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The implementation of Hosoya index and Hosoya polynomial into some graphs related to cycles

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Abstract

The Hosoya index counts the number of independent edge sets in a graph, that is the number of subsets of the edge set such that no two edges in the subset share a vertex. Moreover, the Hosoya index gives important details on a graph's structural properties, including its connectivity. It has applications in a variety of fields, including computational biology, networking, and chemistry. In our article, we study Hosoya indiex of amalgamation of cycles and edge-amalgamation of cycles. Moreover, in this article we study the restricted Hosoya polynomial of amalgamation of cycles and we also give the general form of topological index.

Keywords: Hosoya index, edge-amalgamation of cycles, amalgamation of cycles, Hosoya polynomials.

1. Introduction

The Hosoya index was introduced in 1971 by Hosoya [7]. The purpose of this index is to give a characterization of carbon compounds in organic chemistry. The Hosoya index has been used to measure the variety of the structures and discover structurally related molecules on different chemical graphs [5, 10, 12]. The molecular structures are initially represented as graphs, where the atoms are the vertices and the bonds are the edges, in order to employ the Hosoya index for this purpose. The Hosoya index is then calculated for each graph, producing a number that indicates the structure's topological complexity.

The paper by Ghorbani et al. [20] focuses on the application of partial Hosoya polynomials in chemistry, specifically in the prediction of molecular properties [22, 24]. The authors demonstrate the effectiveness of partial Hosoya polynomials in the prediction of the boiling points of a diverse set of organic compounds. They also compare the performance of partial Hosoya polynomials with other graph-based descriptors and show that partial Hosoya polynomials outperform them in terms of prediction accuracy.

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Although initially defined for chemical compounds, the concept of the Hosoya index has been studied in a wide variety of graphs [1, 2, 15, 21]. One of the families of graphs in which the Hosoya index has been known is the cycle graphs, which have Lucas numbers as their Hosoya indices. **Lucas numbers,** L_n has value 2 for $n = 1$, value 1 for $n = 2$,and recursively defined as $L_n = L_{n-1} + L_{n-2}$ for $n > 2$ [6, 26].

However, the Hosoya index still has not been found for some families of graphs related to cycles. The aim of this paper is to propose an idea for implementing the Hosoya index in both the amalgamation of cycles and the edge amalgamation of cycles. The amalgamation of cycles is formed when one identifies a fixed vertex from a finite collection of cycles, and the edge amalgamation of cycles is formed when one identifies a fixed edge from a finite collection of cycles.

2. Hosoya index of amalgamation of cycles

We start this chapter with the definition of amalgamation of graphs, which is taken from [17].

Definition 2.1. Let $\{G_i\}$ be a finite collection of graphs and each G_i has a fixed vertex v_i called an axis. The amalgamation Amal$\{G_i, v_{0i}\}$ is formed by taking all G_i's and identifying their axis.

For the case when all G_i are cycles, then the choice of the vertex is irrelevant.

Definition 2.2. [13] Let $\{C_{n_i}\}$ be a finite collection of cycles and each C_{n_i} has a fixed vertex v_iw_i called a terminal. The amalgamation of these cycles is formed by taking all C_{n_i}'s and identifying their terminal. We denote this amalgamation by $(C_{n_i})t$, where t denotes the number of cycles.

Some properties of the amalgamation of cycles have been studied, such as its resolving graph [13] and its magic and antimagic decomposition [25].

In this part, we discuss how to find the Hosoya index amalgamation of cycles. The definition of the Hosoya index is taken from [7].

Definition 2.3. Given a graph G, denote $m(G, k)$ as the number of ways k mutually independent edges can be selected in G, that is, the number of k-matching in G. $m(G, 0)$ is defined as 0, and $m(G, 1)$ is clearly 1. The **Hosoya index** of G is the summation of all $m(G, k)$, $\Sigma_{k\geq 1} m(G, k)$, denoted by $Z(G)$.

Our result regarding the Hosoya index of amalgamation of cycles C_n is based on the following theorem about the Hosoya index of cycles, which is the Corollary 11.6.2 in [14].

Theorem 2.4 (Hosoya index of cycle). *[14]*

The Hosoya index of amalgamation of cycles C_n is the Lucas number which is denoted by L_n.

$$L_n = \begin{cases} 2 & n = 1 \\ 1 & n = 2 \\ L_{n-1} + L_{n-2} & n > 2. \end{cases}$$

We also utilize the result concerning the Hosoya number of paths, specifically Corollary 11.6.1 in [14] and supported by [8].

