



SCHULTZ POLYNOMIALS AND THEIR TOPOLOGICAL INDICES OF BOTTLENECK GRAPHS

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ABSTRACT

Let $G = (V, E)$ be a simple connected graph. The degree of a vertex u and the distance between the vertices u and v are denoted by d_u and $d(u, v)$ of a graph G respectively. The Schultz and modified Schultz polynomials are $Sc(G, x) = \sum_{(u,v) \in V(G)} (d_u + d_v) x^{d(u,v)}$

and $Sc^*(G, x) = \sum_{(u,v) \in V(G)} (d_u d_v) x^{d(u,v)}$ respectively. Then their first derivative at x

$= 1$ are equals to $Sc(G) = \sum_{(u,v) \in V(G)} (d_u + d_v) d(u, v)$ and

$Sc^*(G) = \sum_{(u,v) \in V(G)} (d_u d_v) d(u, v)$ are known as Schultz index and modified Schultz

index respectively. In this article, we compute the Schultz and modified Schultz polynomials and their indices for the bottleneck graphs $K_2 \circ K_n, \forall n \in N, K_2 \circ K_{m,n}, \forall m, n \in N$ and $K_2 \circ K_{m,n}, \forall m, n \in N, m \neq n$.

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INTRODUCTION

Let $G(V(G), E(G))$ be a simple connected graph, where $V(G)$ and $E(G)$ are the vertex and edge sets respectively. For vertices $u, v \in V(G)$, u is adjacent to v if they are connected by an edge. The degree of a vertex u is the number of vertices adjacent to u and is denoted as d_u . The distance between vertices u and v is the number of edges in a shortest path connecting them and is denoted as $d(u, v)$. The largest distance between any two vertices of a graph G is called the *diameter* of G and is denoted as $d(G)$.

A Topological index is a numerical quantity derived in an unambiguous manner from the structure graph of a molecule. As a graph structural invariant, i.e., it does not depend on the labelling or the pictorial representation of a graph. Various topological indices usually reflect molecular size and shape.

Distance is an important concept in graph theory and it has numerous applications in Computer science, Biology, Chemistry and a variety of other fields. Using the concept of distances in graph. H. Wiener defined a descriptor for explaining the boiling points of paraffins [16].

$$W(G) = \sum_{(u,v) \in V(G)} d(u, v) \tag{1}$$

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This descriptor is known as Wiener index. A topological index is a real number related to a structural graph of a molecule and it does not depend on the labelling or pictorial representation of a graph. A lot of topological indices have been introduced. Wiener index is one of the topological indices that correlate with some of the physico - chemical properties of the compound [2, 11].

Harry Schultz [15] introduced another distance based topological index known as Schultz index.

$$Sc(G, x) = \sum_{(u,v) \in V(G)} (d_u + d_v) x^{d(u,v)} \tag{2}$$

The Schultz index is closely related to the wiener index in the case of trees with relation [14].

$$Sc(G, x) = 4W(G) - n(n - 1) \tag{3}$$

Gutman et. al. [10] defined the modified Schultz index as,

$$Sc^*(G) = \sum_{(u,v) \in V(G)} (d_u d_v) d(u, v) \tag{4}$$

This topological index is also closely related to wiener index with relation [8].

$$Sc^*(G) = 4W(G) - n(2n - 1) \tag{5}$$

H. Hosoya [13] introduced a distance based polynomial to generate distance distribution for graphs called the Wiener polynomial.

$$H(G, x) = \sum_{(u,v) \in V(G)} x^{d(u,v)} \tag{6}$$

The first derivative of $H(G, x)$ at $x = 1$ is equal to Wiener index of a graph G .

Gutman [9] introduced new polynomials called the Schultz polynomial and the modified schultz polynomial as

$$Sc(G, x) = \sum_{(u,v) \in V(G)} (d_u + d_v) x^{d(u,v)} \tag{7}$$

$$Sc^*(G, x) = \sum_{(u,v) \in V(G)} (d_u d_v) x^{d(u,v)} \tag{8}$$

Such that their derivative at $x = 1$ are equal to the Schultz and modified Schultz indices. He also obtained some connection between these polynomials and Wiener polynomial of tree. For further details, we refer [3, 4, 5, 6, 7, 12].

The **Corona** of two graphs G_1 and G_2 is denoted by $G_1 \circ G_2$ and is obtained by taking one copy of G_1 and n_1 copies of G_2 and joining all vertices of the i^{th} copy of G_2 to the i^{th} vertex of G_1 for $i = 1, 2, \dots, n_1$. Unlike join, corona is a non - commutative operation and its component graphs appear in markedly asymmetric roles. Interesting classes of graphs can also be obtained by specializing the first component in the corona product. For example, for a graph G , the graph $K_2 \circ G$ is called its **bottleneck graph** [1].

Motivated by [9, 10, 15]. In this article, we study the schultz, modified schultz polynomials and their topological indices for bottleneck graphs $K_2 \circ K_n, \forall n \in N, K_2 \circ K_n, n, \forall n \in N$ and $K_2 \circ K_m, n \forall m, n \in N, m \neq n$.

RESULTS

In this section, we calculate the schultz polynomial and modified schultz polynomial and their indices of bottleneck graphs $K_2 \circ K_n, \forall n \in N, K_2 \circ K_n, n, \forall n \in N$ and $K_2 \circ K_m, n \forall m, n \in N, m \neq n$.

