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EXTREMAL F-INDEX OF APEX TREE

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ABSTRACT. A topological index is a numeric quantity that creates a link between molecular graph of compound and its different properties and activities. The forgotten topological index is one of the most used degree based topological indices in the field of chemical graph theory. It is defined as the sum of cubes of degree of all the nodes of a graph. A graph G is called a K-apex tree if K is the smallest integer for which there exists a subset X of $V(G)$ such that $|X| = K$ and $G - X$ is a tree. In this work, the maximum forgotten topological index in the class of all k-apex trees of order n is found and the corresponding extremal graphs are characterized.

1. INTRODUCTION

Chemical graph theory is a branch of graph theory whose focus of interest is to model different structure property relationship/structure activity relationship to predict different properties and activities of molecule. The topological index play key role in such model devising. A topological index is a function from the collection of all molecular graph to the set of real numbers that remains unchanged for isomorphic graphs. A molecular graph [1] is simple connected graph considering vertices as atoms and edges as chemical bonds between them. Let G be a molecular graph with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex $v \in V(G)$ is defined as the number of vertices adjacent to v and is denoted by $d_G(v)$. The forgotten topological index is one of the well-established

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and most utilized degree based indices [2]. The forgotten topological index of a graph G is defined by

$$F(G) = \sum_{v \in V(G)} d_G(v)^3 = \sum_{uv \in E(G)} [d_G(u)^2 + d_G(v)^2].$$

This index was first appeared in 1972 [3] and its chemical significance was established in 2015 [4]. For some more works on the forgotten topological index, readers are referred to [5–7]

Let $X \subset V(G)$, then the sub graph obtained from G deleting the vertices of X is denoted by $G - X$. Note that when we delete the vertices of X, all the edges incident with the vertices of X are also deleted. If $X = \{v\}$, a singleton, then $G - X$ will be written as $G - v$. For any two non-adjacent pair of vertices u and v in a graph G, $G + uv$ denote the graph obtained from adding a new edge $uv \in G$. As usual we denote by K_n the complete graph of order n and the complete bipartite graph $K_{1,n-1}$. The join of G_1 and G_2 having V_1 and V_2 as disjoint vertex sets, is the graph $G_1 + G_2$ which contains $V_1 \cup V_2$ as vertex set and $E_1 \cup E_2 \cup \{uv : u \in V_1, v \in V_2\}$ as edge set.

Definition 1.1. *A graph is called an apex tree if it contains a vertex x such that $(G - x)$ is a tree.*

Definition 1.2. *For any integer $K \geq 1,$ the graph G is called K-apex tree if there exist a subset X of $V(G)$ of cardinality K such that $(G - X)$ is a tree and for any $Y \subset V(G)$ and $|Y| < K$, $(G - Y)$ is not a tree.*

For any $n \geq 3$ and $K \geq 1,$ let
(i) $T(n)$ denotes the set of all non-trivial apex tree of order n.
(ii) $T_K(n)$ denotes the set of all k-apex tree of order $n,$ so that $T_1(n) = T(n)$.
Apex trees and k-apex trees were introduced in [8] under the name quasi-tree graphs and k-generalized quasi-tree graphs, respectively. After that the minimal and maximal matching energies in the class of K-apex tree are computed in [9]. For some more works on the family of K-apex tree, we refer [10–12]. The goal of the present work is to obtain the maximum forgotten topological index in the class of all K-apex trees and characterize the corresponding extremal graphs.

2. MAIN RESULTS

Lemma 2.1. *If T be a tree of order n, then*

$$F(T) \leq (n-1)(n^2-2n+2)$$

with equality holds if and only if $T \cong S_n$, the star graph of order n.

Lemma 2.2. *If $u, v \in V(G)$ are not adjacent, then*

$$F(G+uv) > F(G) .$$

Theorem 2.1. *For any two vertex-disjoint graphs G_1 and G_2, we have*

$$\begin{aligned} F(G_1+G_2) &= F(G_1)+F(G_2)+3|V_2|M_1(G)+3|V_1|M_1(G_2)+6|V_2|^2|E_1| \\ &\quad +6|V_1|^2|E_2|+|V_1||V_2|^3+|V_2||V_1|^3. \end{aligned}$$

Corollary 1. *For any connected graph G with n vertices and m edges,*

$$F(K_1+G) = F(G)+3M_1(G)+n^3+6m+n.$$

Theorem 2.2. *Let G be a apex tree of order n, then*

$$F(G) \leq 2(n^3-3n^2+7n-9),$$

with equality if and only if $G \cong K_1+S_{n-1}$.

