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Topological indices and polynomials in isomers of organic compounds

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Abstract

Let G = (V, E) be a molecular graph .The sets of vertices and edges of are denoted by V = V (G) and E = E (G) respectively. In molecular graph , vertices represent atoms and edges represent bonds. The distance between u and v in V (G)of graph G is the number of edges, a shortest path between them d (u, v). In graph theory, there are many molecular indices and polynomials for a graph G . In this research ,we computing Total adjacency index (A) , Randic index (R) , indices of Zagreb group (M_1 , M_2) and Zagreb polynomial for isomers of pentane ($C_5 H_{12}$) .

Keywords Randic index, Zagreb index,Zagreb polynomial, Adjacency matrix.

Introduction

A graph G (V , E) consists of a set of objects V = { v_1 , v_2--------} called vertices and another set E = { e_1 , e_2 , ----------} whose elements are called edges , such that each edge e_k is identified with an unordered pair (v_i , v_j) of vertices [1].In simple graph , representing the carbon atom skeleton of an hydrocarbon [2], two vertices of G , connected by edge aresaid to adjacent (i.e. u ~v) . The adjacency matrix or connection matrix of a graph G with n vertices and no parallel edges is n by n symmetric binary matrix.

X = [X_{ij}] defined over the ring of integers [1],such that

X ij = 1, if there is an edge between i^{th} and j^{th}vertices, and

= 0, if there is no edge between them.

A topological index is a real number related to the structure of a connected graph G and invariant under graph automorphism.It is graph invariant thus it does not depend on labeling or pictorial representation. The topological indices are used for establishing correlations between the structure of a molecular compounds and its physico-chemical properties or biological activity[2 ,3]. Wiener index and Wiener polynomial in isomers of organic compounds are studied by K.S.Ahire[4]. Wiener index of a graph and chemical applications are studied by A.Vijaya Bharathi [5]. The matrix expression for topological index and molecular topological structure studied by Quan-Nan-Hu [6] , Applications of graph theory for sociological, biological and mathematical problems studied by Sanjeev Kumar [7] and applications of graph theory in chemistry studied by A.T. Balban [8].

Topological indices

Total adjacency index: Total adjacency index is the half sum of entries in the adjacency matrix

(A)and is equal to edges, in graph

$$A = \tfrac{1}{2}\sum_i \sum_j [A]_{ij} \quad (1)$$

Randic index

This topological index is also known branching index or connectivity index, was defined as [9],

$$R = R(G) = \sum_{u \sim v} 1 / [d_u(G) * d_v(G)]^{1/2} \quad (2)$$

with summation going over all pairs of adjacent vertices of the molecular graph G . A recent result about the Randic index is

$$R(G) = n/2 - \tfrac{1}{2} \sum_{1 \le l \le j \le n-1} (1/\sqrt{i} - 1/\sqrt{j})^2 m_{ij} \quad (3)$$

Where G stands for any graph with n-vertices, in which there are m_{ij} edges connecting a vertex of degree i with a vertexof degreej [10].

Zagreb indices Topological indices based on adjacency matrix (i.e. based on connectivity) were introduced by group of Zagreb [11,12].

First Zagreb index $M_1(G) = \sum_{u,v \in E(G)} d_u + d_v$ (4)

Second Zagreb index $M_2(G) = \sum_{e=uv \in E(G)} (d_u * d_v)$ (5)

Where d_u, d_v are the vertex degree for any two adjacent vertices. Pierre Hansen [13] noticed that for numerous graph with n vertices and m edges ,an inequality between first and second Zagreb indices, $M_1(G)/n \le M_2(G)/m$ (6)

is satisfied .He conjectured that, this inequality hold for all graphs and other inequality for a simple connected graph G (without loops and multiple edges) proved by Das and Gutman [14] for n vertices was, $M_1 + 2M_2 \le 4m^2$ (7)

Zagreb polynomials The first and second Zagreb polynomials are defined as [15],

First Zagreb polynomial

$$Z_{g1}(G, x) = \sum_{e=uv \in E(G)} x^{du + dv} \quad (8)$$

Second Zagreb polynomial

$$Z_{g2}(G, x) = \sum_{e=uv \in E(G)} x^{du * dv} \quad (9)$$

Compounds thathave the same molecular formula but a different configuration of atoms are known as isomers. The pentane (C_5H_{12}) has three isomers with linear structure ,iso-pentane and neo-pentane. In this, paper we study Total adjacency index, Randic index, first Zagreb index , second Zagreb index, first Zagreb polynomial and second Zagreb polynomial for isomers of pentane.

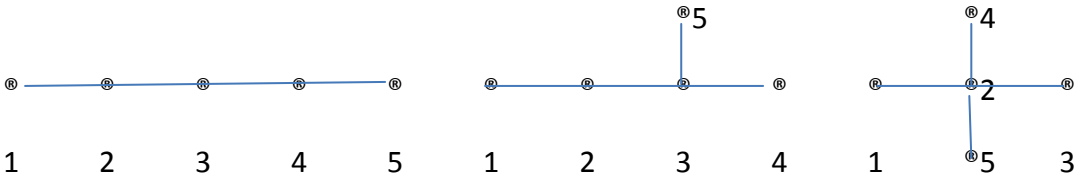
Results and discussion

Alkanes are any of a series of saturated aliphatic hydrocarbons having the general formula C_nH_{2n+2} .Alkanes have only single covalent bonds meaning that the bonds are formed by two carbon atoms sharing a pair of electrons . Pentane is member of this family with formula C_5H_{12} and has three isomers as linear structure, iso-pentane and neo-pentane.

