

The Smallest Hosoya Index of Connected Tricyclic Graphs

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ABSTRACT

The Hosoya index of a graph G is defined as the total number of independent edge subsets of the graph. A connected tricyclic graph is a connected simple graph with n vertices and $n + 2$ edges. In this paper we characterize the $(n, n + 2)$ -graphs with the smallest Hosoya index. We show that the lower bound of the Hosoya index of the $(n, n + 2)$ -graphs, is $4n - 6$.

1. INTRODUCTION AND PRELIMINARIES

The Hosoya index or z -index $z(G)$ of a graph G is the total number of its matchings plus one, where a matching is a non-empty subset $M \subseteq E$ with the property that no two different edges of M share a common vertex. If $m(G, k)$ denotes the number of its k -matchings, matchings consisting of k edges, then $z(G) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} m(G, k)$, where n is the number of the vertices of G . It is convenient to set $m(G, 0) = 1$. By its definition, we deduce that $m(G, k) = 0$ where $k > \lfloor \frac{n}{2} \rfloor$. The Hosoya index is a prominent example of topological indices which are of interest in combinatorial chemistry. The Hosoya index was introduced by Hosoya [6] in 1971,

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and it turned out to be applications with physico-chemical properties such as boiling point, entropy [7] or heat of vaporization are well studied. For more results on Hosoya index see the book [5], the recent papers [8-12] and the references cited therein.

Let $G = (V(G), E(G))$ be a simple connected graph with the vertex set $V(G)$ and the edge set $E(G)$. For any $v \in V(G)$, $N_G(v) = \{u \mid uv \in E(G)\}$ denotes the neighbors of v , and $d_G(v) = |N_G(v)|$ is the degree of v in G . A end-vertex is a vertex of degree one. A pendant edge is an edge incident with a end-vertex. A path consisting exactly one end-vertex is called a pendant path. An $(n, n + 2)$ - graph is a simple connected graph of order n with $n + 2$ edges. Here, its three cycles are very important, so in this paper we call it a tricyclic graph freely. Let $E' \subseteq E(G)$, we denote by $G - E'$ the subgraph of G obtained by deleting the edges of E' . If $W \subseteq V(G)$, $G - W$ denotes the subgraph of G obtained by deleting the vertices in W and the edges incident with them. If $W = \{v\}$ is a singleton set, we use $G - v$ instead of $G - \{v\}$. Let u and v be two distinct vertices of G . By $C_G(u-v, p)$ we mean the set of cycles of length p that contain u but not contain v . The set of edges of $C_G(u-v, p)$ is denoted by $E^{C_p}(u - v)$. By $M_G(v)$ we mean the set of edges incident upon v in G . Let $G = (V(G), E(G))$ and $G' = (V(G'), E(G'))$ be two graphs such that $V(G) \cap V(G') = \emptyset$. Suppose that $v_1, v_2, \dots, v_k \in V(G)$ and $v'_1, v'_2, \dots, v'_k \in V(G')$ ($k \geq 1$) by $G \triangleright v_1 = v'_1, v_2 = v'_2, \dots, v_k = v'_k \triangleleft G'$ we mean the obtained graph of identifying v_i on v'_i for $i = 1, \dots, k$. Suppose that P_n denotes the path on n vertices, C_n is the cycle on n vertices and S_n is the star consisting of one center vertex adjacent to $n - 1$ leaves. Let \mathcal{C}_1 be all unicycle graphs that obtained from attaching a non-trivial path to a cycle. Precisely $\mathcal{C}_1 := \{G \triangleright u = v \triangleleft G' \mid V(G) \cap V(G') = \emptyset, G \cong C_q, G' \cong P_r, deg_{G'}(v) = 1, r \geq 2\}$. Among all n -vertex trees, the path P_n has the greatest Hosoya index and the star S_n has the smallest Hosoya index. This fact was established long time ago [3, 4], that is, for any tree T with n vertices, $n = z(S_n) \leq z(T) \leq z(P_n) = f(n + 1)$, where $f(n)$ is the n th Fibonacci number.

