



RHF AND DFT STUDY OF THE OPTIMIZED MOLECULAR STRUCTURE AND ATOMIC CHARGE DISTRIBUTION OF PENTACENE

*Galadanci, G. S.M., Chifu, E. Ndikilar, Safana A.A. and Sabiu, S. A

Physics Department, Federal University Dutse, P.M.B 7156, Dutse, Jigawa State Nigeria

*Email: gsmgalad@gmail.com Tel: +2348037260380

ABSTRACT

Restricted HartreeFock (RHF) and Density Functional Theory (DFT) studies were carried out on the organic semi conductor material Pentacene. 6-31G and 6-31G* basis sets were used to optimize the molecule and compute the charge distribution at both levels of theory. The results show that the Carbon-Hydrogen bonds in the molecule are the shortest and strongest with average bond length of 1 Å. The C-C bonds were the longest and weakest. On the average the bond angles were all above 90 degrees, giving the molecule a fairly symmetric structure. The bulk positive charges in Pentacene were predicted to reside mostly in the Hydrogen atoms and the Carbon atoms were averagely electronegative in this molecule.

INTRODUCTION

Organic field-effect transistors (FETs) have attracted considerable attention due to their potential in organic thin film transistors (OTFTs) with large-area of application that are mechanically flexible, lightweight (as switching devices for logic gates and memory arrays), organic light emitting diodes (OLEDs), solar cells and low-cost devices (Kitamura, Arakawa, 2008; Hwan et al. 2004; Byoungnan, 2008). Organic semiconductors are materials with semiconducting properties. These include Polycyclic aromatic hydrocarbons such as anthracene, rubrene and pentacene. Among many organic semiconductors, pentacene has been reported to be the most promising applicant, because of its high hole mobility up to $5.5 \text{ cm}^2/\text{Vs}$ that exceed amorphous Silicon (Hwan et al, 2004). Pentacene is a linear acene consisting of five benzene rings with molecular formula $\text{C}_{22}\text{H}_{14}$, molar mass 278.36 g/mol, density 1.3 g/cm^3 and melting point of $> 300 \text{ }^\circ\text{C}$; sublimes at $372 \text{ }^\circ\text{C}$ which behaves as a p-type semiconductor. These kind of materials are important in electrical applications as their band gap is controlled by selecting the number of aromatic rings that is the more rings, the smaller the band gap. Crystallized pentacene has triclinic lattice structure comprising of. Moreover this compound is purple powder which generate exciton upon absorption of Ultraviolet (UV) or visible light that makes it very sensitive to oxidation, this is the reason why the compound degrades upon exposure to air or light (Dan, 2005). With these remarkable properties Pentacene and other derivatives of benzene attract both experimental and theoretical research.

There has been a report on organic p-i-n homojunctions composed of differently doped vacuum-deposited pentacene layers. Where remarkably high built-in voltage of 1.65 V was observed; moreover an analysis of the current-voltage characteristics under dark and illuminated conditions reveals that the open-circuit voltage is directly related to the built-in voltage whereby the recombination process is influenced by the

distinct charge transport properties of electrons and holes in the pentacene film (Harada, 2008). Furthermore, investigation have shown that doping pentacene films with iodine and alkaline metals help in achieving maximum conductivity of 150 S cm^{-1} for highly ordered films heavily doped with iodine, and 2.8 S cm^{-1} for a rubidium-doped film, which turned the film into an n-type Semiconductor (Dan, 2005). Other experimental research include Channel Formation in Single-Mono layer Pentacene Thin Film Transistors, Orientation of Pentacene molecules on SiO_2 by Byoungnam Park (Byoungnan, 2008); Modelling the UV/visible spectrum of etakis (phenylethynyl) benzene by Denis Jacquemin (Jacquemin et al, 2008] Molecular structure, vibrational, UV and NBO analysis of 4-chloro-7-nitrobenzofurazan by DFT calculations by M. Kurta (Kurta et al; Jacquemin et al; 2005).

Nowadays, the molecular modelization techniques offer a competitive alternative for the interpretation of experimental data arising from industrial interest and applications (Jacquemin et al, 2005). In this article, the Gaussian software is used to compute the optimum electronic structure of pentacene and its atomic charge distribution (James, Jan et al, 1991).

