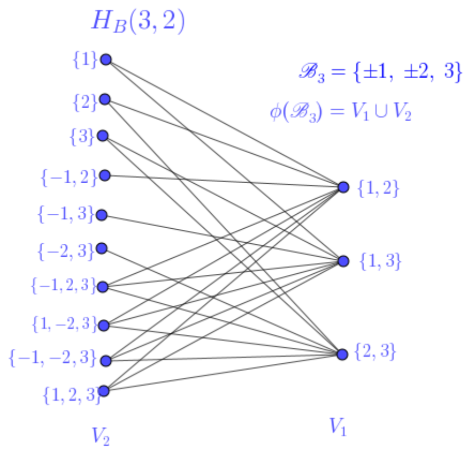

FIGURE 2. $H_B(3,2)$

Example 2.3. *The bipartition of* $H_B(4,2)$ *is given below:*

$$\mathscr{B}_4 = \{\pm 1,\ \pm 2,\ \pm 3,\ 4\}$$
$$V_1 = \big\{\{1,2\},\{1,3\},\{1,4\},\{2,3\},\{2,4\},\{3,4\}\big\}$$
$$\begin{aligned} V_2 = \big\{&\{1\},\{2\},\{3\},\{4\},\{-1,2\},\{-1,3\},\{-1,4\}\\ &\{-2,3\},\{-2,4\},\{-3,4\},\{1,2,3\},\{-1,2,3\},\{1,-2,3\},\{-1,-2,3\},\\ &\{1,2,4\},\{-1,2,4\},\{1,-2,4\},\{-1,-2,4\},\{2,3,4\},\{-2,3,4\},\\ &\{2,-3,4\},\{-2,-3,4\},\{1,3,4\},\{-1,3,4\},\{1,-3,4\},\{-1,-3,4\}\\ &\{1,2,3,4\},\{-1,2,3,4\},\{1,-2,3,4\},\{1,2,-3,4\},\{-1,-2,3,4\}\\ &\{1,-2,-3,4\},\{-1,2,-3,4\},\{-1,-2,-3,4\}\big\}\end{aligned}$$

Here, we summarise certain results proved by Jayakumar *et al.* [3] on $H_B(n,k)$.

Theorem 2.4. [3] *The order and size of* $H_B(n,k)$ *are given by* $|V| = \dfrac{3^n-1}{2}$ *and* $|E| = \binom{n}{k}\left(\dfrac{3^k-3}{2} + 2^{k-1}(3^{n-k}-1)\right)$.

Proposition 2.5. [3] *If* $n > 2$ *and* $1 < k < n$*, for the graph* $H_B(n,k)$*, the eccentricity of a vertex is given by*

$$e(v) = \begin{cases} 3 & \text{if } v \in V_1,\\ 2 & \text{if } v \in V_2 \text{ is an } n\text{-vertex},\\ 4 & \text{if } v \in V_2 \text{ is an } r\text{-vertex, } 1 \le r < n.\end{cases}$$

Proposition 2.6. [3]*Consider the bipartite Kneser B type-k graph $H_B(n,k))$, $n > 2$, $1 < k < n$. Let $d_h(v_i,v_j)$ be the number of unordered pairs of vertices for which $d(v_i,v_j) = h$. Then*

$$d_h(v_i,v_j) = \begin{cases} |E| & \text{if } h = 1, \\ \binom{\binom{n}{k}}{2} & \text{if } h = 2 \text{ and } v_i \text{ and } v_j \text{ are in } V_1, \\ \binom{n}{k}(|V| - \binom{n}{k}) - |E| & \text{if } h = 3, \end{cases}$$

Also, $d_2(v_i,v_j) + d_4(v_i,v_j) = \binom{|V|}{2} - (d_1(v_i,v_j) + d_3(v_i,v_j))$.

The degrees of vertices in $G = H_B(n,k)$ and the number of vertices having a specific degree are determined in [3]. The degree sequence is simply obtained by arranging the sequence.

$$\Big\{d(1)^{N(1)}, d(2)^{N(2)} \ldots, d(k-1)^{N(k-1)},$$
$$d_{V_1}(k)^{N_{V_1}(k)}, d_{V_2}(k)^{N_{V_2}(k)}, d(k+1)^{N(k+1)}, \ldots d(n)^{N(n)}\Big\}$$

of degrees with corresponding multiplicities as a monotonic non-increasing sequence. Here $d(r)$, where $r = 1,2,3,\ldots,k-1,k+1,\ldots n$, denotes the degrees of r-vertices in V_2 and $N(r)$ denotes the number of r-vertices. The values of $d(r)$ and $N(r)$ are given below:

$$d(1) = \binom{n-1}{k-1} \qquad N(1) = 2^0\binom{n}{1}$$
$$d(2) = \binom{n-2}{k-2} \qquad N(2) = 2^1\binom{n}{2}$$
$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$
$$d(k-1) = \binom{n-(k-1)}{k-(k-1)} \qquad N(k-1) = 2^{k-2}\binom{n}{k-1}$$
$$d_{V_1}(k) = \left(\frac{3^k-3}{2} + 2^{k-1}(3^{n-k}-1)\right) \qquad N_{V_1}(k) = \binom{n}{k}$$
$$d_{V_2}(k) = 1 \qquad N_{V_2}(k) = (2^{k-1}-1)\binom{n}{k}$$
$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$
$$d(k+1) = \binom{k+1}{k} \qquad N(k+1) = 2^k\binom{n}{k+1}$$
$$d(n) = \binom{n}{k} \qquad N(n) = 2^{n-1}\binom{n}{n}.$$

3. Topological indices of $H_B(n,k)$

Topological indices form an essential part of chemical graph theory, which correlates the physiochemical properties such as boiling point, melting point, infrared spectrum, electronic parameters, viscosity and density of the underlying chemical graphs. Topological indices are of different types, such as degree-based topological indices, distance-based topological indices, and spectrum-based topological indices. In this paper, we determined some eccentricity, distance, and degree-based topological indices of $G = H_B(n,k)$. They are the total eccentricity index, average eccentricity index, eccentric connectivity index, connective eccentricity index, first Zagreb eccentricity index, second Zagreb eccentricity index, terminal Wiener index, Wiener polarity index, Szeged index, vertex Padmakar-Ivan index and Sombor index. The M-polynomial of $H_B(n,k)$ is also determined.

Definition 3.1. For a simple graph G with vertex set $V(G)$, the total eccentricity index [14] is defined by$T\xi(G) = \sum_{v\in V(G)} e(v)$.

Definition 3.2. The average eccentricity index [2] of a graph G is the mean value of eccentricities of all vertices of a graph, that is,

$$avec(G) = \frac{1}{n} \sum_{v\in V(G)} e(v).$$

Definition 3.3. Let G be a simple graph with vertex set $V(G)$. The eccentric connectivity index [2] is defined by

$$\xi C(G) = \sum_{v\in V(G)} d(v)e(v).$$

Here $e(v)$ and $d(v)$ respectively denote the eccentricity and degree of any vertex v in G.

Definition 3.4. The connective eccentricity index [2] for a graph G is

$$C\xi(G) = \sum_{v\in V(G)} \frac{d(v)}{e(v)}.$$

Definition 3.5. First and second Zagreb eccentricity indices [8] are defined by

$$E_1 = E_1(G) = \sum_{v\in V(G)} [e(u)]^2 \quad \text{and} \quad E_2 = E_2(G) = \sum_{uv\in E(G)} e(u)e(v).$$

Definition 3.6. The Szeged index [10] is defined by

$$Sz(G) = \sum_{e=uv\in E(G)} n_u(e)n_v(e).$$

Here $n_u(e)$ is the number of vertices in G nearer to u than to v, and $n_v(e)$ is the number of vertices in G closer to v than to u.

Definition 3.7. The vertex Padmakar-Ivan index [9]of G denoted by $\mathrm{PI}_v(G)$ is defined by

$$PI_v(G) = \sum_{e=uv\in E(G)} (n_u(e) + n_v(e)).$$

Definition 3.8. The Wiener polarity index [1] is defined by

$$W_P(G) = d(G, 3)$$

where $d(G, 3)$ denotes the number of vertex pairs in G that has distance 3.

Definition 3.9. The terminal Wiener index [7] is defined by

$$TW(G) = \sum_{\{x,y\} \subseteq V_p(G)} d(x, y)$$

where $V_p(G)$ is the set of pendent vertices in G.

Definition 3.10. The Sombor index [5] of a simple graph G with edge set $E(G)$ is defined by

$$SO(G) = \sum_{v_i v_j \in E(G)} \sqrt{(deg(v_i}.$$

Definition 3.11. The M-polynomial of a graph G [6] is defined by

$$M(G; x, y) = \sum_{s \le t} m_{st}(G) x^s y^t,$$

where $m_{st}, (s, t \ge 1)$, is the number of edges uv in G such that $d_G(u) = s$ and $d_G(v) = t$.

4. Main Results

The Total Eccentricity Index (TEI) measures the degree of irregularity of a graph. Molecules with lower TEI values have more stable structures and are less reactive. In social and biological network analysis, TEI is used to quantify the degree of heterogeneity in the network.

