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## THE SCHULTZ INDEX, MODIFIED SCHULTZ INDEX AND GEOMETRIC ARITHMETIC INDEX , THEORETICAL BOND LENGTH AND BOND ANGLE OF CHEMICAL TREES OF PENTANE ISOMERS

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### Abstract

Many organic molecules have a graph representation that is tree. Isomers have same chemical formula but different molecular structure. To determine how two chemical structures are different. In this paper we study a Hausdorff ( $\mathcal{H}^f$ ) distance , Geometrical – Arithmetic index ( $GA(G)$ ), Schultz index ( $S_C(G)$ ), modified Schultz index ( $S_C^*(G)$ ) and Schultz polynomial, Modified Schultz polynomial for tress of pentane ( $C_5H_{12}$ ) and its isomers, isopentane and neopentane, having three different tree graphs (chemical trees). We use Gaussian 0.3 computational chemistry software to interpretate the physical properties of these isomers. The bond length and bond angle are important characteristics of covalent bonding in molecules. The concept of bond length and bond angle permits us to get an immediate insight into the bonding situation in different molecules. The thermodynamic properties show that the intermolecular interactions become weaker as the molecular shape becomes more nearly spherical and the surface area decreases with branching.

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Chemical graph theory;  
Schultz index;  
Modified Schultz index;  
Isomers of Pentane;  
Geometric arithmetic index.

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## 1. Introduction

To determine how two chemical structures are same or how similar they are [1]. The carbon atoms are represented as a vertices and chemical bonds are then represented as a edges in the graph  $G = (V(G), E(G))$  consists of finite set of vertices,  $V(G)$ , and a set of edges,  $E(G)$ . The Geometric Arithmetic (GA(G)) index play an significant role in quantitative structure- property relationship (QSPR) and quantitative structure activity relationship (QSAR) studies. The Geometrical Arithmetic index (GA(G)) index is defined in [2] is

$$GA(G) = \sum_{u,v \in E(G)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)}$$

where the summation goes over all the edges of G,  $d_u$  and  $d_v$  are the degrees of the terminal vertices  $u$  and  $v$  of edge  $uv$ . Also  $d(u, v)$  is the distance between vertices  $u$  and  $v$ .

Consider the following formula [2]:  $\sum_{u,v \in E(G)} (d_u d_v)^\alpha$

If  $\alpha = 1$ , we get Second Zagreb index,  $M_2$  [3]. For  $\alpha = \frac{-1}{2}$  we get Randic connectivity index,  $\chi$  [4] which is one of mostly used topological descriptors today.

If  $\alpha = -1$  we get modified Zagreb indices [5], etc.

The Molecule topological index (Schultz index) was introduced in 1989 [6].

$$S_C(G) = \frac{1}{2} \sum_{\{u,v\} \subset V(G)} (d_u + d_v) d(u, v)$$

The modified Schultz index was defined in 1997 [7].

$$S_C^*(G) = \frac{1}{2} \sum_{\{u,v\} \subset V(G)} (d_u d_v) d(u, v)$$

The Schultz polynomial and Modified Schultz polynomial of graph G are defined respectively as:

$$S_C(G, x) = \frac{1}{2} \sum_{\{u,v\} \subset V(G)} (d_u + d_v) x^{d(u,v)}$$

and

$$S_C^*(G, x) = \frac{1}{2} \sum_{\{u,v\} \subset V(G)} (d_u d_v) x^{d(u,v)}$$

In general the bond length and bond angle parameters may be useful in correlating the quantum mechanics and ordinary chemistry [8]. Gaussian 03(W) has been used to get variety of configurations [9]. The  $R(i, j)$  define a bond coordinate between atoms  $i$  and  $j$  that means bond length between atoms  $i$  and  $j$ .  $A(i, j, k)$  define a non-linear angle coordinates involving atoms  $i, j$  and  $k$ .  $D(i, j, k, l)$  define a dihedral angle between the plane containing atoms  $i, j, k$  and the plane containing atoms  $j, k, l$ .

The bond length is defined to be the average distance between the nuclei of two atoms bonded together in any given molecule. A bond angle is the angle formed between three atoms across at least two bonds. For four atoms bonded together in a chain, the Dihedral (torsional) angle is the angle between the plane formed by the first three atoms and the plane formed by the last three atoms.