COMPUTATIONAL METHOD

The molecular structure of pentacene is modeled with the Gaussian03 package. Geometric optimization of the structure is performed at Restricted HartreeFock (RHF) and Density Functional Theory (DFT) levels of theory using the basis sets 6-31G and 6-31G*. Geometry optimizations usually attempt to locate minima on the potential energy surface, thereby predicting equilibrium structures of molecular systems. At the minima, the first derivative of the energy (gradient) is zero. Since the gradient is the negative of the forces, the forces are also zero at such a point (stationary point). In Gaussian, a geometry optimization begins at the molecular structure specified at the input (in this case from GaussView) and steps along the potential energy surface.

It computes the energy and gradient at that point, and determines which direction to make the next step. The gradient indicates the direction along the surface in which the energy decreases most rapidly from the current point as well as the steepness of that slope. The optimized parameters are the bond lengths (in Angstrom), the bond angles and the dihedral angles (in degrees) for the optimized molecular structure. Atoms in the molecule are numbered according to their order in the molecule specification section of the input. The structures are refined further using Density Functional Theory which is a cost effective method for inclusion of electron correlations with the three-parameter density functional generally known as Becke3LYP (B3LYP).

RESULTS AND DISCUSSION

Optimized Bond lengths

The optimized structure of pentacene is shown in Fig. 1 and the optimized bond lengths at different levels of theory are shown in Table 1. In molecular geometry, the bond length (or bond distance) is the average distance between nuclei of two bonded atoms in a molecule. Bond length is inversely related to bond strength and bond dissociation energy. The predicted shortest bond

lengths are all in the vicinity of 1\AA and these are the C-H bonds: R(2,17), R(7,16), R(8,19), R(13,20), R(14,21), R(15,22), R(23,25), R(26,29), R(27,31), R(30,34), R(32,35) and R(33,36). Thus, since these C-H bonds are shortest it implies they are the strongest bonds in pentacene molecule that will require much energy to be broken. On the other hand, the longest and weakest bonds with bond lengths close to 1.5\AA are the following C-C bonds: R(1,6), R(3,4), R(9,10), R(9,15), R(10,11), R(13,14), R(24,27), R(24,28), R(28,32) and R(30,33). These are all bonds within the fused benzene rings and hence it can be predicted that due to the free electron movements within the rings, the bonds are relatively weaker compared to the C-H bonds. On the average, the 6-31G* basis set results are relatively higher compared to the 6-31G basis set results at both levels of theory. Interestingly, the RHF and DFT results for 6-31G* are the same indicating that electron correlation has very little effect on the bond lengths using this basis set; however, for 6-31G basis set, electron correlation has an effect of expanding the bond and thus the DFT results are slightly higher than those at RHF level of theory.