Theorem 1. Let $K_2 \circ K_n, \forall n \in N$ be the bottleneck graph, then

(i) The schultz polynomial is

$$Sc(K_2 \circ K_n, x) = [2(n^3 + n^2 + 2n + 1)]x^1 + [2n(2n + 1)]x^2 + [2n^3]x^3.$$

(ii) The schultz index is

$$Sc(K_2 \circ K_n) = 2(4n^3 + 5n^2 + 4n + 1).$$

(iii) The modified schultz polynomial is

$$Sc^*(K_2 \circ K_n, x) = [n^3(n + 1) + n(3n + 2) + 1]x^1 + [2n^2(n + 1)]x^2 + [n^4]x^3.$$

(iv) The modified schultz index is

$$Sc^*(K_2 \circ K_n) = n^3(4n + 5) + n(7n + 2) + 1.$$

Proof: Consider the bottleneck graph $K_2 \circ K_n, \forall n \in N$. Then the bottleneck graph of the kind $K_2 \circ K_n$ has $2(n+1)$ vertices and $n(n+1)+1$ edges. Among $2(n+1)$ vertices of $K_2 \circ K_n$, 2 vertices have degree $(n + 1)$ and remaining $2n$ vertices have degree n i.e., $|V_{(n+1)}| = 2$ and $|V_n| = 2n$.

The maximum distance between the vertices of a graph $K_2 \circ K_n$ is 3. Hence diameter of $(K_2 \circ K_n)$ i.e., $d(K_2 \circ K_n) = 3$. Now we compute the schultz and modified schultz polynomials and also the schultz and modified schultz indices of the bottleneck graph $(K_2 \circ K_n)$ by using the contents in table 1.

Now we calculate all 3-cases of $d(u,v)$ edge-paths of $(K_2 \circ K_n)$ by using Table 1.

Table 1

$d(u, v)$ = i	degree of d_u, d_v	Number of i-edges paths	Term of $Sc(G, x)$	Term of $Sc^*(G, x)$
1	$(n + 1), (n + 1)$	1	$2(n + 1)$	$(n + 1)^2$
1	n, n	$n(n - 1)$	$2n^2(n - 1)$	$n^3(n - 1)$
1	$n, (n + 1)$	$2n$	$2n(2n + 1)$	$2n^2(n + 1)$
2	$(n + 1), (n + 1)$	0	0	0
2	n, n	0	0	0
2	$n, (n + 1)$	$2n$	$2n(2n + 1)$	$2n^2(n + 1)$
2	$(n + 1), (n + 1)$	0	0	0
3	n, n	$n2$	$2n^3$	$n4$
3	$n, (n + 1)$	0	0	0

Explanation of Table 1

CASE 1: If $\forall u, v \in V (K_2 \circ K_n), d(u, v) = 1$ then we have following 3-cases to calculate first term of schultz and modified schultz polynomial of $(K_2 \circ K_n)$.

Subcase 1.1. For a vertex $v \in V_{n+1}$, there is one path with length one until a vertex $u \in V_{n+1}$. Thus we have one edge, such that $d_u + d_v = 2(n + 1)$ and $d_u \times d_v = (n + 1)^2$. Therefore we have two terms $2(n + 1)x^1$ and $(n + 1)^2x^1$ of the schultz and modified schultz polynomials of $(K_2 \circ K_n)$ respectively.

Subcase 1.2. Now consider a vertex $v \in V_n$, there are $n(n-1)$ paths with length one until a vertex $u \in V_n$. Thus we have $n(n-1)$ edges, such that $d_u + d_v = 2n$ and $d_u \times d_v = n^2$. Therefore the schultz and modified schultz polynomials of $(K_2 \circ K_n)$ are $2n^2(n-1)x^1$ and $n^3(n-1)x^1$ respectively.

Subcase 1.3. Next consider a vertex $v \in V_n$, there are $2n$ paths with length one until a vertex $u \in V_{n+1}$. Thus we have $2n$ edges, such that $d_u + d_v = 2n + 1$ and $d_u \times d_v = n(n + 1)$. Therefore the schultz and modified schultz polynomials of $(K_2 \circ K_n)$ are $2n(2n + 1)x^1$ and $2n^2(n + 1)x^1$ respectively.

CASE 2. If $\forall u, v \in V (K_2 \circ K_n), d(u, v) = 2$ then we have following 3-subcases to calculate second term of schultz and modified schultz polynomial of $(K_2 \circ K_n)$.

Subcase 2.1. For a vertex $v \in V_{n+1}$, there are no paths of length two until a vertex $u \in V_{n+1}$. Thus we have zero edges, such that the schultz and modified schultz polynomials of $(K_2 \circ K_n)$ are zero.

Subcase 2.2. For a vertex $v \in V_n$, there are no paths of length two until a vertex $u \in V_n$. Thus we have zero edges, such that the schultz and modified schultz polynomials of $(K_2 \circ K_n)$ are zero.

Subcase 2.3. Next consider a vertex $v \in V_n$, there are $2n$ paths with length two until a vertex $u \in V_{n+1}$. Thus we have $2n$ edges, such that $d_u + d_v = 2n + 1$ and $d_u \times d_v = n(n + 1)$. Therefore the second term of schultz and modified schultz polynomials of $(K_2 \circ K_n)$ are $2n(2n + 1)x^2$ and $2n^2(n + 1)x^2$ respectively.

CASE 3. If $\forall u, v \in V (K_2 \circ K_n), d(u, v) = 3$ then we have following 3-subcases to calculate third term of schultz and modified schultz polynomial of $(K_2 \circ K_n)$.

Subcase 3.1. For a vertex $v \in V_{n+1}$, there are no paths of length three until a vertex $u \in V_{n+1}$. Thus we have zero edges, such that the schultz and modified schultz polynomials of $(K_2 \circ K_n)$ are zero.