Bond angle [10] is the internal angle between the orbitals containing electron pairs in the valence shell of the central atom in a covalent molecule. Bond angles give an idea of distribution of the orbitals in three dimensional spaces around the central atom in the molecule and thus give an idea of the shape of the molecule. Bond angle will be the maximum in case if central atom has no lone pair i.e. with the decrease in magnitude of bond pair – bond pair repulsion as well as with decrease of electronegativity. The shorter bond length, the more energy it takes to break that bond. The [11] reported that C-C-C bond angle bending potential energy for neopentane is the largest, with that of isopentane the second largest. The behaviour of C-C bond stretching energies, however, is different from that of C-C-C bond angle bending energies: the C-C bond stretching for neopentane is smaller than normal pentane and isopentane since the C-C bond stretching in neopentane is independent of each other. The thermodynamic properties show that the intermolecular interactions become weaker as the molecular shape approaches that of a sphere and the surface area decreases with branching Ahire and Sawant [12] reported that, Wiener index, Hosoya index and Wiener polynomial of isomers of pentane are follow the order: pentane > isopentane > neopentane. The values of density and boiling point follow the same trend.

2. Preliminaries:

The chemical graphs of pentane, isopentane, neopentane are as below .

Figure- 1:  $T_1$  be the chemical graph of pentane

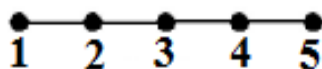


Figure-1

Figure- 2:  $T_2$  be the chemical graph of isopentane

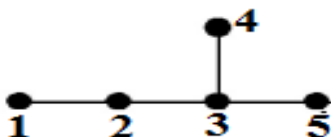


Figure-2

Figure- 3:  $T_3$  be the chemical graph of neopentane

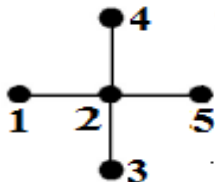


Figure-3

3. Hausdorff distance between trees:

A Hausdorff ( $H$ ) distance, Geometrical –Arithmetic index ( $GA(G)$ ) are studied below. The tree has either exactly one central vertex or exactly two central vertices that adjacent. The tree  $T$  is central if  $|center(T)| = 1$ , otherwise it is bicentral. Also  $diam(T) = 2 \cdot rad(T) - 1$ , if  $T$  is bicentral, and  $diam(T) = 2 \cdot rad(T)$ , if  $T$  is central.

Corollary 1. Let  $T_1, T_2,$  and  $T_3$  be arbitrary trees, Then  $H(T_1, T_2, T_3) \leq \max \left\{ \left\lfloor \frac{diam(T_1)}{2} \right\rfloor, \left\lfloor \frac{diam(T_2)}{2} \right\rfloor, \left\lfloor \frac{diam(T_3)}{2} \right\rfloor \right\}$

Corollary 2. Let  $T_1, T_2,$  and  $T_3$  be arbitrary non trivial trees with,  $diam(T_1) \geq diam(T_2) \geq diam(T_3)$ . For a fixed integer  $k, 0 \leq k \leq rad(T_1)$  then,  $H(T_1, T_2, T_3) > k$ .

Corollary 3. Let  $T_1, T_2$  and  $T_3$  be non- trivial trees with  $diam(T_1) \geq diam(T_2) \geq diam(T_3)$ . If  $T_i (i=1,2,3)$  is bicentral then,  $H(T_1, T_2, T_3) < rad(T_i)$ .