Theorem 2.5 (Hosoya of path). *[14]*

For P_n, the Hosoya index is the Fibonacci number

$$F_n = \frac{1}{\sqrt{5}} \quad \frac{1+\sqrt{5}}{2}\Bigg)^n + \frac{1}{\sqrt{5}} \quad \frac{1-\sqrt{5}}{2}\Bigg)^n.$$

To find the Hosoya index of amalgamation of cycles, we apply the following recursion relations. ([14, Theorem 11.6(a)]).

Theorem 2.6. *[14]*

1. *If e is any edge of a graph G connecting the vertices u and v, then*

$$Z(G) = Z(G - e) + Z(G - u - v).$$

2. *If v is a vertex in G and its neighbours are the vertices $v_1, v_2, \ldots, v_k$, then*

$$Z(G) = Z(G - v) + \sum_{i=1}^{k} Z(G - v - v_i).$$

3. *If the graph G has components $G_1, G_2, \ldots, G_k$, then*

$$Z(G) = Z(G_1).Z(G_2) \ldots Z(G_k).$$

With these recursion relations, we can determine the Hosoya index of a graph by calculating the Hosoya indices of its subgraphs. Another concept of recursion can be found in [9]. Now we are ready to discuss the Hosoya index of the amalgamation of cycles.

Theorem 2.7 (The Hosoya index of the amalgamation of cycles)**.**

The Hosoya index of amalgamation of $C_{n_1}, C_{n_2}, \ldots, C_{n_k}$ is

$$\prod_{i=1}^{k} F_{n_i-2} + 2\sum_{i=1}^{k} F_{n_i-3} \prod_{j=1, j\neq i}^{k} F_{n_j-2}.$$

Proof. Let v be the terminal and G be the graph. We use Lemma 2.6(ii). The deletion of the terminal induced a graph with $P_{n_1-2}, P_{n_2-2}, \ldots, P_{n_k-2}$ as its components. By Lemma 2.6(iii), the Hosoya index for this graph is $\prod_{i=1}^{k} F_{n_i-2}$.

The deletion of the terminal and one of its neighbours in C_{n_i} induced a graph with k components, one is P_{n_i-3} and the others are in the form P_{n_j-2} for $j \neq i$. The Hosoya index of this graph is $F_{n_i-3} \prod_{j=1,j\neq i}^{k} F_{n_j-2}$.

Let $N(v)$ denote the set of all neighbours of the terminal. Since there are two neighbours of v in each C_{n_i}, then $\sigma_{u\in N(v)} Z(G - v - u) = 2\sigma_{i=1}^{k} F_{n_i-3} \prod_{j=1,j\neq i}^{k} F_{n_j-2}$. Therefore, the Hosoya index of the amalgamation of the cycles $C_{n_1}, C_{n_2}, \ldots, C_{n_k}$ is $\prod_{i=1}^{k} F_{n_i-2} + 2\sigma_{i=1}^{k} F_{n_i-3} \prod_{j=1,j\neq i}^{k} F_{n_j-2}$. □

3. Hosoya index of edge amalgamation of cycles

Similar to the previous chapter, we begin this chapter with the definition of edge amalgamation of graphs, which is taken from[23, 4, 3].

Definition 3.1. Let $\{C_{n_i}\}$ be a finite collection of graphs and each C_{n_i} has a fixed vertex $v_i w_i$ called a terminal. The amalgamation of these cycles is formed by taking all C_{n_i}'s and identifying their axis. We denote this amalgamation by $EdgeAmal(C_{n_i})t$, where t denotes the number of cycles.

For the case when all G_i are cycles, then the choice of the terminal is irrelevant.

Definition 3.2. Let $\{C_{n_i}\}$ be a finite collection of cycles and each C_{n_i} has a fixed vertex $v_i w_i$ called a terminal. The amalgamation of these cycles is formed by taking all C_{n_i}'s and identifying their axis. We denote this amalgamation by $(C_n)_t$, where t represents the number of cycles.

