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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 ($\mathscr{H}$) 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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Keywords:

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]: $\sum_{u,v\, \in\, E(G)} (du\ dv)^{\alpha}$

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

If α =-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 distribut- ion 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 thechemical graph of pentane

Figure-1

Figure- 2: T_2 be thechemical graph of isopentane

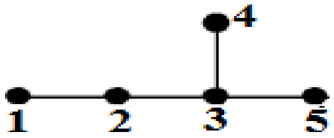

Figure-2

Figure- 3: T_3 be thechemical graph of neopentane

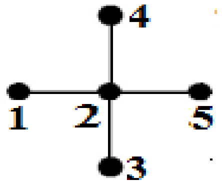

Figure-3

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 rad(T)-1, if T is bicentral, and diam(T)= 2 rad(T), if T is central.

Corollary 1. Let T_1, T_2, and T_3 be arbitrary trees, Then
$H\ (T_1, T_2, T_3) \leq \max \{ [\frac{\text{diam}\ (T1)}{2} , \frac{\text{diam}\ (T2)}{2} , \frac{\text{diam}\ (T3)}{2}] \}$
Corollary 2. Let T_1, T_2, and T_3 be arbitrary non trivial trees with, $\text{diam}(T_1) \geq \text{diam}(T_2) \geq \text{diam}\ (T_3)$.
For a fixed integer k, $0 \leq k \leq \text{rad}(T_1)$ then, $H\ (T_1, T_2, T_3) > k$.
Corollary 3. Let T_1, T_2 andT_3 be non- trivial trees with $\text{diam}(T_1) \geq \text{diam}(T_2) \geq \text{diam}(T_3)$.
If T_i (i=1,2,3) is bicentral then, $H\ (T_1, T_2, T_3) < \text{rad}\ (T_i)$.

