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Cyclohexane based isomers discrimination using topological indices

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Abstract

The isomers are the structures with same molecular formulae but with different structures. Cyclohexane isomers consists of an atom or group of atoms linked to cyclohexane itself. The cyclohexane based isomers are examined and topological indices such as Wiener, Balaban and Randic indices are calculated by using the molecular graphs distance matrix D_S and D_M matrix, where D_M matrix includes the data of the superior distances. In our proposed work, we have analyzed the Wiener index, Balaban index and Randic index of cyclohexane based isomers.

Keywords

Positional isomers, D_S-Matrix, D_M-Matrix, Wiener index, Balaban index, Randic index.

AMS Subject Classification

05C07, 05C10, 05C12.

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Contents

1. Introduction

A graph is a collection of points called as vertices, connected by a number of lines called edges. Let $G = (V,E)$ be a graph with vertices set $V(G)$ and Edge set $E(G)$. The study of graph theory is important in various domains such as mathematics, graph theory and engineering. Chemical graph theory is a discipline of mathematics, links mathematics with chemistry [7, 10, 17–20]. Isomers are the molecules with same structural formula but with different organisation of atoms in a molecule. There are 2 types of isomers known as Structural isomers(Constitutional isomers) and stereo isomers. Structural isomers are molecules with same structural formula but with different atomic organisation pattern where stereo-isomers are molecules in which molecular bonds are of same order but with different spatial arrangements.

Topological index is a numerical descriptor or a number depicting the chemical structure[1, 2, 15, 16]. There are two types of topological indices called degree based and distance

based topological indices. In our proposed work, we study the Wiener index, Balban index and Randic index on isomer called cyclohexane[3, 4, 8, 11–14]. Cyclohexane is a hydrocarbon structure consisting of only carbon and hydrogen atoms with a total of 6 carbon atoms. The chemical formula of cyclohexane is C_6H_{12} and is as shown in Figure 1.

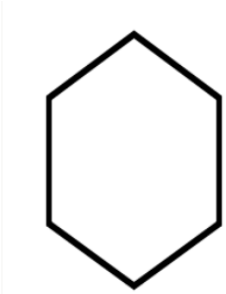

Figure 1. Cyclohexane-C_6H_{12}

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To construct an isomer of cyclohexane, place 3-methyls(CH_3) or 1-ethyl(C_2H_5) and 1-methyl(CH_3) on any carbon atom of cyclohexane. There are 12 isomers of cyclohexane. The molecular graphs are considered for calculation of invariants[5, 6, 9]. They are as shown in below Table 1.

Table 1. Cyclohexane based isomers

$2,3,5-trimethylcyclohexane$	$2,4,6-trimethylcyclohexane$
$2,4,7-trimethylcyclohexane$	$2,3,6-trimethylcyclohexane$
$2,3,3-trimethylcyclohexane$	$2,4,4-trimethylcyclohexane$
$2,5,5-trimethylcyclohexane$	$Isopropylcyclohexane$
$3-ethyl\ 4-methylcyclohexane$	$3-ethyl\ 5-methylcyclohexane$
$3-ethyl\ 6-methylcyclohexane$	$Propylcyclohexane$

2. Preliminaries

2.1 Wiener index

In chemical graph theory, The Wiener index also called as Wiener number proposed by Harry Wiener. It is defined as the sum of the distance between all pairs of vertices of a graph G and is represented as,

$$W(G) = \sum_{\{i,j\}\subseteq V(G)} d(i,j)$$

2.2 Randic index

In the year 1975, Milan Randic proposed the Randic index and is defined as,

$$\chi(G) = \sum_{e=ij} \frac{1}{\sqrt{d_i d_j}}$$

2.3 Balaban index

Balaban introduced the topological index known as Balaban index is the row sums of the distance matrix and is defined as,

$$J(G) = \frac{E}{\mu+1} \sum_{e=ij} (d_i d_j)^{-\frac{1}{2}}$$

Where E and n are the total number of edges and vertices of a graph G and $\mu = E-n+1$ is called the cyclomatic number of G and j is the reciprocal square root of the row sums of the D_M matrix. The Balaban index is widely used topological indices in QSAR and QSPR studies.

2.4 Steps to find the D_M-Matrix

Step 1: Compute D_S-Matrix for molecular graphs of cyclohexane Based isomers. where D_S is the distance matrix and R_u is the largest element in the u^{th} row , C_v be the largest element in the v^{th} column of D_S matrix.

