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Extremal Prism like Graphs with Respect to the F-Index

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Abstract. In this paper, we determine the extremal graphs with respect to the F-index among the classes of connected prism like graphs.

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1. Introduction and Preliminaries

In modern years, a major trend in chemical graph theory is to characterize the extremal (minimal or maximal) on a certain collection of graphs with regard to various distance-based topological indices. It is significant to set up the (upper or lower) bounds for indices and to characterize the consequent extremal graphs at the point where upper or lower bounds are achieved. Topological indices are arithmetical factor of a graph which illustrate its topology. They are generally graph invariant. Topological indices are essential for growth of QSAR/QSPR wherein the biological movement and further characteristics of

molecules are interrelated with their chemical composition.
Only connected and simple graphs G are consider in this paper. $V(G)$ and $E(G)$ are vertex and edge set of graph G respectively. $|V(G)|$ and $|E(G)|$ denotes order and size of a graph respectively. $d(v)$ denotes the degree of the vertex v of G.
The 1st and 2nd Zagreb indices introduced in 1972 (see [10]), among two oldest degree based molecular structure-descriptors. The 1st Zagreb index M_1 and 2nd Zagreb index M_2 are described as:

$$M_1 = \sum_{v \in V(G)} d(v)^2 \text{ and } M_2 = \sum_{uv \in E(G)} d(u)d(v)$$

One can rewrite the 1st Zagreb index as:

$$M_1 = \sum_{uv \in E(G)} [d(u) + d(v)]$$

These indices are examined to discuss chirality, heterosystems, ZE-isomerism and molecular complexity. More about their mathematical properties and physico-chemical applications, we refer to [2], [3], [4], [7], [8], [9], [11], [12], [13], [14] and [15]. In an early work on the total φ-electron energy [10], beside the first Zagreb index, it was indicated that another term on which this energy depends is of the shape

$$F(G) = \sum_{v \in V(G)} d(v)^3.$$

Very recently Furtula and Gutman renamed this topological index as a forgotten index or F-index and they have obtained some interesting results in [5].
Prism graph is actually cartesian product of cycle graph on n edges with a single edge and denoted by Y_n. Let P_k and S_k denotes the path graph and star graph on k edges respectively. Different prism like graphs are constructed by attaching path graphs P_k or star graphs S_k to the vertices of prism graph Y_n. In that way we defined different classes of graphs by slightly modifying prism graph and study the behavior of F-index.
In [1], Shenaz et al. computed the extremal graphs with respect to the F-index among the classes of connected bicyclic and unicyclic graphs. In this paper, we find the extremal graphs with respect to the F-index among the classes of connected prism like graphs.

2. EXTREMAL PRISM LIKE GRAPHS WITH RESPECT TO F-INDEX

The first part of this section is devoted to a necessary lemma that will be useful in the next part of this paper to find out the extremal prism like graphs with respect to the F-index.

Lemma 2.1. *let $x \geq 3$, and $y, z \geq 1$ be the integers, then following functions defined by*

(a): $f(x,y,z) = x[27 - (y+3)^3 - 8y(z-1) - y]$
(b): $g(x,y,z) = x[27 - (y+3)^3 - y(z-1) - yz^3]$
(c): $h(x,y,z) = 27(x-1) - (x-1)(y-2)^3 - y(x-8)(z-1) + y - xyz^3$
(d): $\psi(x,y,z) = 7xy(z-1) + xy(1-z^3)$
(e): $\theta(x,y,z) = (x-1)[27 - (y+3)^3] + y(x+8)(z-1) - xyz^3$
(f): $\phi(x,y,z) = xy - 27(x-1) - (x-1)(y+3)^3 + y(8x-1)(z-1) - yz^3$

are strictly decreasing functions.

Proof. **(a):** Since we have $\frac{\partial f(x,y,z)}{\partial x} = 27-(y+3)^3-8y(z-1)-y < 0$, $\frac{\partial^2 f(x,y,z)}{\partial^2 y} = -6x(y+3) < 0$ and $\frac{\partial f(x,y,z)}{\partial z} = -8xy < 0$ for every $x \geq 3$ and $y, z \geq 1$. Hence $f(x,y,z)$ is a strictly decreasing function.