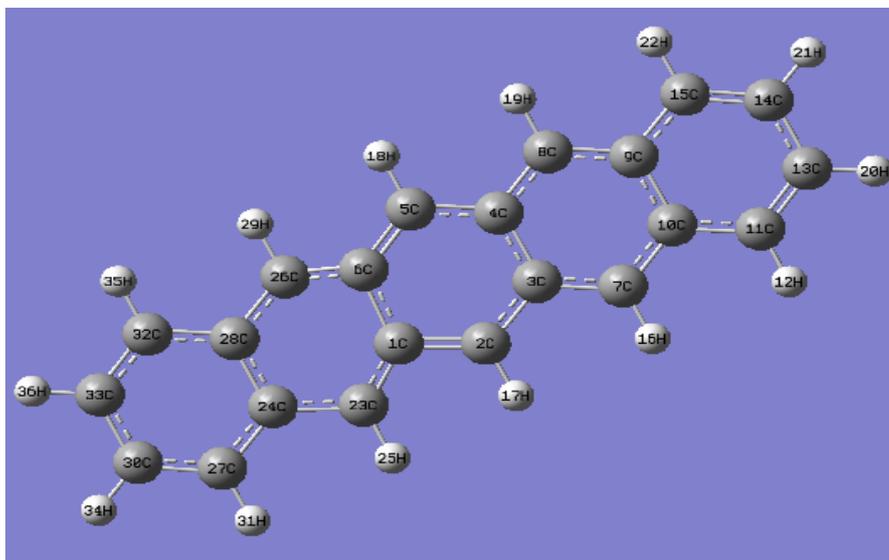


Fig.1: Optimized Structure of Pentacene

Table 1: Optimized bond lengths (Å) of pentacene molecule

Geometrical parameter Bond length (Å)	RHF/6-31G Gas	RHF/6-31G* Gas	B3LYP/6-31G Gas	B3LYP/6-31G* Gas
R(1,2)	1.3930	1.4131	1.4056	1.4131
R(1,6)	1.4371	1.5057	1.4605	1.5057
R(1,23)	1.4180	1.3733	1.4174	1.3733
R(2,3)	1.3929	1.4328	1.4053	1.4328
R(2,17)	1.0745	1.1005	1.0870	1.1005
R(3,4)	1.4371	1.4288	1.4606	1.4288
R(3,7)	1.4181	1.3991	1.4176	1.3991
R(4,5)	1.3929	1.4328	1.4053	1.4328
R(4,8)	1.4181	1.3991	1.4176	1.3991
R(5,6)	1.3930	1.3646	1.4056	1.3646
R(5,18)	1.0745	1.1005	1.0870	1.1005
R(6,26)	1.4180	1.3733	1.4174	1.3733
R(7,10)	1.3693	1.3991	1.3926	1.3991
R(7,16)	1.0746	1.1010	1.0871	1.1010
R(8,9)	1.3693	1.3991	1.3925	1.3991
R(8,19)	1.0746	1.1010	1.0871	1.1010
R(9,10)	1.4464	1.4287	1.4587	1.4287
R(9,15)	1.4459	1.4328	1.4385	1.4328
R(10,11)	1.4459	1.4328	1.4385	1.4328
R(11,12)	1.0738	1.1005	1.0864	1.1005
R(11,13)	1.3452	1.3646	1.3698	1.3646
R(13,14)	1.4421	1.4258	1.4353	1.4258
R(13,20)	1.0729	1.1000	1.0853	1.1000
R(14,15)	1.3452	1.3647	1.3698	1.3647
R(14,21)	1.0729	1.1000	1.0853	1.1000
R(15,22)	1.0738	1.1005	1.0864	1.1005
R(23,24)	1.3694	1.4726	1.3928	1.4726
R(23,25)	1.0746	1.1003	1.0871	1.1003
R(24,27)	1.4458	1.4220	1.4384	1.4220
R(24,28)	1.4463	1.4189	1.4586	1.4189
R(26,28)	1.3694	1.4221	1.3928	1.4221
R(26,29)	1.0746	1.1003	1.0871	1.1003
R(27,30)	1.3453	1.3728	1.3699	1.3728
R(27,31)	1.0738	1.1003	1.0864	1.1003
R(28,32)	1.4458	1.4217	1.4384	1.4217
R(30,33)	1.4421	1.4160	1.4351	1.4160
R(30,34)	1.0729	1.1000	1.0853	1.1000
R(32,33)	1.3453	1.3733	1.3699	1.3733
R(32,35)	1.0738	1.1002	1.0864	1.1002
R(33,36)	1.0729	1.1000	1.0853	1.1000

Optimized Bond Angles

The average angle between the orbital's of the central atom containing the bonding electron pairs in the molecular structure is known as the bond angle between the atoms. The bond angle gives an idea

about the distribution of orbital's about the central atom in a molecule. Table 2 shows the optimized bond angles of pentacene at RHF and DFT levels of theory using 6-31G and 6-31G* basis sets.