Theorem 4.1. *The Total Eccentricity Index of $G = H_B(n, k)$ is given by*

$$T\xi(G) = 3\binom{n}{k} + 4\left(|V| - \binom{n}{k} - 2^{n-1}\right) + 2^n.$$

Proof. We know that $e(u) = 3, 2$ and 4 according to u is a k-vertex in V_1, an n-vertex in V_2, and an r-vertex, $1 \le r < n$ in V_2. Then $\sum_{u \text{ is an n-vertex in } V_2} e(u) = 4(|V| - \binom{n}{k} - 2^{n-1})$, $\sum_{u \in V_1} e(u) = 3\binom{n}{k}$ and $\sum_{u \text{ is an r-vertex in } V_2} e(u) = 2 \times 2^{n-1}$.

Therefore, $T\xi(G) = \sum_{v \in V(G)} e(v) = 3\binom{n}{k} + 4\left(|V| - \binom{n}{k} - 2^{n-1}\right) + 2^n$. □

Corollary 4.2. *The average eccentricity index of $G = H_B(n, k)$ is*

$$avec(G) = \frac{1}{n} \sum_{v \in V(G)} e(v) = \frac{1}{n}\left(3\binom{n}{k} + 4\left(|V| - \binom{n}{k} - 2^{n-1}\right) + 2^n\right).$$

Proof. The proof follows from the above theorem and the definition of the average eccentricity index. □

The eccentric connectivity index has been employed successfully for the development of numerous mathematical models for the prediction of biological activities of diverse nature:

Theorem 4.3. *The eccentric connectivity index of $G = H_B(n,k)$ is*

$$\xi^C(G) = 3\left(\frac{3^k-3}{2} + 2^{k-1}(3^{n-k}-1)\right)\binom{n}{k} + 4\left(\sum_{i=1}^{k-1} 2^{i-1}\binom{n}{i}\binom{n-i}{k-i}) + (2^{k-1}-1)\binom{n}{k} + \sum_{i=k+1}^{n-1} 2^{i-1}\binom{n}{i}\binom{i}{k}\right) + 2^n\binom{n}{k}.$$

Proof. $V(G) = V_1 \cup V_2$ where $V_1 = \{x \in G | x \text{ is a } k\text{-vertex}\}$, $V_2 = (W_1 \cup W_2 \cup \cdots \cup W_k \cup W_{k+1} \cup \cdots W_{n-1}) \cup W_n$. Here, $W_r, 1 \leq r \leq n$ are the sets of r-vertices in V_2.

$$\begin{aligned}
\xi^C(G) &= \sum_{x \in V} e(x)d(x) \\
&= \sum_{x \in V_1} e(x)d(x) + \sum_{x \in W_r, 1 \leq r \leq n-1} e(x)d(x) + \sum_{x \in W_n} e(x)d(x) \\
&= 3\left(\frac{3^k-3}{2} + 2^{k-1}(3^{n-k}-1)\right)\binom{n}{k} + \\
&\quad 4\left(\sum_{i=1}^{k-1} 2^{i-1}\binom{n}{i}\binom{n-i}{k-i} + (2^{k-1}-1)\binom{n}{k} + \sum_{i=k+1}^{n-1} 2^{i-1}\binom{n}{i}\binom{i}{k}\right) + 2^n\binom{n}{k}.
\end{aligned}$$

□

Corollary 4.4. *The connective eccentricity index of $G = H_B(n,k)$ is*

$$C^\xi(G) = \frac{1}{3}\left(\frac{3^k-3}{2} + 2^{k-1}(3^{n-k}-1)\right)\binom{n}{k} + \frac{1}{4}\left(\sum_{i=1}^{k-1} 2^{i-1}\binom{n}{i}\binom{n-i}{k-i} + (2^{k-1}-1)\binom{n}{k} + \sum_{i=k+1}^{n-1} 2^{i-1}\binom{n}{i}\binom{i}{k}\right) + 2^{n-2}\binom{n}{k}.$$

Proof.

$$\begin{aligned}
C^{\xi}(G) &= \sum_{v\in V(G)} \frac{d(v)}{e(v)} \\
&= \sum_{v\in V_1} \frac{d(v)}{e(v)} + \sum_{v\in W_r, 1\le r\le n-1} \frac{d(v)}{e(v)} + \sum_{v\in W_n} \frac{d(v)}{e(v)} \\
&= \frac{1}{3}\left(\frac{3^k-3}{2} + 2^{k-1}(3^{n-k}-1)\right)\binom{n}{k} + \\
&\quad \frac{1}{4}\left(\sum_{i=1}^{k-1} 2^{i-1}\binom{n}{i}\binom{n-i}{k-i} + (2^{k-1}-1)\binom{n}{k} + \sum_{i=k+1}^{n-1} 2^{i-1}\binom{n}{i}\binom{i}{k}\right) + \\
&\quad \frac{1}{2}\times 2^{n-1}\binom{n}{k}.
\end{aligned}$$

