



## Research article

## Conjugated tricyclic graphs with maximum variable sum exdeg index

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## ABSTRACT

The variable sum exdeg index, initially introduced by Vukicevic (2011) [20] for predicting the octanol water partition co-efficient of certain chemical compounds, is an invariant for a graph  $G$  and defined as  $SEI_a(G) = \sum_{v \in V(G)} (d_v a^{d_v})$ , where  $d_v$  is the degree of vertex  $v \in V(G)$ ,  $a$  is a positive real number different from 1. In this paper, we defined sub-collections of tricyclic graphs say  $T_{2m}^3, T_{2m}^4, T_{2m}^6$  and  $T_{2m}^7$ . The graph with maximum variable sum exdeg index is characterized from each collection given above with perfect matching. Consequently, through a comparison among these extremal graphs, we indicate the graph which contains maximum  $SEI_a$ -value from  $T_{2m}$ .

## 1. Introduction

Let  $G = (V, E)$  be a graph which is finite, connected and simple such that  $V$  and  $E$  denote the set of vertices and set of edges respectively. Let  $y \in V(G)$ ,  $d_y$  or  $d_y(G)$  is defined as the degree of the vertex  $y$ . Let  $M(G) \subset E(G)$ , if the degree of each vertex in  $M(G)$  is 1 or 0 then  $M(G)$  is called  $m$ -matching in  $G$  where  $|M(G)| = m$ . In a graph  $G$  if each vertex is incident to exactly one edge of matching set then such matching is called perfect matching such that  $n = 2m$ . Let  $e$  be an edge such that  $e \in M(G)$  and  $u \in V(G)$ , the vertex  $u$  is said to be saturated by  $M(G)$  if  $u$  is incident with  $e$ . A simple and connected graph with  $2m$  vertices and  $2m + 2$  edges is called conjugated tricyclic graph, where  $m$  is the matching number of the graph.

A vertex which possesses degree one is called pendent vertex. A path  $P = x_0x_1 \dots x_s$  is said to be pendent path if  $d_{x_0} \geq 3$ ,  $d_{x_i} = 2$  ( $i = 1, 2, \dots, (s-1)$ ) and  $d_{x_s} = 1$ . A path  $P = x_0x_1 \dots x_s$  is said to be an internal path of a graph if  $d_{x_0} \geq 3$ ,  $d_{x_i} = 2$  ( $i = 1, 2, \dots, (s-1)$ ) and  $d_{x_s} \geq 3$  whereas  $P$  is the shortest path from  $x_0$  to  $x_s$ . We denote the length of the path  $P$  by  $|P|$ . In a graph  $G$ , an induced cycle is an induced sub-graph which has no chords. Set of neighbouring vertices of a vertex  $x$  in  $G$  is denoted by  $N_G(x)$  whereas  $N_G[x] = N_G(x) \cup \{x\}$ .

Set of all conjugated tricyclic graphs is denoted by  $T_{2m}$  where  $2m$  is order of the graph  $T_{2m}$  with  $m \geq 2$ . Since  $T_4 = K_4$  here  $K_4$  denotes the complete graph with order 4. That is why we consider in the following  $m \geq 3$ . From [10] we know that tricyclic graph has minimum 3 and maximum 7 cycles; furthermore there does not exist a graph in  $G$  with five cycles. We define  $T_{2m} = T_{2m}^3 \cup T_{2m}^4 \cup T_{2m}^6 \cup T_{2m}^7$  where  $T_{2m}^k$  ( $k = 3, 4, 6, 7$ ) represents the collection of all tricyclic graphs having  $k$  cycles in  $T_{2m}$ . We organized the rest of the paper as follows. In section 2, we have given some lemmas which help us in proving main result. In section 3, we investigated maximum values of  $SEI_a$  in  $T_{2m}^j$  ( $j = 3, 4, 6, 7$ ) for  $a > 1$ . At the end of this section, we have investigated the graph which contains maximum  $SEI_a$ -value in  $T_{2m}$  for  $a > 1$ . To read about the expressions and definitions related to this paper, the readers can see [2,4].

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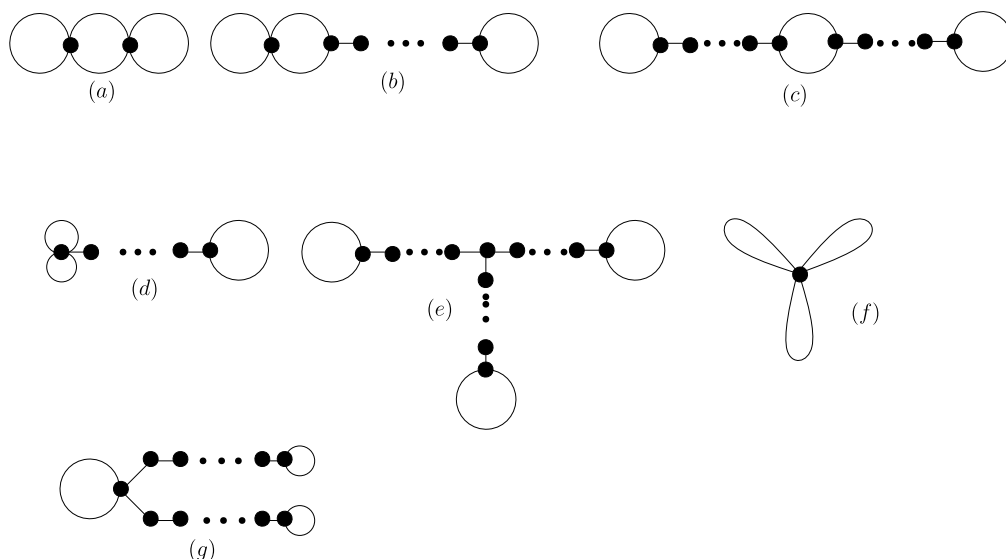


Fig. 1. Possible graphs in  $G \in T_{2m}^3$ .

Graphs help us design the chemical graph in which vertices and edges represent atoms and bonds respectively. Topological indices are used to investigate the physicochemical properties of a molecular graph. The graph invariants are called topological indices [22]. Actually, these topological indices give us the values which are the information about the physicochemical properties of a certain related chemical compound. In this way, we can spare ourselves from a heavy expense of chemical experiments.

Topological indices are used in quantitative structure-property relation (QSPR) and quantitative structure-activity relation (QSAR) studies to model the physicochemical characteristics of chemical compounds including total surface area, melting points, molar refraction, boiling points, acentric factor, octanol-water partition coefficient, motor octane number, and standard enthalpy of formation [5,11,19]. In addition to QSPR and QSAR the topological indices are also used in many fields of knowledge including chemistry, physics, biology, and the social sciences see for more detail [7–9,17,18]. There are a large number of topological indices in literature which have been used to investigate the above mentioned physicochemical properties for their related molecular structure. To investigate these properties researchers find extremal graphs from related class of molecular structures. For instance, in [13], extremal graphs have been characterized by using different graph parameters such as segments and vertices of degree two. Xiaoling Sun et al. [16] investigated extremal values of exdeg index for quasi-tree graphs and unicyclic graphs by using some graph parameters. In [3], the first three maximum and minimum values of  $SEI_a$  have been undersought for  $n$ -vertex trees. Furthermore,  $n$ -vertex trees with given diameter  $d$  have first three largest values of  $SEI_a$ . In [12], lower bounds of some topological indices have been found for some family of graphs. In the following lines we will discuss the topological index related to our current work.