Step 2: compute D_M-Matrix for the molecular graphs such that

$$(D_M)_{uv} = (D_S)_{uv},\ if\ (D_S)_{uv} \geqslant min\{R_u, C_v\}$$
$$(D_M)_{uv} = 0,\ if\ (D_S)_{uv} < min\{R_u, C_v\}$$

3. Evaluation of D_S and D_M-Matrices of Cyclohexane Based Isomers

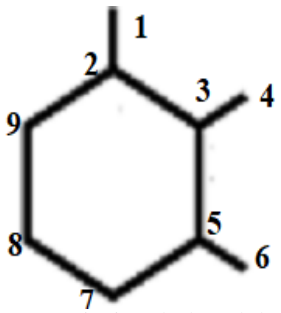

Figure 2. 2,3,5-trimethyl cyclohexane

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D_S-Matrix

$$\begin{pmatrix} 0 & 1 & 2 & 3 & 3 & 4 & 4 & 3 & 2 \\ 1 & 0 & 1 & 2 & 2 & 3 & 3 & 2 & 1 \\ 2 & 1 & 0 & 1 & 1 & 2 & 2 & 3 & 2 \\ 3 & 2 & 1 & 0 & 2 & 3 & 3 & 4 & 3 \\ 3 & 2 & 1 & 2 & 0 & 1 & 1 & 2 & 3 \\ 4 & 3 & 2 & 3 & 1 & 0 & 2 & 3 & 4 \\ 4 & 3 & 2 & 3 & 1 & 2 & 0 & 1 & 2 \\ 3 & 2 & 3 & 4 & 2 & 3 & 1 & 0 & 1 \\ 2 & 1 & 2 & 3 & 3 & 4 & 2 & 1 & 0 \end{pmatrix} \begin{matrix} 22 \\ 15 \\ 14 \\ 21 \\ 15 \\ 22 \\ 18 \\ 19 \\ 18 \end{matrix}$$

D_M-Matrix

$$\begin{pmatrix} 0&0&0&0&3&4&4&0&0 \\ 0&0&0&0&0&3&3&0&0 \\ 0&0&0&0&0&0&0&3&0 \\ 0&0&0&0&0&0&0&4&0 \\ 3&0&0&0&0&0&0&0&3 \\ 4&3&0&0&0&0&0&0&4 \\ 4&3&0&0&0&0&0&0&0 \\ 0&0&3&4&0&0&0&0&0 \\ 0&0&0&0&3&4&0&0&0 \end{pmatrix} \begin{matrix} 11 \\ 6 \\ 3 \\ 4 \\ 6 \\ 11 \\ 7 \\ 7 \\ 7 \end{matrix}$$

$W = 82,\ \ 2,3,5-trimethyl\ cyclohexane,\ \ \chi = 4.2152$		
$C-CBond$	J	j
$1-2$	0.0550	0.1230
$2-3$	0.0690	0.2357
$3-4$	0.0583	0.2886
$3-5$	0.0690	0.2357
$5-6$	0.0550	0.1230
$5-7$	0.0608	0.1543
$7-8$	0.0540	0.1428
$8-9$	0.0540	0.1428
$9-2$	0.0608	0.1139
$TOTAL$	0.5359	1.5598

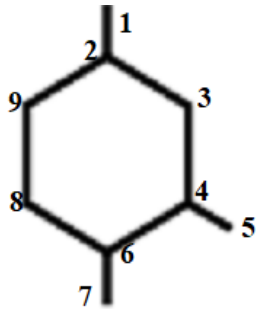

Figure 3. 2,4,6-trimethyl cyclohexane

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D_S-Matrix

$$\begin{pmatrix} 0&1&2&3&4&4&5&3&2 \\ 1&0&1&2&3&3&4&2&1 \\ 2&1&0&1&2&2&3&3&2 \\ 3&2&1&0&1&1&2&2&3 \\ 4&3&2&1&0&2&3&3&4 \\ 4&3&2&1&2&0&1&1&2 \\ 5&4&3&2&3&1&0&2&3 \\ 3&2&3&2&3&1&2&0&1 \\ 2&1&2&3&4&2&3&1&0 \end{pmatrix} \begin{matrix} 24 \\ 17 \\ 16 \\ 15 \\ 22 \\ 16 \\ 23 \\ 17 \\ 18 \end{matrix}$$

D_M-Matrix

$$\begin{pmatrix} 0&0&0&3&4&4&5&3&0 \\ 0&0&0&0&0&0&4&0&0 \\ 0&0&0&0&0&0&3&3&0 \\ 3&0&0&0&0&0&0&0&3 \\ 4&0&0&0&0&0&0&3&4 \\ 4&0&0&0&0&0&0&0&0 \\ 5&4&3&0&0&0&0&0&0 \\ 3&0&3&0&3&0&0&0&0 \\ 0&0&0&3&4&0&0&0&0 \end{pmatrix} \begin{matrix} 19 \\ 4 \\ 6 \\ 6 \\ 11 \\ 4 \\ 12 \\ 9 \\ 7 \end{matrix}$$