4. Optimized Symmetries of Molecules

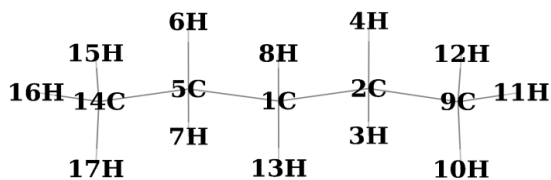


Fig. 4. Chemical Structure of Pentane Structure

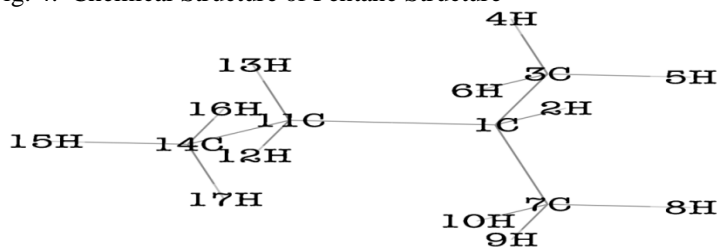


Fig. 5. Chemical Structure of Isopentane Structure

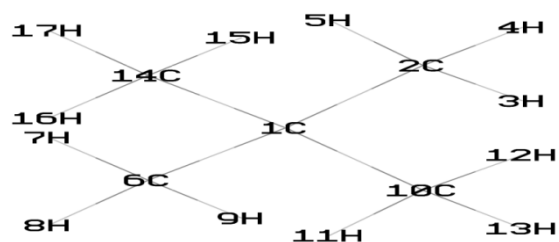


Fig. 6. Chemical Structure of Neopentane Structure

Name	Definition	Value	Name	Definition	Value
R <sub>1</sub>	R(1,2)	1.5327	A <sub>26</sub>	R(5,14,16)	111.4606
R <sub>2</sub>	R(1,5)	1.5327	A <sub>27</sub>	R(5,14,17)	111.1174
R <sub>3</sub>	R(1,8)	1.0982	A <sub>28</sub>	R(15,14,16)	107.693
R <sub>4</sub>	R(1,13)	1.0982	A <sub>29</sub>	R(15,14,17)	107.5777
R <sub>5</sub>	R(2,3)	1.097	A <sub>30</sub>	R(16,14,17)	107.6927
R <sub>6</sub>	R(2,4)	1.097	D <sub>1</sub>	D(5,1,2,3)	-57.7909
R <sub>7</sub>	R(2,9)	1.5315	D <sub>2</sub>	D(5,1,2,4)	57.8027
R <sub>8</sub>	R(5,6)	1.097	D <sub>3</sub>	D(5,1,2,9)	-179.9942
R <sub>9</sub>	R(5,7)	1.097	D <sub>4</sub>	D(8,1,2,3)	179.9971
R <sub>10</sub>	R(5,14)	1.5315	D <sub>5</sub>	D(8,1,2,4)	-64.4093
R <sub>11</sub>	R(9,10)	1.0949	D <sub>6</sub>	D(8,1,2,9)	57.7938
R <sub>12</sub>	R(9,11)	1.0938	D <sub>7</sub>	D(13,1,2,3)	64.4205
R <sub>13</sub>	R(9,12)	1.0949	D <sub>8</sub>	D(13,1,2,4)	-179.9859
R <sub>14</sub>	R(14,15)	1.0949	D <sub>9</sub>	D(13,1,2,9)	-57.7828
R <sub>15</sub>	R(14,16)	1.0938	D <sub>10</sub>	D(2,1,5,6)	-57.7888
R <sub>16</sub>	R(14,17)	1.0949	D <sub>11</sub>	D(2,1,5,7)	57.8041
A <sub>1</sub>	R(2,1,5)	113.7467	D <sub>12</sub>	D(2,1,5,14)	-179.9925
A <sub>2</sub>	R(2,1,8)	109.1793	D <sub>13</sub>	D(8,1,5,6)	64.4225
A <sub>3</sub>	R(2,1,13)	109.1798	D <sub>14</sub>	D(8,1,5,7)	-179.9845