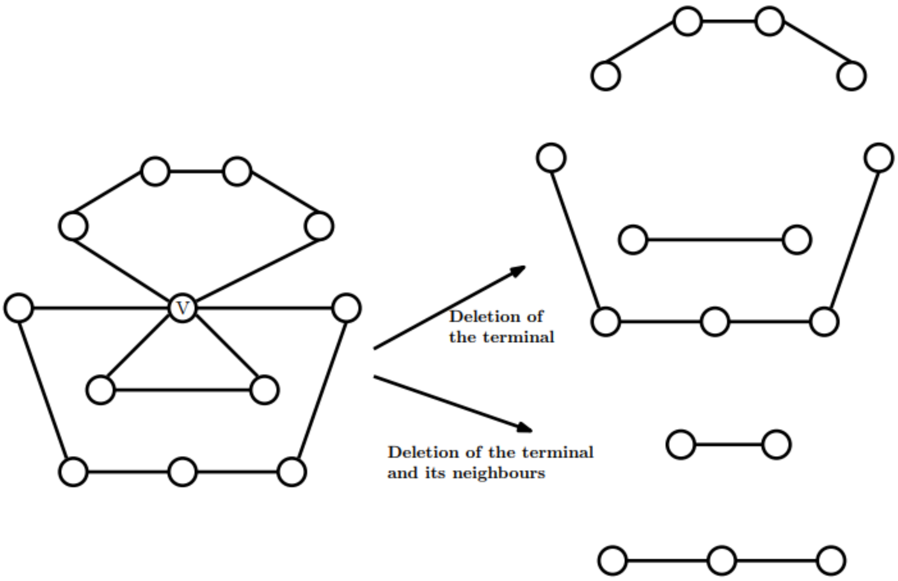

Figure 1: The deletion of vertices for the recurrence relation of Hosoya index of the amalgamation of cycles.

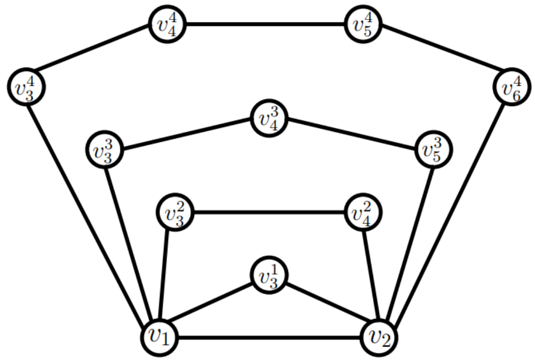

Figure 2: Edge amalgamation of cycles

Similar to the previous chapter, we find the Hosoya index of the edge amalgamation of cycles by repeatedly using Lemma 2.6 to the edge amalgamation of cycles. In the process, some classes of graphs arise. We first find the Hosoya indices of these classes before finding the Hosoya index of edge amalgamation of cycles.

First, we find the Hosoya index of amalgamation of paths where the terminal is formed by identifying an endpoint of paths (Figure 3). We denote this graph by Amal$\{P_i, v_i\}$.

Lemma 3.3. *Let $Amal\{P_i, v_i\}$ be the graph formed when an endpoint of the paths $P_{n_1}, P_{n_2}, \ldots, P_{n_k}$ are identified. Then,*

$$Z(Amal\{P_i, v_i\}) = \prod_{i=1}^{k} F_{n_i-1} + \sum_{i=1}^{k} F_{n_i-2} \prod_{j=1, j\neq i}^{k} F_{n_j-1}.$$

Proof. We again use Lemma 2.6(ii). The deletion of the terminal induced a graph with $P_{n_1-1}, P_{n_2-1}, \ldots, P_{n_k-1}$ as its components. The Hosoya index for this graph is $\prod_{i=1}^{k} F_{n_i-1}$.

The deletion of the terminal and its neighbours in P_{n_i} induced a graph with k components, one is P_{n_i-2} and the others are in the form P_{n_j-1} for $j \neq i$. The Hosoya index of this graph is $F_{n_i-2} \prod_{j=1, j\neq i}^{k} F_{n_j-1}$.