□

The first and second Zagreb eccentricity indices have been used in the development of Quantitative Structure Activity Relationship (QSAR) models for drug design and other applications in the pharmaceutical industry:

Theorem 4.5. *The first Zagreb eccentricity index of $G = H_B(n,k)$ is given by*

$$E_1(G) = 9\binom{n}{k} + 16\left(|V| - \binom{n}{k} - 2^{n-1}\right) + 2^{n+1}.$$

Proof.

$$\begin{aligned}
E_1(G) &= \sum_{u\in V(G)} [e(u)]^2 \\
&= \sum_{u\in V_1} [e(u)]^2 + \sum_{\substack{u \text{ is an } r\text{-vertex in } V_2 \\ 1\le r\le n-1}} [e(u)]^2 + \sum_{u \text{ is an } n\text{-vertex in } V_2} [e(u)]^2 \\
&= 3^2 \times \binom{n}{k} + 4^2 \times \left(|V| - \binom{n}{k} - 2^{n-1}\right) + 2^2 \times 2^{n-1} \\
&= 9\binom{n}{k} + 16\left(|V| - \binom{n}{k} - 2^{n-1}\right) + 2^{n+1}.
\end{aligned}$$

□

Theorem 4.6. *The second Zagreb eccentricity index of $G = H_B(n,k)$ is given by*

$$E_2(G) = 6(3^k-1) - 12 + 6\times 2^k(3^{n-k} - 2^{n-k} - 1) + 3\times 2^n.$$

Proof.

$$\begin{aligned}
E_2(G) &= \sum_{uv\in E(G)} e(u)e(v)\\
&= \sum_{\substack{uv\in E(G)\\ u\in V_1\\ v\in V_2 \text{is an } r\text{-vertex}\\ 1\le r\le n-1}} e(u)e(v) + \sum_{\substack{uv\in E(G)\\ u\in V_1\\ v\in V_2 \text{is an } n\text{-vertex}}} e(u)e(v)\\
&= (3\times 4)\left(2^0\binom{k}{1} + 2^1\binom{k}{2} + \cdots + 2^{k-1} - 1 + 2^k\binom{n-k}{1} + \cdots +\right.\\
&\quad \left. 2^{n-2}\binom{n-k}{n-k-1}\right) + (3\times 2)2^{n-1}\\
&= 12\left(\frac{3^k-1}{2}\right) - 12 + 12\times 2^k\left(\frac{3^{n-k}-2^{n-k}-1}{2}\right) + 3\times 2^n\\
&= 6(3^k-1) - 12 + 6\times 2^k(3^{n-k}-2^{n-k}-1) + 3\times 2^n.
\end{aligned}$$

□

Theorem 4.7. *The terminal Wiener index of* $G = H_B(n,k)$ *is*

$$TW(G) = 2\binom{2^{k-1}-1}{2}\binom{n}{k} + 4\left(\binom{(2^{k-1}-1)\binom{n}{k}}{2} - \binom{2^{k-1}-1}{2}\binom{n}{k}\right).$$

Proof. The set of pendant vertices in G is $T(G) = \{u \mid u \text{ is a } k\text{-vertex in } V_2\}$. Any k-vertex in V_2 is of degree 1 and $|T(G)| = (2^{k-1}-1)\binom{n}{k}$. The number of unordered pairs of vertices which are at distance 2 in $T(G)$ is $d_2(u,v) = \binom{2^{k-1}-1}{2}\binom{n}{k}$. The number of unordered pairs of vertices which are at distance 4 in $T(G)$ is $d_4(u,v) = \binom{(2^{k-1}-1)\binom{n}{k}}{2} - \binom{2^{k-1}-1}{2}\binom{n}{k}$. Therefore,

$$\begin{aligned}
TW(G) &= \sum_{\{u,v\}\in T(G)} d(u,v)\\
&= 2d_2(u,v) + 4d_4(u,v)\\
&= 2\binom{2^{k-1}-1}{2}\binom{n}{k} + 4\left(\binom{(2^{k-1}-1)\binom{n}{k}}{2} - \binom{2^{k-1}-1}{2}\binom{n}{k}\right).
\end{aligned}$$

□

In organic compounds like paraffin, the Wiener polarity index is the number of pairs of carbon atoms which are separated by three carbon-carbon bonds. Based on the Wiener index $W(G)$ and the Wiener polarity index $W_p(G)$, the formula $t_B = aW(G) + bW_p(G) + c$ was used to calculate the boiling points t_b of the paraffins where a, b and c are constants for a given isometry group.

