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F-indices and F-polynomials for Carbon Nanocones $CNC_k[n]$

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Abstract: *Let G = (V, E) be a connected graph with the vertex set V= V(G) and the edge set E = E(G), without loops and multiple edges. In this paper F-index, minus F-index, F-Revan index, F-reverse index and line version of F-index polynomials and their corresponding topological indices for carbon nanocones $CNC_k[n]$ are investigated.*

Keywords: *F-index, F-polynomial, inverse index, molecular graph, nanocones, Revan index, topological index.*

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I. Introduction

Let G = (V, E) be a molecular graph. The set of vertex and edge are denoted by V=V(G) and E=E(G) respectively. The number of vertices of G, adjacent to a given vertex v, is the degree of this vertex and will be denoted by $d_v(G)$ or d_v. A topological index for a graph is a numerical quantity which is invariant under automorphisms of the graph. An automorphism is a permutation ϕ : V → V that preserves the adjacency relation, that is, (u, v) ∈ E ⇔ (ϕ(u), ϕ(v)) ∈ E. The Carbon nanocones were accidentally discovered in 1994 and firstly synthesized in 1997. The reverse index, Revan index, F-index and Zagreb polynomials for molecular graphs are studied by [1-16]. Zagreb polynomials and Redefined Zagreb indices for the line graph of Carbon nanocones are studied by [17]. The reverse vertex degree vertex v in G is defined as $c_v = \Delta(G) - d_G(v) + 1$. The Revan vertex degree of a vertex u in G is defined as $r_G(u)$=ΔG+$\delta(G)$-$d_G(u)$. The edge of molecular graph G e = uv ∈ E(G) is defined as, $d_G(e) = d_G(u) + d_G(v) - 2$ [18].The symbols used in this paper are mainly taken from standards books of Graph theory.

The degree is defined as the number of edges with that vertex. In [19] F-index and F-polynomial of a graph are defined as, F(G) = $\sum_{u\,v\,\in\,V(G)} d_G{}^3(u) = \sum_{u\,v\,\in\,E(G)}(d_G{}^2(u) + d_G{}^2(v))$ and

F(G,x)=$\sum_{u\,v\,\epsilon\,E(G)} x^{(du^2+dv^2)}$.

The molecular graph of $CNC_k[n]$ nanocones have conical structures with a cycle of length k at its core and n layers of hexagons placed at the conical surface around its center as shown in figure (1) .The first and second Revan indices of a graph G are studied by [20] and are defined as,

$r_1(G) = \sum_{u\,v\,\in(G)}(r(u) + r(v))$;and $r_2(G) = \sum_{u\,v\,\in(G)}(r(u)r(v))$. The minus F-index of a graph G is studied by [21] and is defined as,

$FM_i(G) = \sum_{u\,v\,\in(G)} |d_G(u)^2 - d_G(u)^2|$, and the minus F-index polynomial of a graph G can be defined as, $FM_i(G,x)=\sum_{uv\in(G)} x^{|d_G(u)^2 - d_G(v)^2|}$.

The F-reverse index of a graph G is defined as, $FC(G)=\sum_{uv\in E(G)}[c_u{}^2 + c_v{}^2]$ and

the F-reverse polynomial of a graph G is defined as, $FC(G,x)=\sum_{uv\in E(G)} x^{[c_u^2 + c_v^2]}$.

The reverse edge connecting the reverse vertices u and v will be denoted by uv [22-24]. One can see that the number of vertices of CNCn(k) is n(k + 1) 2 and the number of edges of CNCn(k) is n* 2 (k + 1)(3k + 2). The F-Revan index of a graph *G* is defined as:

$FR(G)=\sum_{uv\in(G)}[r_G(u)^2+r_G(v)^2]$ and the F-Revan polynomial of a graph *G* is defined as [25] ,

$FR(G,x) = \sum_{uv\in(G)}[r_G(u)^2 + r_G(u)^2]$.