Thus, the Hosoya index of the graph Amal$\{P_i, v_i\}$ is

$$\prod_{i=1}^{k} F_{n_i-1} + \sum_{i=1}^{k} F_{n_i-2} \prod_{j=1, j\neq i}^{k} F_{n_j-1}$$

. □

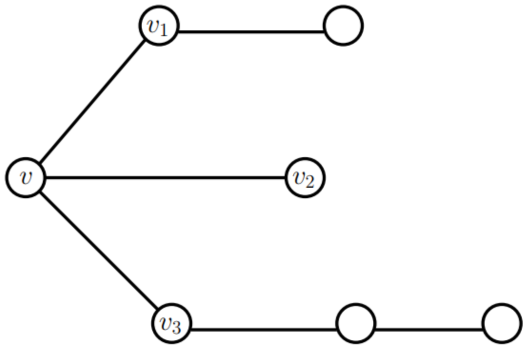

Figure 3: Amalgamation of paths with an endpoint as the terminal

Next, we need to find the Hosoya index of the amalgamation of the graphs formed by identifying the endpoints of several paths. We denote this kind of amalgamation by Amal$\{P_i, v_i w_i\}$

Lemma 3.4. *Hosoya index of amalgamation of paths Let $P_{n_1}, P_{n_2}, \ldots, P_{n_k}$ be paths with length $n_1, n_2, \ldots, n_k$ respectively, all n_i's greater than 1. Let Amal $\{P_i, v_i w_i\}$ be the graph formed when both endpoints of the paths are identified. Then,*

$$\begin{aligned} Z(Amal\{P_i, v_i w_i\}) = & \prod_{i=1}^{k} F_{n_i-2} + \sum_{i=1}^{k} F_{n_i-3} \prod_{j=1, j\neq i}^{k} F_{n_j-2} \\ & + \sum_{i=1}^{k}((F_{n_i-3}) \prod_{\substack{j=1 \\ j\neq i}}^{k} F_{n_j-2} + \sum_{i}^{k}((F_{n_i^*-4}) \prod_{\substack{j=1 \\ j\neq i}}^{k} F_{n_j-2} + (F_{n*_i-4})(F_{n_m^*-3}) \prod_{\substack{j=1 \\ j\neq i \\ j\neq m}}^{k} F_{n_j-2}) \end{aligned}$$

where $n_i^* - 4 = max\{n_i - 4, 0\}$ and $n_m^* - 3 = max\{n_m - 3, 0\}$.

Proof. We also use Lemma 2.6(ii) for this proof. Let v and w be the identified endpoints of $P_{n_1}, \ldots, P_{n_k}$. The deletion of v induces an endpoint amalgamation of paths, Amal$\{P_i, v_i\}$, the graph class in the Lemma 3.3, where the paths are $P_{n_1-1}, \ldots, P_{n_k-1}$. The Hosoya index of this graph is $\prod_{i=1}^{k} F_{n_i-2} + \sum_{i=1}^{k} F_{n_i-3} \prod_{j=1, j\neq i}^{k} F_{n_j-2}$.

Suppose the paths are $P_{n_1-1}, \ldots, P_{n_{i-1}-1}, P_{n_i-2}, P_{n_{i+1}-1}, \ldots, P_{n_k-1}$, the deletion of v and its neighbour in C_{n_i} induces Amal$\{P_i, v_i\}$. In this graph, the deletion of v induced graph with k components, one is P_{n_i-3} and all the others are in the form $P_{n_j-2}, j \neq i$. Thus, the Hosoya index is $(F_{n_i-3}) \prod_{\substack{j=1 \\ j\neq i}}^{k} F_{n_j-2}$. Meanwhile, for the deletion of v and one of its neighbours, we shall consider two cases. If we delete v and its neighbour in P_{n_i-2}, then the Hosoya index is $F_{n*_i} \prod_{\substack{j=1 \\ j\neq i}}^{k} F_{n_j-2}$, where $n*_i = max\{n_i - 4, 0\}$. If we delete v and its neighbour in one of the paths other than P_{n_i-2}, says in P_{n_m-1}, then the Hosoya index is $(F_{n_i^*-4}) F_{n_m^*-3} \prod_{\substack{j=1 \\ j\neq i \\ j\neq m}}^{k} F_{n_j-2}$, where $n_i^* - 4 = max\{n_i - 4, 0\}$ and $n_m^* - 3 = max\{n_m - 3, 0\}$.