The variable sum exdeg index of a graph  $G$  is denoted by Vukicevic as,

$$SEI_a(G) = \sum_{uv \in E(G)} (a^{d_u} + a^{d_v}) = \sum_{u \in V(G)} (d_u a^{d_u}) \quad (1)$$

where  $a > 0$  but  $a \neq 1$ . The above mentioned molecular structure descriptor/topological index having a good correlation with octane-water partition coefficient [19] and octane isomers is studied very well by this index, see [20]. The role of this index in nanoscience can be seen in [23]. Rizwan et al. investigated sharp lower and upper bounds on  $SEI_a$  for conjugated uni cyclic graphs with respect to the length of its cycle [15]. In [14], the author investigated sharp lower and upper bounds on  $SEI_a$  for conjugated bicyclic graphs. The author et al. investigated extremal values of  $SEI_a$  for cactus graphs with fixed number of cycles [6]. We refer the following papers to see mathematical properties and chemical application of this index [1,19,21]. In the below sections of this paper we apply some graph operations or transformation on a graph  $G$  and the resulting graph is depicted by  $G'$ . In such case whenever we discuss the degree of a vertex  $x$  say  $d_x$ , it means the degree of the vertex  $x$  in  $G$  i.e.,  $|V(G)| = |V(G')|$ .

## 2. Some lemmas

Here we will put some lemmas for supporting our main goal. Let  $G \in T_{2m}^j$  ( $j = 3, 4, 6, 7$ ) (with perfect matching) be a connected graph having minimal connected subgraph  $H$  with  $j$  cycles ( $j = 3, 4, 6, 7$ ) and some trees. Let  $G'_j$  ( $j = 3, 4, 6, 7$ ) contain maximum  $SEI_a$  which means for all  $G \in T_{2m}^j$  ( $j = 3, 4, 6, 7$ ) we have  $SEI_a(G'_j) \geq SEI_a(G)$  where  $a > 1$ . For a graph  $G'_j$  ( $j = 3, 4, 6, 7$ ), minimal subgraph and perfect matching are depicted by  $H'_j$  and  $M'_j$  respectively. By [10], the arrangement of  $j$  cycles of the graph from  $T_{2m}^j$  ( $j = 3, 4, 6, 7$ ) contains 7, 4, 3 and 1 possible cases respectively, as depicted in Fig. 1, Fig. 2, and Fig. 3, respectively.

**Lemma 1.** For any pendent path  $P$  from  $G'_j$  ( $j = 3, 4, 6, 7$ ) we have the following results:

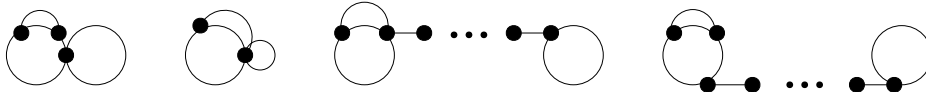


Fig. 2. Possible graphs in  $G \in T_{2m}^4$ .



Fig. 3. Possible graphs in  $G \in T_{2m}^6$  and one graph in  $G \in T_{2m}^7$ .

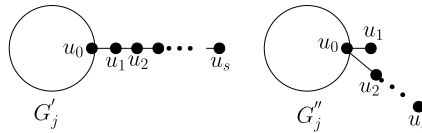


Fig. 4.  $G'_j$  and  $G''_j$  in (1).

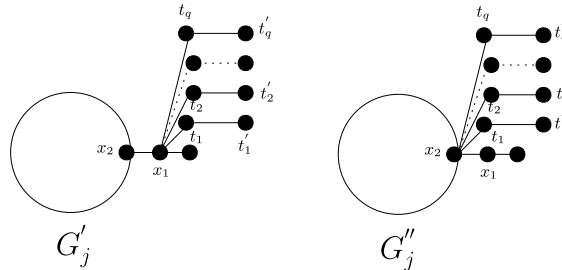


Fig. 5.  $G'_j$  and  $G''_j$  in (2).

1. The length of the pendent path  $P$  is less or equal to two.
2. In  $G'_j$  every pendent path of length two (if there exists) is attached to the vertex  $u$  where the vertex  $u$  has maximum degree in  $H'_j$ .

**Proof.** (1) We suppose on the contrary that  $P = u_0u_1\dots u_s$  where  $s \geq 3$  be a pendent path where  $d_{u_0} \geq 3$ ,  $d_{u_s} = 1$  and  $d_{u_i} = 2(i = 1, 2, \dots, (s - 1))$ . We define  $G''_j = G'_j - u_{s-2}u_{s-1} + u_0u_{s-1}$  clearly  $G''_j \in T_{2m}^j$  ( $j = 3, 4, 6, 7$ ). For instance we show  $G''_j$  in Fig. 4. So we have,

$$SEI_a(G''_j) - SEI_a(G'_j) = \left[ (d_{u_0} + 1)a^{d_{u_0}+1} - (d_{u_0})a^{d_{u_0}} \right] - \left[ (d_{u_{s-2}})a^{d_{u_{s-2}}} - (d_{u_{s-2}} - 1)a^{d_{u_{s-2}-1}} \right] = \left[ a^{\mu_2}(1 + \mu_2 \ln a) - a^{\mu_1}(1 + \mu_1 \ln a) \right], \tag{2}$$

from  $a > 1$ ,  $\mu_1 \in (d_{u_{s-2}} - 1, d_{u_{s-2}})$ ,  $\mu_2 \in (d_{u_0}, d_{u_0} + 1)$  and  $\mu_2 > \mu_1$ , we have  $SEI_a(G''_j) > SEI_a(G'_j)$ , a contradiction.