4. Optimized Symmetries of Molecules

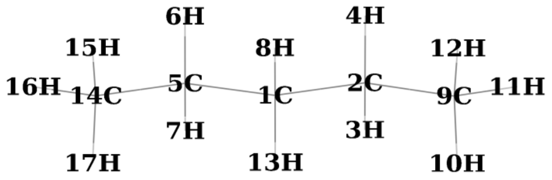

Fig. 4. Chemical Structure of Pentane Structure

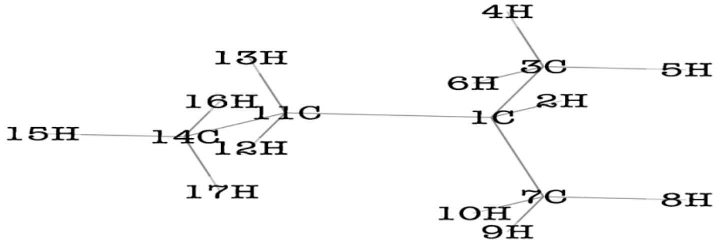

Fig. 5. Chemical Structure of Isopentane Structure

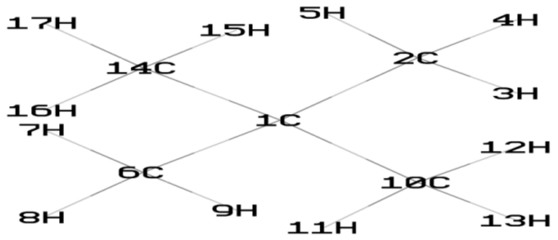

Fig. 6. Chemical Structure of Neopentane Structure

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

Name	Definition	Value	Name	Definition	Value
R_1	R(1,2)	1.5327	A_{26}	R(5,14,16)	111.4606
R_2	R(1,5)	1.5327	A_{27}	R(5,14,17)	111.1174
R_3	R(1,8)	1.0982	A_{28}	R(15,14,16)	107.693
R_4	R(1,13)	1.0982	A_{29}	R(15,14,17)	107.5777
R_5	R(2,3)	1.097	A_{30}	R(16,14,17)	107.6927
R_6	R(2,4)	1.097	D_1	D(5,1,2,3)	-57.7909
R_7	R(2,9)	1.5315	D_2	D(5,1,2,4)	57.8027
R_8	R(5,6)	1.097	D_3	D(5,1,2,9)	-179.9942
R_9	R(5,7)	1.097	D_4	D(8,1,2,3)	179.9971
R_{10}	R(5,14)	1.5315	D_5	D(8,1,2,4)	-64.4093
R_{11}	R(9,10)	1.0949	D_6	D(8,1,2,9)	57.7938
R_{12}	R(9,11)	1.0938	D_7	D(13,1,2,3)	64.4205
R_{13}	R(9,12)	1.0949	D_8	D(13,1,2,4)	-179.9859
R_{14}	R(14,15)	1.0949	D_9	D(13,1,2,9)	-57.7828
R_{15}	R(14,16)	1.0938	D_{10}	D(2,1,5,6)	-57.7888
R_{16}	R(14,17)	1.0949	D_{11}	D(2,1,5,7)	57.8041
A_1	R(2,1,5)	113.7467	D_{12}	D(2,1,5,14)	-179.9925
A_2	R(2,1,8)	109.1793	D_{13}	D(8,1,5,6)	64.4225
A_3	R(2,1,13)	109.1798	D_{14}	D(8,1,5,7)	-179.9845
A_4	R(5,1,8)	109.1805	D_{15}	D(8,1,5,14)	-57.7812
A_5	R(5,1,13)	109.1797	D_{16}	D(13,1,5,6)	179.9997
A_6	R(8,1,13)	105.0926	D_{17}	D(13,1,5,7)	-64.4073
A_7	R(1,2,3)	109.1497	D_{18}	D(13,1,5,14)	57.796
A_8	R(1,2,4)	109.1492	D_{19}	D(1,2,9,10)	59.8875
A_9	R(1,2,9)	113.2931	D_{20}	D(1,2,9,11)	-179.987
A_{10}	R(3,2,4)	106.1346	D_{21}	D(1,2,9,12)	-59.862
A_{11}	R(3,2,9)	109.4348	D_{22}	D(3,2,9,10)	-62.1585
A_{12}	R(4,2,9)	109.432	D_{23}	D(3,2,9,11)	57.967
A_{13}	R(1,5,6)	109.1494	D_{24}	D(3,2,9,12)	178.092
A_{14}	R(1,5,7)	109.1495	D_{25}	D(4,2,9,10)	-178.0671
A_{15}	R(1,5,14)	113.2936	D_{26}	D(4,2,9,11)	-57.9416
A_{16}	R(6,5,7)	106.1341	D_{27}	D(4,2,9,12)	62.1834
A_{17}	R(6,5,14)	109.4321	D_{28}	D(1,5,14,15)	59.8814
A_{18}	R(7,5,14)	109.4317	D_{29}	D(1,5,14,16)	-179.9932
A_{19}	R(2,9,10)	111.1176	D_{30}	D(1,5,14,17)	-59.8681
A_{20}	R(2,9,11)	111.4603	D_{31}	D(6,5,14,15)	-62.1648
A_{21}	R(2,9,12)	111.1167	D_{32}	D(6,5,14,16)	57.9606
A_{22}	R(10,9,11)	107.6932	D_{33}	D(6,5,14,17)	178.0857
A_{23}	R(10,9,12)	107.578	D_{34}	D(7,5,14,15)	-178.0726
A_{24}	R(11,9,12)	107.6932	D_{35}	D(7,5,14,16)	-57.9472
A_{25}	R(5,14,15)	111.1174	D_{36}	D(7,5,14,17)	62.1779