Subcase 3.2. Next consider a vertex $v \in V_n$, there are n^2 paths with length three until a vertex $u \in V_n$. Thus we have n^2 edges, such that $d_u + d_v = 2n$ and $d_u \times d_v = n^2$. Therefore the schultz and modified schultz polynomials of $(K_2 \circ K_n)$ are $2n^3x^3$ and n^4x^3 respectively.

Subcase 3.3. For a vertex $v \in V_n$, there are no paths of length three until a vertex $u \in V_{n+1}$. Thus we have zero edges, such that the schultz and modified schultz polynomials of $(K_2 \circ K_n)$ are zero.

From the definition of schultz, modified schultz polynomial and above mentions, we have following results.

$$\begin{aligned} Sc(K_2 \circ K_n, x) &= \sum_{(u,v) \in V(K_2 \circ K_n)} (d_u + d_v) x^{d(u,v)} \\ &= [2(n+1) + 2n^2(n-1) + 2n(2n+1)]x^1 + [2n(2n+1)]x^2 + [2n^3]x^3 \\ &= [2(n^3 + n^2 + 2n + 1)]x^1 + [2n(2n+1)]x^2 + [2n^3]x^3. \end{aligned}$$

From the definition of schultz index, we can compute the schultz index of $(K_2 \circ K_n)$ by the first derivative of schultz polynomial of $(K_2 \circ K_n)$ [evaluating at $x = 1$] as follows:

$$\begin{aligned} Sc(K_2 \circ K_n) &= \left. \frac{\partial Sc(K_2 \circ K_n, x)}{\partial x} \right|_{x=1} \\ &= \left. \frac{\partial}{\partial x} ([2(n^3 + n^2 + 2n + 1)]x^1 + [2n(2n+1)]x^2 + [2n^3]x^3) \right|_{x=1} \\ &= 2[4n^3 + 5n^2 + 4n + 1] \end{aligned}$$

And also from equation (8), the modified schultz polynomial of $(K_2 \circ K_n)$ is,

$$\begin{aligned} Sc^*(K_2 \circ K_n, x) &= \sum_{(u,v) \in V(K_2 \circ K_n)} (d_u d_v) x^{d(u,v)} \\ &= [(n+1)^2 + n^3(n-1) + 2n^2(n+1)]x^1 + [2n^2(n+1)]x^2 + [n^4]x^3 \\ &= [n^3(n+1) + n(3n+2) + 1]x^1 + [2n^2(n+1)]x^2 + [n^4]x^3. \end{aligned}$$

Again we can compute modified schultz index of $(K_2 \circ K_n)$ by first derivative of modified schultz polynomial of $(K_2 \circ K_n)$ [evaluated at $x = 1$] as follows:

$$\begin{aligned} Sc^*(K_2 \circ K_n) &= \left. \frac{\partial Sc^*(K_2 \circ K_n, x)}{\partial x} \right|_{x=1} \\ &= \left. \frac{\partial}{\partial x} ([n^3(n+1) + n(3n+2) + 1]x^1 + [2n^2(n+1)]x^2 + [n^4]x^3) \right|_{x=1} \\ &= n^3[4n + 5] + n[7n + 2] + 1. \end{aligned}$$

Theorem 2: Let $K_2 \circ K_n, \forall n \in \mathbb{N}$ be the bottleneck graph, then,

(i) The schultz polynomial is

$$Sc(K_2 \circ K_n, x) = [2(2n^3 + 1) + 4n(4n+3)]x^1 + [4n(n^2 + 3n+1)]x^2 + [8n^2(n+1)]x^3.$$

(ii) The schultz index is

$$Sc(K_2 \circ K_n) = 36n^3 + 64n^2 + 20n + 2.$$

(iii) The modified schultz polynomial is

$$Sc^*(K_2 \circ K_n, x) = [2n^4 + 12n^3 + 18n^2 + 8n + 1]x^1 + 2n[n^3 + 5n(n+1) + 1]x^2 + [4n^2(n+1)^2]x^3.$$

(iv) The modified schultz index is

$$Sc^*(K_2 \circ K_n) = 18n^4 + 56n^3 + 50n^2 + 12n + 1.$$

Proof: Consider the bottleneck graph $K_2 \circ K_n, \forall n \in \mathbb{N}$. Then the bottleneck graph of this kind contains $2(2n+1)$ vertices and $2n(n+2) + 1$ edges. Among $2(2n+1)$ vertices of $K_2 \circ K_n$, 2 vertices have degree $(2n+1)$ and remaining $4n$ vertices have

degree $(n+1)$ i.e., $|V_{(2n+1)}| = 2$ and $|V_{(n+1)}| = 4n$.

Here the distance between vertices of the graph $(K_2 \circ K_n)$ are upto 3 and diameter i.e., $d(K_2 \circ K_n) = 3$.

Now we have calculate all cases of $d(u,v)$ edge paths $d(u,v) = 1, 2, 3$ of $(K_2 \circ K_n)$ for the term of schultz and modified schultz polynomial in table 2.