$W = 84,\ \ 2,4,6-trimethyl\ cyclohexane,\ \ \chi = 4.1984$		
$C-CBond$	J	j
$1-2$	0.0495	0.1147
$2-3$	0.0606	0.2041
$3-4$	0.0645	0.1666
$4-5$	0.0550	0.1230
$4-6$	0.0645	0.2041
$6-7$	0.0521	0.1443
$6-8$	0.0606	0.1666
$8-9$	0.0571	0.1259
$9-2$	0.0571	0.1889
$TOTAL$	0.521	1.4382

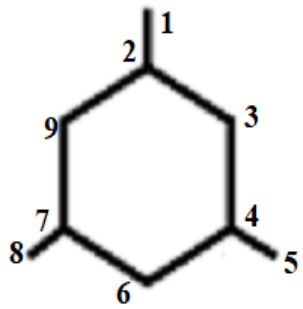

Figure 4. 2,4,7-trimethyl cyclohexane

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D_S-Matrix

$$\begin{pmatrix} 0&1&2&3&4&4&3&4&2 \\ 1&0&1&2&3&3&2&3&1 \\ 2&1&0&1&2&2&3&4&2 \\ 3&2&1&0&1&1&2&3&3 \\ 4&3&2&1&0&2&3&4&4 \\ 4&3&2&1&2&0&1&2&2 \\ 3&2&3&2&3&1&0&1&1 \\ 4&3&4&3&4&2&1&0&2 \\ 2&1&2&3&4&2&1&2&0 \end{pmatrix} \begin{matrix} 23 \\ 16 \\ 17 \\ 16 \\ 23 \\ 17 \\ 16 \\ 23 \\ 17 \end{matrix}$$

D_M-Matrix

$$\begin{pmatrix} 0&0&0&3&4&4&3&4&0 \\ 0&0&0&0&3&3&0&3&0 \\ 0&0&0&0&0&0&3&4&0 \\ 3&0&0&0&0&0&0&3&3 \\ 4&3&0&0&0&0&3&4&4 \\ 4&3&0&0&0&0&0&0&0 \\ 3&0&3&0&3&0&0&0&0 \\ 4&3&4&3&4&0&0&0&0 \\ 0&0&0&3&4&0&0&0&0 \end{pmatrix} \begin{matrix} 18 \\ 9 \\ 7 \\ 9 \\ 18 \\ 7 \\ 9 \\ 18 \\ 7 \end{matrix}$$

$W=84,\ \ 2,4,7-trimethyl\ cyclohexane,\ \ \chi=4.1815$		
$C-CBond$	J	j
$1-2$	0.0521	0.0785
$2-3$	0.0606	0.1259
$3-4$	0.0606	0.1259
$4-5$	0.0521	0.0785
$4-6$	0.0606	0.1259
$6-7$	0.0606	0.1259
$7-8$	0.0521	0.0785
$7-9$	0.0606	0.0785
$9-2$	0.0606	0.0785
$TOTAL$	0.5199	0.8961

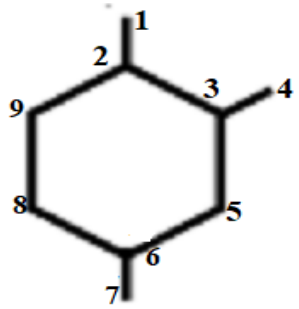

Figure 5. 2,3,6-trimethyl cyclohexane

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D_M-Matrix

$$\begin{pmatrix} 0&0&0&0&3&4&5&0&0 \\ 0&0&0&0&0&0&4&0&0 \\ 0&0&0&0&0&0&3&3&0 \\ 0&0&0&0&0&0&4&4&3 \\ 3&0&0&0&0&0&0&0&3 \\ 4&0&0&0&0&0&0&0&0 \\ 5&4&3&4&0&0&0&0&3 \\ 0&0&3&4&0&0&0&0&0 \\ 0&0&0&3&3&0&3&0&0 \end{pmatrix} \begin{matrix} 12 \\ 4 \\ 6 \\ 11 \\ 6 \\ 4 \\ 19 \\ 7 \\ 9 \end{matrix}$$