It has been reported in the literature [26], the edge version of geometric-arithmetic index introduced based on the end-vertex degrees of edges in a line graph of G which is a graph such that each vertex of L(G) represents an edge of G, and two vertices of L(G) are adjacent if and only if their corresponding edges share a common endpoint in G, as follows:

$$GA_e(G) = \sum_{ef\in(L(G))} \frac{2\sqrt{d_{L(G)}(e)d_{L(G)}(f)}}{d_{L(G)}(e)+d_{L(G)}(f)} .$$

The edge version of F-index [27-29] and polynomial are defined as,

$F_e(G) = \sum_{e\,f\,\in\,L(G)}(d_{L(G)}(e)^2 + d_{L(G)}(f)^2)$ and $F_e(G,x)=\sum_{ef\in L(G)} x^{(d_{L(G)}(e)^2+d_{L(G)}(f)^2)}$.

Where $d_{L(G)}$ denotes the degree of the edge x in G.

The graph L(G) of a graph G is the each of whose vertex represents an edge of G and two of its vertices are adjacent if their corresponding edges are adjacent in G. Topological indices derived from graph theory are used as structural descriptors in QSPR/QSAR models.

In this paper F-index, minus F-index, F-Revan index, F-reverse index and line version of F-index polynomials and corresponding topological indices for carbon nanocones $CNC_k[n]$. are investigated.

II. Materials and Methods

A molecular graph is constructed by representing each atom of a molecule by a vertex and bonds between atoms by edges. The degree of each vertex equals the valence of the corresponding atom. The basic parameters used in the computation of F-polynomials and corresponding indices for carbon nanocones are as follows. Let G be a graph, u ∈ V(G) and e = uv ∈ E(G). Then d(e) = d(u) + d(v) − 2.The reverse vertex degree of a vertex v in G is defined as $c_v = \Delta(G) - d_G(v) + 1$. The Revan vertex degree of a vertex u in G is defined as $r_G(u)=\Delta G+\delta(G)-d_G(u)$.

If the total number of vertices V(G) and total number of edges in a 2-dimensional graph are known for nanomaterials then the topological polynomials and the corresponding topological indices can be computed. The molecular graph and line graph of carbon nanocones $CNC_k[n]$ are shown in figure (1) and (2) respectively.

III. Results And Discussion

The degree $d_G(v)$ of vertex v is the number of vertices adjacent to v. In this section we compute the F-polynomials and F-indices of Carbon nanocones $CNC_k[n]$.

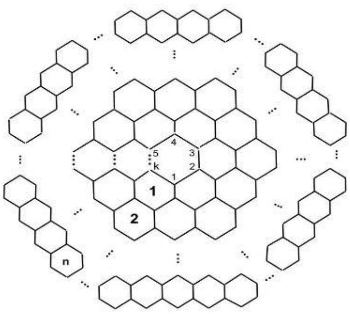

Fig.1. Carbon nanocone $CNC_k[n]$.

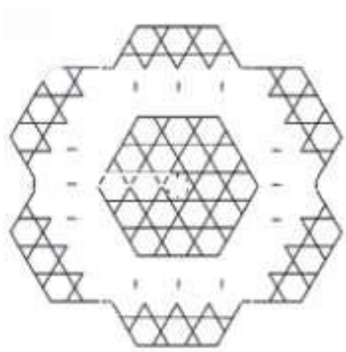

Fig.2. Line graph of the carbon nanocone $CNC_k[n]$.

It is observed from figure (1) there are three edge partitions for carbon nanocones $CNC_k[n]$.

$E_{(2,2)} = \{e = uv \in E(G) | d_u = 2 \& d_v = 2\} \rightarrow |E_{(2,2)}| = k$,

$E_{(2,3)} = \{e = uv \in E(G) | d_u = 2 \& d_v = 3\} \rightarrow |E_{(2,3)}| = 2k(n-1)$,

$E_{(3,3)} = \{e = uv \in E(G) | d_u = 2 \& d_v = 3\} \rightarrow |E_{(3,3)}| = \frac{k}{2}(n-1)(3n-2)$.

The F-polynomial:

$F(G,x) = \sum_{u v \in E(G)} x^{(du^2 + dv^2)}$.

$= \sum_{u v \in E_{(2,2)}(G)} x^{(du^2 + dv^2)} + \sum_{u v \in E_{(2,3)}(G)} x^{(du^2 + dv^2)} + \sum_{u v \in E_{(3,3)}(G)} x^{(du^2 + dv^2)}$.

$= k\ x^{(2^2 + 2^2)} + 2k(n-1)\ x^{(2^2 + 3^2)} + \frac{k}{2}\ (n-1)(3n-2)\ x^{(3^2 + 3^2)}$.