Table 2

$d=i$	degree of d_u, d_v	No. of i -edge paths	Term of $Sc(G,x)$	Term of $Sc^*(G,x)$
1	$(2n+1), (2n+1)$	1	$2(2n+1)$	$(2n+1)^2$
1	$(n+1), (n+1)$	$2n^2$	$4n^2(n+1)$	$2n^2(n+1)^2$
1	$(2n+1), (n+1)$	$4n$	$4n(3n+2)$	$4n(2n+1)(n+1)$
2	$(2n+1), (2n+1)$	0	0	0
2	$(n+1), (n+1)$	$2n(n-1)$	$4n(n^2-1)$	$2n(n-1)(n+1)^2$
2	$(2n+1), (n+1)$	$4n$	$4n(3n+2)$	$4n(n+1)(2n+1)$
3	$(2n+1), (2n+1)$	0	0	0
3	$(n+1), (n+1)$	$4n^2$	$8n^2(n+1)$	$4n^2(n+1)^2$
3	$(2n+1), (n+1)$	0	0	0

Explanation of Table 2

CASE 1. If $\forall u,v \in V (K_2 \circ K_{n,n}), d(u,v) = 1$ then we have following 3-cases to calculate first term of schultz and modified schultz polynomial of $(K_2 \circ K_{n,n})$.

Subcase 1.1. For a vertex $v \in V_{2n+1}$, there is one path with length one untill a vertex $u \in V_{2n+1}$. Thus we have one edge, such that $d_u + d_v = 2(2n+1)$ and $d_u \times d_v = (2n+1)^2$. Therefore the first terms of the schultz and modified schultz polynomials of $(K_2 \circ K_{n,n})$ is $2(2n+1)x^1$ and $(2n+1)^2x^1$ respectively.

Subcase 1.2. Now consider a vertex $v \in V_{n+1}$, there are $2n^2$ paths with length one untill a vertex $u \in V_{n+1}$. Thus we have $2n^2$ edges, such that $d_u + d_v = 2(n+1)$ and $d_u \times d_v = (n+1)^2$. Therefore the first term of schultz and modified schultz polynomials of $(K_2 \circ K_{n,n})$ are $[4n^2(n+1)]x^1$ and $[2n^2(n+1)^2]x^1$ respectively.

Subcase 1.3. Next consider a vertex $v \in V_{2n+1}$, there are $4n$ paths with length one untill a vertex $u \in V_{n+1}$. Thus we have $4n$ edges, such that $d_u + d_v = 3n+2$ and $d_u \times d_v = (2n+1)(n+1)$. Then the first term schultz and modified schultz polynomials of $(K_2 \circ K_{n,n})$ are $[4n(3n+2)]x^1$ and $[4n(2n+1)(n+1)]x^1$ respectively.

CASE 2. If $\forall u,v \in V (K_2 \circ K_{n,n}), d(u,v) = 2$ then we have following 3-subcases to calculate second term of schultz and modified schultz polynomial of $(K_2 \circ K_{n,n})$.

Subcase 2.1. For a vertex $v \in V_{2n+1}$, there are no paths of length two untill a vertex $u \in V_{2n+1}$. Thus we have zero edges, such that the schultz and modified schultz polynomials of $(K_2 \circ K_{n,n})$ are zero.

Subcase 2.2. Now consider a vertex $v \in V_{n+1}$, there are $2n(n-1)$ paths with length two untill a vertex $u \in V_{n+1}$. Thus we have $2n(n-1)$ edges, such that $d_u + d_v = 2(n+1)$ and $d_u \times d_v = (n+1)^2$. Therefore the second term of schultz and modified schultz polynomials of $(K_2 \circ K_{n,n})$ are $[4n(n^2-1)]x^2$ and $[2n(n-1)(n+1)^2]x^2$ respectively.

Subcase 2.3. Next consider a vertex $v \in V_{2n+1}$, there are $4n$ paths with length two untill a vertex $u \in V_{n+1}$. Thus we have $4n$ edges, such that $d_u + d_v = (3n+2)$ and $d_u \times d_v = (2n+1)(n+1)$. Then the second term of schultz and modified schultz polynomials of $(K_2 \circ K_{n,n})$ are $[4n(3n+2)]x^2$ and $[4n(2n+1)(n+1)]x^2$ respectively.

CASE 3: If $\forall u,v \in V (K_2 \circ K_{n,n}), d(u,v) = 3$ then we have following 3-subcases to calculate third term of schultz and modified schultz polynomial of $(K_2 \circ K_{n,n})$.

Subcase 3.1. For a vertex $v \in V_{2n+1}$, there are no paths of length three untill a vertex $u \in V_{2n+1}$. Thus we have zero edges,

such that the schultz and modified schultz polynomials of $(K_2 \circ K_{n,n})$ are zero.

Subcase 3.2. Next consider a vertex $v \in V_{n+1}$, there are $4n^2$ paths with length three untill a vertex $u \in V_{n+1}$. Thus we have $4n^2$ edges, such that $d_u + d_v = 2(n+1)$ and $d_u \times d_v = (n+1)^2$. Therefore the third term of schultz and modified schultz polynomials of $(K_2 \circ K_{n,n})$ are $[8n^2(n+1)]x^3$ and $[4n^2(n+1)^2]x^3$ respectively.

Subcase 3.3. For a vertex $v \in V_{2n+1}$, there are no paths of length three untill a vertex $u \in V_{n+1}$. Thus we have zero edges, such that the schultz and modified schultz polynomials of $(K_2 \circ K_{n,n})$ are zero.