$W=84,\ \ 2,3,6-trimethyl\ cyclohexane,\ \ \chi=4.1984$		
$C-CBond$	J	j
$1-2$	0.0521	0.1443
$2-3$	0.0645	0.2041
$3-4$	0.0550	0.1230
$3-5$	0.0645	0.1666
$5-6$	0.0606	0.2041
$6-7$	0.0495	0.1147
$6-8$	0.0571	0.1889
$8-9$	0.0571	0.1259
$9-2$	0.0606	0.1666
$TOTAL$	0.521	1.4382

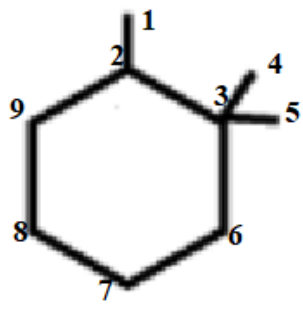

Figure 6. 2,3,3-trimethyl cyclohexane

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D_S-Matrix

$$\begin{pmatrix} 0&1&2&3&3&4&5&3&2 \\ 1&0&1&2&2&3&4&2&1 \\ 2&1&0&1&1&2&3&3&2 \\ 3&2&1&0&2&3&4&4&3 \\ 3&2&1&2&0&1&2&2&3 \\ 4&3&2&3&1&0&1&1&2 \\ 5&4&3&4&2&1&0&2&3 \\ 3&2&3&4&2&1&2&0&1 \\ 2&1&2&3&3&2&3&1&0 \end{pmatrix} \begin{matrix} 23 \\ 16 \\ 15 \\ 22 \\ 16 \\ 17 \\ 24 \\ 18 \\ 17 \end{matrix}$$

D_S-Matrix

$$\begin{pmatrix} 0&1&2&3&3&3&4&3&2 \\ 1&0&1&2&2&2&3&2&1 \\ 2&1&0&1&1&1&2&3&2 \\ 3&2&1&0&2&2&3&4&3 \\ 3&2&1&2&0&2&3&4&3 \\ 3&2&1&2&2&0&1&2&3 \\ 4&3&2&3&3&1&0&1&2 \\ 3&2&3&4&4&2&1&0&1 \\ 2&1&2&3&3&3&2&1&0 \end{pmatrix} \begin{matrix} 21 \\ 14 \\ 13 \\ 20 \\ 20 \\ 16 \\ 19 \\ 20 \\ 17 \end{matrix}$$

D_M-Matrix

$$\begin{pmatrix} 0&0&0&0&0&3&4&0&0 \\ 0&0&0&0&0&0&3&0&0 \\ 0&0&0&0&0&0&0&3&0 \\ 0&0&0&0&0&0&0&4&3 \\ 0&0&0&0&0&0&0&4&3 \\ 3&0&0&0&0&0&0&0&3 \\ 4&3&0&0&0&0&0&0&0 \\ 0&0&3&4&4&0&0&0&0 \\ 0&0&0&3&3&3&0&0&0 \end{pmatrix} \begin{matrix} 7 \\ 3 \\ 3 \\ 7 \\ 7 \\ 6 \\ 7 \\ 11 \\ 9 \end{matrix}$$

$W = 80,\ \ 2,3,3-trimethyl\ cyclohexane,\ \ \chi = 4.1278$		
$C-CBond$	J	j
$1-2$	0.0583	0.218
$2-3$	0.0741	0.333
$3-4$	0.0620	0.2182
$3-5$	0.0620	0.2182
$3-6$	0.0693	0.2357
$6-7$	0.0573	0.1543
$7-8$	0.0512	0.1139
$8-9$	0.0542	0.1005
$9-2$	0.0648	0.1924
$TOTAL$	0.5532	1.7842

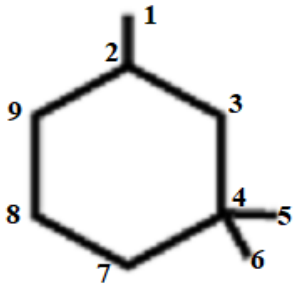

Figure 7. 2,4,4-trimethyl cyclohexane

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D_S-Matrix

$$\begin{pmatrix} 0&1&2&3&4&4&4&3&2 \\ 1&0&1&2&3&3&3&2&1 \\ 2&1&0&1&2&2&2&3&2 \\ 3&2&1&0&1&1&1&2&3 \\ 4&3&2&1&0&2&2&3&4 \\ 4&3&2&1&2&0&2&3&4 \\ 4&3&2&1&2&2&0&1&2 \\ 3&2&3&2&3&3&1&0&1 \\ 2&1&2&3&4&4&2&1&0 \end{pmatrix} \begin{matrix} 23 \\ 16 \\ 15 \\ 14 \\ 21 \\ 21 \\ 17 \\ 18 \\ 19 \end{matrix}$$