Theorem 4.8. *The Wiener polarity index of $G = H_B(n,k)$ is*

$$W_P(G) = d(G,3) = \binom{n}{k}(\frac{3^n-1}{2} - \binom{n}{k}) - \binom{n}{k}\left(\frac{3^k-3}{2} + 2^{k-1}(3^{n-k}-1)\right).$$

Here $d(G,3)$ denotes the number of vertex pairs in G that are at distance 3.

Proof. The distance between a vertex in V_1 and a vertex in V_2 is either 1 or 3. The number of unordered pairs of vertices at distance 3 is $d_3(u,v) = \binom{n}{k}\left(|V| - \binom{n}{k}\right) - |E|$. Then the Wiener polarity index of G is $W_p(G) = d(G,3) = d_3(u,v) = \binom{n}{k}(\frac{3^n-1}{2} - \binom{n}{k}) - \binom{n}{k}\left(\frac{3^k-3}{2} + 2^{k-1}(3^{n-k}-1)\right)$. □

Theorem 4.9. *The Szeged index of $G = H_B(n,k)$ is*

$$\begin{aligned} Sz(G) = \binom{n}{k} d_{V_1}(k)\Bigg(& 2^0\binom{k}{1}\binom{n-1}{k-1} + 2^1\binom{k}{2}\binom{n-2}{k-2} + \cdots + \\ & 2^{k-2}\binom{k}{k-1}\binom{n-(k-1)}{k-(k-1)} + (2^{k-1}-1) + \\ & 2^k\binom{n-k}{1}\binom{k+1}{k} + \cdots 2^{n-1}\binom{n-k}{n-k}\binom{n}{k}\Bigg). \end{aligned}$$

Here the degree of a k-vertex u in V_1 is $d_{V_1}(k) = \left(\frac{3^k-3}{2} + 2^{k-1}(3^{n-k}-1)\right)$.

Proof. Let $u \in V_1$. Any vertex in V_1 has maximum degree

$d_{V_1}(k) = \left(\frac{3^k-3}{2} + 2^{k-1}(3^{n-k}-1)\right)$. Consider the edge $e = uv$.

Let $uv_1, uv_2, \ldots, uv_{d_{V_1}(k)-1}$ be the other edges having u as one end vertex. Then, the vertices in G nearer to u than to v are $u, v_1, v_2, \ldots, v_{d_{V_1}(k)-1}$. Therefore, $n_u(e) = d_{V_1}(k)$. Let n_r be the number of r-vertices, $1 \le r \le n$, adjacent to u in V_2. Then, the values of n_r are $2^0\binom{k}{1}, 2^1\binom{k}{2}, \ldots, 2^{k-1}-1, 2^k\binom{n-k}{1}, 2^{k+1}\binom{n-k}{2}, \ldots, 2^{n-1}$. Let $d(r)$ denote the degree of any r-vertex, $1 \le r \le n$, adjacent to u. The values of $d(r)$ are $\binom{n-1}{k-1}, \binom{n-2}{k-2}, \ldots, \binom{n-(k-1)}{k-(k-1)}, 1, \binom{k+1}{k}, \ldots, \binom{n}{k}$. The number of vertices in G closer to

v than to u is $n_v(e)$. For edges $uv_1, uv_2, \ldots, uv_{d_{V_1}(k)-1}$,

$$\sum_{e=uv_i\in E(G)} n_u(e)n_{v_i}(e) = d_{V_1}(k)\Bigg(\underbrace{(d(1)+d(1)+\ldots+d(1))}_{n_1}+\underbrace{(d(2)+d(2)+\ldots+d(2))}_{n_2}$$
$$+\ldots\underbrace{(d(k)+d(k)+\ldots+d(k))}_{n_k}+\ldots+$$
$$\underbrace{(d(n)+d(n)+\ldots+d(n))}_{n_n}\Bigg)$$
$$= d_{V_1}(k)\big(n_1d(1)+n_2d(2)+\ldots+n_{k-1}d(k-1)+$$
$$n_kd(k)+\ldots+n_nd(n)\big)$$
$$= d_{V_1}(k)\Bigg(2^0\binom{k}{1}\binom{n-1}{k-1}+2^1\binom{k}{2}\binom{n-2}{k-2}+\cdots+$$
$$2^{k-2}\binom{k}{k-1}\binom{n-(k-1)}{k-(k-1)}+(2^{k-1}-1)+$$
$$2^k\binom{n-k}{1}\binom{k+1}{k}+\cdots+2^{n-1}\binom{n-k}{n-k}\binom{n}{k}\Bigg).$$