(b): Similarly $\frac{\partial g(x,y,z)}{\partial x} = 27-(y+3)^3-y(z-1)-yz^3 < 0$, $\frac{\partial^2 g(x,y,z)}{\partial^2 y} = -6x(y+3) < 0$ and $\frac{\partial^2 g(x,y,z)}{\partial^2 z} = -6xyz < 0$ for every $x \geq 3$ and $y, z \geq 1$. Hence $g(x,y,z)$ is a strictly decreasing function.

(c): We have $\frac{\partial h(x,y,z)}{\partial x} = 27-(y-2)^3-y(z-1)+y-yz^3 < 0$, $\frac{\partial^2 h(x,y,z)}{\partial^2 y} = -6(x-1)(y-3) < 0$ and $\frac{\partial^2 h(x,y,z)}{\partial^2 z} = -6xyz < 0$ for every $x \geq 3$ and $y, z \geq 1$. Hence $h(x,y,z)$ is a strictly decreasing function.

(d): Since we have $\frac{\partial \psi(x,y,z)}{\partial x} = 7y(z-1)+y(1-z^3) < 0$; $\frac{\partial \psi(x,y,z)}{\partial y} = 7x(z-1)+x(1-z^3) < 0$; and $\frac{\partial^2 \psi(x,y,z)}{\partial^2 z} = -6xyz < 0$; for every $x \geq 3$ and $y, z \geq 1$. Hence $\psi(x,y,z)$ is a strictly decreasing function.

(e): We have $\frac{\partial \theta(x,y,z)}{\partial x} = 27-(y+3)^3+y(z-1)-yz^3 < 0$, $\frac{\partial^2 \theta(x,y,z)}{\partial^2 y} = -6(x-1)(y-3) < 0$ and $\frac{\partial^2 \theta(x,y,z)}{\partial^2 z} = -6xyz < 0$ for every $x \geq 3$ and $y, z \geq 1$. Hence $\theta(x,y,z)$ is a strictly decreasing function.

(f): Since we have $\frac{\partial \phi(x,y,z)}{\partial x} = y-27-(y+3)^3+8y(z-1) < 0$, $\frac{\partial^2 \phi(x,y,z)}{\partial^2 y} = -6(x-1)(y+3) < 0$ and $\frac{\partial^2 \phi(x,y,z)}{\partial^2 z} = -6yz < 0$ for every $x \geq 3$ and $y, z \geq 1$. Hence $\phi(x,y,z)$ is a strictly decreasing function.

□

Now our main goal is to define different prism like graphs which are actually constructed by attaching path graphs or star graphs to the vertices of prism graph and than characterize extremal prism like graphs with respect to F-index. The first class of these classes is prism Y_n of order n (see Fig. 1). For the graphs in which the prism Y_n and l copies of path P_k are incident with a unique vertex of Y_n, are denoted by $A(n,k,l)$, where $n \geq 3$, $k \geq 1$ and $l \geq 1$. The prism like graph $A(5,3,2)$ is shown in Fig. 2.

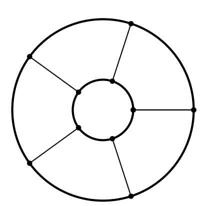

FIGURE 1. Y_5

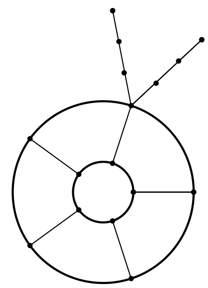

FIGURE 2. $A(5,3,2)$

Now we introduce another class of prism like graphs. Suppose $B(n,k,l)$ is graph of order n consisting of a prism Y_n and l copies of path P_k are incident to every vertex of the prism Y_n. The prism like graph $B(5,3,2)$ is shown in Fig. 3.

