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Quantum Mechanic Studies of Natural Bond Orbital & Stabilities of $[CuCH_2SiMe_3]_4$Complexes With Different Halogens

Arezo Batebi, somaieh kopaiee malek

Department of Inorganic Chemistry, Faculty of Chemistry, University College of Science, University of Tehran, Tehran, Iran P.O. Box 14155-6455, Tehran, Iran

*Corresponding Author e-mail Address: Arezobatebi@hotmail.com

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Abstract

The asymmetric unit of the title compound, $[CuCH_2SiMe_3]_4$ Contains two independent molecules. The Cu atoms are four coordinated in distorted tetrahedral configuration by two N atoms from 5,5`-dimethyl-2,2`- bipyridine and two terminal Cl atoms. In the Cuystal structure, inter molecular $C-H...Cl$ hydrogen bonds link the molecules. The are $C-H....\pi$ contacts between the methyl groups and the pyridine and five member rings containing Cu atoms. $\pi-\pi$ Contacts also exist between the pyridine rings. (Fig 1)

Keywords: Complexes, Halogens, Chemical potential, 5,5`-dimethyl-2,2`- bipyridine.

1. Introduction

The studies show that the stability of complexes after changing Cl with $F\ \&Br$ has been varied. Also amount of coefficient factors of p orbital in $\sigma\&\pi$ bonds, the different of energy between HOMO & LUMO orbital, and another factors in bond like the distance of bonds and bond angles in the same bonds in the different complexes have been researched. The (core/charge) of, Cu complexes with different ligands, calculated by NBO method at the levels of HF/6-31G(d) in the GAUSSIAN 98. All calculations have been done in gas phase.The calculations for C,H,N,O atoms have been performed by the standard $6-31G*$ basis set, and for Cu standard LANL2DZ basis sets have been considered(Fig 1)[1-6].