The above summation is with respect to any vertex u in V_1. As there are $\binom{n}{k}$ vertices in V_1, we get the Szeged index as $Sz(G) = \binom{n}{k}\sum_{e=uv_i\in E(G)} n_u(e)n_{v_i}(e)$. □

Corollary 4.10. *An upper bound for the Wiener index of* $G = H_B(n,k)$ *is* $W(G) \leq \binom{n}{k}d_{V_1}(k)\Bigg(2^0\binom{k}{1}\binom{n-1}{k-1}+2^1\binom{k}{2}\binom{n-2}{k-2}+\cdots+2^{k-2}\binom{k}{k-1}\binom{n-(k-1)}{k-(k-1)}+(2^{k-1}-1)+$

$$2^k\binom{n-k}{1}\binom{k+1}{k}+\cdots+2^{n-1}\binom{n-k}{n-k}\binom{n}{k}\Bigg).$$

Proof. The proof follows from the inequality $W(G) \leq Sz(G)$ in [10] for a connected graph G. □

Theorem 4.11. *The vertex Padmakar-Ivan index of* $G = H_B(n,k)$ *is*

$$PI_v(G) = \sum_{e=uv\in E(G)} (n_u(e)+n_v(e))$$
$$= \binom{n}{k}\Bigg((d_{V_1}(k))^2+2^0\binom{k}{1}\binom{n-1}{k-1}+2^1\binom{k}{2}\binom{n-2}{k-2}+\cdots+$$
$$2^{k-2}\binom{k}{k-1}\binom{n-(k-1)}{k-(k-1)}+(2^{k-1}-1)+$$
$$2^k\binom{n-k}{1}\binom{k+1}{k}+\cdots+2^{n-1}\binom{n-k}{n-k}\binom{n}{k}\Bigg).$$

Proof. For the edges $uv_1, uv_2, \dots, uv_{d_{V_1}(k)-1}$,

$$\sum_{uv_i \in E(G)} (n_u(e) + n_{v_i}(e)) = d_{V_1}(k)(n_1 + n_2 + \dots + n_{k-1} + n_k + \dots + n_n) + n_1 d(1) + n_2 d(2) + \ldots + n_{k-1} d(k-1) + n_k d(k) + \ldots + n_n d(n)$$
$$= d_{V_1}(k) \times d_{V_1}(k) + 2^0 \binom{k}{1}\binom{n-1}{k-1} + 2^1 \binom{k}{2}\binom{n-2}{k-2} + \cdots + 2^{k-2}\binom{k}{k-1}\binom{n-(k-1)}{k-(k-1)} + (2^{k-1}-1) + 2^k \binom{n-k}{1}\binom{k+1}{k} + \cdots + 2^{n-1}\binom{n-k}{n-k}\binom{n}{k}.$$

Because of the existence of $\binom{n}{k}$ vertices in V_1, the vertex Padmakar-Ivan index of G is

$$PI_v(G) = \binom{n}{k}\left(\sum_{uv_i \in E(G)} (n_u(e) + n_{v_i}(e))\right)$$
$$= \binom{n}{k}\Bigg((d_{V_1}(k))^2 + 2^0 \binom{k}{1}\binom{n-1}{k-1} + 2^1 \binom{k}{2}\binom{n-2}{k-2} + \cdots + 2^{k-2}\binom{k}{k-1}\binom{n-(k-1)}{k-(k-1)} + (2^{k-1}-1) + 2^k \binom{n-k}{1}\binom{k+1}{k} + \cdots + 2^{n-1}\binom{n-k}{n-k}\binom{n}{k}\Bigg).$$

□

Theorem 4.12. *The Sombor index of $G = H_B(n,k)$ satisfies the inequality*

$$SO(G) \le \binom{n}{k}\Bigg[(d_{V_1}(k))^2 + (\sqrt{2}-1)\Bigg(2^0 \binom{k}{1}\binom{n-1}{k-1} + 2^1 \binom{k}{2}\binom{n-2}{k-2} + \cdots + 2^{k-2}\binom{k}{k-1}\binom{n-(k-1)}{k-(k-1)} + (2^{k-1}-1)\binom{n}{k} + 2^k \binom{n-k}{1}\binom{k+1}{k} + \cdots + 2^{n-1}\binom{n-k}{n-k}\binom{n}{k}\Bigg)\Bigg].$$

Proof. We know that the degree of any k-vertex in V_1 is $d_{V_1}(k)$. Also, the degree of any r-vertex where $1 \le r \le n$ in V_2 is $d(r)$. Let n_r be the number of r-vertices, $1 \le r \le n$ in V_2 adjacent to any k-vertex u of degree $d_{V_1}(k)$ in V_1. For $deg(v_i) \ge deg(v_j)$, the Sombor index of G will be $SO(G) = \sum_{v_i v_j \in E(G)} \sqrt{(deg(v_i))^2 + deg(v_j))^2} \le$