From the definition of schultz, modified schultz polynomial and above mentions cases we have following results.

$$\begin{aligned}
 Sc(K_2 \circ K_{n,n}, x) &= \sum_{(u,v) \in V(K_2 \circ K_{n,n})} (d_u + d_v) x^{d(u,v)} \\
 &= [2(2n+1) + 4n^2(n+1) + 4n(3n+2)]x^1 + [4n(n^2-1) \\
 &\quad + 4n(3n+2)]x^2 + [8n^2(n+1)]x^3 \\
 &= [2(2n^3+1) + 4n(4n+3)]x^1 + [4n(n^2+3n+1)]x^2 + [8n^2(n+1)]x^3.
 \end{aligned}$$

From the definition of schultz index, we compute the schultz index of $(K_2 \circ K_{n,n})$ by the first derivative of schultz polynomial of $(K_2 \circ K_{n,n})$ [evaluating at $x = 1$] as follows:

$$\begin{aligned}
 Sc(K_2 \circ K_{n,n}) &= \frac{\partial Sc(K_2 \circ K_{n,n}, x)}{\partial x} \Big|_{x=1} \\
 &= \frac{\partial}{\partial x} \left([2(2n^3+1) + 4n(4n+3)]x^1 + [4n(n^2+3n+1)]x^2 \right. \\
 &\quad \left. + [8n^2(n+1)]x^3 \right) \Big|_{x=1} \\
 &= 36n^3 + 64n^2 + 20n + 2.
 \end{aligned}$$

And also modified schultz polynomial of $(K_2 \circ K_{n,n})$ is,

$$\begin{aligned}
 Sc^*(K_2 \circ K_{n,n}, x) &= \sum_{(u,v) \in V(K_2 \circ K_{n,n})} (d_u d_v) x^{d(u,v)} \\
 &= [(2n+1)^2 + 2n^2(n+1)^2 + 4n(2n+1)(n+1)]x^1 + [2n(n-1)(n+1) \\
 &\quad + 4n(n+1)(2n+1)]x^2 + [4n^2(n+1)^2]x^3 \\
 &= [2n^4 + 12n^3 + 18n^2 + 8n + 1]x^1 + 2n[n^3 + 5n(n+1) + 1]x^2 + [4n^2(n+1)^2]x^3.
 \end{aligned}$$

Now we compute modified schultz index of $(K_2 \circ K_{n,n})$ by first derivative of modified schultz polynomial of $(K_2 \circ K_{n,n})$ [evaluated at $x = 1$] as follows:

$$\begin{aligned}
 Sc^*(K_2 \circ K_{n,n}) &= \frac{\partial Sc^*(K_2 \circ K_{n,n}, x)}{\partial x} \Big|_{x=1} \\
 &= \frac{\partial}{\partial x} \left([2n^4 + 12n^3 + 18n^2 + 8n + 1]x^1 + 2n[n^3 + 5n(n+1) + 1]x^2 \right. \\
 &\quad \left. + [4n^2(n+1)^2]x^3 \right) \Big|_{x=1} \\
 &= 18n^4 + 56n^3 + 50n^2 + 12n + 1.
 \end{aligned}$$

Theorem 3: Let $K_2 \circ K_{m,n} \forall m, n \in \mathbb{N}, m \neq n$. be the bottleneck graph, then

(i) The schultz polynomial is

$$Sc(K_2 \circ K_{m,n}, x) = 2[(m^2 + n^2) + (m+n)(mn+3) + 6mn + 1]x^1 + 2[2(m^2 + n^2) + (m+n)(mn+1) + 2mn]x^2 + 2[(m^2 + n^2) + 2mn(m+n+1)]x^3.$$

(ii) The schultz index is

$$Sc(K_2 \circ K_{m,n}) = 2[8(m^2 + n^2) + 16mn + 1 + (m+n)(9mn + 5)].$$

(iii) The modified schultz polynomial is

$$\begin{aligned}
 Sc^*(K_2 \circ K_{m,n}, x) &= [3(m^2 + n^2) + (6mn + 4)(m+n) + 2mn(mn+6) + 1]x^1 + [3(m^2 + n^2) \\
 &\quad + (m+n)[5mn + 1] + 2mn(mn+2)]x^2 + [4mn(mn+m+n) + (m+n)^2]x^3.
 \end{aligned}$$

(iv) The modified schultz index is

$$Sc^*(K_2 \circ K_{m,n}) = 12(m^2 + n^2) + 2mn(9mn + 13) + (28mn + 6)(m + n) + 1.$$

Proof: Consider the bottleneck graph $K_2 \circ K_{m,n} \forall m, n \in \mathbb{N}, m \neq n$. Then the bottleneck graph of this kind contains $2(m + n) + 2$ vertices and $[2(m + n + mn) + 1]$ edges. Among $2(m + n) + 2$ vertices of $K_2 \circ K_{m,n}$, 2 vertices have degree $(m + n + 1)$, $2m$ vertices have degree $(n + 1)$ and $2n$ vertices have degree $m + 1$ i.e., $|V_{(m+n+1)}| = 2, |V_{(n+1)}| = 2m$ and $|V_{(m+1)}| = 2n$.

Here the distance between vertices of the graph $(K_2 \circ K_{m,n})$ are upto 3 and diameter i.e., $d(K_2 \circ K_{m,n}) = 3$. Now we compute the terms of schultz, modified schultz polynomial of the bottleneck graph $(K_2 \circ K_{m,n})$ by using the table 3.