Proof. Using Theorem 2.1, we have for a graph G with n vertices and m edges,

$$F(K_1+G) = F(G)+3M_1(G)+n^3+6m+n.$$

Let, $G = T_{n-1}$ is a tree of order $(n-1)$. Then, from above

$$F(K_1+T_{n-1} = F(T_{n-1}+3M_1(T_{n-1}+(n-1)^3+6(n-2)+(n-1).$$

Now, using lemma 2.1, for T_{n-1}, we have

$$M_1(T_{n-1}) \leq (n-1)(n-2)$$

and

$$F(T_{n-1} \leq (n-2)((n-1)^2-2(n-1)+2) = (n-2)(n^2-4n+5).$$

Therefore,

$$F(G) \leq (n-2)(n^2-4n+5)+3(n-1)(n-2)+(n-1)^3+6(n-2)+(n-1)$$

from where the desired result follows clearly in the above inequality, equality holds if and only if $G = K_1+S_{n-1}$. □

Lemma 2.3. *Let* $G \in T(n, K)$, *then*

$$|E(G-v)| = K(n-1) - \frac{K(K+1)}{2}.$$

Lemma 2.4. *Let* $G \in T(n, K)$. *Then*

$$M_1(G-v) \leq K[(n-2)^2 + K(n-K-1)]$$

with equality if and only if $G = K_K + S_{n-K}$.

Theorem 2.3. *Let* $G \in T(n, K)$, *then*

$$F(G) \leq (K+1)(n-1)^3 + (n-K-1)(K+1)^3,$$

with equality if and only if G *is isomorphic to* $S_{n-K} + K_K$.

Proof. We will prove this theorem using mathematical induction on K. The result is already proved for $K = 1$ in Theorem 2.2. Now as induction hypothesis, let us assume that the result is true for $(K-1)$ apex tree. Let $G \in T_K(n)$ be the graph with maximum $F(G)$. Let v be a K-apex vertex of G. Then using Lemma 2.3, we have $d_G(v) = n-1$. Then, we can write

$$|E(G-v)| = K(n-1) - \frac{1}{2}K(K+1). \tag{2.1}$$

Also,since $d_G(v) = n-1$, then $d_G(u) = d_{G-v}(u) + 1$ for all $u \in V(G)$, with $u \neq v$. Thus, we have

$$\begin{aligned} F(G) &= \sum_{u \in V(G)} d_G(u)^3 \\ &= \sum_{u \in V(G-v)} (d_{G-v}(u)+1)^3 + d_G(v)^3 \\ &= \sum_{u \in V(G-v)} [d_{G-v}(u)^3 + 3d_{G-v}(u)^2 + 3d_{G-v}(u) + 1] + d_G(v)^3 \\ &= F(G-v) + 3M_1(G-v) + 6|E(G-v)| + (n-1) + (n-1)^3. \qquad (2.2) \end{aligned}$$

Now, since $G - v \in T_{K-1}(n-1)$, so by induction hypothesis, we have

$$F(G-v) \leq K(n-2)^3 + K^3(n-K-1) \tag{2.3}$$

and

$$M_1(G-v) \leq K(n-2)^2 + K^2(n-K-1). \tag{2.4}$$

So, by using (2.1), (2.3), and (2.4) in (2.2), we have

$$\begin{aligned} F(G) &\leq K(n-2)^3 + K^3(n-K-1) + 3K(n-2)^2 + 3K^2(n-K-1) \\ &\quad +6K(n-1) - 3K(K+1) + (n-1)(n^2-2n+2). \end{aligned}$$

From above after simplification we get

$$F(G) \leq (K+1)(n-1)^3 + (n-K-1)(K+1)^3. \tag{2.5}$$

Thus, from mathematical induction we get the desired result. Also, from induction hypothesis the inequality (2.3) holds if and only if $G-v$ is isomorphic to $S_{n-K}+K_{K-1}$. Hence, the equality in (2.5) if and only if G is isomorphic to $S_{n-K}+K_K$. □

3. CONCLUSIONS

In this report, we obtained the maximum forgotten topological index of apex tree with n nodes and the class of K-apex trees with n nodes. Also we characterized the graphs for which the forgotten topological index is maximum. In future such work for apex trees can be done for other topological indices that are not investigated till now.

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