We use the following results throughout the paper.

Lemma 1.1. [6] If v is a vertex and $e = uv$ is an edge of G , then

$$z(G) = z(G - \{e\}) + z(G - \{u, v\})$$

$$z(G) = z(G - \{v\}) + \sum_{x \in N_G(v)} z(G - \{v, x\})$$

Lemma 1.2. [5] If G is a graph with components $G_1, G_2, G_3, \dots, G_k$ then $z(G) = \prod z(G_i)$.

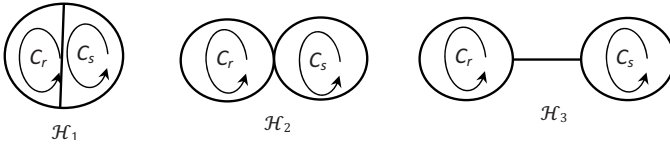


Figure 1: Three different classes of bicyclic graphs.

Some properties of the Fibonacci number are in the following lemma.

Lemma 1.3. [1] $f(n) = f(k)f(n - k + 1) + f(k - 1)f(n - k) \quad 1 \leq k \leq n$

2. TRICYCLIC GRAPHS

In this section, we present the some lemma and methods by which one can construct a $k+1$ -cyclic graph from k -cyclic graph.

Lemma 2.1. Let $G = (V(G), E(G))$ be a connected k -cyclic graph. Suppose that $C_q : u_1 u_2 \dots u_q u_1$ and $P_r : v_1 v_2 \dots v_r$ are a cycle graph and a path graph, respectively, such that $V(G) \cap V(C_q) = \emptyset$ and $V(G) \cap V(P_r) = \emptyset$. Suppose that u and v are two distinct vertices of G . All the following graphs are $k+1$ -cyclic graphs.

i) $G' = G \triangleright u = v_1, v = v_r \triangleleft P_r$, where $r \geq 3$ or $uv \notin E(G)$

ii) $G' = G \triangleright u = u_i \triangleleft C_q$, for $i = 1, 2, \dots, q$

iii) $G' = G \triangleright u = v_H \triangleleft H$, where $H \in \mathcal{C}_1$ and v_H is the single end-vertex of H

In the rest of the section, we refer to the items i, ii and iii as the methods i, ii , and iii , respectively. Note that, all the tricyclic graphs are constructed by applying the above lemma on the bicyclic graphs. Indeed the above lemma inspires an algorithm to construct a $(k+1)$ -cyclic graph from a k -cyclic graph. Therefore, by using the lemma we have the following theorem.

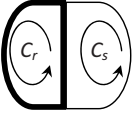
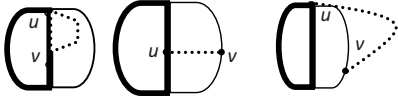
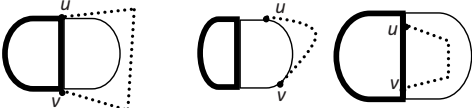
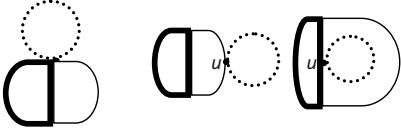
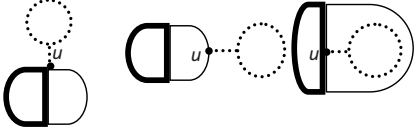
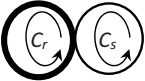


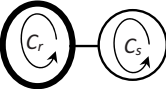
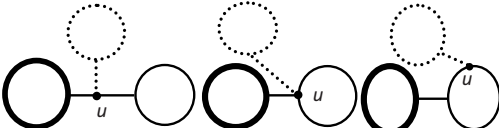
Class of bicyclic	Method In Lemma2.1	Constructed tricyclic graphs
\mathcal{H}_1 	<i>i</i>	
		
	<i>ii</i>	
<i>iii</i>		
\mathcal{H}_2 	<i>ii</i>	
	<i>iii</i>	
\mathcal{H}_3 	<i>iii</i>	

Figure 2: All the classes of tricyclic graphs which are constructed from the bicyclic graphs.