(2) We suppose on the contrary there exist  $x_1$  and  $x_2$  vertices in  $H'_j$  such that  $d_{x_2} \geq d_{x_1} \geq 2$ . Let  $x_1$  be the end vertex of some pendent paths of length two, say  $P_1 = x_1t_1t'_1$ ,  $P_2 = x_1t_2t'_2$ , ...  $P_q = x_1t_qt'_q$ . We define  $G''_j = G'_j - \sum_{i=1}^q(x_1t_i) + \sum_{i=1}^q(x_2t_i)$  clearly  $G''_j \in T_{2m}^j$ . For instance, we show  $G''_j$  in Fig. 5. From  $G'_j$  and  $G''_j$  we have,

$$SEI_a(G''_j) - SEI_a(G'_j) = \left[ (d_{x_2} + q)a^{d_{x_2}+q} - (d_{x_2})a^{d_{x_2}} \right] - \left[ (d_{x_1})a^{d_{x_1}} - (d_{x_1} - q)a^{d_{x_1}-q} \right] = \left[ a^{\mu_2}(1 + \mu_2 \ln a) - a^{\mu_1}(1 + \mu_1 \ln a) \right], \tag{3}$$

from  $a > 1$ ,  $\mu_1 \in (d_{x_1} - q, d_{x_1})$ ,  $\mu_2 \in (d_{x_2}, d_{x_2} + q)$  and  $\mu_2 > \mu_1$ , we have  $SEI_a(G''_j) > SEI_a(G'_j)$ , a contradiction.  $\square$

**Lemma 2.** If  $P_1 \in G'_j \in T_{2m}^j$  ( $j = 3, 4, 6, 7$ ) is an internal path and  $P_2 \in G'_j \in T_{2m}^j$  ( $j = 3, 4, 6, 7$ ) is the shortest path between the vertices  $w_1$  and  $w_2$  where  $w_1$  and  $w_2$  are the common vertices of any two cycles, then

1. Length of the path  $P_1$  is exactly one and both the vertices of  $P_1$  exist in the same cycle.
2. Length of the path  $P_2$  is exactly one.

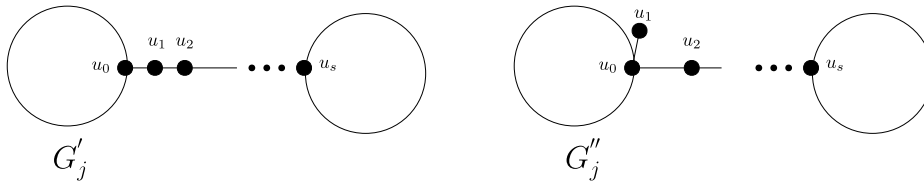


Fig. 6.  $G'_j$  and  $G''_j$  in (1).

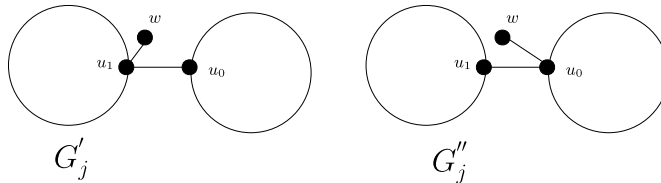


Fig. 7.  $G'_j$  and  $G''_j$  in Lemma 2, Subcase-2.

**Proof.** (1) Let  $P = u_0u_1 \dots u_s$  where  $s \geq 1$  be an internal path in  $G'_j$  ( $j = 3, 4, 6, 7$ ) where  $d_{u_0} \geq 3$ ,  $d_{u_s} \geq 3$  and  $d_{u_i} = 2$  ( $i = 1, 2, \dots, (s - 1)$ ).

Case-1: when  $s \geq 2$

Subcase-1.1: if  $u_0u_1 \in M'_j$  ( $j = 3, 4, 6, 7$ ).

We define  $G''_j = G'_j - u_1u_2 + u_0u_2$  clearly  $G''_j \in T_{2m}^j$ , as  $G''_j$  is shown in Fig. 6. We calculate,

$$SEI_a(G''_j) - SEI_a(G'_j) = \left[ (d_{u_0} + 1)a^{d_{u_0}+1} - (d_{u_0})a^{d_{u_0}} \right] - \left[ (d_{u_1})a^{d_{u_1}} - (d_{u_1} - 1)a^{d_{u_1}-1} \right] \\ = \left[ a^{\mu_2}(1 + \mu_2 \ln a) - a^{\mu_1}(1 + \mu_1 \ln a) \right], \tag{4}$$

from  $a > 1$ ,  $\mu_1 \in (d_{u_1} - 1, d_{u_1})$ ,  $\mu_2 \in (d_{u_0}, d_{u_0} + 1)$  and  $\mu_2 > \mu_1$ , we conclude  $SEI_a(G''_j) > SEI_a(G'_j)$ , a contradiction.

Subcase-1.2: if  $u_0u_1 \notin M'_j$  ( $j = 3, 4, 6, 7$ ).

We define  $G''_j = G'_j - u_0u_1 + u_0u_k$  clearly  $G''_j \in T_{2m}^j$ .

$$SEI_a(G''_j) - SEI_a(G'_j) = \left[ (d_{u_k} + 1)a^{d_{u_k}+1} - (d_{u_k})a^{d_{u_k}} \right] - \left[ (d_{u_1})a^{d_{u_1}} - (d_{u_1} - 1)a^{d_{u_1}-1} \right] \\ = \left[ a^{\mu_2}(1 + \mu_2 \ln a) - a^{\mu_1}(1 + \mu_1 \ln a) \right], \tag{5}$$

from  $a > 1$ ,  $\mu_1 \in (d_{u_1} - 1, d_{u_1})$ ,  $\mu_2 \in (d_{u_k}, d_{u_k} + 1)$  and  $\mu_2 > \mu_1$ , we conclude  $SEI_a(G''_j) > SEI_a(G'_j)$ , a contradiction.

Subcase-2: if  $s = 1$  but  $u_0$  and  $u_1$  does not exist on same cycle.

As we know that  $s = 1$ ,  $d_{u_1} \geq 3$ . Here we let  $d_{u_0} \geq d_{u_1}$  then there must exist a vertex  $w \in N_{G'_j}(u_1) - N_{G'_j}(u_0)$  such that  $u_1w \notin M'_j$  ( $j = 3, 4, 6, 7$ ).

We define  $G''_j = G'_j - u_1w + u_0w$  clearly  $G''_j \in T_{2m}^j$  as shown in Fig. 7.

$$SEI_a(G''_j) - SEI_a(G'_j) = \left[ (d_{u_0} + 1)a^{d_{u_0}+1} - (d_{u_0})a^{d_{u_0}} \right] - \left[ (d_{u_1})a^{d_{u_1}} - (d_{u_1} - 1)a^{d_{u_1}-1} \right] \\ = \left[ a^{\mu_2}(1 + \mu_2 \ln a) - a^{\mu_1}(1 + \mu_1 \ln a) \right], \tag{6}$$

from  $a > 1$ ,  $\mu_1 \in (d_{u_1} - 1, d_{u_1})$ ,  $\mu_2 \in (d_{u_0}, d_{u_0} + 1)$  and  $\mu_2 > \mu_1$ , we have  $SEI_a(G''_j) > SEI_a(G'_j)$ , a contradiction.