D_M-Matrix

$$\begin{pmatrix} 0&0&0&3&4&4&4&3&0 \\ 0&0&0&0&3&3&3&0&0 \\ 0&0&0&0&0&0&0&3&0 \\ 3&0&0&0&0&0&0&0&3 \\ 4&3&0&0&0&0&0&3&4 \\ 4&3&0&0&0&0&0&3&4 \\ 4&3&0&0&0&0&0&0&0 \\ 3&0&3&0&3&3&0&0&0 \\ 0&0&0&3&4&4&0&0&0 \end{pmatrix} \begin{matrix} 18 \\ 9 \\ 3 \\ 6 \\ 14 \\ 14 \\ 7 \\ 12 \\ 11 \end{matrix}$$

$W = 82,\ \ 2,4,4-trimethyl\ cyclohexane,\ \ \chi = 4.1009$		
$C-CBond$	J	j
$1-2$	0.0521	0.0785
$2-3$	0.0645	0.1924
$3-4$	0.06900	0.2357
$4-5$	0.0583	0.1091
$4-6$	0.0583	0.1091
$4-7$	0.0648	0.1543
$7-8$	0.0571	0.1091
$8-9$	0.0540	0.0870
$9-2$	0.0573	0.1005
$TOTAL$	0.5354	1.1757

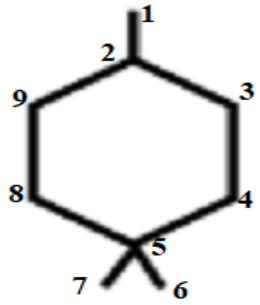

Figure 8. 2,5,5-trimethyl cyclohexane

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D_S-Matrix

$$\begin{pmatrix} 0&1&2&3&4&5&5&3&2 \\ 1&0&1&2&3&4&4&2&1 \\ 2&1&0&1&2&3&3&3&2 \\ 3&2&1&0&1&2&2&2&3 \\ 4&3&2&1&0&1&1&1&2 \\ 5&4&3&2&1&0&2&2&3 \\ 5&4&3&2&1&2&0&2&3 \\ 3&2&3&2&1&2&2&0&1 \\ 2&1&2&3&2&3&3&1&0 \end{pmatrix} \begin{matrix} 25 \\ 18 \\ 17 \\ 16 \\ 15 \\ 22 \\ 22 \\ 16 \\ 17 \end{matrix}$$

D_M-Matrix

$$\begin{pmatrix} 0 & 0 & 0 & 3 & 4 & 5 & 5 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 & 3 & 3 & 0 \\ 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 \\ 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 5 & 4 & 3 & 0 & 0 & 0 & 0 & 0 & 3 \\ 5 & 4 & 3 & 0 & 0 & 0 & 0 & 0 & 3 \\ 3 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 3 & 3 & 0 & 0 \end{pmatrix} \begin{matrix} 20 \\ 8 \\ 9 \\ 6 \\ 4 \\ 15 \\ 15 \\ 6 \\ 9 \end{matrix}$$

$W = 84$, $2,5,5-trimethyl\ cyclohexane$, $\chi = 4.1009$		
$C-CBond$	J	j
$1-2$	0.0471	0.0790
$2-3$	0.0571	0.1178
$3-4$	0.0606	0.1360
$4-5$	0.0645	0.2041
$5-6$	0.0550	0.1290
$5-7$	0.0550	0.1290
$5-8$	0.0645	0.2041
$8-9$	0.0606	0.1360
$9-2$	0.0571	0.1178
$TOTAL$	0.5215	1.2528

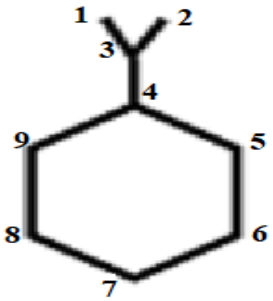

Figure 9. ISO propyl cyclohexane

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D_S-Matrix

$$\begin{pmatrix} 0 & 1 & 2 & 2 & 3 & 4 & 5 & 4 & 3 \\ 1 & 0 & 1 & 1 & 2 & 3 & 4 & 3 & 2 \\ 2 & 1 & 0 & 2 & 3 & 4 & 5 & 4 & 3 \\ 2 & 1 & 2 & 0 & 1 & 2 & 3 & 2 & 1 \\ 3 & 2 & 3 & 1 & 0 & 1 & 2 & 3 & 2 \\ 4 & 3 & 4 & 2 & 1 & 0 & 1 & 2 & 3 \\ 5 & 4 & 5 & 3 & 2 & 1 & 0 & 1 & 2 \\ 4 & 3 & 4 & 2 & 3 & 2 & 1 & 0 & 1 \\ 3 & 2 & 3 & 1 & 2 & 3 & 2 & 1 & 0 \end{pmatrix} \begin{matrix} 24 \\ 17 \\ 24 \\ 14 \\ 17 \\ 20 \\ 23 \\ 20 \\ 17 \end{matrix}$$

