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Schultz, Modified Schultz and Hosoya polynomials and their indices in 2, 3-dimethyl hexane an isomer of octane

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Abstract:

Let G be a molecular graph. The Schultz and modified Schultz polynomials are defined as

$$S_c(G, x)= ½\sum_{u,v \subset (G)} (du + dv)\ x^{d(u,v)} \quad \text{and}$$

$$S_c^*(G,x) = ½\sum_{u,v \subset (G)} (du\ dv)\ x^{d(u,v)}$$

Where du (ordv)denote the degree of the vertex u (orv), respectively. In this paper ,Schultz, Modified Schultz, Hosoya polynomials and their indices for 2,3-dimethyl hexane an isomer of octane are presented.

Keywords: Topological indices, Schultz polynomial, Hosoyapolynomial, molecular graph.

Introduction

Molecular graph is a simple graph representing the carbon –carbon skeleton of an organic molecule (usually hydrocarbons) . The vertices of a molecular graph represent the carbon atoms, and the edges carbon-carbon bonds [1]. A molecular graph G (V,E) is constructed by representing each atom of molecule by vertex and bonds between by edges. Let V (G) be vertex set and E (G) be the edge set. In chemical graph theory, we have invariants polynomials for any graph , that they have usually integer coefficients. A topological index (or molecular descriptor) is a numerical value associated with chemical constitution for correlation of chemical structure with various physical properties , chemical reactivity . The graph theory has a wide range of applications in engineering, physical, social and biological sciences, linguistics and numerous other areas [2].

A quantitative measure of branching is needful for finding connections between molecular structure and physico – chemical properties of chemical compounds. Isomers are molecules that have the same molecular formula, but a have different arrangement of the atoms in space [3].

The degree is defined as number of edges with that vertex. For a linear graph G = (V ,E),the sum of degrees of all vertices is equal to $2n_e$. Where n_e is the number of vertices of edges. The degree of vertex equals valence of the corresponding atom. LetV Є G be a graph G . The neighborhood of v is the set of

$N_G(V) = \{u \in G \mid v\ u \in G\}$

The degree of v is the number of its neighbors[4].

$d_G(V) = dv = | N_G(V) |$

The Schultz, Modified Schultz polynomial and their indices are defined as [5, 6, 7, 8, and 9],

$$S_c(G,x) = ½ \sum_{u,v \subset (G)} (du + dv)\ x^{d(u,v)} \quad (1)$$

$$S_c^*(G,x) = ½ \sum_{u,v \subset (G)} (du\ dv)\ x^{d(u,v)} \quad (2)$$ and

$$S_c(G,x) = ½ \sum_{u,v \subset (G)} (du + dv) d(u,v) \quad (3)$$

$$S_c^*(G,x) = ½ \sum_{u,v \subset (G)} (du\ dv) d(u,v) \quad (4)$$

The Hosoya polynomial and Wiener index are defined as [10, 11, 12, 13, 14, 15],

$$H(G, x) = ½ \quad \Sigma_{v \in V(G)} \sum_{u \in V(G)} x^{d(v,u)} \quad (5)$$

$$W(G, x) = ½ \quad \Sigma_{v \in V(G)} \sum_{u \in V(G)} d(v,u) \quad (6)$$

In this paper, Schultz polynomial, Modified Schultz polynomial, Hosoya polynomial and their indices for 2,3-dimethyl hexane, an isomer of octane are studied.

Results and **discussion**:

There are eighteen isomers of octane, 2,3-dimethyl hexane (2,3-dmh) is an isomer of octane with molecular formula $C_8 H_{18}$. The degree of vertex u Є V (G) is the number of vertices joining to u and denoted by d(u). The degrees of different vertices of (2,3-dimethyl hexane) are shown in figure (1).

The molecular graph with suppressed hydrogen atoms of 2,3-dimethyl hexane is given in fig.(2)

In this section we compute topologicalindices and their polynomials for 2,3-dmh with formula C_8H_{18}.

Theorem: Let 2,3-dimethyl hexane be an isomer of octane .Then , the Schultz polynomial of 2,3-dmh is equal to

$S_c(G,x) = 140x^1 + 224x^2 + 188x^3 + 60x^4 + 22x^5$

The modified Schultz polynomial of 2,3-dmh is equal to

$S_c^*(G,x) = 91x^1 + 240x^2 + 15x^3 + 44x^4 + 14x^5$

Hosoyapolynomial, $H(G,x) = 7x^1 + 8x^2 + 7x^3 + 4x^4 + 2x^5$

and then respectively ,the Schultz, Modified Schultz and Wiener indices of 2,3-dmh are equal to

$S_c(G) = 1502$, $S_c^* = 862$, and $W(G) = 70$

Proof:

Schultz polynomial:

The matrix for 2,3-dmh is given in fig.(3).