(2) We assume that  $P_2 = u_0u_1 \dots u_s$  where  $s \geq 1$ ,  $w_1 = u_0$  and  $u_s = w_2$ . Let  $P_2$  be the shortest path between the vertices  $w_1$  and  $w_2$  with  $d_{w_1} \geq 3$  and  $d_{w_2} \geq 3$ . We suppose on the contrary  $|P_2| = s \geq 2$  then by proof (1) and Lemma 1 we can find a vertex of degree one adjacent to  $u_1$  and  $u_1u_2 \notin M'_j$  ( $j = 3, 4, 6, 7$ ), so it becomes clear that  $d_{u_1} = 3$ . We define  $G''_j = G'_j - u_1u_2 + u_2w_1$  clearly  $G''_j \in T_{2m}^j$ .

$$SEI_a(G''_j) - SEI_a(G'_j) = \left[ (d_{w_1} + 1)a^{d_{w_1}+1} - (d_{w_1})a^{d_{w_1}} \right] - \left[ (d_{u_1})a^{d_{u_1}} - (d_{u_1} - 1)a^{d_{u_1}-1} \right] \\ = \left[ a^{\mu_2}(1 + \mu_2 \ln a) - a^{\mu_1}(1 + \mu_1 \ln a) \right], \tag{7}$$

from  $a > 1$ ,  $\mu_1 \in (d_{u_1} - 1, d_{u_1})$ ,  $\mu_2 \in (d_{w_1}, d_{w_1} + 1)$  and  $\mu_2 > \mu_1$ , we derive the relation  $SEI_a(G''_j) > SEI_a(G'_j)$ , a contradiction.  $\square$

**Lemma 3.** For any induced cycle say  $C$  from  $G'_j \in T_{2m}^j$  ( $j = 3, 4, 6, 7$ ) the length of this cycle is 3 such that  $|C| = 3$ .

**Proof.** From Lemma 2 we are sure that all induced cycles which belong to  $G'_j \in T_{2m}^j$  having exactly three vertices in it. That is why we discuss the graph  $G'_j \in T_{2m}^j$  ( $j = 3, 4, 6$ ) only. We suppose on the contrary,  $|C| \geq 4$ . Let  $x$  and  $y$  be the vertices in  $C$  where  $x$  has the maximum degree and  $y$  be at the farthest distance from  $x$ . Let  $P : x = x_0x_1 \dots x_s (= y)$ , be the shortest path and the vertices  $x_1, x_2, \dots, x_{s-1}$  are not common between any two cycles. Length of the path  $P$  can be greater or equal to 2 such that  $|P| = s \geq 2$ .

Case-1: when  $s = 2$

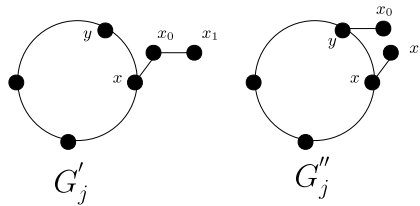


Fig. 8.  $G'_j$  and  $G''_j$  in Lemma 4, Case-1.

Subcase-1.1: if  $x_1x_2 \notin M'_j (j = 3, 4, 6)$ .

We define  $G''_j = G'_j - x_1x_2 + xx_2$  clearly  $G''_j \in T_{2m}^j (j = 3, 4, 6)$ .

$$SEI_a(G''_j) - SEI_a(G'_j) = [(d_x + 1)a^{d_x+1} - (d_x)a^{d_x}] - [(d_{x_1})a^{d_{x_1}} - (d_{x_1} - 1)a^{d_{x_1}-1}] = [a^{\mu_2}(1 + \mu_2 \ln a) - a^{\mu_1}(1 + \mu_1 \ln a)], \tag{8}$$

from  $a > 1, \mu_1 \in (d_{x_1} - 1, d_{x_1}), \mu_2 \in (d_x, d_x + 1)$  and  $\mu_2 > \mu_1$ , we conclude  $SEI_a(G''_j) > SEI_a(G'_j)$ , a contradiction.

Subcase-1.2: if  $x_1x_2 \in M'_j (j = 3, 4, 6)$ .

As we know that  $M'_j (j = 3, 4, 6)$  so Lemma 1 and Lemma 2 ensure that  $d_{x_1} = 2$ . Let  $G''_j = G'_j - xx_1 + xx_2$  clearly  $G''_j \in T_{2m}^j (j = 3, 4, 6)$ .

$$SEI_a(G''_j) - SEI_a(G'_j) = [(d_{x_2} + 1)a^{d_{x_2}+1} - (d_{x_2})a^{d_{x_2}}] - [(d_{x_1})a^{d_{x_1}} - (d_{x_1} - 1)a^{d_{x_1}-1}] = [a^{\mu_2}(1 + \mu_2 \ln a) - a^{\mu_1}(1 + \mu_1 \ln a)], \tag{9}$$

from  $a > 1, \mu_1 \in (d_{x_1} - 1, d_{x_1}), \mu_2 \in (d_{x_2}, d_{x_2} + 1)$  and  $\mu_2 > \mu_1$ , we get  $SEI_a(G''_j) > SEI_a(G'_j)$ , a contradiction.

Subcase-2: if  $s \geq 3$

Subcase-2.1: if  $x_2x_3 \in M'_j (j = 3, 4, 6)$ .

We define  $G''_j = G'_j - x_1x_2 + xx_2$  clearly  $G''_j \in T_{2m}^j$ . We have,

$$SEI_a(G''_j) - SEI_a(G'_j) = [(d_x + 1)a^{d_x+1} - (d_x)a^{d_x}] - [(d_{x_1})a^{d_{x_1}} - (d_{x_1} - 1)a^{d_{x_1}-1}] = [a^{\mu_2}(1 + \mu_2 \ln a) - a^{\mu_1}(1 + \mu_1 \ln a)], \tag{10}$$

from  $a > 1, \mu_1 \in (d_{x_1} - 1, d_{x_1}), \mu_2 \in (d_x, d_x + 1)$  and  $\mu_2 > \mu_1$ , we have  $SEI_a(G''_j) > SEI_a(G'_j)$ , a contradiction.

Subcase-2.2: if  $x_2x_3 \notin M'_j (j = 3, 4, 6)$ .

Let  $G''_j = G'_j - x_2x_3 + xx_3$  clearly  $G''_j \in T_{2m}^j$ .

$$SEI_a(G''_j) - SEI_a(G'_j) = [(d_x + 1)a^{d_x+1} - (d_x)a^{d_x}] - [(d_{x_2})a^{d_{x_2}} - (d_{x_2} - 1)a^{d_{x_2}-1}] = [a^{\mu_2}(1 + \mu_2 \ln a) - a^{\mu_1}(1 + \mu_1 \ln a)], \tag{11}$$

since  $a > 1, \mu_1 \in (d_{x_2} - 1, d_{x_2}), \mu_2 \in (d_x, d_x + 1)$  and  $\mu_2 > \mu_1$ , and we get  $SEI_a(G''_j) > SEI_a(G'_j)$ , a contradiction.  $\square$

**Lemma 4.** Let  $P_1, P_2, \dots, P_r$  be the pendent paths of length two in  $G'_j$ . All these pendent paths are attached to the vertex  $x \in V(H'_j)$  where  $x$  be the vertex of maximum degree. Then the graph  $G'_j \in T_{2m}^j (j = 3, 4, 6, 7)$  contains a unique vertex of degree one adjacent to  $x$  such that  $m \geq 4$ .