A <sub>4</sub>	R(5,1,8)	109.1805	D <sub>15</sub>	D(8,1,5,14)	-57.7812
A <sub>5</sub>	R(5,1,13)	109.1797	D <sub>16</sub>	D(13,1,5,6)	179.9997
A <sub>6</sub>	R(8,1,13)	105.0926	D <sub>17</sub>	D(13,1,5,7)	-64.4073
A <sub>7</sub>	R(1,2,3)	109.1497	D <sub>18</sub>	D(13,1,5,14)	57.796
A <sub>8</sub>	R(1,2,4)	109.1492	D <sub>19</sub>	D(1,2,9,10)	59.8875
A <sub>9</sub>	R(1,2,9)	113.2931	D <sub>20</sub>	D(1,2,9,11)	-179.987
A <sub>10</sub>	R(3,2,4)	106.1346	D <sub>21</sub>	D(1,2,9,12)	-59.862
A <sub>11</sub>	R(3,2,9)	109.4348	D <sub>22</sub>	D(3,2,9,10)	-62.1585
A <sub>12</sub>	R(4,2,9)	109.432	D <sub>23</sub>	D(3,2,9,11)	57.967
A <sub>13</sub>	R(1,5,6)	109.1494	D <sub>24</sub>	D(3,2,9,12)	178.092
A <sub>14</sub>	R(1,5,7)	109.1495	D <sub>25</sub>	D(4,2,9,10)	-178.0671
A <sub>15</sub>	R(1,5,14)	113.2936	D <sub>26</sub>	D(4,2,9,11)	-57.9416
A <sub>16</sub>	R(6,5,7)	106.1341	D <sub>27</sub>	D(4,2,9,12)	62.1834
A <sub>17</sub>	R(6,5,14)	109.4321	D <sub>28</sub>	D(1,5,14,15)	59.8814
A <sub>18</sub>	R(7,5,14)	109.4317	D <sub>29</sub>	D(1,5,14,16)	-179.9932
A <sub>19</sub>	R(2,9,10)	111.1176	D <sub>30</sub>	D(1,5,14,17)	-59.8681
A <sub>20</sub>	R(2,9,11)	111.4603	D <sub>31</sub>	D(6,5,14,15)	-62.1648
A <sub>21</sub>	R(2,9,12)	111.1167	D <sub>32</sub>	D(6,5,14,16)	57.9606
A <sub>22</sub>	R(10,9,11)	107.6932	D <sub>33</sub>	D(6,5,14,17)	178.0857
A <sub>23</sub>	R(10,9,12)	107.578	D <sub>34</sub>	D(7,5,14,15)	-178.0726
A <sub>24</sub>	R(11,9,12)	107.6932	D <sub>35</sub>	D(7,5,14,16)	-57.9472
A <sub>25</sub>	R(5,14,15)	111.1174	D <sub>36</sub>	D(7,5,14,17)	62.1779