Table 2: Optimized bond angles (°) of pentacene molecule

Geometrical parameter	RHF/6-31G Gas	RHF/6-31G* Gas	B3LYP/6-31G Gas	B3LYP/6-31G* Gas
A(2,1,6)	119.1271	112.1259	118.9965	112.1259
A(2,1,23)	122.2267	114.5151	122.2946	114.5151
A(6,1,23)	118.6462	130.1766	118.7089	130.1766
A(1,2,3)	121.7445	125.3768	122.0032	125.3768
A(1,2,17)	119.1260	116.5158	118.9912	116.5158
A(3,2,17)	119.1296	118.0813	119.0057	118.0813
A(2,3,4)	119.1285	118.7901	119.0004	118.7901
A(2,3,7)	122.2270	121.7006	122.2963	121.7006
A(4,3,7)	118.6445	119.5092	118.7032	119.5092
A(3,4,5)	119.1284	118.7868	119.0013	118.7868
A(3,4,8)	118.6445	119.5145	118.7022	119.5145
A(5,4,8)	122.2270	121.6986	122.2966	121.6986
A(4,5,6)	121.7445	120.7650	122.0034	120.7650
A(4,5,18)	119.1295	118.0759	119.0099	118.0759
A(6,5,18)	119.1260	121.1591	118.9868	121.1591
A(1,6,5)	119.1271	124.0525	118.9952	124.0525
A(1,6,26)	118.6462	103.5659	118.7091	103.5659
A(5,6,26)	122.2267	126.7466	122.2956	126.7466
A(3,7,10)	121.8140	120.9763	121.9843	120.9763
A(3,7,16)	118.5427	119.4985	118.6825	119.4985
A(10,7,16)	119.6433	119.5252	119.3331	119.5252
A(4,8,9)	121.8140	120.9759	121.9845	120.9759
A(4,8,19)	118.5427	119.4990	118.6819	119.4990
A(9,8,19)	119.6433	119.5251	119.3336	119.5251
A(8,9,10)	119.5415	119.5096	119.3130	119.5096
A(8,9,15)	122.2483	121.6954	122.2921	121.6954
A(10,9,15)	118.2103	118.7949	118.3949	118.7949
A(7,10,9)	119.5415	119.5142	119.3128	119.5142
A(7,10,11)	122.2483	121.7035	122.2921	121.7035
A(9,10,11)	118.2103	118.7822	118.3951	118.7822
A(10,11,12)	118.0966	118.0746	118.2627	118.0746
A(10,11,13)	121.1503	120.7675	121.0774	120.7675
A(12,11,13)	120.7531	121.1578	120.6599	121.1578
A(11,13,14)	120.6395	120.4489	120.5275	120.4489
A(11,13,20)	120.4923	120.9732	120.2867	120.9732
A(14,13,20)	118.8683	118.5779	119.1858	118.5779
A(13,14,15)	120.6395	120.4423	120.5275	120.4423
A(13,14,21)	118.8683	118.5802	119.1858	118.5802
A(15,14,21)	120.4923	120.9774	120.2867	120.9774
A(9,15,14)	121.1503	120.7641	121.0775	120.7641
A(9,15,22)	118.0966	118.0731	118.2627	118.0731
A(14,15,22)	120.7531	121.1628	120.6598	121.1628
A(1,23,24)	121.8132	115.3929	121.9791	115.3929
A(1,23,25)	118.5459	126.8252	118.6997	126.8252
A(24,23,25)	119.6409	114.2224	119.3212	114.2224
A(23,24,27)	122.2478	126.0912	122.2879	126.0912
A(23,24,28)	119.5406	114.7844	119.3122	114.7844
A(27,24,28)	118.2116	119.0959	118.3999	119.0959
A(6,26,28)	121.8132	128.0747	121.9807	128.0747
A(6,26,29)	118.5459	107.8530	118.6991	107.8530
A(28,26,29)	119.6409	118.5913	119.3203	118.5913
A(24,27,30)	121.1495	120.5099	121.0732	120.5099
A(24,27,31)	118.0983	118.6069	118.2727	118.6069
A(30,27,31)	120.7522	120.8832	120.6542	120.8832
A(24,28,26)	119.5407	119.0596	119.3100	119.0596
A(24,28,32)	118.2115	119.2103	118.4002	119.2103
A(26,28,32)	122.2478	121.7300	122.2898	121.7300
A(27,30,33)	120.6389	120.3763	120.5268	120.3763
A(27,30,34)	120.4915	120.6477	120.2782	120.6477
A(33,30,34)	118.8696	118.9760	119.1950	118.9760
A(28,32,33)	121.1495	120.4559	121.0736	120.4559
A(28,32,35)	118.0983	118.6441	118.2735	118.6441
A(33,32,35)	120.7522	120.8999	120.6529	120.8999
A(30,33,32)	120.6389	120.3516	120.5263	120.3516
A(30,33,36)	118.8696	119.0027	119.1956	119.0027
A(32,33,36)	120.4915	120.6457	120.2781	120.6457