D_M-Matrix

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 3 & 4 & 5 & 4 & 3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 4 & 5 & 4 & 3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 \\ 3 & 0 & 3 & 0 & 0 & 0 & 0 & 3 & 0 \\ 4 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 3 \\ 5 & 4 & 5 & 3 & 0 & 0 & 0 & 0 & 0 \\ 4 & 0 & 4 & 0 & 3 & 0 & 0 & 0 & 0 \\ 3 & 0 & 3 & 0 & 0 & 3 & 0 & 0 & 0 \end{pmatrix} \begin{matrix} 19 \\ 4 \\ 19 \\ 3 \\ 9 \\ 11 \\ 17 \\ 11 \\ 9 \end{matrix}$$

$W = 88$, $ISO\ propyl\ cyclohexane$, $\chi = 4.3045$		
$C-CBond$	J	j
$1-2$	0.0495	0.1147
$2-3$	0.0495	0.1147
$2-4$	0.0648	0.2886
$4-5$	0.0648	0.1924
$5-6$	0.0542	0.1005
$6-7$	0.0466	0.0730
$7-8$	0.0466	0.0730
$8-9$	0.0542	0.1005
$9-4$	0.0648	0.1924
$TOTAL$	0.495	1.2498

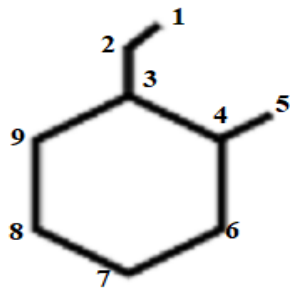

Figure 10. 3-ethyl-4-methyl cyclohexane

.

D_S-Matrix

$$\begin{pmatrix} 0 & 1 & 2 & 3 & 4 & 4 & 5 & 4 & 3 \\ 1 & 0 & 1 & 2 & 3 & 3 & 4 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 2 & 3 & 2 & 1 \\ 3 & 2 & 1 & 0 & 1 & 1 & 2 & 3 & 2 \\ 4 & 3 & 2 & 1 & 0 & 2 & 3 & 4 & 3 \\ 4 & 3 & 2 & 1 & 2 & 0 & 1 & 2 & 3 \\ 5 & 4 & 3 & 2 & 3 & 1 & 0 & 1 & 2 \\ 4 & 3 & 2 & 3 & 4 & 2 & 1 & 0 & 1 \\ 3 & 2 & 1 & 2 & 3 & 3 & 2 & 1 & 0 \end{pmatrix} \begin{matrix} 26 \\ 19 \\ 14 \\ 15 \\ 22 \\ 18 \\ 21 \\ 20 \\ 17 \end{matrix}$$

D_M-Matrix

$$\begin{pmatrix} 0 & 0 & 0 & 3 & 4 & 4 & 5 & 4 & 3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 \\ 3 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 4 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 3 \\ 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 \\ 5 & 4 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 4 & 0 & 0 & 3 & 4 & 0 & 0 & 0 & 0 \\ 3 & 0 & 0 & 0 & 3 & 3 & 0 & 0 & 0 \end{pmatrix} \begin{matrix} 23 \\ 4 \\ 3 \\ 6 \\ 11 \\ 7 \\ 12 \\ 11 \\ 9 \end{matrix}$$

$W = 86,\ \ 3-ethyl-4-methyl\ cyclohexane,\ \ \chi = 4.6413$		
$C-CBond$	J	j
$1-2$	0.0449	0.1042
$2-3$	0.0613	0.2886
$3-4$	0.0690	0.2357
$4-5$	0.0550	0.1230
$4-6$	0.0608	0.1543
$6-7$	0.0514	0.1091
$7-8$	0.0487	0.0870
$8-9$	0.0542	0.1005
$9-3$	0.0648	0.1924
$TOTAL$	0.5101	1.3948

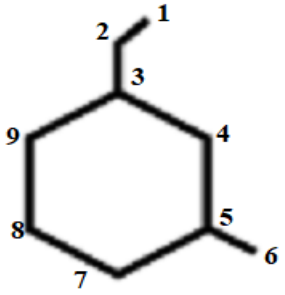

Figure 11. 3-ethyl-5-methyl cyclohexane

.