Table 3

$d=i$	degree of d_u, d_v	No. of i -edge paths	Term of $Sc(G, x)$	Term of $Sc^*(G, x)$
1	$(m + n + 1), (m + n + 1)$	1	$2(m + n + 1)$	$(m + n + 1)^2$
1	$(m + n + 1), (n + 1)$	$2m$	$2m(m + 2n + 2)$	$2m(m + n + 1)(n + 1)$
1	$(m + n + 1), (m + 1)$	$2n$	$2n(2m + n + 2)$	$2n(m + n + 1)(m + 1)$
1	$(n + 1), (n + 1)$	0	0	0
1	$(n + 1), (m + 1)$	$2mn$	$2mn(m + n + 2)$	$2mn(n + 1)(m + 1)$
1	$(m + 1), (m + 1)$	0	0	0
2	$(m + n + 1), (m + n + 1)$	0	0	0
2	$(m + n + 1), (n + 1)$	$2m$	$2m(m + 2n + 2)$	$2m(m + n + 1)(n + 1)$
2	$(m + n + 1), (m + 1)$	$2n$	$2n(2m + n + 2)$	$2n(m + n + 1)(m + 1)$
2	$(n + 1), (n + 1)$	$m(m - 1)$	$2m(m - 1)(n + 1)$	$m(m - 1)(n + 1)^2$
2	$(n + 1), (m + 1)$	0	0	0
2	$(m + 1), (m + 1)$	$n(n - 1)$	$2n(n - 1)(m + 1)$	$n(n - 1)(m + 1)^2$
3	$(m + n + 1), (m + n + 1)$	0	0	0
3	$(m + n + 1), (n + 1)$	0	0	0
3	$(m + n + 1), (m + 1)$	0	0	0
3	$(n + 1), (n + 1)$	m^2	$2m^2(n + 1)$	$m^2(n + 1)^2$
3	$(n + 1), (m + 1)$	$2mn$	$2mn(m + n + 2)$	$2mn(n + 1)(m + 1)$
3	$(m + 1), (m + 1)$	n^2	$2n^2(m + 1)$	$n^2(m + 1)^2$

Explanation of the table 3

Case 1. If $\forall u, v \in V (K_2 \circ K_{m,n}), d(u, v) = 1$ then we have following 3-cases to calculate first term of schultz and modified schultz polynomial of $(K_2 \circ K_{m,n})$.

Subcase 1.1. For a vertex $v \in V_{m+n+1}$, there is one path with length one until a vertex $u \in V_{m+n+1}$. Thus we have one edge, such that $d_u + d_v = 2(m+n+1)$ and $d_u \times d_v = (m+n+1)^2$. Therefore the first terms of the schultz and modified schultz polynomials of $(K_2 \circ K_{m,n})$ is $2(m + n + 1)x^1$ and $(m + n + 1)^2x^1$ respectively.

Subcase 1.2. For a vertex $v \in V_{m+n+1}$, there is $2m$ path with length one until a vertex $u \in V_{n+1}$. Thus we have $2m$ edge, such that $d_u + d_v = (m+2n+2)$ and $d_u \times d_v = (m+n+1)(n+1)$. Therefore the first terms of the schultz and modified schultz polynomials of $(K_2 \circ K_{m,n})$ is $[2m(m + 2n + 2)]x^1$ and $[2m(m + n + 1)(n + 1)]x^1$ respectively.

Subcase 1.3. For a vertex $v \in V_{m+n+1}$, there is $2n$ path with length one until a vertex $u \in V_{m+1}$. Thus we have $2n$ edge, such that $d_u + d_v = (2m+n+2)$ and $d_u \times d_v = (m+n+1)(m+1)$. Therefore the first terms of the schultz and modified schultz polynomials of $(K_2 \circ K_{m,n})$ is $[2n(2m + n + 2)]x^1$ and $[2n(m + n + 1)(m + 1)]x^1$ respectively.

Subcase 1.4. For a vertex $v \in V_{n+1}$, there are no paths of length one until a vertex $u \in V_{n+1}$. Thus we have zero edges, such that the schultz and modified schultz polynomials of $(K_2 \circ K_{m,n})$ are zero.

Subcase 1.5. For a vertex $v \in V_{n+1}$, there is $2mn$ paths with length one until a vertex $u \in V_{m+1}$. Thus we have $2mn$ edge, such that $d_u + d_v = (m+n+2)$ and $d_u \times d_v = (m+1)(n+1)$. Therefore the first terms of the schultz and modified schultz polynomials of $(K_2 \circ K_{m,n})$ is $[2mn(m + n + 2)]x^1$ and $[2mn(n + 1)(m + 1)]x^1$ respectively.

Subcase 1.6. For a vertex $v \in V_{m+1}$, there are no paths of length one until a vertex $u \in V_{m+1}$. Thus we have zero edges, such that the schultz and modified schultz polynomials of $(K_2 \circ K_{m,n})$ are zero.

CASE 2: If $\forall u, v \in V (K_2 \circ K_{m,n}), d(u, v) = 2$ then we have following 3-cases to calculate first term of schultz and modified schultz polynomial of $(K_2 \circ K_{m,n})$.

Subcase 2.1. For a vertex $v \in V_{m+n+1}$, there are no paths of length two until a vertex $u \in V_{m+n+1}$. Thus we have zero edges, such that the schultz and modified schultz polynomials of $(K_2 \circ K_{m,n})$ are zero.

Subcase 2.2. For a vertex $v \in V_{m+n+1}$, there is $2m$ path with length two until a vertex $u \in V_{n+1}$. Thus we have $2m$ edge, such that $d_u + d_v = (m+2n+2)$ and $d_u \times d_v = (m+n+1)(n+1)$. Therefore the second terms of the schultz and modified schultz polynomials of $(K_2 \circ K_{m,n})$ is $[2m(m + 2n + 2)]x^2$ and $[2m(m + n + 1)(n + 1)]x^2$ respectively.