$\sum\limits_{v_iv_j\in E(G)}(deg(v_i)+(\sqrt{2}-1)deg(v_j))$. Also, $\sum\limits_{v_iv_j\in E(G)}(deg(v_i)+(\sqrt{2}-1)deg(v_j)) = \binom{n}{k}(\sum\limits_{r=1}^{n} d_{V_1}(k)+(\sqrt{2}-1)n_rd(r))$. Here,

$$\begin{aligned}\sum_{r=1}^{n} d_{V_1}(k)+(\sqrt{2}-1)n_rd(r) =& d_{V_1}(k)+(\sqrt{2}-1)n_1d(1)+d_{V_1}(k)+(\sqrt{2}-1)n_2d(2)+\\ & \cdots + d_{V_1}(k)+(\sqrt{2}-1)n_{k-1}d(k-1)+\\ & d_{V_1}(k)+(\sqrt{2}-1)n_kd(k)\\ & + d_{V_1}(k)+(\sqrt{2}-1)n_{k+1}d(k+1)+\cdots\\ & + d_{V_1}(k)+(\sqrt{2}-1)n_nd(n).\\ & = (d_{V_1}(k))^2+(\sqrt{2}-1)\Big(n_1d(1)+n_2d(2)+\cdots\\ & + n_{k-1}d(k-1)+\\ & n_kd(k)+n_{k+1}d(k+1)+\cdots+n_nd(n)\Big).\\ & = (d_{V_1}(k))^2+(\sqrt{2}-1)\Bigg(2^0\binom{k}{1}\binom{n-1}{k-1}+\\ & 2^1\binom{k}{2}\binom{n-2}{k-2}+\cdots+\\ & 2^{k-2}\binom{k}{k-1}\binom{n-(k-1)}{k-(k-1)}+(2^{k-1}-1)\binom{n}{k}+\\ & 2^k\binom{n-k}{1}\binom{k+1}{k}+\cdots+2^{n-1}\binom{n-k}{n-k}\binom{n}{k}\Bigg).\end{aligned}$$

Therefore,

$$\begin{aligned}SO(G)\leq \binom{n}{k}\Bigg[&(d_{V_1}(k))^2+(\sqrt{2}-1)\Bigg(2^0\binom{k}{1}\binom{n-1}{k-1}+2^1\binom{k}{2}\binom{n-2}{k-2}+\cdots+\\ & 2^{k-2}\binom{k}{k-1}\binom{n-(k-1)}{k-(k-1)}+(2^{k-1}-1)\binom{n}{k}+\\ & 2^k\binom{n-k}{1}\binom{k+1}{k}+\cdots+2^{n-1}\binom{n-k}{n-k}\binom{n}{k}\Bigg)\Bigg].\end{aligned}$$

□

Theorem 4.13. *The M-polynomial of $G=H_B(n,k)$ is*

$M(G;x,y)=\sum\limits_{d(i)\leq d_{V_1}(k)} m_{d(i)d_{V_1}(k)}(G)x^{d(i)}y^{d_{V_1}(k)}$, where $m_{d(i)d_{V_1}(k)}$ is the number of edges uv in G such that $d_G(u)=d_{V_1}(k)$ and $d_G(v)=d(i)$. Here $d(i)$ is the degree of an i-vertex in V_2 for $1\leq i\leq n$.

Proof. In the formula of M-polynomial, we replace s with $d(i)$ and t with $d_{V_1}(k)$. $M(G;x,y) = \sum_{s\leq t} m_{st}(G)x^s y^t = \sum_{d(i)\leq d_{V_1}(k)} m_{d(i)d_{V_1}(k)}(G)x^{d(i)}y^{d_{V_1}(k)}$. The degrees of the vertices in V_2 follow the order $d(1) > d(2) > \ldots > d(k-1) > d(k) = 1$ and $d(k) = 1 < d(k+1) < \ldots < d(n-1) < d(n)$. Here $d(i)$ represents the degree of the i-vertex in V_2 for $1 \leq i \leq n$. Also, every vertex in V_1 has a unique maximum degree $d_{V_1}(k)$. Number of edges having end vertices of degrees $d(i)$ and $d_{V_1}(k)$ is $m_{d(i)d_{V_1}(k)}(G) = d(i)N(i)$ where $N(i)$ is the number of i-vertices. □

