

# Degree Based Topological Indices of Isomers of Organic Compounds

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**Abstract-** Let  $G(V,E)$  be a connected graph. The sets of vertices and edges of  $G$  are denoted by  $V=V(G)$  and  $E=E(G)$  respectively. In such a molecular graph, vertices represent atoms and edges represent bonds. The number of edges incident on a  $v_i$  is called the degree  $d(v_i)$  of vertex  $v_i$ . The sum of degrees of all vertices in  $G$  is twice the number of edges in  $G$  [1]. In molecular graph we have many topological indices. In this research, we computing Randic index, Molecular topological index, Augmented Zagreb index, Geometric-Arithmetic index, Atom-bond connectivity index, Harmonic index, Sum-connectivity index of n-decane, 3,4,4-Trimethyl heptane and 2,4-dimethyl-4-ethyl hexane.

**Index Terms-** Randic index, Molecular topological index, Augmented Zagreb index, Geometric-arithmetic index, Harmonic index, Sum-connectivity index.

## Randic index

The first degree-based topological index was put forward in 1975 by Milan Randic, in paper, on characterization of molecular branching. This index was defined as

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

with summation going over all of adjacent vertices of the molecular graph  $G$ . This is called Randic index or branching index [2].

**Molecular topological index** Molecular topological index (MTI) is defined as

$$MTI = MTI(G) = \sum_{i=1}^N [V(A+D)]_i \quad (2)$$

Here  $A$  is adjacent matrix of graph,  $D$  is distance matrix of graph  $G$  and  $V$  is vector of degrees of vertices in the molecular graph [3].

## Augmented Zagreb index

Augmented Zagreb index abbreviated as AZI ( $G$ ). It is defined as

$$AZI(G) = \sum_{u \sim v} [d_u(G) * d_v(G) / (d_u(G) + d_v(G) - 2)]^3 \quad (3)$$

## Geometric-arithmetic index

Vukicevic and Furtula (2009) proposed a topological index named geometric-arithmetic index (GAI). The GAI is defined as

$$GAI = \sum_{u,v \in E(G)} 2 (d_u + d_v)^{1/2} / (d_u + d_v) \quad (4)$$

where  $d_u$  (or  $d_v$ ) denote the degree the vertex  $u$  (or  $v$ ) [4,5].

## Atom-bond connectivity index

The atom-bond connectivity index of graph  $G$ , is defined as

$$ABC(G) = \sum_{u,v \in E(G)} [(d_u + d_v - 2) / (d_u * d_v)]^{1/2} \quad (5)$$

where  $d_u$  (or  $d_v$ ) denote the degree the vertex  $u$  (or  $v$ ) has [4,5].

## Harmonic index

Harmonic index is defined as [2],

$$H(G) = \sum_{u,v} 2 / [d_u(G) + d_v(G)] \quad (6)$$

and the sum-connectivity index is defined as

## I. INTRODUCTION

Let  $G$  be a molecular graph. The vertex-set and edge-set of  $G$  denoted by  $V(G)$  and  $E(G)$  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  $d_v$ . The concept of degree in graph theory is closely related to valence in chemistry [2]. Chemical graphs are mathematical objects that represent chemical compounds.

A topological index is a structural descriptor (derived from molecular graph) that represents an efficient way to express in a numerical form the molecular size, shape, cyclicality, and branching. The topological indices of molecular graphs are widely used for establishing correlations between the structure of a molecular compound and its physico-chemical properties or biological activity.

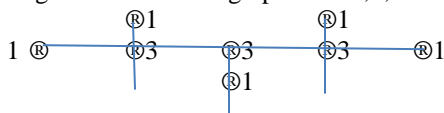
**Sum-connectivity index**

$$SCI(G) = \sum_{u \sim v} 1 / [d_u(G) + d_v(G)]^{1/2} \tag{7}$$

The purpose of this paper is computing the Randic index, Molecular topological index, Augmented Zagreb index, Geometric–arithmetic index, Atom-bond connectivity, Harmonic and Sum-connectivity index of n-decane, 3,4,4-trimethyl heptane and 2,4-dimethyl-4-ethyl hexane, some members of isomers of decane with molecular formula (C<sub>10</sub>H<sub>22</sub>).