Thus, the Hosoya index from the graph that formed after the deletion of v and its neighbour in C_{n_i} is $(F_{n_i-3}) \prod_{\substack{j=1 \\ j\neq i}}^{k} F_{n_j-2} + \sum_{i}^{k}((F_{n_i^*-4}) \prod_{\substack{j=1 \\ j\neq i}}^{k} F_{n_j-2} + (F_{n*_i-4})(F_{n_m^*-3}) \prod_{\substack{j=1 \\ j\neq i \\ j\neq m}}^{k} F_{n_j-2}$, where $n_i^* - 4 = max\{n_i - 4, 0\}$ and $n_m^* - 3 = max\{n_m - 3, 0\}$.

Hence, the Hosoya index of Amal$\{P_i, v_i w_i\}$ satisfies

$$\prod_{i=1}^{k} F_{n_i-2} + \sum_{i=1}^{k} F_{n_i-3} \prod_{j=1,j\neq i}^{k} F_{n_j-2} + \sum_{i=1}^{k}((F_{n_i-3}) \prod_{\substack{j=1\\ j\neq i}}^{k} F_{n_j-2} + \sum_{i}((F_{n_i^*-4})$$

$$\prod_{\substack{j=1\\ j\neq i}}^{k} F_{n_j-2} + (F_{n*_i-4})(F_{n_m^*-3}) \prod_{\substack{j=1\\ j\neq i\\ j\neq m}}^{k} F_{n_j-2})$$

, where $n_i^* - 4 = max\{n_i - 4, 0\}$ and $n_m^* - 3 = max\{n_m - 3, 0\}$. □

Now we are ready to discuss the Hosoya index of the edge amalgamation of cycles.

Theorem 3.5 (The Hosoya index of the edge amalgamation of cycles)**.** *The Hosoya index of edge amalgamation of the cycles $C_{n_1}, C_{n_2}, \ldots, C_{n_k}$ is*

$$\prod_{i=1}^{k} F_{n_i-3} + \prod_{i=1}^{k} F_{n_i-3} + \sum_{i=1}^{k} F_{n_i^*-4} \prod_{j=1,j\neq i}^{k} F_{n_j-3} + \sum_{i=1}^{k}(F_{n_i^*-4})$$

$$\prod_{\substack{j=1\\ j\neq i}}^{k} F_{n_j-3} + \sum_{i=1}^{k}(F_{n_i^*-5}) \prod_{\substack{j=1\\ j\neq i}}^{k} F_{n_j-3} + (F_{n_i^*-5})(F_{n_m^*-4}) \prod_{\substack{j=1\\ j\neq i\\ j\neq m}}^{k} F_{n_j-3}),$$

where $n_\alpha^* - c = max\{n_i - c, 0\}$ for any positive integer c and α is any of the indexes i, j, m.

Proof. Let v and w be the endpoints of the axis of the edge amalgamation of cycles. We use Lemma 2.6(i) for the proof. The deletion of v and w turns the graph into k numbers of paths $P_{n_1-3}, P_{n_2-3}, \ldots, P_{n_k-3}$. The Hosoya index of this graph is $\prod_{i=1}^{k} F_{n_i}$.

The deletion of the axis turns the graphs into the graph Amal$\{P_i, v_i w_i\}$ discussed in Lemma 3.4 with paths $P_{n_k-1}, \ldots, P_{n_k-1}$. The Hosoya index of this graph is $\prod_{i=1}^{k} F_{n_i-3} + \sum_{i=1}^{k} F_{n_i^*-4} \prod_{j=1,j\neq i}^{k} F_{n_j-3} + \sum_{i=1}^{k}((F_{n_i^*-4}) \prod_{\substack{j=1\\ j\neq i}}^{k} F_{n_j-3} + \sum_{i}^{k}((F_{n_i^*-5}) \prod_{\substack{j=1\\ j\neq i}}^{k} F_{n_j-3} + (F_{n*_i-5})(F_{n_m^*-4}) \prod_{\substack{j=1\\ j\neq i\\ j\neq m}}^{k} F_{n_j-3})$, where $n_\alpha^* - c = max$ $\{n_i - c, 0\}$ for any positive integer c and α is any of the indexes i, j, m. □