Example 4.14. *We find the M-polynomial of $H_B(3,2)$. The values of $d(i)$ are $d(1) = 2,\ d(2) = 1,\ d(3) = 3$ and $d_{V_1}(k) = 7$. Values of $m_{d(i)d_{V_1}(k)}(G)$ are $m_{17} = 3,\ m_{27} = 6,\ m_{37} = 12$. Therefore, the M-polynomial of $G = H_B(3,2)$ is*

$$\begin{aligned} M(G;x,y) &= \sum_{d(i)\leq d_{V_1}(k)} m_{d(i)d_{V_1}(k)}(G)x^{d(i)}y^{d_{V_1}(k)} \\ &= 3xy^7 + 6x^2y^7 + 12x^3y^7. \end{aligned}$$

5. Conclusion

In this paper, we determined some eccentricity, distance, and degree-based topological indices of $G = H_B(n,k)$. They are the total eccentricity index, average eccentricity index, eccentric connectivity index, connective eccentricity index, first Zagreb eccentricity index, second Zagreb eccentricity index, terminal Wiener index, Wiener polarity index, Szeged index, vertex Padmakar-Ivan index and Sombor index. The M-polynomial of $H_B(n,k)$ is also determined.

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

Acknowledgement. The first author is a doctoral fellow in mathematics at University College, Thiruvananthapuram. This research has been promoted/supported by the University of Kerala.

References

[1] Adnan, Syed Ahtsham Ul Haq Bokhary, and Muhammad Imran, *On Wiener polarity index and Wiener index of certain triangular networks*, Journal of Chemistry (2021).

[2] Zaheer Ahmad, Abdul Qudair Baig, Muhammad Razwan Azhar, and Muhammad Imran, *Total eccentricity and average eccentricity indices of some chemical graphs: Carbon graphite and copper oxide*, Journal of Information and Optimization Sciences 41 (2020), 905–924.

[3] Jayakumar C., Sreekumar K.G., Manilal K., and Ismail Naci Cangul, *Invariants of Bipartite Kneser B type-k graphs.*, arXiv:2409.09317, 2024.

[4] Tamal Chowdhury and Ankita Pramanik, *LDPC Code Construction from Bipartite Kneser Graphs*, Proceedings of the 2nd International Conference on Communication, Devices and Computing, Springer, 2020, pp. 1-12.

[5] Kinkar Chandra Das, Ahmet Sinan Cevik, Ismail Naci Cangul, and Yilun Shang,*On Sombor index*, Symmetry 13 (2021), 1–12.

[6] Emeric Deutch and Sandi Klavzar, *M-Polynomial and degree-based topological indices*, arXiv:1407.1592 [math.CO], 2014.

[7] Ivan Gutman, Boris Furtula, and Miroslav Petrović, *Terminal Wiener index*, Journal Of Mathematical Chemistry 46 (2009), 522–531.

[8] Nazeran Idrees, Muhammad Saiff,Asia Rauf,and Saba Mustafa, *First and second Zagreb eccentricity indices of thorny graphs*, Symmetry 9 (2017), pp. 1-9.

[9] Padmakar V. Khadikar, Sneha Karmarkar, and Vijay K. Agrawal, *A Novel PI Index and its Applications to QSPR/QSAR Studies*, Journal of Chemical Information and Computer Sciences 41 (2001), 934–949.

[10] S. Klavzar and A. Rajapakse, *The Szeged and the Wiener index of graphs*, Appl. Math. Lett. 9 (1996), no. 5, 45–49.

[11] K. G. Sreekumar, Jayakumar C., Preenu C.S. & Manilal K., *A Study on Topological Indices of Bipartite Kneser B Type-1 Graphs*, Mathematics Of Intelligent Computing And Data Science, Springer Nature, pp. 117-129 (2025).

[12] K. G. Sreekumar and K. Manilal, *Automorphism groups of some families of bipartite graphs*, Electronic Journal of Graph Theory and Applications 9 (2021), no. 1, 65–75.

[13] K. G. Sreekumar, Suresh Singh G., and Preenu C.S., *Elliptic curves obtained from bipartite Kneser B type-k graphs*, TWMS J. Appl. Eng. Math. Special Issue -1 (2023), no. 01, 102–111.

[14] Kexiang Xu, Yaser Alizadeh, and Kinkar Chandra Das*On two eccentricity-based topological indices of graphs*, Discrete Applied Mathematics 233 (2017), 240–251.

Department of Mathematics, University College, University Of Kerala, Thiruvananthapuram, Kerala, India

Email address: jkcwarrier@gmail.com

Department of Mathematics,Karyavattom, University of Kerala, Thiruvananthapuram, Kerala, India

Email address: sreekumar3121@gmail.com

Department of Mathematics, University College, University of Kerala,Thiruvananthapuram, Kerala, India

Email address: manilalvarkala@gmail.com