**II. RESULTS AND DISCUSSION**

Graph is a data structure which consists of two things, The Set V: vertices and the set E: edges, i.e. graph G = (V,E). Such that each edge is identified with unique pair of vertices in V. Here e = [u,v], where u,v ∈ V, u and v may be called the end points of the edge e. The degree is defined as the number of edges with that vertex. The sum of degrees over all vertices = 2n<sub>e</sub>, where n<sub>e</sub> is the number of edges [6,7]. The degree in molecular graph G of 2,3,4-trimethyl propane with its vertex degrees shown in fig.(1).

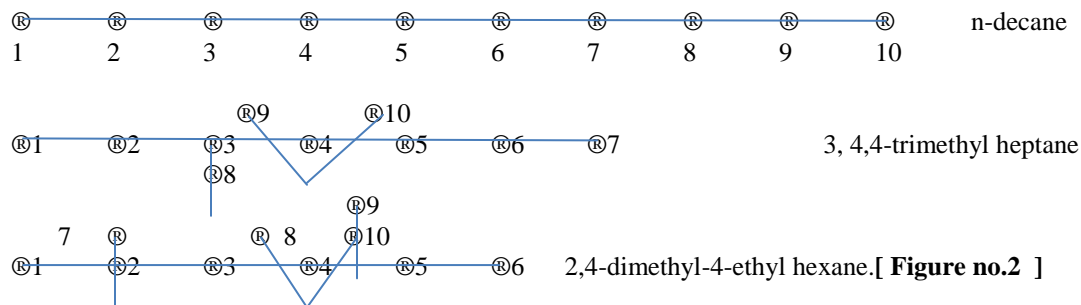


**Fig.(1) : The molecular graph of 2,3,4-methyl propane with its vertex degrees .**

**Randic index or connectivity index**

A molecular graph is constructed by representing each atom of a molecule by a vertex and bonds between atoms by edges [8].

Molecular graphs of n-decane, 3,4,4-trimethyl heptane and 2,4-dimethyl-4-ethyl hexane are given in fig.(2) and referred for computing the topological indices.



The Randic index of 3,4,4-trimethyl heptane from equation (1) and fig.(2) are computed as, the first bond (between atoms 1 and 2) connects vertices of the first and of two degree, the second of (2) and third (3) degree etc. .

$$R(G) = 1/\sqrt{1*2} + 1/\sqrt{2*3} + 1/\sqrt{3*4} + 1/\sqrt{4*2} + 1/\sqrt{2*2} + 1/\sqrt{2*1} + 1/\sqrt{3*1} + 1/\sqrt{4*1} + 1/\sqrt{4*1} = 4.5439$$

The Randic index for n-decane, 3,4,4-trimethyl heptane and 2,4 dimethyl-4-ethyl hexane are given in table (1).

**Molecular topological index**

Molecular topological index (MTI) from equation (2) and fig(2) are computed by constructing distance matrix (D), adjacency matrix(A) and vector the (V) valances (degrees) of vertices of molecular graph. The D, A and V for 3,4,4-trimethyl heptane constructed as

$$\begin{array}{c}
 \text{Distance matrix (D)} \\
 \begin{bmatrix}
 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\
 0 & 1 & 2 & 3 & 4 & 5 & 6 & 3 & 4 & 4 \\
 1 & 0 & 1 & 2 & 3 & 4 & 5 & 2 & 3 & 3 \\
 2 & 1 & 0 & 1 & 2 & 3 & 4 & 1 & 2 & 2 \\
 3 & 2 & 1 & 0 & 1 & 2 & 3 & 2 & 1 & 1 \\
 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 2 & 2 \\
 5 & 4 & 3 & 2 & 1 & 0 & 1 & 4 & 3 & 3 \\
 6 & 5 & 4 & 3 & 2 & 1 & 0 & 5 & 4 & 4 \\
 7 & 6 & 5 & 4 & 3 & 2 & 1 & 0 & 3 & 3 \\
 8 & 3 & 2 & 1 & 2 & 3 & 4 & 5 & 0 & 2 \\
 9 & 4 & 3 & 2 & 1 & 2 & 3 & 4 & 3 & 0 \\
 10 & 4 & 3 & 2 & 1 & 2 & 3 & 4 & 3 & 2 & 0
 \end{bmatrix}
 \end{array}
 \quad
 \begin{array}{c}
 \text{Adjacency matrix (A)} \\
 \begin{bmatrix}
 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\
 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 1 \\
 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0
 \end{bmatrix}
 \end{array}$$

and V [ 2 2 3 4 2 2 1 1 1 1 ].

$$MTI(G) = 440$$

The values of molecular topological index for n-decane 3,4,4-trimethyl heptane and 2,4,dimethyl-4-ethyl hexane, are represented in table(1).MTI (G) value of n-decane is more than other two members due to linear chain of carbon atoms .The 3,4,4-trimethyl heptane and 2,4-dimethyl -4- ethyl hexane share the same value 440.