**Proof.** We suppose on the contrary that vertex  $x$  has no pendent edge adjacent to it. According to Lemma 1, Lemma 2, and Lemma 3 there will be two cases below.

Case-1:

We suppose that  $P = xx_0x_1$  is one of the pendent paths which are adjacent to the vertex  $x$ . Let  $y \in N_{H'_j}(x)$  such that  $(d_y \geq d_{x_0} = 2)$  with  $xy \in M'_j$ . We define  $G''_j = G'_j - x_0x_1 + yx_1$  clearly  $G''_j \in T_{2m}^j (j = 3, 4, 6, 7)$  for our convenience we show  $G''_j$  in Fig. 8. Since  $M''_j = M'_j - \{x_0x_1, xy\} + \{yx_0, yx_1\}$  is a perfect matching of  $G''_j (j = 3, 4, 6, 7)$ . We have,

$$SEI_a(G''_j) - SEI_a(G'_j) = [(d_y + 1)a^{d_y+1} - (d_y)a^{d_y}] - [(d_{x_0})a^{d_{x_0}} - (d_{x_0} - 1)a^{d_{x_0}-1}] = [a^{\mu_2}(1 + \mu_2 \ln a) - a^{\mu_1}(1 + \mu_1 \ln a)], \tag{12}$$

from  $a > 1, \mu_1 \in (d_{x_0} - 1, d_{x_0}), \mu_2 \in (d_y, d_y + 1)$  and  $\mu_2 > \mu_1$ , we have  $SEI_a(G''_j) > SEI_a(G'_j)$ , a contradiction.

Case-2: if pendent path of length 2 does not exist.

Lemma 2 and Lemma 3 guarantee that the vertex  $x$  must be common in at least two induced cycles of length 3 in  $G'_j (3, 4, 6, 7)$ . As we know that  $m \geq 4$ , so we consider  $w_1$  is a pendent vertex adjacent to  $w_2 \in V(H'_j) - x$  where  $w_2 \in N_{H'_j}(x)$ . We consider the vertex

$w_3 \in H'_j$  with  $xw_3 \in M'_j (d_{w_3} \geq 2)$ . Here we make two sub-cases.

Subcase-2.1: if  $w_3 \in N_{H'_j}(x) \cap N_{H'_j}(w_2)$

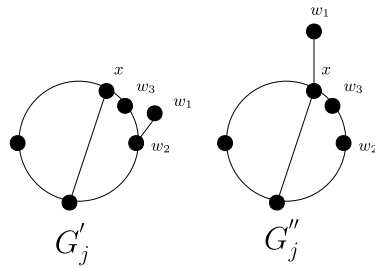


Fig. 9.  $G'_j$  and  $G''_j$  in Lemma 4, Case-2.1.

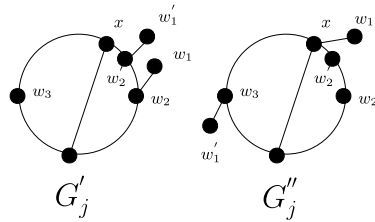


Fig. 10.  $G'_j$  and  $G''_j$  in Lemma 4, Subcase-2.2.

We define  $G''_j = G'_j - w_1w_2 + w_1x$  clearly  $G''_j \in T_{2m}^j$  for our convenience we show  $G''_j$  in Fig. 9. Since  $M''_j = M'_j - \{xw_3, w_1w_2\} + \{xw_1, w_2w_3\}$  is a perfect matching of  $G''_j$  ( $j = 3, 4, 6, 7$ ). We have,

$$SEI_a(G''_j) - SEI_a(G'_j) = [(d_x + 1)a^{d_x+1} - (d_x)a^{d_x}] - [(d_{w_2})a^{d_{w_2}} - (d_{w_2} - 1)a^{d_{w_2}-1}] = [a^{\mu_2}(1 + \mu_2 \ln a) - a^{\mu_1}(1 + \mu_1 \ln a)], \tag{13}$$

from  $a > 1$ ,  $\mu_1 \in (d_{w_2} - 1, d_{w_2})$ ,  $\mu_2 \in (d_x, d_x + 1)$  and  $\mu_2 > \mu_1$ , we have  $SEI_a(G''_j) > SEI_a(G'_j)$ , a contradiction.

Subcase-2.2: if  $w_3 \notin N_{H'_j}(x) \cap N_{H'_j}(w_2)$

Lemma 2 and Lemma 3 guarantee that there exists a vertex  $w'_1$  adjacent to  $w'_2 \notin N_{H'_j}(x) \cap N_{H'_j}(w_2)$  such that  $d_{w'_1=1}$  and one of  $\{w_2, w'_2\}$  has degree 3. We assume that  $d_{w'_2} = 3$ . We define  $G''_j = G'_j - w_1w_2 - w'_2w'_1 + xw_1 + w_3w'_1$  clearly  $G''_j \in T_{2m}^j$  because  $M''_j = M'_j - \{w_1w_2, w'_2w'_1, xw_3\} + \{xw_1, w_2w'_2, w_3w'_1\}$  is a perfect matching of  $G''_j$  ( $j = 3, 4, 6, 7$ ). For instance we define  $G''_j$  in Fig. 10. We have,

$$SEI_a(G''_j) - SEI_a(G'_j) = [(d_x + 1)a^{d_x+1} - (d_x)a^{d_x}] - [(d_{w_2})a^{d_{w_2}} - (d_{w_2} - 1)a^{d_{w_2}-1}] + [(d_{w_3} + 1)a^{d_{w_3}+1} - (d_{w_3})a^{d_{w_3}}] - [(d_{w'_2})a^{d_{w'_2}} - (d_{w'_2} - 1)a^{d_{w'_2}-1}] = [a^{\mu_2}(1 + \mu_2 \ln a) - a^{\mu_1}(1 + \mu_1 \ln a)] + [a^{\mu_4}(1 + \mu_4 \ln a) - a^{\mu_3}(1 + \mu_3 \ln a)], \tag{14}$$

from  $a > 1$ ,  $\mu_1 \in (d_{w_2} - 1, d_{w_2})$ ,  $\mu_2 \in (d_x, d_x + 1)$ ,  $\mu_3 \in (d_{w'_2} - 1, d_{w'_2})$ ,  $\mu_4 \in (d_{w_3}, d_{w_3} + 1)$  and  $\mu_2 > \mu_1$ ,  $\mu_4 > \mu_3$ , we have  $SEI_a(G''_j) > SEI_a(G'_j)$ , a contradiction.  $\square$

### 3. Main results

In the current section, we have investigated the graph from  $T_{2m}^j$  ( $j = 3, 4, 6, 7$ ) which has maximum  $SEI_a$  where  $a > 1$ . Following this, we also described the unique graph in  $T_{2m}$  having the highest  $SEI_a$ -value.