$= k\ x^8 + 2k(n-1)\ x^{13} + \frac{k}{2}\ (n-1)(3n-2)\ x^{18}$.

and the F-index:

$F(G) = \frac{\partial F(G,x)}{\partial x}/_{x=1} = 8k + 26k(n-1) + 9\ k\ (n-1)(3n-2)$.

The line graph L(G) of a graph G is the graph whose vertex set corresponds to the edges of G such that two vertices of L(G) are adjacent if the corresponding edges are adjacent.

Let L(CNCk[n]) be the line graph of carbon nanocones CNCk[n] . The degree of an edge e = uv in G defined as $d_{(G)}(e)= d_{(G)}(u)+d_{(G)}(v)-2$.From the line graph of CNCk[n], we can see that the total number of vertices are 8k + 2kn and total number of edges are k(n + 1)(3n + 1). The edge set of L(CNCk[n]) has following four partitions

$E_1 = E_{\{2,3\}} = \{e = uv \in L(CNCk[n]) : d_u = 2, d_v = 3\}$,

$E_2 = E_{\{3,3\}} = \{e = uv \in L(CNCk[n]) : d_u = 3, d_v = 3\}$,

$E_3 = E_{\{3,4\}} = \{e = uv \in L(CNCk[n]) : d_u = 3, d_v = 4\}$,

and $E_4 = E_{\{4,4\}} = \{e = uv \in L(CNCk[n]) : d_u = 4, d_v = 4\}$.

Now $|E_1(L(CNC_k[n]|=2k$, $|E_2(L(CNC_k[n]|=k(2n-1)$, $|E_3(L(CNC_k[n]|=2kn$, and $|E_4(L(CNC_k[n]|=3kn^2$.
The F-index polynomial of line graph of $CNC_k[n]$ can be computed as:

$F(L(CNC_k[n],x)= \sum_{uv\in E(L(CNC_k[n])} x^{(d_{L(G)}(e)^2+d_{L(G)}(f)^2)}$

$= \sum_{uv\in E_1(CNC_k[n])} x^{(2)^2+(3)^2} + \sum_{uv\in E_2(L(CNC_k[n])} x^{(3)^2+(3)^2} + \sum_{uv\in E_3(L(CNC_k[n])} x^{(3)^2+(4)^2} + \sum_{uv\in E_4 L(L(CNC_k[n])} x^{(4)^2+(4)^2}$.

$=E_1(L(CNC_k[n])\, x^{13}+ E_2(L(CNC_k[n])\, x^{18} +E_3(L(CNC_k[n])\, x^{25}+E_4(L(CNC_k[n])\, x^{32}$.

$=2kx^{13}+k(2n-1)x^{18}+2knx^{25}+3kn^2x^{32}$.

and F-index for line graph of $CNC_k[n]$:

$F(L(CNC_k[n]) = \frac{\partial F(G,x)}{\partial x}/_{x=1} = 26k+18k(2n-1)+50kn+96kn^2$.

The values of F-index polynomials are computed for carbon nanocones CNCk[n] are given in table number (1).

Table 1. F-index polynomials for carbon nanocones CNCk[n].

Topological polynomials	**F-polynomials for carbon nanocones CNCk[n]**
F-index polynomial F(G,x)	$k\,x^8 + 2k(n-1)\,x^{13} + \frac{k}{2}(n-1)(3n-2)\,x^{18}$
minus F-index polynomial $M_iF(G,x)$	$k+\frac{k}{2}(n-1)(3n-2)+2k(n-1)x^5$
F-Revan index polynomial FR(G,x)	$\frac{k}{2}(n-1)(3n-2)x^8+Kx^{18}+2k(n-1)x^{13}$
F-reverse index polynomial FC(G,x)	$\frac{k}{2}(n-1)(3n-2)x^2+2k(n-1)x^5+kx^8$
F-index polynomial line graph $F(L(CNC_k[n])$	$2kx^{13}+k(2n-1)x^{18}+2knx^{25}+3kn^2x^{32}$

IV. Conclusion

The degree based topological indices are important in the study of topological indices of molecular topology. The F-polynomials and corresponding topological indices are studied for carbon nanocones CNCk[n]. Topological indices derived from graph theory are used as structural descriptors in QSPR/QSAR models.

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