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

Name	**Definition**	**Value**	**Name**	**Definition**	**Value**
R_1	R(1,2)	1.0993	A_{26}	R(11,14,16)	111.8425
R_2	R(1,3)	1.5361	A_{27}	R(11,14,17)	111.8426
R_3	R(1,7)	1.5361	A_{28}	R(15,14,16)	107.3703
R_4	R(1,11)	1.5452	A_{29}	R(15,14,17)	107.3705
R_5	R(3,4)	1.0948	A_{30}	R(16,14,17)	107.7545
R_6	R(3,5)	1.0944	D_1	D(2,1,3,4)	-62.3248
R_7	R(3,6)	1.0946	D_2	D(2,1,3,5)	57.5562
R_8	R(7,8)	1.0944	D_3	D(2,1,3,6)	177.1882
R_9	R(7,9)	1.0948	D_4	D(7,1,3,4)	-179.0575
R_{10}	R(7,10)	1.0946	D_5	D(7,1,3,5)	-59.1765
R_{11}	R(11,12)	1.0971	D_6	D(7,1,3,6)	60.4556
R_{12}	R(11,13)	1.0971	D_7	D(11,1,3,4)	53.8336
R_{13}	R(11,14)	1.5345	D_8	D(11,1,3,5)	173.7146
R_{14}	R(14,15)	1.094	D_9	D(11,1,3,6)	-66.6533
R_{15}	R(14,16)	1.0936	D_{10}	D(2,1,7,8)	-57.5422
R_{16}	R(14,17)	1.0936	D_{11}	D(2,1,7,9)	62.3396
A_1	R(2,1,3)	107.161	D_{12}	D(2,1,7,10)	-177.1741
A_2	R(2,1,7)	107.1601	D_{13}	D(3,1,7,8)	59.191
A_3	R(2,1,11)	106.0371	D_{14}	D(3,1,7,9)	179.0728
A_4	R(3,1,7)	111.063	D_{15}	D(3,1,7,10)	-60.4409
A_5	R(3,1,11)	112.4986	D_{16}	D(11,1,7,8)	-173.6995
A_6	R(7,1,11)	112.4974	D_{17}	D(11,1,7,8)	-53.8177
A_7	R(1,3,4)	111.2816	D_{18}	D(11,1,7,9)	66.6686
A_8	R(1,3,5)	110.8041	D_{19}	D(2,1,11,12)	-57.3636
A_9	R(1,3,6)	111.6619	D_{20}	D(2,1,11,13)	57.2515
A_{10}	R(4,3,5)	107.7611	D_{21}	D(2,1,11,14)	179.9447
A_{11}	R(4,3,6)	107.7812	D_{22}	D(3,1,11,12)	-174.1942
A_{12}	R(5,3,6)	107.3643	D_{23}	D(3,1,11,13)	-59.579
A_{13}	R(1,7,8)	110.8044	D_{24}	D(3,1,11,14)	63.1142
A_{14}	R(1,7,9)	111.2814	D_{25}	D(7,1,11,12)	59.4652
A_{15}	R(1,7,10)	111.6613	D_{26}	D(7,1,11,13)	174.0804
A_{16}	R(8,7,9)	107.7616	D_{27}	D(7,1,11,14)	-63.2264
A_{17}	R(8,7,10)	107.3643	D_{28}	D(1,11,14,15)	180.0038
A_{18}	R(9,7,10)	107.7811	D_{29}	D(1,11,14,16)	-60.4817
A_{19}	R(1,11,12)	108.2709	D_{30}	D(1,11,14,17)	60.4891
A_{20}	R(1,11,13)	108.2717	D_{31}	D(12,11,14,15)	57.6276
A_{21}	R(1,11,14)	106.0144	D_{32}	D(12,11,14,16)	177.1421
A_{22}	R(12,11,13)	106.0984	D_{33}	D(12,11,14,17)	-61.8872
A_{23}	R(12,11,14)	108.8698	D_{34}	D(13,11,14,15)	-57.8168
A_{24}	R(13,11,14)	107.8705	D_{35}	D(13,11,14,16)	61.8961
A_{25}	R(11,14,15)	110.4409	D_{36}	D(13,11,14,17)	-177.1331

