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F-Polynomial and Fourth Zagreb Polynomial of a Molecular Graph

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Abstract: ***Let G = (V, E) be molecular graphs. The set of vertex and edge are denoted by V= V(G) and E= E(G) respectively. F-index and fourth Zagreb index can be found from respective polynomials of F-polynomial and fourth Zagreb polynomial. In this paper F-polynomial and fourth Zagreb polynomial of 7-phenacene are studied.***

Keywords: F-index, F-polynomial, fourth Zagreb polynomial, fourth Zagreb index, eccentricity.

1. Introduction

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. 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. Zagreb group indices are vertex degree-based topological indices in which degree of each vertex of the molecular graph counted. A topological index for a graph is a numerical quantity which is invariant under automorphisms of the graph. In this paper F-polynomial and fourth Zagreb polynomial of 7-phenacene are studied.

2. 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. 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 2-dimensional graph of 7-phenacene is shown in figure1.

The first and second Zagreb indices are denoted by $M_1(G)$ and $M_2(G)$ .The fourth Zagreb index was formulated as [1].

$Zg_4(G) = \sum_{u,v \in E(G)}(ec(u)+ ec(v))$.

The fourth Zagreb polynomial can be defined [2,3] as,

$Z_{g4}(G,x) = \sum_{u v \in E(G)} x^{(ec(u)+ ec(v))}$

F-index is vertex degree based topological index. Furtula and Gutman studied the forgotten topological index or F-index and defined it as the sum of cubes of vertex degrees [4-6],

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

In [7], De et al. defined F-polynomial of a molecular graph as,

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

And the forgotten topological coindex is defined [8] as,

$\bar{F}(G) = \sum_{u v \notin E(G)}(d_G^2(u) + d_G^2(v))$,

And the corresponding F-coindex polynomial is,

$\bar{F}(G,x) = \sum_{u v \notin E(G)} x^{(d_G^2(u) + d_G^2(v))}$

Reformulated first Zagreb index in terms of edge degrees instead of vertex degrees, where the degree on edge e = uv is defined as, $d_G(e) = d_G(u) + d_G(v)-2$.

Reformulated version of the general first Zagreb index is defined by [9],

$EM_1 \lambda (G) = \sum_{e \in E(G)} {}^{d}{}_G(e)^{\lambda}$ for $\lambda \in \mathbb{R} - \{0,1\}$

For the special case λ= 3, RF (G) is called reformulated F-index.

The degree of each vertex of 2-dimensional graph of 7-phenacene are counted from figure 1.The maximum entry for a given row/column of the distance matrix of an undirected (strongly connected directed) graph is known as the eccentricity of the node. We constructed row - column symmetric matrix to count the eccentricity of each vertex for 7-phenacene.

3. Results and Discussion

The degree is defined as the number of edges with that vertex. A vertex with degree 1 is called pendent vertex. We compute some degree-based and eccentricity-based topological indices of this network .The fourth Zagreb index was formulated as [10],

$Zg_4(G) = \sum_{u,v \in E(G)}(ec(u) + ec(v))$.

Where ec(u) is eccentricity of u, the summation is taken over all edges of a molecular graph.

The fourth Zagreb polynomial can be defined [2, 3 and 11] as,

$Z_{g4}(G,x) = \sum_{u v \in E(G)} x^{(ec(u)+ ec(v))}$

The forgotten topological index or F-index is defined as [13,14].

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

F-polynomial

In [14] F-polynomial of a graph is defined as,

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

And the forgotten topological coindex is defined [8] as,

$\bar{F}(G) = \sum_{u v \notin E(G)}(d_G^2(u) + d_G^2(v))$.

And corresponding F-coindex polynomial is,
$F^{-}(G,x)=\sum_{uv\notin E(G)} x^{(d_G^{2}(u)+d_G^{2}(v))}$

We compute in this section the F-index polynomial, F-coindex and fourth Zagreb polynomial for 7-phenacene, which belong to the family of $C_{4n+2}H_{2n+4}$ where n≥3.We compute the F-polynomial by two methods : 1) If p and q are the number of degrees 2 and 3 in the family of phenacenes [6], N is number of vertices in the molecular graph of phenacene, then
p = (N/2) + 3 and q = (N/2) – 3.

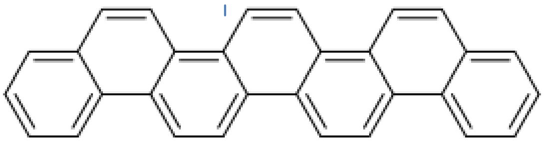

Figure 1: 2-dimensional graph of 7-phenacene

$F(G) = p(2)^3 + q(3)^3 = 18(8) + 12(27) =144+324 = 468.$
And 2) by algebraic method, the edge partitions of 7-phenacene are,
$E_4 = \{uv \in E(G) \mid d_u = 2, d_v = 2\}, |E_4| = 11.$
$E_5 = \{uv \in E(G) \mid d_u = 2, d_v = 3\}, |E_5| =14.$
$E_6 = \{uv \in E(G) \mid d_u = 3, d_v = 3\}, |E_6| =11.$
$F(G,x) = \sum_{uv\in E(G)} x^{(du^2 + dv^2)}$
$=11x^{18}+14x^{13}+11x^{8}.$
$F(G) = \frac{\partial F(G,x)}{\partial x}/_{x=1} = 11*18+14*13+11*8 = 468.$
The F-index computed from two methods [6] and [12 and 14] has same value in the case of 7-phenacene as 468.

F-coindex
To compute F-coindex we use Lemma-3 [8], Let G be connected graph with n vertices and m edges. The value of $M_1(G)$ for 7-phenacene is 180 [6].Then
$F^{-}(G) = (n-1)M_1(G) – F(G)$
$= (30-1)180-468 = 5220-468=4752.$
It is observed that values of F-index < F-coindex for 7-phenacene.

Fourth Zagreb polynomial
To compute eccentricity based fourth Zagreb polynomial we have constructed 30 x 30 matrix [16] and counted the maximum distance between a vertex and the other vertex for the vertices
1-30.The Zagreb polynomial,
$Zg_4(G,x) = \sum_{uv\in E(G)} x^{(ec(u)+ ec(v))}$
$= 4x^{29} + 4x^{27} + 6x^{25} + 4x^{23} + 6x^{21} + 4x^{19} + 6x^{17} + 2x^{16}.$

The fourth Zagreb index is,
$Zg_4(G) = \frac{\partial Zg_4(G,x)}{\partial x}/_{x=1}$
$= 4*29+4*27+6*25+ 4*23 +6 *21+ 4*19+6*17+2*16 = 802.$

4. Conclusion

The distance, degree and eccentricity are important in the study of topological indices of molecular graphs. The degree-based and eccentricity-based topological indices have many applications in QSPR and QSAR study. The F-polynomial and fourth Zagreb polynomial with corresponding indices are computed from degree and eccentricity of 7-phenacene. F-index computed by two methods has the same value for this molecular graph.

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