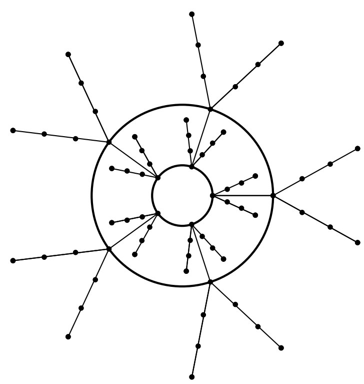

FIGURE 3. $B(5,3,2)$

The connected graphs in which a prism Y_n and l copies of star graph S_k that are incident with a unique vertex of Y_n are denoted by $C(n,k,l)$, where $n \geq 3, k \geq 1$ and $l \geq 1$. The graph $C(5,4,2)$ is represented in Fig. 4.

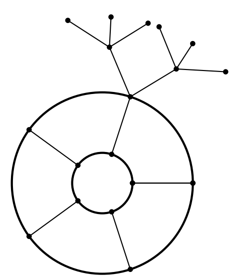

FIGURE 4. $C(5,4,2)$

We now introduce another class of prism like graphs. Suppose $D(n,k,l)$ is graph of order n consisting of a prism Y_n and l copies of star graph S_k incident to every vertex of prism Y_n. The graph $D(5,4,2)$ is shown in Fig. 5.

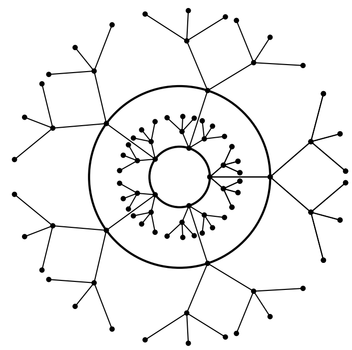

FIGURE 5. $D(5,4,2)$

Lemma 2.2. *Let $n \geq 3$, $k \geq 1$ and $l \geq 1$; then the F-index of prism like graphs are following.*

1: $F(Y_n) = 54n$
2: $F(A(n,k,l) = 27(2n-1) + (l+3)^3 + 8l(k-1) + l$.
3: $F(B(n,k,l) = 2[nl + n(l+3)^3 + 8nl(k-1)]$.
4: $F(C(n,k,l)) = 27(2n-1) + l(k-1) + (l+3)^3 + lk^3$.
5: $F(D(n,k,l)) = 2[n(l+3)^3 + nlk^3 + nl(k-1)]$.

Proof. **1:** The graph Y_n contains $2n$ vertices and all vertices are of degree 3. Hence we get $F(Y_n) = 2n(3)^3 = 54n$.

2: The graph $A(n,k,l)$ contains $2n + lk$ vertices among which degree 3 vertices are $2n-1$, 1 vertex of degree $l+3$, l vertices of degree 1 and $l(k-1)$ vertices of degree 2. Hence we get $F(A(n,k,l))$ = $27(2n-1) + (l+3)^3 + 8l(k-1) + l$.

3: The graph $B(n,k,l)$ contains $2n(kl+1)$ vertices among which $2n$ vertices are of degree $l+3$, $2nl$ vertices of degree 1 and $2nl(k-1)$ vertices of degree 2. Hence we get $F(B(n,k,l))$ = $2nl + 2n(l+3)^3 + 16nl(k-1)$.

4: The graph $C(n,k,l)$ contains $2n + lk$ vertices among which $2n-1$ vertices are of degree 3, 1 vertex of degree $l+3$, l vertices of degree k and $l(k-1)$ vertices of degree 1. Hence we get $F(C(n,k,l))$ = $27(2n-1) + l(k-1) + (l+3)^3 + lk^3$.

5: The graph $D(n,k,l)$ contains $2n(kl+1)$ vertices among which $2n$ vertices are of degree $l+3$, $2nl$ vertices of degree 1 and $2nl(k-1)$ vertices of degree k. Hence we get $F(D(n,k,l))$ = $2(n(l+3)^3 + nlk^3 + nl(k-1)$.