Theorem 2.2. There are exactly nineteen different classes of the tricyclic graphs.

Proof. For proving the theorem we apply the Methods *i*, *ii*, and *iii* of the Lemma 2.1 on the graphs of classes \mathcal{H}_1 , \mathcal{H}_2 , and \mathcal{H}_3 of bicyclic graphs (see Fig.1).

At first let $G \in \mathcal{H}_1$:

Let P be a common path of two cycles C_r and C_s of G (see Fig. 2). We partition the vertices of G into three types as follow.

Type 1: $V_1 = \{v \in V(G) \mid \deg(v) = 2 \text{ and } v \in V(P)\}$.

Type 2: $V_2 = \{v \in V(G) \mid \deg(v) = 3\}$.

Type 3: $V_3 = \{v \in V(G) \mid \deg(v) = 2 \text{ and } v \notin V(P)\}$.

By selecting two vertices of two different types of G for using Method *i* we have three different classes of tricyclic graphs. If the selected two vertices are in the same type of vertices of G for using Method *i*, then we have three other different classes of tricyclic graphs. Now, if we apply Method *ii* on G , then three other different classes are produced. Finally if we apply Method *iii* on graph G , then we have three new different classes for tricyclic graphs (see Fig. 2).

Now, let $G \in \mathcal{H}_2$:

For this class we partition the set $V(G)$ as follows.

Type 1: $V_1 = \{v \in V(G) \mid \deg(v) = 2\}$.

Type 2: $V_2 = \{v \in V(G) \mid \deg(v) \neq 2\}$.

Obviously, V_2 is a singleton set whose element is a vertex of degree four. Since we already have applied the methods of Lemma 2.1 on bicyclic graphs in class \mathcal{H}_1 we do not need apply Method *i* on class \mathcal{H}_2 . By using each of Methods *ii* and *iii* on \mathcal{H}_2 we have two other different classes of tricyclic graphs, because the bicyclic graphs in \mathcal{H}_2 have two types of vertices (see Fig. 2).

Finally, let $G \in \mathcal{H}_3$:

Suppose that P is that path of G that connects two cycles C_r and C_s of G (see Fig. 2). Let us partition the vertices of G as follows.

Type 1: $V_1 = \{v \in V(G) \mid \deg(v) = 2 \text{ and } v \in V(P)\}$

Type 2: $V_2 = \{v \in V(G) \mid \deg(v) = 3\}$

Type 3: $V_3 = \{v \in V(G) \mid \deg(v) = 2 \text{ and } v \notin V(P)\}$

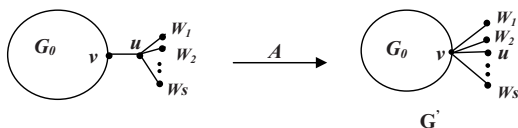


Figure 3. Transformation A.

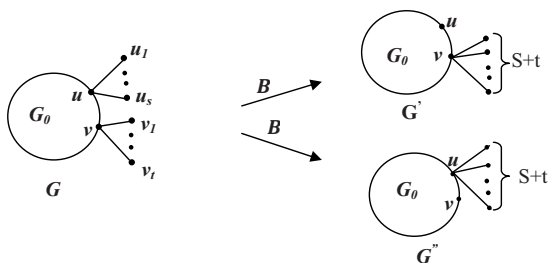


Figure 4. Transformation B.

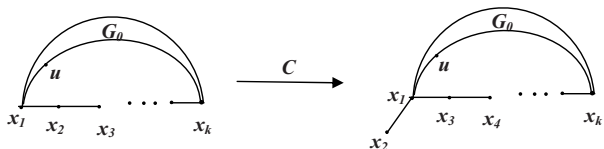


Figure 5. Transformation C.