D_S-Matrix

$$\begin{pmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 5 & 4 & 3 \\ 1 & 0 & 1 & 2 & 3 & 4 & 4 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 & 3 & 2 & 1 \\ 3 & 2 & 1 & 0 & 1 & 2 & 2 & 3 & 2 \\ 4 & 3 & 2 & 1 & 0 & 1 & 1 & 2 & 3 \\ 5 & 4 & 3 & 2 & 1 & 0 & 2 & 3 & 4 \\ 5 & 4 & 3 & 2 & 1 & 2 & 0 & 1 & 2 \\ 4 & 3 & 2 & 3 & 2 & 3 & 1 & 0 & 1 \\ 3 & 2 & 1 & 2 & 3 & 4 & 2 & 1 & 0 \end{pmatrix} \begin{matrix} 27 \\ 20 \\ 15 \\ 16 \\ 17 \\ 24 \\ 20 \\ 19 \\ 18 \end{matrix}$$

D_M-Matrix

$$\begin{pmatrix} 0 & 0 & 0 & 3 & 4 & 5 & 5 & 4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 & 3 & 0 & 0 \\ 3 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 5 & 4 & 3 & 0 & 0 & 0 & 0 & 0 & 4 \\ 5 & 4 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 4 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 \end{pmatrix} \begin{matrix} 21 \\ 8 \\ 6 \\ 6 \\ 4 \\ 16 \\ 12 \\ 7 \\ 4 \end{matrix}$$

$W = 88,\ \ 3-ethyl-5-methyl\ cyclohexane,\ \ \chi = 4.3256$		
$C-CBond$	J	j
$1-2$	0.0430	0.0771
$2-3$	0.0577	0.1443
$3-4$	0.0645	0.1666
$4-5$	0.0606	0.2041
$5-6$	0.0495	0.125
$5-7$	0.0542	0.1443
$7-8$	0.0512	0.1091
$8-9$	0.0540	0.1889
$9-3$	0.0608	0.2041
$TOTAL$	0.4955	1.3635

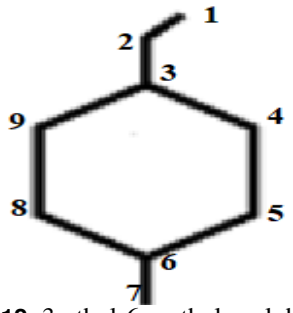

Figure 12. 3-ethyl-6-methyl cyclohexane

.

D_S-Matrix

$$\begin{pmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 4 & 3 \\ 1 & 0 & 1 & 2 & 3 & 4 & 5 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 & 4 & 2 & 1 \\ 3 & 2 & 1 & 0 & 1 & 2 & 3 & 3 & 2 \\ 4 & 3 & 2 & 1 & 0 & 1 & 2 & 2 & 3 \\ 5 & 4 & 3 & 2 & 1 & 0 & 1 & 1 & 2 \\ 6 & 5 & 4 & 3 & 2 & 1 & 0 & 2 & 3 \\ 4 & 3 & 2 & 3 & 2 & 1 & 2 & 0 & 1 \\ 3 & 2 & 1 & 2 & 3 & 2 & 3 & 1 & 0 \end{pmatrix} \begin{matrix} 28 \\ 21 \\ 16 \\ 17 \\ 18 \\ 19 \\ 26 \\ 18 \\ 17 \end{matrix}$$

D_M-Matrix

$$\begin{pmatrix} 0&0&0&3&4&5&6&4&3 \\ 0&0&0&0&0&0&5&0&0 \\ 0&0&0&0&0&0&4&0&0 \\ 3&0&0&0&0&0&3&3&0 \\ 4&0&0&0&0&0&0&0&3 \\ 5&0&0&0&0&0&0&0&0 \\ 6&5&4&3&0&0&0&0&3 \\ 4&0&0&3&0&0&0&0&0 \\ 3&0&0&0&3&0&3&0&0 \end{pmatrix} \begin{matrix} 25 \\ 5 \\ 4 \\ 9 \\ 7 \\ 5 \\ 21 \\ 7 \\ 9 \end{matrix}$$

$W=90,\ 3-ethyl-6-methyl\ cyclohexane,\ \chi=4.3256$		
$C-CBond$	J	j
$1-2$	0.0412	0.0894
$2-3$	0.0545	0.2236
$3-4$	0.0606	0.1666
$4-5$	0.0571	0.1259
$5-6$	0.0540	0.1690
$6-7$	0.0449	0.0975
$6-8$	0.0540	0.1690
$8-9$	0.0571	0.1259
$9-3$	0.0606	0.1666
$TOTAL$	0.4840	1.3335

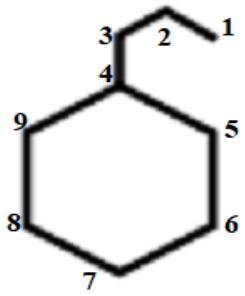

Figure 13. propyl cyclohexane

.