**Theorem 1.** Let  $m \geq 4$ ,  $a > 1$  and  $G \in T_{2m}^3$  then  $SEI_a(G) \leq SEI_a(F_3(2m))$  and the equality in the bound is attained if and only if  $G \cong F_3(2m)$  where  $F_3(2m)$  is depicted in Fig. 11.

**Proof.** From Lemma 1, Lemma 2 and Lemma 3, it is easy to understand that  $H'_3 \cong F_3$  or  $H'_3 \cong F'_3$  (depicted in Fig. 11). Let  $M'_3$  be the perfect matching in  $G'_3$ . Here we claim that  $H'_3 \cong F_3$ .

We suppose on the contrary that  $H'_3 \cong F'_3$ . Let  $x, y, x_1$  and  $x_2$  be the vertices depicted in Fig. 11. In Fig. 11,  $x$  and  $y$  are the only vertices which have maximum degree. Lemma 4 and Lemma 1 ensure the existence of a pendent vertex which is adjacent to  $y$  where all the pendent paths of length two end at the vertex  $y$ . From above discussion we can say  $xy \notin M'_3$ .

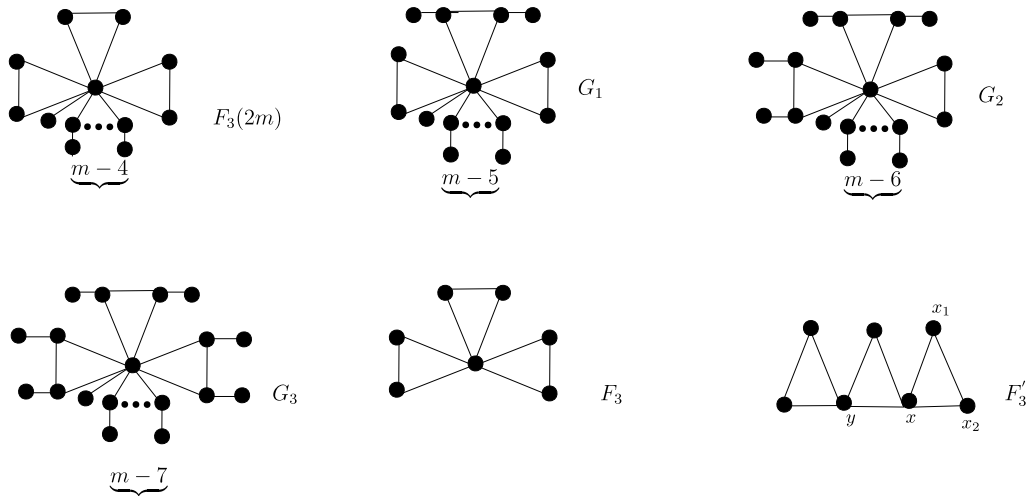


Fig. 11.  $F_3(2m)$ ,  $F_3$ ,  $F'_3$  and  $G_i(i = 1, 2, 3)$ .

Case-1: if  $xx_1 \notin M'_3$  and  $xx_2 \notin M'_3$ .

We define  $G''_3 = G'_3 - xx_1 - xx_2 + yx_1 + yx_2$  clearly  $G''_3 \in T^3_{2m}$ . We have,

$$SEI_a(G''_3) - SEI_a(G'_3) = [(d_y + 2)a^{d_y+2} - (d_y)a^{d_y}] - [(d_x)a^{d_x} - (d_x - 2)a^{d_x-2}] = 2 \cdot [a^{\mu_2}(1 + \mu_2 \ln a) - a^{\mu_1}(1 + \mu_1 \ln a)], \tag{15}$$

from  $a > 1$ ,  $\mu_1 \in (d_x - 2, d_x)$ ,  $\mu_2 \in (d_y, d_y + 2)$  and  $\mu_2 > \mu_1$ , we have  $SEI_a(G''_3) > SEI_a(G'_3)$ , a contradiction.

Case-2: if  $xx_1 \in M'_3$  or  $xx_2 \in M'_3$ .

If  $xx_1 \in M'_3$  then there exists a vertex of degree one say  $x_3$  adjacent to  $x_2$  such that  $x_2x_3 \in M'_3$ . We define  $G''_3 = G'_3 - x_2x_3 + xx_3$  clearly  $G''_3 \in T^3_{2m}$  because  $M''_3 = M'_3 - \{xx_1, x_2x_3\} + \{xx_3, x_1x_2\}$ , and  $M''_3$  belongs to the perfect matching in  $G''_3$ .

$$SEI_a(G''_3) - SEI_a(G'_3) = [(d_x + 1)a^{d_x+1} - (d_x)a^{d_x}] - [(d_{x_2})a^{d_{x_2}} - (d_{x_2} - 1)a^{d_{x_2}-1}] = [a^{\mu_2}(1 + \mu_2 \ln a) - a^{\mu_1}(1 + \mu_1 \ln a)], \tag{16}$$

from  $a > 1$ ,  $\mu_1 \in (d_{x_2} - 1, d_{x_2})$ ,  $\mu_2 \in (d_x, d_x + 1)$  and  $\mu_2 > \mu_1$ , we obtain  $SEI_a(G''_3) > SEI_a(G'_3)$ , a contradiction.

For  $m \geq 4$  there exist some graphs (depicted in Fig. 11). These graphs fulfil (characterized by Lemma 1, Lemma 2, Lemma 3, and Lemma 4) the properties of the graph for maximum  $SEI_a$ . We calculate the difference,

$$SEI_a(F_3(2m)) - SEI_a(G_1) = [(m + 3)a^{m+3} - (m + 2)a^{m+2} - 2.3a^3 + 3.2a^2 - a] > [4a^4 - 3a^3 - 2.3a^3 + 3.2a^2 - a] > 0 \tag{17}$$

In the same way, we can show that  $SEI_a(G_1) > SEI_a(G_2) > SEI_a(G_3)$ . Hence the graph  $F_3(2m)$  contains maximum  $SEI_a$ -value in  $T^3_{2m}$ .  $\square$

**Theorem 2.** Let  $m \geq 3$ ,  $a > 1$  and  $G \in T^4_{2m}$  then  $SEI_a(G) \leq SEI_a(F_4(2m))$  and the equality in the bound is attained if and only if  $G \cong F_4(2m)$ . Particularly when  $m = 3$  then  $F_4$  contains maximum  $SEI_a$  where  $F_4(2m)$  and  $F_4$  are depicted in Fig. 12.

**Proof.** From Lemma 1, Lemma 2, and Lemma 3, it is easy to understand that  $H'_4 \cong F_4$  or  $H'_4 \cong F'_4$  (depicted in Fig. 12). Let  $G'_4$  contain a perfect matching say  $M'_4$ . Here we claim that  $H'_4 \cong F_4$ .