**Augmented Zagreb index**

AZI (G) computed from fig.(2) and equation (3) for 3,4,4-trimethyl heptane as

$$\begin{aligned}
 AZI(G) = & (1 * 2 / 3 - 2)^3 + (2 * 3 / 5 - 2)^3 + (3 * 4 / 7 - 2)^3 + (4 * 2 / 6 - 2)^3 + (2 * 2 / 4 - 2)^3 \\
 & + (2 * 1 / 3 - 2)^3 + (3 * 1 / 4 - 2)^3 + (4 * 1 / 5 - 1)^3 + (4 * 1 / 5 - 1)^3 = 4019.7
 \end{aligned}$$

AZI (G) values of other members are given in table (1).

**Geometric-arithmetic index**

Geometric-arithmetic index (GAI) is computed from equation (4), referring fig(2) ,for 3,4,4-trimethyl heptane as

$$\begin{aligned}
 GAI = & 2\sqrt{1*2} / 3 + 2\sqrt{2*3} / 5 + 2\sqrt{3*4} / 7 + 2\sqrt{4*2} / 6 + 2\sqrt{2*2} / 4 + 2\sqrt{2*1} / 3 + 2\sqrt{3*1} / 4 + \\
 & 2\sqrt{4*1} / 5 + 2\sqrt{4*1} / 5 = 8.8142 \quad (\text{table 1}).
 \end{aligned}$$

**Atom-bond connectivity index** ABCI for 3,4,4-trimethyl heptane ( equation 5,fig.2)

$$\begin{aligned}
 ABCI = & \sqrt{\frac{2+1-2}{2*1}} + \sqrt{\frac{3+2-2}{3*2}} + \sqrt{\frac{4+3-2}{4*3}} + \sqrt{\frac{4+2-2}{4*2}} + \sqrt{\frac{2+2-2}{2*2}} + \sqrt{\frac{2+1-2}{2*1}} + \sqrt{\frac{(3+1-2)}{3*1}} + \sqrt{\frac{4+1-2}{4*1}} + \sqrt{\frac{4+1-2}{4*1}} \\
 = & 5.7716
 \end{aligned}$$

**Harmonic index** H (G) For 3,4,4-trimethyl heptane

$$= 2/3 + 2/5 + 2/7 + 2/6 + 2/4 + 2/3 + 2/4 + 2/5 + 2/5 = 4.152$$

The values of H(G) for other two members , tabulated ( table 1 ).

**Sum-connectivity index** :For 3,4,4-trimethyl heptane from equation(7),fig(2),SCI(G) =

$$\begin{aligned}
 & \sqrt{1/(1+2)} + \sqrt{1/(2+3)} + \sqrt{1/(3+4)} + \sqrt{1/(4+3)} + \sqrt{1/(2+2)} + \sqrt{1/(2+1)} \\
 & + \sqrt{1/(3+1)} + \sqrt{1/(4+1)} + \sqrt{1/(4+1)} = 4.2824 \quad (\text{table 1}).
 \end{aligned}$$

**Table (1):** Values of Randic index, Molecular topological index, Augmented Zagreb index, Geometric-arithmetic index, Atom-bond connectivity index, Harmonic index and Sum-connectivity index for n-decane,3,4,4-trimethyl heptane and 2,4-dimethyl-4-ethylhexane.

Topological indices	n-decane	3,4,4-trimethyl heptane	2,4-dimethyl-4-ethyl hexane
R(G)	4.9161	4.5439	4.5378
MTI(G)	590	440	440
AZI (G)	5832	4019.7	3518.3
GAI(G)	8.8856	8.8142	8.2257
ABC(G)	6.9497	5.7716	5.9113
H(G)	4.8332	4.152	4.1333
SCI(G)	4.6547	4.2824	4.2741

### III. CONCLUSION

The topological indices are determined for some members of isomers of decane .Randic index has higher value for n-decane and it decreases with branching in the structure and the same case is followed for degree- based topological indices, AZI(G),GAI(G),ABC(G),H(G) and SCI(G).Molecular topological index for 3,4,4-trimethyl heptane and 2,4-dimethyl-4-hexane share the same value (440) but in n-decane it is more due to linear chain of carbon atoms.

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