Subcase 2.3. For a vertex $v \in V_{m+n+1}$, there is $2n$ path with length one until a vertex $u \in V_{m+1}$. Thus we have $2n$ edge, such that $d_u + d_v = (2m+n+2)$ and $d_u \times d_v = (m+n+1)(m+1)$. Therefore the second terms of the schultz and modified schultz polynomials of $(K_2 \circ K_{m,n})$ is $[2n(2m + n + 2)]x^2$ and $[2n(m + n + 1)(m + 1)]x^2$ respectively.

Subcase 2.4. For a vertex $v \in V_{n+1}$, there is $m(m-1)$ paths with length two until a vertex $u \in V_{n+1}$. Thus we have $m(m - 1)$ edges, such that $d_u + d_v = 2(n + 1)$ and $d_u \times d_v = (n + 1)^2$. Therefore the second terms of the schultz and modified schultz polynomials of $(K_2 \circ K_{m,n})$ is $[2m(m - 1)(n + 1)]x^2$ and $[m(m - 1)(n + 1)^2]x^2$ respectively.

Subcase 2.5. For a vertex $v \in V_{n+1}$, there are no paths of length two until a vertex $u \in V_{m+1}$. Thus we have zero edges, such that the schultz and modified schultz polynomials of $(K_2 \circ K_{m,n})$ are zero.

Subcase 2.6. For a vertex $v \in V_{m+1}$, there is $n(n-1)$ paths with length two until a vertex $u \in V_{m+1}$. Thus we have $n(n - 1)$ edges, such that $d_u + d_v = 2(m + 1)$ and $d_u \times d_v = (m + 1)^2$. Therefore the second terms of the schultz and modified schultz polynomials of $(K_2 \circ K_{m,n})$ is $[2m(n - 1)(m + 1)]x^2$ and $[n(n - 1)(m + 1)^2]x^2$ respectively.

CASE 3. If $\forall u, v \in V (K_2 \circ K_{m,n}), d(u, v) = 2$ then we have following 3-cases to calculate first term of schultz and modified schultz polynomial of $(K_2 \circ K_{m,n})$.

Subcase 3.1. For a vertex $v \in V_{m+n+1}$, there are no paths of length three until a vertex $u \in V_{m+n+1}$. Thus we have zero edges, such that the schultz and modified schultz polynomials of $(K_2 \circ K_{m,n})$ are zero.

Subcase 3.2. For a vertex $v \in V_{m+n+1}$, there are no paths of length three until a vertex $u \in V_{n+1}$. Thus we have zero edges, such that the schultz and modified schultz polynomials of $(K_2 \circ K_{m,n})$ are zero.

Subcase 3.3. For a vertex $v \in V_{m+n+1}$, there are no paths of length three until a vertex $u \in V_{m+1}$. Thus we have zero edges, such that the schultz and modified schultz polynomials of $(K_2 \circ K_{m,n})$ are zero.

Subcase 3.4. For a vertex $v \in V_{n+1}$, there is m^2 paths with length three until a vertex $u \in V_{n+1}$. Thus we have m^2 edges, such that $d_u+d_v = 2(n+1)$ and $d_u \times d_v = (n+1)^2$. Therefore the third terms of the schultz and modified schultz polynomials of $(K_2 \circ K_{m,n})$ is $[2m^2(n+1)]x^3$ and $[m^2(n+1)^2]x^3$ respectively.

Subcase 3.5. For a vertex $v \in V_{n+1}$, there is $2mn$ paths with length three until a vertex $u \in V_{m+1}$. Thus we have $2mn$ edges, such that $d_u+d_v = (m+n+2)$ and $d_u \times d_v = (n+1)(m+1)$. Therefore the third terms of the schultz and modified schultz polynomials of $(K_2 \circ K_{m,n})$ is $[2mn(m+n+2)]x^3$ and $[2mn(n+1)(m+1)]x^3$ respectively.

Subcase 3.6. For a vertex $v \in V_{m+1}$, there is n^2 paths with length three until a vertex $u \in V_{m+1}$. Thus we have n^2 edges, such that $d_u+d_v = 2(m+1)$ and $d_u \times d_v = (m+1)^2$. Therefore the third terms of the schultz and modified schultz polynomials of $(K_2 \circ K_{m,n})$ is $[2n^2(m+1)]x^3$ and $[n^2(m+1)^2]x^3$ respectively.

From the definition of schultz, modified schultz polynomial and above mentioned cases we have following results.

$$\begin{aligned} Sc(K_2 \circ K_{m,n}, x) &= \sum_{(u,v) \in V(K_2 \circ K_{m,n})} (d_u + d_v) x^{d(u,v)} \\ &= [2(m+n+1) + 2m(m+2n+2) + 2n(2m+n+2) \\ &\quad + 2mn(m+n+2)]x^1 + [2m(m+2n+1) + 2n(2m+n+2) \\ &\quad + 2m(m-1)(n-1) + 2n(n-1)(m+1)]x^2 + [2m^2(n+1) \\ &\quad + 2n^2(m+1) + 2mn(m+n+2)]x^3 \\ &= 2[(m^2+n^2) + (m+n)(mn+3) + 6mn+1]x^1 + 2[2(m^2+n^2) \\ &\quad + (m+n)(mn+1) + 2mn]x^2 + 2[(m^2+n^2) + 2mn(m+n+1)]x^3. \end{aligned}$$