Let **U** denote the set of all unlabeled prism like graphs of order $n \geq 3$, where **U** is defined as follows:

$$\mathbf{U} = \{Y_n, A(n,k,l), B(n,k,l), C(n,k,l), D(n,k,l)\}.$$

The next theorem determines the extremal connected prism like graphs having first, second, third and fourth minimum F-index among the class of graphs **U**. □

Theorem 2.3. *For every $n \geq 3$,$k \geq 1$ and $l \geq 1$ among all the classes of prism like graphs of **U** having the minimum F-index are Y_n, $A(n,k,l)$, $B(n,k,l)$, $C(n,k,l)$ and $D(n,k,l)$ (in this order).*

Proof. Here we have four cases.

Case I: First we will show that Y_n attains the minimum of F-index in the class of graphs **U**.
Consider $F(Y_n) - F(A(n,k,l)) = [27 - (l+3)^3 - 8l(k-1) - l]$. By Lemma 2.1(a), it follows that the class of extremal unicycles in this case is $A(n,k,l)$ with respect to the minimum F-index.
Now consider $F(Y_n) - F(B(n,k,l)) = 2n[27-(l+3)^3-8l(k-1)-l]$. By Lemma 2.1(a), it follows that the class of extremal prism is $B(n,k,l)$ having minimum F-index.
Now consider $F(Y_n) - F(C(n,k,l)) = 27-(l+2)^3 - l(k-1) - lk^3$. By Lemma 2.1(a), it follows that $C(n,k,l)$ is the class of extremal prism like graphs having minimum F-index.
Now consider $F(Y_n) - F(D(n,k,l)) = 2n[27 - (l+3)^3 - l(k-1) - lk^3]$. By Lemma 2.1(b), in this case it follows that $D(n,k,l)$ is the class of extremal prism like graphs having minimum F-index.

Case II: In order to obtain the second minimum F-index, it is necessary to compare the value of F-index of $A(n,k,l)$ with the F-index of other classes of prism graphs **U**.
Consider $F(A(n,k,l)) - F(B(n,k,l)) = (2n-1)[27-(l+3)^3+8l(k-1)-l]$. By Lemma 2.1(b), $B(n,k,l)$ is the class of extremal prism like graphs having minimum F-index.
Now consider $F(A(n,k,l)) - F(C(n,k,l)) = 7l(k-1) + l(1-k^3)$.
By Lemma 2.1(d), $C(n,k,l)$ is the class of extremal prism like graphs having minimum F-index.
Now consider $F(A(n,k,l)) - F(D(n,k,l)) = (2n-1)27 - (l+3)^3 + 2l(4+n)(k-1) - 2nlk^3$. By Lemma 2.1(e), it follows that $D(n,k,l)$ is the class of extremal prism like graphs having minimum F-index.

Case III: In order to obtain the third minimum F-index, it is necessary to compare the F-index of $B(n,k,l)$ with the F-index of other classes of prism graphs in **U**.
Consider $F(B(n,k,l)) - F(C(n,k,l)) = 2nl - 27(2n-1)(l+3)^3 + l(16n-1)(k-1) - lk^3$. By Lemma 2.1(f), it follows that $B(n,k,l)$ is the class of extremal prism like graphs having minimum F-index.
Now consider$F(B(n,k,l)) - F(D(n,k,l)) = 7(2n)l(k-1) + 2nl(1-k^3)$. By Lemma 2.1(d), in this case $D(n,k,l)$ is the class of extremal prism like graphs having minimum F-index.

Case IV: The fourth minimum F-index in the class of prism graphs is attained by $D(n,k,l)$.
Consider $F(C(n,k,l)) - F(D(n,k,l)) = (2n-1)[27-(l+3)^3 - l(k-1) - lk^3$. By Lemma 2.1(b), it follows in this case that $E(n,k,l)$ is the class of extremal prism like graphs having minimum F-index.

From all the above cases and discussions, it follows that $Y_n, A(n,k,l), B(n,k,l), C(n,k,l)$ and $D(n,k,l)$ are the classes of connected prism graphs having the first, second, third and fourth minimum F-index, which conclude the proof.

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□

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