hence there is an overall spread in the molecular structure as the atoms are not close to each other.

The bond angles with the highest value at both levels of theory using the two basis sets are all in the vicinity of 120° as shown in Table 2. These include A(32,33,36), A(30,33,32), A(33,30, 34), A(7,10,11), A(26,28,32), A(23,24,27), A(4,8,9), A(4,5,6), A(2,1,23) etc. Interestingly, all these angles are C-C-C angles within the benzene rings; thus accounting for the more symmetric shape observed in pentacene. All angles in the molecule are predicted to be more than 90° and

Optimized Dihedral Angles

The structure of a molecule can be defined with high precision by the dihedral angles between three successive chemical bond vectors. The dihedral angle varies only the distance between the first and the fourth atoms; the other interatomic distances are constrained by the chemical bond lengths bond angles. The optimized dihedral angles are shown in Table 3.

Table 3: Optimized Dihedral angles (°) of pentacene molecule

Geometrical parameter	RHF/6-31G Gas	RHF/6-31G* Gas	B3LYP/6-31G Gas	B3LYP/6-31G* Gas
D(6,1,2,3)	0.0002	-3.5256	0.0064	-3.5256
D(6,1,2,17)	-179.9989	178.3750	-180.0176	178.3750
D(23,1,2,3)	179.9962	158.4370	179.9924	158.4370
D(23,1,2,17)	-0.0028	-19.6624	0.0036	-19.6624
D(2,1,6,5)	-0.0006	3.6366	-0.0038	3.6366
D(2,1,6,26)	179.9981	158.5815	179.9914	158.5815
D(23,1,6,5)	-179.9968	-154.7266	-179.9903	-154.7266
D(23,1,6,26)	0.0019	0.2183	0.0049	0.2183
D(2,1,23,24)	179.9990	179.5457	-180.0017	179.5457
D(2,1,23,25)	0.0046	22.2073	0.0159	22.2073
D(6,1,23,24)	-0.0049	-22.5040	-0.0157	-22.5040
D(6,1,23,25)	-179.9993	-179.8423	180.0019	-179.8423
D(1,2,3,4)	0.0006	1.8585	-0.0028	1.8585
D(1,2,3,7)	180.0001	-178.1247	-180.0064	-178.1247
D(17,2,3,4)	179.9996	179.9308	-180.0141	179.9308
D(17,2,3,7)	-0.0009	-0.0524	-0.0176	-0.0524
D(2,3,4,5)	-0.0009	0.1839	-0.0033	0.1839
D(2,3,4,8)	179.9995	-179.9227	-180.0048	-179.9227
D(7,3,4,5)	179.9996	-179.8326	-179.9999	-179.8326
D(7,3,4,8)	0.0000	0.0609	-0.0014	0.0609
D(2,3,7,10)	-179.9994	-179.9531	180.0064	-179.9531
D(2,3,7,16)	0.0001	-0.0210	0.0037	-0.0210
D(4,3,7,10)	0.0001	0.0639	0.0028	0.0639
D(4,3,7,16)	179.9996	179.9960	180.0002	179.9960
D(3,4,5,6)	0.0004	-0.0283	0.0059	-0.0283
D(3,4,5,18)	-179.9996	-179.9800	180.0141	-179.9800
D(8,4,5,6)	-180.0000	-179.9193	180.0074	-179.9193
D(8,4,5,18)	0.0000	0.1290	0.0156	0.1290
D(3,4,8,9)	-0.0001	-0.0966	-0.0013	-0.0966
D(3,4,8,19)	-180.0001	180.0000	-180.0000	180.0000
D(5,4,8,9)	180.0003	179.7937	-180.0029	179.7937
D(5,4,8,19)	0.0003	-0.1098	-0.0015	-0.1098
D(4,5,6,1)	0.0003	-2.0317	-0.0024	-2.0317
D(4,5,6,26)	-179.9984	-151.1167	-179.9974	-151.1167
D(18,5,6,1)	180.0003	177.9185	-180.0105	177.9185
D(18,5,6,26)	0.0016	28.8335	-0.0055	28.8335
D(1,6,26,28)	0.0027	26.6944	0.0095	26.6944
D(1,6,26,29)	179.9984	179.6927	-180.0040	179.6927
D(5,6,26,28)	-179.9986	-179.2746	180.0045	-179.2746
D(5,6,26,29)	-0.0029	-26.2762	-0.0090	-26.2762
D(3,7,10,9)	0.0000	-0.1515	-0.0016	-0.1515
D(3,7,10,11)	179.9999	179.9003	-180.0029	179.9003
D(16,7,10,9)	-179.9995	179.9164	-179.9989	179.9164
D(16,7,10,11)	0.0004	-0.0317	-0.0002	-0.0317
D(4,8,9,10)	0.0002	0.0089	0.0026	0.0089
D(4,8,9,15)	-180.0003	-179.9202	180.0018	-179.9202
D(19,8,9,10)	-179.9998	179.9123	180.0012	179.9123
D(19,8,9,15)	-0.0003	-0.0168	0.0005	-0.0168
D(8,9,10,7)	-0.0002	0.1150	-0.0011	0.1150
D(8,9,10,11)	179.9999	-179.9353	-179.9999	-179.9353