Chemical graphs are mathematical objects that are a convenient way for expressing in a numerical form the chemical structure enclosed in the chemical graphs.

Total adjacency index

The hydrogen suppressed graphs of isomers of pentane, with linear structure, iso- pentane and neo-pentane are given fig.(1)



Linear structure ($G_{4,0}$) iso-pentane ($G_{4,1}$) neo-pentane ($G_{4,2}$)

Fig.(1) Molecular graphs for isomers of pentane .

The adjacency matrix for isomers of pentane are shown in fig.(2). The total adjacency index is equal to number of edges in graph.

	1	2	3	4	5
1	0	1	0	1	0
2	1	0	1	0	1
3	0	1	0	1	1
4	1	0	1	0	1
5	0	1	0	1	0

	1	2	3	4	5
1	0	1	0	0	0
2	1	0	1	0	0
3	0	1	0	1	0
4	0	0	1	0	0
5	0	0	0	0	0

	1	2	3	4	5
1	0	1	1	1	0
2	1	0	0	0	0
3	1	0	0	0	0
4	1	0	0	0	0
5	0	0	0	0	0

5000 1 00 0 1 0 0 0 1 0 0 0

Linear structure ($G_{4,0}$)iso-pentane ($G_{4,1}$) neo-pentane ($G_{4,2}$)

Fig.(2) Adjacency matrices for isomers of pentane with linear structure , iso-pentane and neo-pentane. From adjacency matrices for isomers of pentane,A ($G_{4,0}$) = 1+1+1+1 = 4

A ($G_{4,1}$) = 1+1+1+1 = 4 and A ($G_{4,2}$) = 1+1+1+1 = 4

The total adjacency index is equal to number of edges in pentane,for these structures, the number of edges is 4.

Randic index The Randic or connectivity index was introduced for characterizing the branching in graphs, is calculated on edge, by using the vertex degrees of its end points .Randic index from equations (2,3)

$$R(G_{4,0}) = \sqrt{\frac{1}{1*2}} + \sqrt{\frac{1}{2*2}} + \sqrt{\frac{1}{2*2}} + \sqrt{\frac{1}{2*1}} = 2.4144$$

$$R(G_{4,1}) = \sqrt{\frac{1}{1*2}} + \sqrt{\frac{1}{2*3}} + \sqrt{\frac{1}{3*1}} + \sqrt{\frac{1}{1*3}} = 2.27$$

$$R(G_{4,2}) = \sqrt{\frac{1}{1*4}} + \sqrt{\frac{1}{4*1}} + \sqrt{\frac{1}{4*1}} + \sqrt{\frac{1}{1*4}} = 2$$

Randic index values decrease as the branching increases within a set of pentane isomers . The linear structure has R (G) maximal value and neo-pentane has minimal value agreeing well with G.Caporossi et al [16]. This index was shown to correlate with various physico-chemical (e.g. enthalpy of formation, molar refraction, van der Waal's areas and volumes, chromatographic retention index etc. .) and biological properties .In this case n = 5 and m_{ij} , from equation (3) , R has to be less than n/2, are observed for isomers of pentane [10].

Zagreb index

From fig.(1),first Zagreb index for molecular graphs of isomers of pentane ,using algorithm for M_1 and M_2 determination given by G.F.Tabar [17] are

$M_1(G_{4,0}) = 2*1^2 + 3*2^2 = 14$, $M_1(G_{4,1}) = 3*1^2 + 1*2^2 + 1*3^2 = 16$

$M_1(G_{4,2}) = 4*1^2 + 1*4^2 = 20$

The second Zagreb index, fig.(1) and equation (5) for isomers of pentane are computed as $M_2(G_{4,0}) = 2(1*2)+2(2*2) = 12$, $M_2(G_{4,1}) = 2(1*3)+1(1*2)+1(2*3) = 14$ $M_2(G_{4,2}) = 4(1*4) = 16$

Inequality in Zagreb indices

1) An equality in case of M_1 and $M_2$for isomers of pentane

$M_1(G)/n \leq M_2(G)/m$, $n = 5$, $m = 4$

$G_{(4,0)}$----- 2.8 ≤ 3 ,$G_{(4,1)}$---3.2 ≤ 3.5 and $G_{(4,2)}$ ----4 ≤ 4

This inequality between M_1 and M_2 is observed for isomers of pentane [13].

2) An another inequality for simple connected graph G (without loops and multiple edges) proved by Das and Gutman [14] for n vertices from equation (7) is

$G_{(4,0)}$ ---- 38 ≤ 100, $G_{(4,1)}$ ----- 44 ≤ 100 , and $G_{(4,2)}$ ------ 52 ≤ 100.

confirms the result of proved by Das and Gutman [14].

Zagreb polynomials:First Zagreb polynomial, from fig.(1) and equation(8) expressed as

$Z(G_{4,0}) = 2x^3 + 2x^4$, $Z(G_{4,1}) = x^5 + 2x^4 + x^3$ and $Z(G_{4,2}) = 4x^5$

Second Zagreb polynomials

$Z(G_{4,0}) = 2x^4 + 2x^2$, $Z(G_{4,1}) = 2x^6 + x^3 + x^2$ and $Z(G_{4,2}) = x^4$

Conclusions

From adjacency matrix, the total adjacency index is equal to number of edges. The connectivity index values decrease as branching increases within a set of pentane isomers. First and second Zagreb indices increase with structure of isomers of pentane and first, second Zagreb polynomials is determined along with testing of two inequalities about Zagreb indices.

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