Table 1. Optimized parameters: (Angstrom &amp; Degrees) of pentane

**Table 2. Optimized parameters : (Angstrom & Degrees) of isopentane**

Name	Definition	Value	Name	Definition	Value
R <sub>1</sub>	R(1,2)	1.0993	A <sub>26</sub>	R(11,14,16)	111.8425
R <sub>2</sub>	R(1,3)	1.5361	A <sub>27</sub>	R(11,14,17)	111.8426
R <sub>3</sub>	R(1,7)	1.5361	A <sub>28</sub>	R(15,14,16)	107.3703
R <sub>4</sub>	R(1,11)	1.5452	A <sub>29</sub>	R(15,14,17)	107.3705
R <sub>5</sub>	R(3,4)	1.0948	A <sub>30</sub>	R(16,14,17)	107.7545
R <sub>6</sub>	R(3,5)	1.0944	D <sub>1</sub>	D(2,1,3,4)	-62.3248
R <sub>7</sub>	R(3,6)	1.0946	D <sub>2</sub>	D(2,1,3,5)	57.5562
R <sub>8</sub>	R(7,8)	1.0944	D <sub>3</sub>	D(2,1,3,6)	177.1882
R <sub>9</sub>	R(7,9)	1.0948	D <sub>4</sub>	D(7,1,3,4)	-179.0575
R <sub>10</sub>	R(7,10)	1.0946	D <sub>5</sub>	D(7,1,3,5)	-59.1765
R <sub>11</sub>	R(11,12)	1.0971	D <sub>6</sub>	D(7,1,3,6)	60.4556
R <sub>12</sub>	R(11,13)	1.0971	D <sub>7</sub>	D(11,1,3,4)	53.8336
R <sub>13</sub>	R(11,14)	1.5345	D <sub>8</sub>	D(11,1,3,5)	173.7146
R <sub>14</sub>	R(14,15)	1.094	D <sub>9</sub>	D(11,1,3,6)	-66.6533
R <sub>15</sub>	R(14,16)	1.0936	D <sub>10</sub>	D(2,1,7,8)	-57.5422
R <sub>16</sub>	R(14,17)	1.0936	D <sub>11</sub>	D(2,1,7,9)	62.3396
A <sub>1</sub>	R(2,1,3)	107.161	D <sub>12</sub>	D(2,1,7,10)	-177.1741
A <sub>2</sub>	R(2,1,7)	107.1601	D <sub>13</sub>	D(3,1,7,8)	59.191
A <sub>3</sub>	R(2,1,11)	106.0371	D <sub>14</sub>	D(3,1,7,9)	179.0728
A <sub>4</sub>	R(3,1,7)	111.063	D <sub>15</sub>	D(3,1,7,10)	-60.4409
A <sub>5</sub>	R(3,1,11)	112.4986	D <sub>16</sub>	D(11,1,7,8)	-173.6995
A <sub>6</sub>	R(7,1,11)	112.4974	D <sub>17</sub>	D(11,1,7,8)	-53.8177
A <sub>7</sub>	R(1,3,4)	111.2816	D <sub>18</sub>	D(11,1,7,9)	66.6686
A <sub>8</sub>	R(1,3,5)	110.8041	D <sub>19</sub>	D(2,1,11,12)	-57.3636
A <sub>9</sub>	R(1,3,6)	111.6619	D <sub>20</sub>	D(2,1,11,13)	57.2515
A <sub>10</sub>	R(4,3,5)	107.7611	D <sub>21</sub>	D(2,1,11,14)	179.9447
A <sub>11</sub>	R(4,3,6)	107.7812	D <sub>22</sub>	D(3,1,11,12)	-174.1942
A <sub>12</sub>	R(5,3,6)	107.3643	D <sub>23</sub>	D(3,1,11,13)	-59.579
A <sub>13</sub>	R(1,7,8)	110.8044	D <sub>24</sub>	D(3,1,11,14)	63.1142
A <sub>14</sub>	R(1,7,9)	111.2814	D <sub>25</sub>	D(7,1,11,12)	59.4652
A <sub>15</sub>	R(1,7,10)	111.6613	D <sub>26</sub>	D(7,1,11,13)	174.0804
A <sub>16</sub>	R(8,7,9)	107.7616	D <sub>27</sub>	D(7,1,11,14)	-63.2264
A <sub>17</sub>	R(8,7,10)	107.3643	D <sub>28</sub>	D(1,11,14,15)	180.0038
A <sub>18</sub>	R(9,7,10)	107.7811	D <sub>29</sub>	D(1,11,14,16)	-60.4817
A <sub>19</sub>	R(1,11,12)	108.2709	D <sub>30</sub>	D(1,11,14,17)	60.4891
A <sub>20</sub>	R(1,11,13)	108.2717	D <sub>31</sub>	D(12,11,14,15)	57.6276
A <sub>21</sub>	R(1,11,14)	106.0144	D <sub>32</sub>	D(12,11,14,16)	177.1421
A <sub>22</sub>	R(12,11,13)	106.0984	D <sub>33</sub>	D(12,11,14,17)	-61.8872
A <sub>23</sub>	R(12,11,14)	108.8698	D <sub>34</sub>	D(13,11,14,15)	-57.8168
A <sub>24</sub>	R(13,11,14)	107.8705	D <sub>35</sub>	D(13,11,14,16)	61.8961
A <sub>25</sub>	R(11,14,15)	110.4409	D <sub>36</sub>	D(13,11,14,17)	-177.1331