D(15,9,10,7)	180.0003	-179.9538	179.9996	-179.9538
D(15,9,10,11)	0.0004	-0.0041	0.0008	-0.0041
D(8,9,15,14)	-179.9999	72 179.9107	180.0002	179.9107
D(8,9,15,22)	0.0003	-0.1009	0.0016	-0.1009
D(10,9,15,14)	-0.0004	-0.0189	-0.0005	-0.0189
D(10,9,15,22)	-180.0002	179.9695	-179.9991	179.9695
D(7,10,11,12)	-0.0001	-0.1060	0.0003	-0.1060
D(7,10,11,13)	-180.0002	-179.9865	-179.9999	-179.9865
D(9,10,11,12)	179.9998	179.9455	179.9991	179.9455
D(9,10,11,13)	-0.0003	0.0650	-0.0012	0.0650
D(10,11,13,14)	0.0001	-0.1018	0.0012	-0.1018
D(10,11,13,20)	-180.0000	179.9569	-179.9995	179.9569
D(12,11,13,14)	-180.0000	-179.9786	-179.9991	-179.9786
D(12,11,13,20)	-0.0001	0.0801	0.0003	0.0801
D(11,13,14,15)	0.0000	0.0780	-0.0008	0.0780
D(11,13,14,21)	180.0000	180.0000	179.9987	180.0000
D(20,13,14,15)	-179.9999	-179.9793	179.9998	-179.9793
D(20,13,14,21)	0.0001	-0.0573	-0.0006	-0.0573
D(13,14,15,9)	0.0002	-0.0166	0.0005	-0.0166
D(13,14,15,22)	180.0000	179.9954	179.9991	179.9954
D(21,14,15,9)	-179.9998	-179.9366	-179.9991	-179.9366
D(21,14,15,22)	0.0000	0.0753	-0.0005	0.0753
D(1,23,24,27)	-179.9934	-158.2993	180.0235	-158.2993
D(1,23,24,28)	0.0033	19.7293	0.0121	19.7293
D(25,23,24,27)	0.0010	1.9344	0.0058	1.9344
D(25,23,24,28)	179.9976	179.9629	-180.0057	179.9629
D(23,24,27,30)	-179.9981	177.9688	180.0083	177.9688
D(23,24,27,31)	-0.0039	-2.0448	-0.0098	-2.0448
D(28,24,27,30)	0.0052	0.0171	0.0197	0.0171
D(28,24,27,31)	-180.0006	-179.9964	180.0016	-179.9964
D(23,24,28,26)	0.0014	1.8178	0.0025	1.8178
D(23,24,28,32)	-179.9988	-178.1865	-179.9971	-178.1865
D(27,24,28,26)	179.9982	179.9947	-180.0085	179.9947
D(27,24,28,32)	-0.0020	-0.0096	-0.0082	-0.0096
D(6,26,28,24)	-0.0044	-29.4850	-0.0133	-29.4850
D(6,26,28,32)	179.9958	150.5193	179.9864	150.5193
D(29,26,28,24)	179.9999	179.9984	180.0003	179.9984
D(29,26,28,32)	0.0002	0.0027	-0.0001	0.0027
D(24,27,30,33)	-0.0043	-0.0110	-0.0155	-0.0110
D(24,27,30,34)	179.9948	179.9952	-180.0170	179.9952
D(31,27,30,33)	-179.9985	-179.9971	180.0031	-179.9971
D(31,27,30,34)	0.0007	0.0090	0.0016	0.0090
D(24,28,32,33)	-0.0019	-0.0040	-0.0075	-0.0040
D(24,28,32,35)	-179.9982	-179.9878	180.0052	-179.9878
D(26,28,32,33)	179.9978	179.9916	-180.0072	179.9916
D(26,28,32,35)	0.0016	0.0078	0.0056	0.0078
D(27,30,33,32)	0.0002	-0.0029	-0.0008	-0.0029
D(27,30,33,36)	179.9998	-179.9927	-180.0023	-179.9927
D(34,30,33,32)	180.0010	179.9910	180.0007	179.9910
D(34,30,33,36)	0.0006	0.0013	-0.0008	0.0013
D(28,32,33,30)	0.0029	0.0104	0.0123	0.0104
D(28,32,33,36)	-179.9967	-180.0000	180.0138	-180.0000
D(35,32,33,30)	179.9991	179.9938	-180.0008	179.9938
D(35,32,33,36)	-0.0005	-0.0166	0.0008	-0.0166