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

Name	Definition	Value	Name	Definition	Value
R_1	R(1,2)	1.5396	A_{26}	R(1,14,16)	111.1312
R_2	R(1,6)	1.5396	A_{27}	R(1,14,17)	111.1312
R_3	R(1,10)	1.5396	A_{28}	R(15,14,16)	107.7615
R_4	R(1,14)	1.5396	A_{29}	R(15,14,17)	107.7615
R_5	R(2,3)	1.0974	A_{30}	R(16,14,17)	107.7615
R_6	R(2,4)	1.0974	D_1	D(6,1,2,3)	60.0
R_7	R(2,5)	1.0974	D_2	D(6,1,2,4)	180.0
R_8	R(6,7)	1.0974	D_3	D(6,1,2,5)	-60.0
R_9	R(6,8)	1.0974	D_4	D(10,1,2,3)	-60.0
R_{10}	R(6,9)	1.0974	D_5	D(10,1,2,4)	60.0
R_{11}	R(10,11)	1.0974	D_6	D(10,1,2,5)	180.0
R_{12}	R(10,12)	1.0974	D_7	D(14,1,2,3)	180.0
R_{13}	R(10,13)	1.0974	D_8	D(14,1,2,4)	-60.0
R_{14}	R(14,15)	1.0974	D_9	D(14,1,2,5)	60.0
R_{15}	R(14,16)	1.0974	D_{10}	D(2,1,6,7)	60.0
R_{16}	R(14,17)	1.0974	D_{11}	D(2,1,6,8)	180.0
A_1	R(2,1,6)	109.4712	D_{12}	D(2,1,6,9)	-60.0
A_2	R(2,1,10)	109.4712	D_{13}	D(10,1,6,7)	180.0
A_3	R(2,1,14)	109.4712	D_{14}	D(10,1,6,8)	-60.0
A_4	R(6,1,10)	109.4712	D_{15}	D(10,1,6,9)	60.0
A_5	R(6,1,14)	109.4712	D_{16}	D(14,1,6,7)	-60.0
A_6	R(10,1,14)	109.4712	D_{17}	D(14,1,6,8)	60.0
A_7	R(1,2,3)	111.1312	D_{18}	D(14,1,6,9)	180.0
A_8	R(1,2,4)	111.1312	D_{19}	D(2,1,10,11)	180.0
A_9	R(1,2,5)	111.1312	D_{20}	D(2,1,10,12)	-60.0
A_{10}	R(3,2,4)	107.7615	D_{21}	D(2,1,10,13)	60.0
A_{11}	R(3,2,5)	107.7615	D_{22}	D(6,1,10,11)	60.0
A_{12}	R(4,2,5)	107.7615	D_{23}	D(6,1,10,12)	180.0
A_{13}	R(1,6,7)	111.1312	D_{24}	D(6,1,10,13)	-60.0
A_{14}	R(1,6,8)	111.1312	D_{25}	D(14,1,10,11)	-60.0
A_{15}	R(1,6,9)	111.1312	D_{26}	D(14,1,10,12)	60.0
A_{16}	R(7,6,8)	107.7615	D_{27}	D(14,1,10,13)	180.0
A_{17}	R(7,6,9)	107.7615	D_{28}	D(2,1,14,15)	60.0
A_{18}	R(8,6,9)	107.7615	D_{29}	D(2,1,14,16)	180.0
A_{19}	R(1,10,11)	111.1312	D_{30}	D(2,1,14,17)	-60.0
A_{20}	R(1,10,12)	111.1312	D_{31}	D(6,1,14,15)	180.0
A_{21}	R(1,10,13)	111.1312	D_{32}	D(6,1,14,16)	-60.0
A_{22}	R(11,10,12)	107.7615	D_{33}	D(6,1,14,17)	60.0
A_{23}	R(11,10,13)	107.7615	D_{34}	D(10,1,14,15)	-60.0
A_{24}	R(12,10,13)	107.7615	D_{35}	D(10,1,14,16)	60.0
A_{25}	R(1,14,15)	111.1312	D_{36}	D(10,1,14,17)	180.0

4. Results and Discussion

From fig 1 $diam(T_1) = 2\,rad(T_1) = 2(2) = 4$, From fig 2 $diam(T_2) = 2\,rad(T_2) - 1 = 2(2) - 1 = 3$ (having centers 2 and 3.), From fig 3 $diam(T_3) = 2\,rad(T_3) = 2(1) = 2$.
From corollary 1 we get $H\ (T_1, T_2, T_3) \leq 2$.
From corollary 2 we get $diam(T_1) = 4 \geq diam(T_2) = 3 \geq diam(T_3) = 2$. For a fixed integer k, $0 \leq k \leq rad(T_1)$ hence ,$H\ (T_1, T_2, T_3) > k = 0,1$.
From corollary 3 we get $diam(T_1) = 4 \geq diam(T_2) = 3 \geq diam(T_3) = 2$. Here T_2 is bicentral .
Hence $H\ (T_1, T_2, T_3) \leq rad\,(T_2) = 2$
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 Å which is maximum means electronegativity between these atoms will be minimum as compare to C_2-C_9 andC_5-C_{14} having bond length 1.5315Å. In isopentane C_1-C_{11} has maximum bond length which is 1.5452 Å, and minimum value is 1.5345 ÅatC_{11}-C_{14}. In neopentane all four C-C bonds having same bond length which is 1.5396Å, all twelve C-H bonds having same bond length which is 1.0947Å.

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 3the neopentane has no C-C-C-C dihedral states.

6. Conclusion:

T_1, T_2, and T_3 follows the relation: rad (T_i) ≤ diam (T_i) ≤ 2 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 ≥ C-C-H > H-C-H ≥ H-C-C ; C-C-H > C-C-C > H-C-H. The C-C-C-C Diherdral angle in pentane is more than isopentane.

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