We suppose on the contrary that  $H'_4 \cong F'_4$ . Let  $x, y$  be the vertices in  $F'_4$  depicted in Fig. 12. As we know that  $d_x = 2$  in  $F'_4$  so there will exist a vertex  $x_1 \in F'_4(d_{x_1} \geq 2)$  such that  $yx_1 \notin M'_4$ . We define  $G''_4 = G'_4 - yx_1 + xy$  clearly  $G''_4 \in T^4_{2m}$ .

$$SEI_a(G''_4) - SEI_a(G'_4) = [(d_y + 1)a^{d_y+1} - (d_y)a^{d_y}] - [(d_{x_1})a^{d_{x_1}} - (d_{x_1} - 1)a^{d_{x_1}-1}] = [a^{\mu_2}(1 + \mu_2 \ln a) - a^{\mu_1}(1 + \mu_1 \ln a)], \tag{18}$$

from  $a > 1$ ,  $\mu_1 \in (d_{x_1} - 1, d_{x_1})$ ,  $\mu_2 \in (d_y, d_y + 1)$  and  $\mu_2 > \mu_1$ , we have  $SEI_a(G''_4) > SEI_a(G'_4)$ , a contradiction.

It is easy to calculate that  $(F_4)$  contains maximum  $SEI_a$ -value for  $m = 3$ . For  $m \geq 4$  there are only four possible graphs (depicted in Fig. 12). These graphs fulfil the properties of the graph for maximum  $SEI_a$ . We calculate the difference,

$$SEI_a(F_4(2m)) - SEI_a(G_1) = [(m + 2)a^{m+2} - (m + 1)a^{m+1} - 4a^4 + 2.2a^2 - a]$$

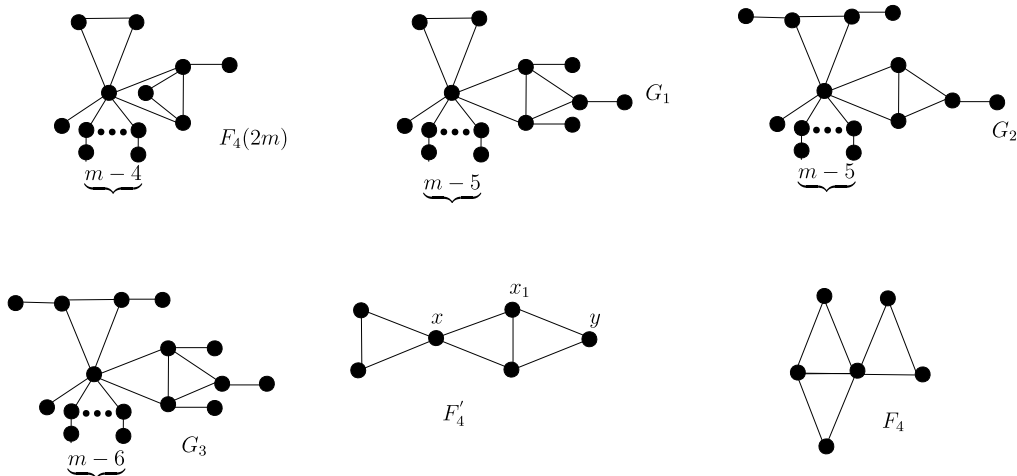


Fig. 12.  $F_4(2m)$ ,  $F_4$ ,  $F_4'$  and  $G_i(i = 1, 2, 3)$ .

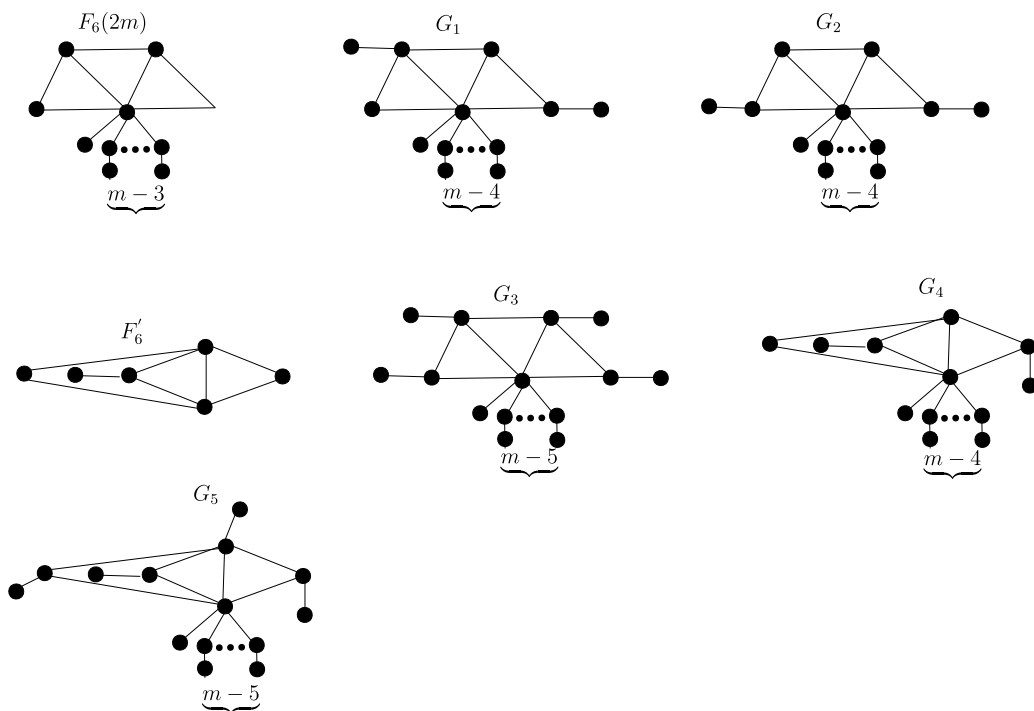


Fig. 13.  $F_6(2m)$ ,  $F_6'$  and  $G_i(i = 1, 2, 3, 4, 5)$ .

$$> [5a^5 - 2.4a^4 + 2.2a^2 - a] > 0 \tag{19}$$

Similarly, we may demonstrate that  $SEI_a(G_1) > SEI_a(G_2) > SEI_a(G_3)$ . Hence the graph  $F_4(2m)$  contains maximum  $SEI_a$ -value in  $T_{2m}^4$ .  $\square$

**Theorem 3.** Let  $m \geq 3$ ,  $a > 1$  and  $G \in T_{2m}^6$  then  $SEI_a(G) \leq SEI_a(F_6(2m))$  and the equality in the bound is attained if and only if  $G \cong F_6(2m)$  where  $F_6(2m)$  is depicted in Fig. 13.