As shown in Table 3, there is slight variation in the predicted dihedral angles for some bonds as we move from RHF to DFT level. However, the variation is very minimal except in some particular cases where the two basis sets predict different orientations to the angles. At both levels of theory, the angles are either too small

(approaching zero) or almost 180° similarly The dihedral angle is considered to be positive if a clockwise rotation is performed with the molecule and it will be negative when an anti clockwise rotation is performed with the molecule in its plane.

Atomic Charge Distribution

Within molecular system, atoms can be treated as a quantum mechanical system. On the basis of the topology of the electron density the atomic charges in

the molecule can be explained. The electrostatic potential derived charges using the CHelpG scheme of Breneman at different atomic positions in gas phase are computed at RHF and DFT levels of theory using 6-31G

and 6-31G* basis sets. The Mulliken population analysis partitions the charges among the atoms of the molecule by dividing orbital overlap evenly between two atoms. Whereas the electrostatic potential derived charges assign point charges to fit the computed electrostatic potential at a number of points on or near the Van Der Waal surface. Hence, it is appropriate to consider the charges calculated by CHelpG scheme of Breneman instead of Mulliken population analysis.

Table 4 shows the electrostatic potential derived atomic charges of pentacene molecule. The charges are almost evenly distributed with the Carbon atoms retaining most of the bulk negative charge and the Hydrogen atoms retaining the bulk positive charge. This can be expected due to the free movement of electrons between the Carbon atoms in the five fused benzene rings.