**Table 3. Optimized parameters: (Angstrom & Degrees) of Neopentane**

Name	Definition	Value	Name	Definition	Value
R <sub>1</sub>	R(1,2)	1.5396	A <sub>26</sub>	R(1,14,16)	111.1312
R <sub>2</sub>	R(1,6)	1.5396	A <sub>27</sub>	R(1,14,17)	111.1312
R <sub>3</sub>	R(1,10)	1.5396	A <sub>28</sub>	R(15,14,16)	107.7615
R <sub>4</sub>	R(1,14)	1.5396	A <sub>29</sub>	R(15,14,17)	107.7615
R <sub>5</sub>	R(2,3)	1.0974	A <sub>30</sub>	R(16,14,17)	107.7615
R <sub>6</sub>	R(2,4)	1.0974	D <sub>1</sub>	D(6,1,2,3)	60.0
R <sub>7</sub>	R(2,5)	1.0974	D <sub>2</sub>	D(6,1,2,4)	180.0
R <sub>8</sub>	R(6,7)	1.0974	D <sub>3</sub>	D(6,1,2,5)	-60.0
R <sub>9</sub>	R(6,8)	1.0974	D <sub>4</sub>	D(10,1,2,3)	-60.0
R <sub>10</sub>	R(6,9)	1.0974	D <sub>5</sub>	D(10,1,2,4)	60.0
R <sub>11</sub>	R(10,11)	1.0974	D <sub>6</sub>	D(10,1,2,5)	180.0
R <sub>12</sub>	R(10,12)	1.0974	D <sub>7</sub>	D(14,1,2,3)	180.0
R <sub>13</sub>	R(10,13)	1.0974	D <sub>8</sub>	D(14,1,2,4)	-60.0
R <sub>14</sub>	R(14,15)	1.0974	D <sub>9</sub>	D(14,1,2,5)	60.0
R <sub>15</sub>	R(14,16)	1.0974	D <sub>10</sub>	D(2,1,6,7)	60.0
R <sub>16</sub>	R(14,17)	1.0974	D <sub>11</sub>	D(2,1,6,8)	180.0
A <sub>1</sub>	R(2,1,6)	109.4712	D <sub>12</sub>	D(2,1,6,9)	-60.0
A <sub>2</sub>	R(2,1,10)	109.4712	D <sub>13</sub>	D(10,1,6,7)	180.0
A <sub>3</sub>	R(2,1,14)	109.4712	D <sub>14</sub>	D(10,1,6,8)	-60.0
A <sub>4</sub>	R(6,1,10)	109.4712	D <sub>15</sub>	D(10,1,6,9)	60.0
A <sub>5</sub>	R(6,1,14)	109.4712	D <sub>16</sub>	D(14,1,6,7)	-60.0
A <sub>6</sub>	R(10,1,14)	109.4712	D <sub>17</sub>	D(14,1,6,8)	60.0
A <sub>7</sub>	R(1,2,3)	111.1312	D <sub>18</sub>	D(14,1,6,9)	180.0
A <sub>8</sub>	R(1,2,4)	111.1312	D <sub>19</sub>	D(2,1,10,11)	180.0
A <sub>9</sub>	R(1,2,5)	111.1312	D <sub>20</sub>	D(2,1,10,12)	-60.0
A <sub>10</sub>	R(3,2,4)	107.7615	D <sub>21</sub>	D(2,1,10,13)	60.0
A <sub>11</sub>	R(3,2,5)	107.7615	D <sub>22</sub>	D(6,1,10,11)	60.0
A <sub>12</sub>	R(4,2,5)	107.7615	D <sub>23</sub>	D(6,1,10,12)	180.0
A <sub>13</sub>	R(1,6,7)	111.1312	D <sub>24</sub>	D(6,1,10,13)	-60.0
A <sub>14</sub>	R(1,6,8)	111.1312	D <sub>25</sub>	D(14,1,10,11)	-60.0
A <sub>15</sub>	R(1,6,9)	111.1312	D <sub>26</sub>	D(14,1,10,12)	60.0
A <sub>16</sub>	R(7,6,8)	107.7615	D <sub>27</sub>	D(14,1,10,13)	180.0
A <sub>17</sub>	R(7,6,9)	107.7615	D <sub>28</sub>	D(2,1,14,15)	60.0
A <sub>18</sub>	R(8,6,9)	107.7615	D <sub>29</sub>	D(2,1,14,16)	180.0
A <sub>19</sub>	R(1,10,11)	111.1312	D <sub>30</sub>	D(2,1,14,17)	-60.0
A <sub>20</sub>	R(1,10,12)	111.1312	D <sub>31</sub>	D(6,1,14,15)	180.0
A <sub>21</sub>	R(1,10,13)	111.1312	D <sub>32</sub>	D(6,1,14,16)	-60.0
A <sub>22</sub>	R(11,10,12)	107.7615	D <sub>33</sub>	D(6,1,14,17)	60.0
A <sub>23</sub>	R(11,10,13)	107.7615	D <sub>34</sub>	D(10,1,14,15)	-60.0
A <sub>24</sub>	R(12,10,13)	107.7615	D <sub>35</sub>	D(10,1,14,16)	60.0
A <sub>25</sub>	R(1,14,15)	111.1312	D <sub>36</sub>	D(10,1,14,17)	180.0

#### 4. Results and Discussion

From fig 1  $\text{diam}(T_1) = 2$   $\text{rad}(T_1) = 2(2) = 4$ , From fig 2  $\text{diam}(T_2) = 2$   $\text{rad}(T_2) - 1 = 2(2) - 1 = 3$  (having centers 2 and 3.), From fig 3  $\text{diam}(T_3) = 2$   $\text{rad}(T_3) = 2(1) = 2$ .

From corollary 1 we get  $H(T_1, T_2, T_3) \leq 2$ .

From corollary 2 we get  $\text{diam}(T_1) = 4 \geq \text{diam}(T_2) = 3 \geq \text{diam}(T_3) = 2$ . For a fixed integer  $k$ ,  $0 \leq k \leq \text{rad}(T_1)$  hence  $H(T_1, T_2, T_3) > k = 0, 1$ .