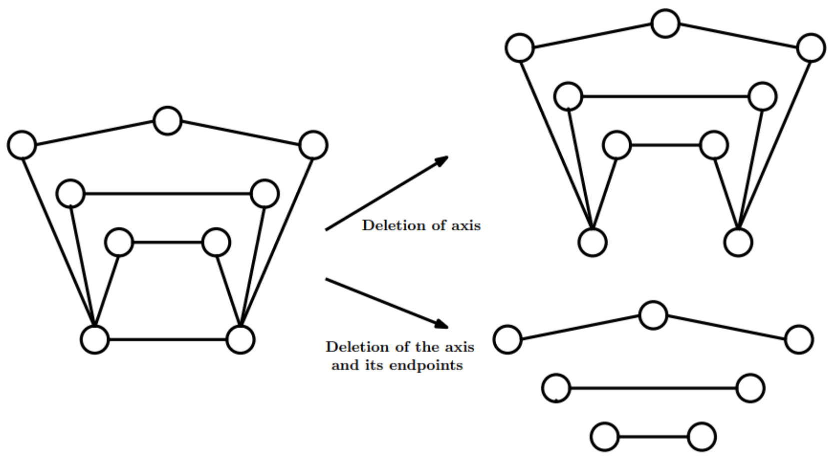

Figure 4: Graph induced by deletion of axis and graph induced by deletion of axis and its endpoints on the edge-amalgamation of cycles.

G	Order	Size	$H(G,\lambda)$	$W(G)$
C_1^1	3	3	3λ	3
C_1^2	5	6	$6\lambda + 8\lambda^2$	22
C_1^3	8	10	$10\lambda + 13\lambda^2 + 5\lambda^3$	51
C_1^4	12	15	$15\lambda + 25\lambda^2 + 20\lambda^3 + 6\lambda^4$	149
C_1^5	17	21	$21\lambda + 40\lambda^2 + 45\lambda^3 + 25\lambda^4 + 5\lambda^5$	361
C_1^6	23	28	$28\lambda + 58\lambda^2 + 77\lambda^3 + 59\lambda^4 + 25\lambda^5 + 6\lambda^6$	772
C_1^7	30	36	$36\lambda + 79\lambda^2 + 116\lambda^3 + 108\lambda^4 + 66\lambda^5 + 25\lambda^6$ $+5\lambda^7$	1489
C_1^8	38	45	$45\lambda + 103\lambda^2 + 162\lambda^3 + 168\lambda^4 + 127\lambda^5$ $+67\lambda^6 + 25\lambda^7 + 6\lambda^8$	2669
C_1^9	47	55	$55\lambda + 130\lambda^2 + 215\lambda^3 + 239\lambda^4 + 208\lambda^5$ $+138\lambda^6 + 66\lambda^7 + 25\lambda^8 + 5\lambda^9$	4491
C_1^{10}	57	66	$66\lambda + 160\lambda^2 + 275\lambda^3 + 321\lambda^4 + 304\lambda^5$ $+234\lambda^6 + 138\lambda^7 + 67\lambda^8 + 25\lambda^9 + 6\lambda^{10}$	7260

Table 1: Hosoya polynomials of edge amalgamation of cycle graphs

4. Hosoya Polynomial and Wiener Index

The Hosoya polynomial and Wiener index have a powerful relationship, hence why it is also sometimes called the Wiener-Hosoya polynomial. The relationship is that the first derivative of the Hosoya polynomial at $\lambda = 1$ gives the Wiener index.

Definition 4.1. The Hosoya polynomial of a graph G was introduced by Hosoya in 1988 [11]. It was previously known as the "Wiener polynomial", but nowadays it is called the Hosoya polynomial. Hosoya polynomial is a distance-based polynomial denoted by $H(G;\lambda)$. It is defined as follows [18]:

$$H(G,\lambda) = \sum_{k\geq 1} d(G,k)\lambda^k = \sum_{1\leq i<j\leq n} \lambda^{d(v_i,v_j|G)}$$

Table 1 gives the calculation of Hosoya polynomials of edge amalgamation of several types of cycle graphs.

5. Conclusion

In our study of Hosoya index, we obtain results for the amalgamation of cycles and the edge amalgamation of cycles. In addition, we obtain the Hosoya index of amalgamation of paths where the identified vertex is an endpoint.

Our results are primarily by counting the Hosoya index of the subgraphs that arise by the deletion of an edge or some vertices. We only consider the cycles, in case of path graph P_n the Hosoya index is just the Fibonacci number F_n this is because the deletion of edge or vertices in a cycle gives the path. We also worked out Hosoya polynomial for some edge amalgamation of cycles given in Table 1. In our further work we would like to work on Hosoya Index of some newly constructed graphs and we will get some computational result for the Hosoya polynomial.

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