For this class by using Method *iii* we have three new classes of tricyclic graphs. After that applying Methods *i* and *ii* on this class of bicyclic graphs do not produce a new class of tricyclic graphs. Thus applying the methods of Lemma 2.1 on bicyclic graphs produces nineteen classes of tricyclic graphs (see Fig. 2). ■

3. DECREASING TRANSFORMATIONS

In this section, we present some results and decreasing transformations for the Hosoya index of graphs. At first we recall the following two decreasing transformations which have been presented in [2].

Transformation A: Let uv be an edge of G , $N_G(u) = \{v, w_1, w_2, \dots, w_s\}$, and uw_1, uw_2, \dots, uw_s are pendant edges. $G' = G + \{vw_1, vw_2, \dots, vw_s\} - \{uw_1, uw_2, \dots, uw_s\}$, as shown in Figure 3.

Lemma 3.1. If G' is obtained from G by Transformation A, then $z(G') < z(G)$ [2].

Transformation B: Let u and v be two vertices in G . Suppose that uu_1, uu_2, \dots, uu_s are the pendant edges incident with u and vv_1, vv_2, \dots, vv_t are the pendant edges incident with v . $G' = G - \{uu_1, uu_2, \dots, uu_s\} + \{vu_1, vu_2, \dots, vu_s\}$,

$G'' = G - \{vv_1, vv_2, \dots, vv_t\} + \{uv_1, uv_2, \dots, uv_t\}$, (see Figure 4).

Lemma 3.2. If G' and G'' are obtained from G by Transformation B, then either $z(G') < z(G)$ or $z(G'') < z(G)$ [2].

In the rest of the section, we present some new results and some new decreasing transformations for the Hosoya index.

Lemma 3.3. Let G_0 be a simple graph and u and v be two distinct vertices of G_0 . Suppose that $P_k = x_1x_2 \dots x_k$ be a path of order k (for $k \geq 2$) such that $V(G_0) \cap V(P_k) = \emptyset$, then the Hosoya index of $(G_0 \triangleright u = x_1, v = x_k \triangleleft P_k)$ is as follows.

$$\begin{cases} z(G_0) + z(G_0 - \{x_1, x_2\}) & k = 2 \text{ and } uv \notin E(G) \\ z(G_0) + z(G_0 - \{x_1\}) + z(G_0 - \{x_3\}) & k = 3 \\ f(k-1)z(G_0) + f(k-2)z(G_0 - \{x_k\}) + \\ f(k-2)z(G_0 - \{x_1\}) + f(k-3)z(G_0 - \{x_1, x_k\}) & k \geq 4 \end{cases}$$

Proof. By using the first part of Lemma 1.1 and deleting the edges $x_1x_2, x_{k-1}x_k$ the result follows. ■

By using Lemma 3.3, we introduce the following decreasing transformation for the Hosoya index.

Transformation C. Let $= x_1x_2 \dots x_k$ ($k \geq 3$), be an internal path in G , such that $deg_G(x_i) = 2$, for $i = 2 \dots, k - 1$. The graph G' is obtained from G by deleting x_2x_3 and adding x_1x_3 .

Lemma 3.4. If G' is obtained from G by Transformation C, then $z(G') \leq z(G)$.