From corollary 3 we get  $\text{diam}(T_1) = 4 \geq \text{diam}(T_2) = 3 \geq \text{diam}(T_3) = 2$ . Here  $T_2$  is bicentral.

Hence  $H(T_1, T_2, T_3) \leq \text{rad}(T_2) = 2$

The Geometrical-Arithmetic index: The  $(GA(T_1)) \approx 3.885$ ;  $(GA(T_2)) \approx 3.884$  and  $(GA(T_3)) \approx 3.20$

From fig. 1. The Schultz index :  $S_C(T_1) = 30$ ; The Modified Schultz index :  $S_C^*(T_1) = 22$

The Schultz polynomial :  $S_C(T_1, x) = x^4 + 3x^3 + 5x^2 + 7x$

The modified Schultz polynomial  $S_C^*(T_1, x) : \frac{1}{2}x^4 + 2x^3 + 4x^2 + 6x$

From fig. 2. The Schultz index:  $S_C(T_2) = 24.5$ ; The Modified Schultz index :  $S_C^*(T_2) = 17.5$

The Schultz polynomial :  $S_C(T_2, x) = 2x^3 + 5x^2 + 9x$

The modified Schultz polynomial  $S_C^*(T_2, x)$ :  $x^3 + \frac{7}{2}x^2 + \frac{15}{2}x$

From fig. 3. The Schultz index :  $S_C(T_3) = 22$ ; The Modified Schultz index :  $S_C^*(T_3) = 14$

The Schultz polynomial :  $S_C(T_3, x) = x^4 + 6x^2 + 10x$

The modified Schultz polynomial  $S_C^*(T_3, x)$ :  $\frac{1}{2}x^4 + \frac{7}{2}x^2 + 8x$ .

In pentane bond length of  $C_1-C_2$  and  $C_1-C_5$  are  $1.5327 \text{ \AA}$  which is maximum means electronegativity between these atoms will be minimum as compare to  $C_2-C_9$  and  $C_5-C_{14}$  having bond length  $1.5315 \text{ \AA}$ . In isopentane  $C_1-C_{11}$  has maximum bond length which is  $1.5452 \text{ \AA}$ , and minimum value is  $1.5345 \text{ \AA}$  at  $C_{11}-C_{14}$ . In neopentane all four C-C bonds having same bond length which is  $1.5396 \text{ \AA}$ , all twelve C-H bonds having same bond length which is  $1.0947 \text{ \AA}$ .

From table 1 the pentane has two C-C-C-C dihedral states which are  $D(5,1,2,9)$  and  $D(2,1,5,4)$ . From table 2, the isopentane has two C-C-C-C dihedral states which are  $D(3,1,11,14)$  and  $D(7,11,14,16)$ . From table 3 the neopentane has no C-C-C-C dihedral states.

## 6. Conclusion:

$T_1, T_2,$  and  $T_3$  follows the relation:  $\text{rad}(T_i) \leq \text{diam}(T_i) \leq 2 \text{rad}(T_i)$  for each  $i=1, 2, 3$ .

The  $GA(T)$  values are follows the trend :  $GA(T_1) > GA(T_2) > GA(T_3)$ .

The Schultz index :  $S_C(T_1) > S_C(T_2) > S_C(T_3)$

The Modified Schultz index:  $S_C^*(T_1) > S_C^*(T_2) > S_C^*(T_3)$

The bond length between C-C and C-H atoms in pentane, isopentane and neopentane are in the order: C-C > C-H. Hence electronegativity difference between C-H bonding is maximum.

The average of C-C bond length values follows the trend : neopentane > isopentane > pentane. The average of C-H bond length values follows the trend : pentane > isopentane > neopentane.

The average of C-C-C bond angles values follows the trend : pentane > isopentane > neopentane. The average of C-C-H bond angles values follows the trend : neopentane > isopentane > pentane. The average of H-C-H bond angles values follows the trend : neopentane > isopentane > pentane. The average of H-C-C bond angles values follows the trend: pentane > isopentane.

The bond angles between different bonds of pentane, isopentane, neopentane, respectively are in the order : C-C-C > H-C-C > C-C-H > H-C-H; C-C-C  $\geq$  C-C-H > H-C-H  $\geq$  H-C-C ; C-C-H > C-C-C > H-C-H. The C-C-C-C Dihedral angle in pentane is more than isopentane.

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