From the definition of schultz index, we compute the schultz index of $(K_2 \circ K_{m,n})$ by the first derivative of schultz polynomial of $(K_2 \circ K_{m,n})$ [evaluating at $x = 1$] as follows:

$$\begin{aligned} Sc(K_2 \circ K_{m,n}) &= \frac{\partial Sc(K_2 \circ K_{m,n}, x)}{\partial x} \Big|_{x=1} \\ &= \frac{\partial}{\partial x} \left(2[(m^2+n^2) + (m+n)(mn+3) + 6mn+1]x^1 + 2[2(m^2+n^2) \right. \\ &\quad \left. + (m+n)(mn+1) + 2mn]x^2 + 2[(m^2+n^2) + 2mn(m+n+1)]x^3 \right) \Big|_{x=1} \\ &= 2[8(m^2+n^2) + 16mn+1 + (m+n)(9mn+5)] \end{aligned}$$

And also modified schultz polynomial of $(K_2 \circ K_{m,n})$ is,

$$\begin{aligned} Sc^*(K_2 \circ K_{m,n}, x) &= \sum_{(u,v) \in V(K_2 \circ K_{m,n})} (d_u d_v) x^{d(u,v)} \\ &= [(m+n+1)^2 + 2m(m+n+1)(n+1) + 2n(m+n+1)(m+1) \\ &\quad + 2mn(n+1)(m+1)]x^1 + [2m(m+n+1)(n+1) + 2n(m+n+1) \\ &\quad (m+1) + m(m-1)(n+1)^2 + n(n-1)(m+1)^2]x^2 + [m^2(n+1)^2 \\ &\quad + 2mn(n+1)(m+1) + n^2(m+1)^2]x^3 \\ &= [3(m^2+n^2) + (6mn+4)(m+n) + 2mn(mn+6) + 1]x^1 \\ &\quad + [3(m^2+n^2) + (m+n)(6mn+1) + 2mn(mn+2)]x^2 \\ &\quad + [4mn(mn+m+n) + (m+n)^2]x^3. \end{aligned}$$

Now we compute modified schultz index of $(K_2 \circ K_n)$ by first derivative of modified schultz polynomial of $(K_2 \circ K_{m,n})$ [evaluated at $x = 1$] as follows:

$$\begin{aligned} Sc^*(K_2 \circ K_{m,n}) &= \frac{\partial Sc^*(K_2 \circ K_{m,n}, x)}{\partial x} \Big|_{x=1} \\ &= \frac{\partial}{\partial x} \left([3(m^2+n^2) + (6mn+4)(m+n) + 2mn(mn+6) + 1]x^1 \right. \\ &\quad \left. + [3(m^2+n^2) + (m+n)(6mn+1) + 2mn(mn+2)]x^2 \right. \\ &\quad \left. + [4mn(mn+m+n) + (m+n)^2]x^3 \right) \Big|_{x=1} \\ &= 12(m^2+n^2) + 2mn(9mn+13) + (28mn+6)(m+n) + 1. \end{aligned}$$

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References

1. Y. Alizadeh, A. Iranmanesh, T. Doslic and M. Azari, 2014, The edge wiener index of suspensions, bottlenecks and thorny graphs, *GlasnikMatematicki*, 49(1), 1-12.

2. A. A. Dobrynin, R. Entringer, I. Gutman, 2001, Wiener index of trees; Theory and applications, *Acta. Appl. Math.*, 66, 211-249.
3. M. Eliasi and B. Taeri, 2008, Shultz polynomials of composite graphs, *Applicable Analysis and Discrete Mathematics*, 2, 285-296.
4. M. R. Farahani and Hosoya, 2013, Schultz, Modified schultz polynomials and their topological indices of benzene molecules: First members of polycyclic Aromatic hydrocarbons[PAHs], *International journal of theoretical chemistry*, 1(2), 9-16.
5. M. R. Farahani, 2013, Shultz, Modified schultz polynomial, Hosoya polynomial and wiener index of circumcoronene series of Bezenoid, *Applied mathematics and information sciences*, 31(5-6), 595-608.
6. M. R. Farahani, 2014, Schultz indices and schultz polynomials of Harary graph, *Pacific Journal of Applied Mathematics*, 6(3), 77-84.
7. M. R. Farhani, W. Gao and M. R. Rajesh Kanna, 2015, The schultz, modified schultz indices and their polynomials of the jahangir graphs $J_{n,m}$ for integer numbers $n=3$, $m > 3$, *Asian journal of applied sciences*, 3(6), 823-827.
8. I. Gutman, 1994, Selected properties of the schultz molecular topological index, *J. chem. Inf. Comput. Sci.*, 34, 1087-1089.
9. I. Gutman, 2005, Some Relations between Distance-based polynomials of trees, *Sciences Mathematiques*, 30, 1-7.
10. I. Gutman, S. Klavzar, 1997, Wiener number of vertex-weighted graphs and a chemical application, *Disc. Appl. Math.*, 80, 73-81.
11. I. Gutman, O. E. Polansky, 1986, Mathematical concepts in organic chemistry, Springer, Berlin.
12. F. Hassani, A. Iranmanesh, S. Mirzaie, 2013, Schultz and modified schultz polynomials of C_{100} fullerence, *MATCH Commun. Math. Comput. Chem.*, 69, 87-92.
13. H. Hosoya, 1988, On some counting polynomials in chemistry. *Discrete Applied Mathematics*, 19, 239-257.
14. D. J. Klein, Z. Mihali'c, D. Plav'si'c, N. Trinjasti'c, 1992, Molecular topological index: A relation with the wiener index, *J. Chem. Inf. Comput. Sci.*, 32, 304-305.
15. H. P. Schultz, 1989, Topological organic chemistry 1. Graph theory and topological indices of alkanes, *J. Chem. Inf. Comput. Sci.*, 29, 227-228.
16. H. Wiener, 1947, Structural determination of paraffin boiling points, *J. Amer. Chem. Soc.*, 69, 17-20.

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