Proof. Suppose that the length of the path in Transformation C is k . At first we prove the assertion for $k \geq 5$.

$$\begin{aligned}
 z(G') &= z(G' - \{x_1x_2\}) + z(G' - \{x_1, x_2\}) \\
 &= z(G' - \{x_1x_2\}) + z(G' - \{x_1, x_2, x_{k-1}x_k\}) \\
 &\quad + z(G' - \{x_1, x_2, x_{k-1}, x_k\}) \\
 &= f(k-2)z(G_0) + f(k-3)z(G_0 - \{x_k\}) \\
 &\quad + f(k-3)z(G_0 - \{x_1\}) + f(k-4)z(G_0 - \{x_1, x_k\}) \\
 &\quad + f(k-2)z(G_0 - \{x_1\}) + f(k-3)z(G_0 - \{x_1, x_k\}) \\
 &= f(k-2)z(G_0) + f(k-3)z(G_0 - \{x_k\}) \\
 &\quad + f(k-1)z(G_0 - \{x_1\}) + f(k-2)z(G_0 - \{x_1, x_k\})
 \end{aligned}$$

Now, by the above calculations and Lemma 3.3 we have

$$\begin{aligned}
 \Delta &= z(G) - z(G') \\
 &= f(k-3)(z(G_0) - z(G_0 - \{x_1\})) + f(k-4)(z(G_0 - \{x_k\}) \\
 &\quad - z(G_0 - \{x_1, x_k\}))
 \end{aligned}$$

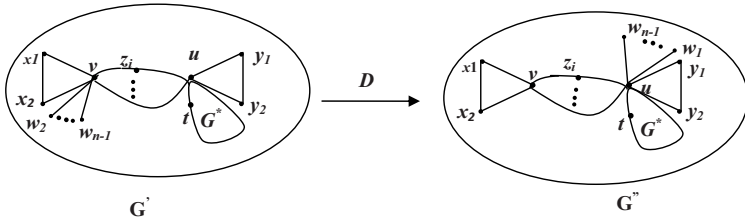
Since $z(G_0) > z(G_0 - \{x_1\})$ and $z(G_0 - \{x_k\}) > z(G_0 - \{x_1, x_k\})$

$z(G) > z(G')$ for $k = 5$.

Now, suppose that $k = 4$.

$$\begin{aligned}
 z(G') &= z(G' - \{x_1x_2\}) + z(G' - \{x_1, x_2\}) \\
 &= z(G' - \{x_1x_2\}) + z(G' - \{x_1, x_2, x_3x_4\}) \\
 &\quad + z(G' - \{x_1, x_2, x_3, x_4\}) \\
 &= z(G_0) + z(G_0 - \{x_1\}) + z(G_0 - \{x_4\})
 \end{aligned}$$

$$\begin{aligned}
 & +z(G_0 - \{x_1\}) + z(G_0 - \{x_1, x_4\}) \\
 \Delta = z(G) - z(G') & \\
 & = f(4 - 1)z(G_0) + f(4 - 2)z(G_0 - \{x_4\}) \\
 & + f(4 - 2)z(G_0 - \{x_1\}) + f(4 - 3)z(G_0 - \{x_1, x_4\}) \\
 & - z(G_0) - z(G_0 - \{x_4\}) - 2z(G_0 - \{x_1\}) - z(G_0 - \{x_1, x_4\}) \\
 & = z(G_0) - z(G_0 - \{x_1\})
 \end{aligned}$$



Since $z(G_0) > z(G_0 - \{x_1\})$, $z(G) > z(G')$ for $k=4$. Finally, suppose that $k=3$.

$$\begin{aligned}
 z(G') & = z(G_0) + z(G_0 - \{x_1, x_3\}) + z(G_0 - \{x_1\}) \\
 \Delta = z(G) - z(G') & \\
 & = z(G_0 - \{x_3\}) - z(G_0 - \{x_1, x_3\})
 \end{aligned}$$

Since $z(G_0 - \{x_3\}) > z(G_0 - \{x_1, x_3\})$ we conclude that $z(G) > z(G')$ for $k=3$ too. That means the assertion is true for all values of k . ■

The following lemma inspires a decreasing transformation.