Schultz polynomial is computed by adding the entries in upper triangular part of distance matrix of a graph along with number of degrees of u and v –vertices for each of and number of k-element independent edge sets of the graph G. Denoted by m(G,k) the number of k-element independent set of the graph G.

According tofig(1)-(3), the distances d(u,v) along with corresponding degrees of

u,v-vertices (du + dv) are:

1(4)+2(3)+3(3)+4(2)+5(2)+2(2)+1(4)+

1(6)+2(5)+3(5)+4(4)+1(4)+2(4)+

1(5)+2(5)+3(4)+2(4)+1(4)+

1(4)+2(3)+3(3)+2(3)+

1(3)+4(3)+3(3)+

5(2)+4(2)+3(2)

The Schultz polynomial is $S_c(G,x) = 140x^1 + 224x^2 + 188x^3 + 60x^4 + 22x^5$andthe Schultz index is

$S_c(G) = \frac{\partial Sc\ (G,x)}{\partial x}/_{x=1}$ =140*1+224*2+188*3+60*4+22*5 = 1502.

Modified Schultz polynomial:

Modified Schultz polynomial is computed by adding number of entries in upper triangular part of distance matrix of the graph,d(u,v) along with number of degrees of u and v-vertices for number of edges in the graph.

The distances in upper triangular part of distance matrix along with corresponding (du dv) degrees are:

1(3)+2(3)+3(2)+4(2)+5(1)+2(1)+3(1)+

1(9)+2(6)+3(6)+4(3)+1(3)+2(3)+

1(6)+2(6)+3(3)+2(3)+1(3)+

1(4)+2(2)+3(2)+2(2)+

1(2)+4(2)+3(2)+

5(1)+4(1)+

3(1).

By equation (2),the modified Schultz polynomial

$S_c^* (G,x) = 91x^1 + 240x^2 + 15x^3 + 44x^4 + 14x^5$ and

Modified Schultz index

$S_c^*(G) = \frac{\partial Sc\,(G,x)}{\partial x}/_{x=1} = 91*1+240*2+15*3+44*4+14*5 = 862.$

Hosoya polynomial:

Hosoya polynomial is computed by adding the entries in upper (or lower) triangular part of distance matrix of a molecular graph. The distanced(u,v) between two vertices u and v is minimum of the lengths of u-v paths of G,that is d(u,v) is the number of edges in a geodesic.d(G,o)=n,d(G,1)=e,where n-number of edges of vertices in graph G, e-number of edges,d(G)- topological diameter. Using algorithm [3] and fig. (3),we have

$(G_{2,6}, 1) = 7$, $(G_{2,6}, 2) = 8$, $(G_{2,6}, 3) = 7$, $(G_{2,6}, 4) = 4$, $(G_{2,6}, 5) = 5$.

The Hosoya polynomial for 2,3-dmh is

$H(G,x) = 7x^1 + 8x^2 + 7x^3 + 4x^4 + 2x^5$. and

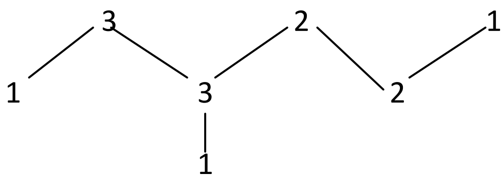
Wiener index is equal to:

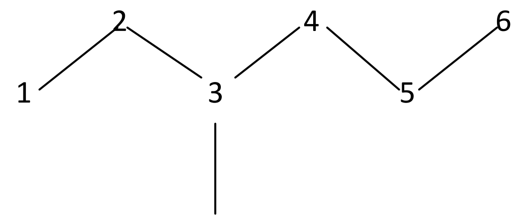
$W(G) = \frac{\partial H(G,x)}{\partial x}/_{x=1} = 7*1+8*2+7*3+4*4+2*5 = 70.$

That completes the proof.

Conclusion:

In this paper, we count the topological indices and their polynomials of 2,3-dimehyl hexane. These topological indices are useful in studying physico-chemical properties of organic compounds of molecular graph, which have relation with degrees of its vertices.





Fig(1):Molecular graph G of 2,3-dmh

with its vertex degrees indicatedFig (2):Molecular graph for 2,3-dmh (G_2 , 6).

	1	2	3	4	5	6	7	8
1	0	1	2	3	4	5	2	3
2	1	0	1	2	3	4	1	2
3	2	1	0	1	2	3	2	1
4	3	2	1	0	1	2	3	2
5	4	3	2	1	0	1	4	3
6	5	4	3	2	1	0	5	4
7	2	1	2	3	4	5	0	3
8	3	2	1	2	3	4	3	0

Fig (3): Distancematrix for 2,3-dmh.

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