D_S-Matrix

$$\begin{pmatrix} 0&1&2&3&4&5&6&5&4 \\ 1&0&1&2&3&4&5&4&3 \\ 2&1&0&1&2&3&4&3&2 \\ 3&2&1&0&1&2&3&2&1 \\ 4&3&2&1&0&1&2&3&2 \\ 5&4&3&2&1&0&1&2&3 \\ 6&5&4&3&2&1&0&1&2 \\ 5&4&3&2&3&2&1&0&1 \\ 4&3&2&1&2&3&2&1&0 \end{pmatrix} \begin{matrix} 30 \\ 23 \\ 18 \\ 15 \\ 18 \\ 21 \\ 24 \\ 21 \\ 18 \end{matrix}$$

D_M-Matrix

$$\begin{pmatrix} 0&0&0&3&4&5&6&5&4 \\ 0&0&0&0&0&0&5&0&0 \\ 0&0&0&0&0&0&4&0&0 \\ 3&0&0&0&0&0&3&0&0 \\ 4&0&0&0&0&0&0&0&0 \\ 5&0&0&0&0&0&0&0&0 \\ 6&5&4&3&0&0&0&0&0 \\ 5&0&0&0&0&0&0&0&0 \\ 4&0&0&0&0&0&0&0&0 \end{pmatrix} \begin{matrix} 27 \\ 5 \\ 4 \\ 6 \\ 4 \\ 5 \\ 18 \\ 5 \\ 4 \end{matrix}$$

$W=94,\ propyl\ cyclohexane,\ \chi=4.4318$		
$C-CBond$	J	j
$1-2$	0.0380	0.0860
$2-3$	0.0491	0.2236
$3-4$	0.0608	0.2041
$4-5$	0.0608	0.2041
$5-6$	0.0514	0.2236
$6-7$	0.0445	0.1054
$7-8$	0.0445	0.1054
$8-9$	0.0514	0.2236
$9-4$	0.0589	0.2041
$TOTAL$	0.4594	1.5798

$Name$	W	χ	J	j
$2,3,5-trimethyl\ cyclohexane$	82	4.2152	0.5359	1.5598
$2,4,6-trimethyl\ cyclohexane$	84	4.1984	0.521	1.4382
$2,4,7-trimethyl\ cyclohexane$	84	4.1815	0.5199	0.8961
$2,3,6-trimethyl\ cyclohexane$	84	4.1984	0.521	1.4382
$2,3,3-trimethyl\ cyclohexane$	80	4.1278	0.5532	1.7842
$2,4,4-trimethyl\ cyclohexane$	82	4.1009	0.5354	1.1757
$2,5,5-trimethyl\ cyclohexane$	84	4.1009	0.5215	1.2528
$ISO\ propyl\ cyclohexane$	88	4.3045	0.495	1.2498
$3-ethyl-4-methyl\ cyclohexane$	86	4.6413	0.5101	1.3948
$3-ethyl-5-methyl\ cyclohexane$	88	4.3256	0.4955	1.3635
$3-ethyl-6-methyl\ cyclohexane$	90	4.3256	0.4840	1.3335
$Propyl\ cyclohexane$	94	4.4318	0.4594	1.5798

4. Results and Discussions

$SI.No.$	$Name\ of\ Indices$	$Mean$	SD	CV
1	$Wiener\ index$	85.5	3.92	4.58%
2	$Randic\ index$	4.263	0.1565	3.67%
3	$Balaban\ index$	0.5126	0.0256	5%
4	j	1.3722	0.2242	16.3%

Based on the analysis carried out above for cyclohexane based isomers on several indices considered in this study, it is observed that mean value is highest for Wiener index i.e. 85.5. But when coefficient of variation(CV) is considered, it has least variation with Randic index. Hence it can be concluded that the data obtained by using Randic index is more consistent when compared to other indices.

5. Conclusion

For all cyclohexane based isomers Wiener index, Balaban index and Randic index are computed. It is observed that, standard deviation alone will not help to make the selection of topological indices but also coefficient of variation plays an important role in decision making process.

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