Transformatin D: Let G be a tricyclic graph. Suppose that u and v are two distinct vertices of G , such that $d(u) > d(v)$ and $|C(u - v, 3)| \geq |C(v - u, 3)|$. Moreover, suppose that for each edge $e \in M_G(v) \setminus E^{C_3}(v - u)$ there is a v - u path of lengths 1 or 2, such that the mentioned paths above are internally disjoint. Let H be a star tree whose center is denoted by w . By this transformation we obtain $G'' = G \triangleright u = w \triangleleft H$ from $G' = G \triangleright v = w \triangleleft H$ (see Figure 6).

Lemma 3.5. The Transformation D is a decreasing transformation.

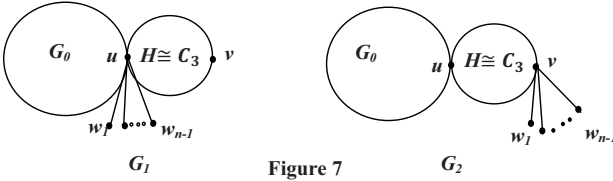


Figure 7

Proof. Suppose that the order of H is n and $\{w_1, w_2, \dots, w_{n-1}\}$ is the set of its leaves. Obviously, $|C_G(v - u, 3)| \leq 1$; we denote the single edge in $E^{C_3}(v - u) \setminus M_G(v)$ for the equality case by x_1x_2 . In this case, since $1 = |C_G(v - u, 3)| \leq |C_G(u - v, 3)| \leq 2$, we denote one arbitrary edge in $E^{C_3}(u - v) \setminus M_G(u)$ by y_1y_2 . Since $d_G(u) > d_G(v)$ so there exists a vertex $t \in N_G(u) \setminus N_G(v)$. If the v - u path P_i from the mentioned paths in Transformation **D** is of length 2, we denote the common vertex in $N_G(u)$ and $N_G(v)$ of P_i by z_i . Suppose that $M(G')$ and $M(G'')$ are the families of the all matchings of G' and G'' , respectively. We can show that $z(G'') < z(G')$ by constructing an injective, non-surjective mapping h from $M(G'')$ to $M(G')$ as follow. Suppose that $M_{G'}(v) \cap E^{C_3}(v - u) = \{vx_1, vx_2\}$

$$h: M(G'') \rightarrow M(G')$$

$$h(B) = \begin{cases} (B - \{vz_i, uw_j\}) \cup \{z_iu, vw_j\} & vz_i, uw_j \in B, \text{ for some } i \text{ and } j \\ (B - \{uw_j\}) \cup \{vw_j\} & uw_j \in B, B \cap M_G(v) = \emptyset \text{ for some } j \\ (B - \{vx_i, uw_j\}) \cup \{uy_i, vw_j\} & vx_i \in B, y_1y_2 \notin B, i=1,2 \\ (B - \{vx_i, uw_j, y_1y_2\}) \cup \{uy_i, vw_j, x_1x_2\} & vx_i \in B, y_1y_2 \in B, i=1,2 \\ B & o.w. \end{cases}$$



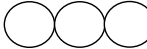

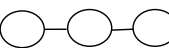

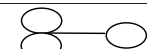



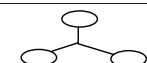
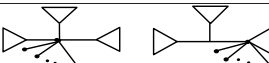

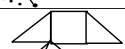

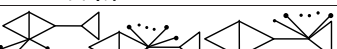
















The mapping h is injective. However, there is no $B \in M(G'')$ with $h(B) = \{vw_j, ut\}$. So, $z(G'') < z(G')$ ■

Corollary 3.6. Let $G_0 = (V(G_0), E(G_0))$ be a non-trivial connected graph and $u_0 \in V(G_0)$. Assume that $H \cong C_3$ and $u, v \in V(H)$. Suppose that $G = G_0 \triangleright u_0 = u \triangleleft H$. Suppose that T is a star tree of order n , whose center vertex is w . If $G_1 = (G \triangleright u = w \triangleleft T)$ and $G_2 = (G \triangleright v = w \triangleleft T)$ (see Figure 7), then $z(G_1) < z(G_2)$.