Table 4: Electrostatic potential derived charges

S/N	Atom	RHF/6-31G Gas	RHF/6-31G* Gas	B3LYP/6-31G Gas	B3LYP/6-31G* Gas
1	C	0.062240	0.107974	0.091598	0.16648
2	C	-0.172484	-0.278425	-0.228535	-0.30156
3	C	0.062225	0.178206	0.091629	0.16649
4	C	0.062225	0.141149	0.091630	0.16648
5	C	-0.172484	-0.234382	-0.228535	-0.30157
6	C	-0.062240	0.117416	0.091624	0.16650
7	C	-0.172319	-0.294388	-0.225408	-0.29822
8	C	-0.172320	-0.295986	-0.225401	-0.29822
9	C	-0.066066	0.146512	0.075625	0.14771
10	C	-0.066066	0.144103	0.075625	0.14772
11	C	-0.135957	-0.179701	-0.143134	-0.17949
12	H	0.209939	0.131178	0.129479	0.13054
13	C	-0.216068	-0.142957	-0.136443	-0.14152
14	C	-0.216068	-0.283655	-0.136443	-0.14152
15	C	-0.135957	0.181247	-0.143132	-0.17949
16	H	0.218690	0.134039	0.131364	0.12959
17	H	0.219254	0.122794	0.131221	0.12946
18	H	0.219254	0.132107	0.131221	0.12946
19	H	0.218690	0.131107	0.131363	0.12959
20	H	0.200651	0.131047	0.125608	0.13095
21	H	0.200651	0.131635	0.125608	0.13095
22	H	0.209939	0.131311	0.129479	0.13054
23	C	-0.172325	-0.233291	-0.225398	-0.29822
24	C	-0.066087	0.106285	0.075585	0.14772
25	H	0.218692	0.135856	0.131370	0.12959
26	C	-0.172325	-0.273691	-0.225431	-0.29823
27	C	-0.135985	-0.184688	-0.143236	-0.17950
28	C	-0.066087	0.134561	0.075613	0.14772
29	H	0.218692	0.104486	0.131369	0.12959
30	C	-0.216062	-0.133115	-0.136421	-0.14151
31	H	0.209939	0.128114	0.129479	0.13054
32	C	-0.135985	-0.176900	-0.143243	-0.17950
33	C	-0.216062	-0.137127	-0.136417	-0.14151
34	H	0.200652	0.132043	0.125604	0.13095
35	H	0.209939	0.133349	0.129480	0.13054
36	H	0.200652	0.131323	0.125605	0.13095

CONCLUSION

The optimized structure and atomic charge distribution of the organic semi-conductor molecule pentacene has been studied using the Gaussian software package at the RHF and DFT levels of theory. Basically, it is

predicted that the bond lengths are relatively short and strong with the C-H bonds being the strongest and the C-C bonds being the weakest. The charge distribution is fairly symmetric with the hydrogen atoms being slightly electropositive and the carbon atoms electronegative.

REFERENCES

- Byoungnam Park,(2008).Channel Formation in single-monolayer pentacene thin film transistors electronic and structural properties of pentacene at organic/inorganic interfaces materials science thesis at the university of wisconsin-madison
- Dan Kolb,(2005). Pentacene-based organic transistors, School of Engineering, University of Durham
- Harada K., Riede M., Leo K., Hild O.R., and Elliott C.M. (2008)., Pentacenehomojunctions: Electron and hole transport properties and related photovoltaic responses Phys. Rev. B 77, 195212.
- Hwan S.K., Young H. C., Hoon S.H and Jang J.pentacene (2004).Thin Film with Large Grain on Plastic Substrate by Organic Vapor Phase Deposition Journal of the Korean Physical Society, Vol. 45 2004. 760-762
- Jacquemin D., Perpète E.A., Adamo C., (2008). Modelling the UV/visible spectrum of tetrakis(phenylethynyl)benzene . Journal of Molecular Structure 863 123–127
- Jacquemin D., Preat J., Wathelet V., Marie Andre J., Perpete E.A. (2005). Substitution effects on the visible spectra of 1,4-diNHP-9,10-anthraquinonesChemical Physics Letters 405 429–433
- Jan A. and Wimmer E. (1991); Optimization of Gaussian-type basis sets for local spin density functional calculations. Part I. Boron through neon, optimization technique and validation
- Kitamura M., and Yasuhiko Arakawa (2008);Pentacene-based organic field-effect transistors *J. Phys.: Condense. Matter***20** 184011.
- M. Kurta, P. ChinnaBabub, N.Sundaraganesanb, M. Chinarc, M. Karabacak. Molecular structure,Vibrational UV and NBO analysis of 4-chloro-7-nitrobenzofuran by DFT calculations.