**Proof.** For  $m = 3$  from Lemma 1, Lemma 2, and Lemma 3, it becomes easy to understand that  $G_6' \cong F_6(6)$  or  $G_6' \cong F_6'$  (depicted in Fig. 13).

$$SEI_a(F_6(6)) - SEI_a(F_6') = [5a^5 - 4a^4] - [4a^4 - 3a^3]$$



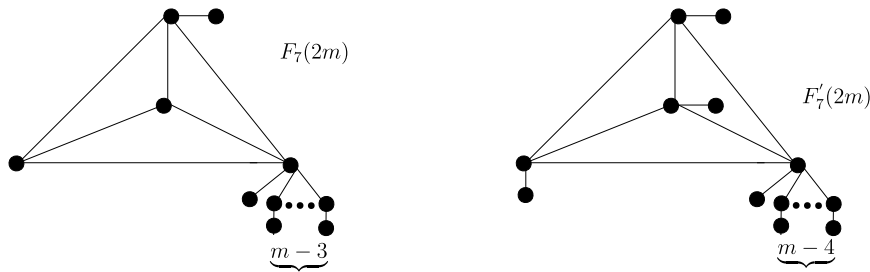


Fig. 14.  $F_7(2m)$  and  $F'_7(2m)$ .

$$= [a^{\mu_2}(1 + \mu_2 \ln a) - a^{\mu_1}(1 + \mu_1 \ln a)], \tag{20}$$

from  $a > 1$ ,  $\mu_1 \in (3, 4)$ ,  $\mu_2 \in (4, 5)$  and  $\mu_2 > \mu_1$ , we get  $SEI_a(F_6(6)) > SEI_a(F'_6)$ , a contradiction.

For  $m \geq 4$  there are only six possible graphs (depicted in Fig. 13). These graphs fulfil (characterized by Lemma 1 to Lemma 4) the properties of the graph for maximum  $SEI_a$ . We calculate the difference,

$$\begin{aligned} SEI_a(F_6(2m)) - SEI_a(G_1) &= [(m + 2)a^{m+2} - (m + 1)a^{m+1} - 4a^4 + 2.2a^2 - a] \\ &> [5a^5 - 2.4a^4 + 2.2a^2 - a] > 0. \end{aligned} \tag{21}$$

Hence,  $SEI_a(F_6(2m)) > SEI_a(G_1)$ . In the same way, we can show that  $SEI_a(G_1) > SEI_a(G_2) > SEI_a(G_3)$  and  $SEI_a(G_4) > SEI_a(G_5)$ . We also notice that  $SEI_a(G_1) = SEI_a(G_4)$  because  $G_1$  and  $G_4$  have the same degree sequence. Hence the graph  $F_6(2m)$  contains maximum  $SEI_a$ -value in  $T_{2m}^6$ .  $\square$

**Theorem 4.** Let  $m \geq 3$ ,  $m \neq 4$ ,  $a > 1$  and  $G \in T_{2m}^7$  then  $SEI_a(G) \leq SEI_a(F_7(2m))$  and the equality in the bound is attained if and only if  $G \cong F_7(2m)$  where  $F_7(2m)$  is depicted in Fig. 14.

**Proof.** For  $m = 3$ , Lemma 4 ensures that  $F_7(6)$  contains maximum  $SEI_a$ -value.

For  $m \geq 5$  there exist some graphs (depicted in Fig. 14). These graphs fulfil the properties (characterized by Lemma 1 to Lemma 4) of the graph for maximum  $SEI_a$ -value in  $T_{2m}^7$ . We calculate the difference,

$$\begin{aligned} SEI_a(F_7(2m)) - SEI_a(F'_7(2m)) &= [(m + 1)a^{m+1} - (m)a^m - 2.4a^4 + 2.3a^3 + 2a^2 - a] \\ &\geq [6a^6 - 5a^5 - 2.4a^4 + 2.3a^3 + 2a^2 - a] > 0 \end{aligned} \tag{22}$$

Finally, we conclude  $F_7(2m)$  has maximum  $SEI_a$ -value in  $T_{2m}^7$ .  $\square$

**Theorem 5.** For  $a > 1$ ,  $F_6(6)$  and  $F_3(2m)$  maximize  $SEI_a$  in  $T_{2m}$  when  $m = 3$  and  $m \geq 4$  respectively.

**Proof.** For  $m = 3$ , we have the graphs  $F_6(6)$ ,  $F_4$  and  $F_7(6)$ . We calculate the following difference.

$$SEI_a(F_6(6)) - SEI_a(F_4) = [3a^3 + a - 2a + 2a^2] > 0, \tag{23}$$

and

$$SEI_a(F_6(6)) - SEI_a(F_7(6)) = [5a^5 + 2.2a^2 - 2.4a^4 - a] > 0. \tag{24}$$

This implies that  $F_6(6)$  has the maximum  $SEI_a$ -value.

For  $m = 4$  we have the graphs  $F_3(8)$ ,  $F_4(8)$  and  $F_6(8)$ ,  $F_7(8)$  and  $F'_7(8)$ . We calculate the following difference.

$$SEI_a(F_3(8)) - SEI_a(F_4(8)) = [7a^7 - 6a^6 - 2.3a^3 + 3.2a^2 - a] > 0, \tag{25}$$

and

$$SEI_a(F_6(8)) - SEI_a(F_7(8)) = [6a^6 - 5a^5 - 4a^4 + 2.2a^2 - a] > 0, \tag{26}$$

and

$$SEI_a(F_6(8)) - SEI_a(F'_7(8)) = [6a^6 - 4.4a^4 + 2.3a^3 + 3.2a^2 - 2a] > 0. \tag{27}$$

As we know that  $SEI_a(F_4(8)) = SEI_a(F_6(8))$ ,  $F_3(8)$  contains maximum  $SEI_a$ -value.

For  $m \geq 5$

$$\begin{aligned} SEI_a(F_3(2m)) - SEI_a(F_4(2m)) &= [(m+3)a^{m+3} - (m+2)a^{m+2} - 2.3a^3 + 3.2a^2 - a] \\ &> [4a^4 - 3a^3 - 2.3a^3 + 3.2a^2 - a] > 0, \end{aligned} \quad (28)$$

and

$$\begin{aligned} SEI_a(F_6(2m)) - SEI_a(F_7(2m)) &= [(m+2)a^{m+2} - (m+1)a^{m+1} - 4a^4 + 2.2a^2 - a] \\ &> [5a^5 - 2.4a^4 + 2.2a^2 - a] > 0. \end{aligned} \quad (29)$$

Since  $SEI_a(F_4(2m)) = SEI_a(F_6(2m))$ , we conclude that  $F_3(2m)$  contains maximum  $SEI_a$ -value in  $T_{2m}$ .  $\square$

#### 4. Conclusion

In this paper, the extremal values of variable sum exdeg index  $SEI_a$  have been investigated for the class of tricyclic graphs. Therefore, the extremal values of variable sum exdeg index for multicyclic graphs are still an open problem for different values of  $a$ .

#### CRediT authorship contribution statement

Muhammad Rizwan: Conceived and designed the experiments; Performed the experiments; Wrote the paper. Akhlaq Ahmad Bhatti, Muhammad Javaid, Yilun Shang: Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data.

#### Declaration of competing interest

The authors declare the following conflict of interests: We declare that Yilun Shang is a Section Editor of Heliyon.

#### Data availability

No data was used for the research described in the article.

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