4. SMALLEST TRICYCLIC GRAPH

In section 2 we have shown that a tricyclic graph has 19 classes, according to its cycles. In this section, we find the smallest Hosoya index of the tricyclic graphs without changing their orders. This is done by applying some decreasing transformations on the 19 classes of the tricyclic graphs. Let $G(n, n + 2)$ be the set of simple connected graphs with n vertices and $n + 2$ edges-the set of connected tricyclic graphs of order n . We use the decreasing Transformations **A**, **B**, **C**, and **D**. We repeat these transformations to decrease the Hosoya index of $(n, n + 2)$ -graphs as much as possible. Let $G_0 \in G(n, n + 2)$ be a tricyclic graph. At first by repeating Transformation **A** on G_0 we construct a tricyclic graph G_1 which $z(G_1) \leq z(G_0)$ and all pendant paths of G_1 are of length one. In the second step, by using Transformation **B**, we reach the tricyclic graph G_2 in which these pendant edges are attached to the same vertex. Then we apply the Transformation **C** as the third step. We repeat this step until we obtain a tricyclic graph G_3 which has no the conditions of the Transformation **C**. Note that, after each applying of the Transformation **C** we may use the Transformation **B** to achieve the conditions of the Transformation **C** (reducing the degree of the vertices of the internal paths to two). Now, we have a graph that all its pendant edges are attached to a finite set of vertices. Once again, by applying the Transformation **B**, we reach a graph in which these pendant edges are attached to the same vertex. Now, by applying three steps above we have some candidate graphs for each class to be smallest. Then for class number i ($i=1, \dots, 19$ and $i \neq 12$) we use the Transformation **D** to select the smallest graphs among the candidate graphs. For class 12 we select the smallest one by directly comparison. Finally, we find the smallest Hosoya index of $G(n, n + 2)$ by comparison the smallest Hosoya index among all obtained smallest graph for each class. A summary is depicted as a table in Fig. 8. In this figure all classes are shown in the second column of the given table. The third column represents the obtained graph (or graphs) of using and repeating the decreasing transformations for each class. Finally, the fourth column represents the Smallest Hosoya index of each class. By comparison the smallest Hosoya index of the obtained graphs, we find the smallest Hosoya index of $G(n, n + 2)$ which is $4n - 6$ and are related to classes number 13 and 15.

Consequently, in the following theorem we present a lower bound for the Hosoya index of the tricyclic graphs of order n . Moreover, we show that the depicted graphs in Figure 9 are the extremal graphs.

class	Main graph	Smallest graph in the the class	The smallest index
1			$z(G) = 8n - 24$
2			$12n - 48$
3			$40n - 260$
4			$16n - 72$
5			$20n - 100$
6			$64n - 480$
7			$10n - 25$
8			$16n - 72$
9			$12n - 46$
10			$6n - 14$
11			$8n - 24$
12			$8n - 24$
13			$4n - 6$
14			$5n - 10$
15			$4n - 6$
16			$10n - 35$


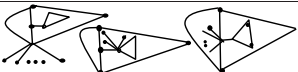
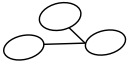

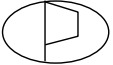
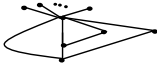
17			$16n - 72$
18			$32n - 192$
19			$5n - 10$

Figure 8. Smallest graph (or graphs) with respect to the Hosoya index and the smallest Hosoya index for each class.

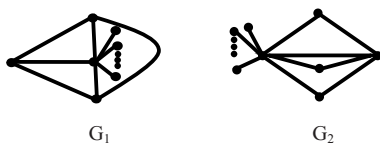


Figure 9. The smallest tricyclic graphs with respect to the Hosoya index

Theorem 4.1. If G is an arbitrary tricyclic graph of order $n \geq 5$ then $z(G) \geq 4n - 6$. Equality holds if and only if $G \in \{G_1, G_2\}$, where G_1 and G_2 are the depicted graphs in Figure 9.

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