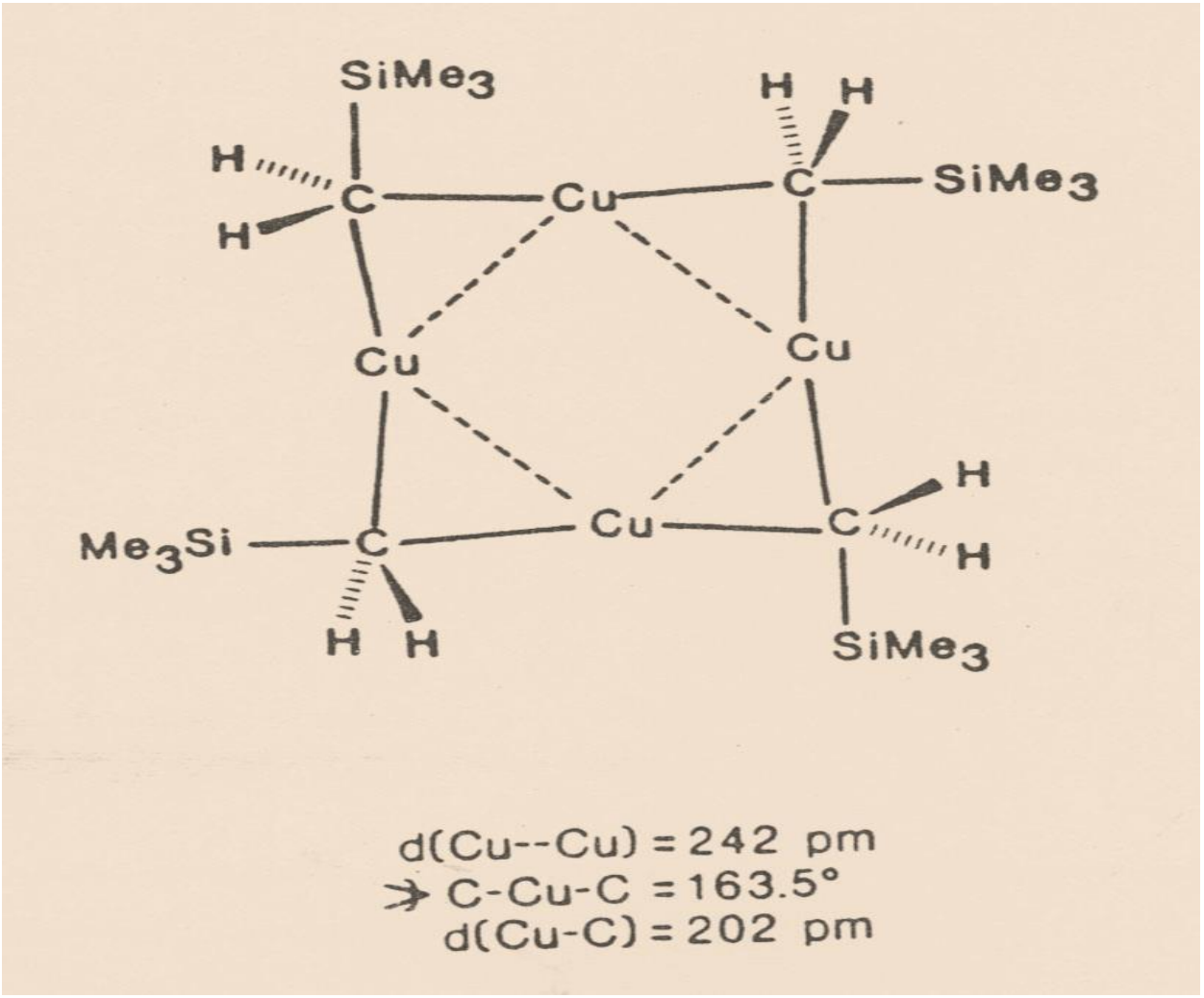

Fig 1.

Table 1. Dipole moments Value for complexes in 2 methods of HF,DFT

	Energy(a.u)	*Hartree* *Energy(kcal/mol)*	*Dipole moment(Debye)*
B3LYP- Cu-Cl	-3380.201574	-2121091.699	18.819
B3LYP- Cu-Br	-5491.726113	-3446082.849	19.5355
B3LYP-Cu-F	-3000.379101	-1882751.388	44.1118
HF-Cu-Cl	-3367.613098	-2113192.373	21.3454
HF-Cu-Br	-5477.841435	-3437370.151	33.7405
HF-Cu-F	-3007.412686	-1887164.994	26.1615
HF-Cu-CH3	-2947.562735	-1849608.88	24.483
HF-Cu-C2H5	-2986.786173	-1874221.764	22.6707
HF-Cu-C3H7	-3025.683589	-1898630.068	22.6438
HF-Cu-C4H9	-3064.488549	-1898630.068	15.3742
HF-Cu-COOH	-3096.353871	-1942975.988	19.8566
HF-Cu-CO	-3020.565291	-1895418.313	31.8739
HF-Cu-CN	-3000.499067	-1882826.667	18.8065
HF-Cu-NO2	-3112.230163	-1952938.432	18.2325
HF-Cu-OH	-2983.576041	-1872207.392	

2. Computational details

All Computations are performed by means of GAUSSIAN 03 packing [9]. Geometries for all compounds are computed by means of the density functional theory (DFT) with Becke's three-parameter functional (B3) plus Lee, Yang, and Parr (LYP) correlation functional. For all atoms, the standard 6-31G basis set is utilized. The structures of complexs were designed primarily using of Gauss View 5.0.8 and nanotube modeler 1.3.0.3 soft wares. The interaction effects of Fluoxetine on Fullerene were investigated

Through attachment to three different base positions. All these calculations are done under the assumption of standard state of gas phase, pressure of 1 atmosphere, and temperature of 25 degrees centigrade. The calculations are performed, using a Pentium 4 PC with a Windows 7 OS and a Core i5 processor[7-9] .

3. Results

Table 2. Show total electrons (Total) to the partial charge of the atom in the complex Cu-NO, Cu-NO2 Base Series 6-31G * Two methods of HF, DFT

HF , B3LYP(6-31G)				
Atom	Cu-NO		Cu-NO2	
	Charge	Total	Charge	Total
	0.37878	14.12122	1.01484	13.48516
Cu 1	0.92657	13.57343	0.67678	13.82322
	-0.40552	4.40552	-0.4038	4.4038
O 5	-0.33625	4.33625	0.09173	3.90827
	-0.46768	4.46768	0.06247	3.93753
O 6	-0.22333	4.22333	-0.25715	4.25715
	0.2053	3.7947	-0.43663	4.43663
O 8	-0.25412	4.25412	-0.32812	4.32812
	0.25204	3.74796	-0.3409	4.3409
O 9	-0.14991	4.14991	-0.20346	4.20346
	-0.44803	4.44803	-0.3756	4.3756
O 10	-0.35756	4.35756	-0.35504	4.35504
	-0.35371	4.35371	-0.30742	4.30742
O 11	-0.34366	4.34366	-0.24714	4.24714
	0.4481	3.5519	-0.21038	4.21038
O32	-0.10175	4.10175	-0.163	4.163
			-0.19894	4.19894
O33			-0.16433	4.16433
	0.1415	2.8585	0.1269	2.8731
C 23	0.07511	2.92489	0.07974	2.92026
	-0.14776	3.14776	-0.11014	3.11014
C 24	-0.09457	3.09457	-0.08658	3.08658
	0.09041	2.90959	0.12166	2.87834
C 26	0.0659	2.9341	0.06815	2.93185
	-0.10398	3.10398	-0.11521	3.11521
C 27	-0.09802	3.09802	-0.08779	3.08779
	0.17207	2.82793	0.12895	2.87105
C 29	0.0812	2.9188	0.08424	2.91576
C 30	0.45225	2.54775	0.44035	2.55965

	0.39938	2.60062	0.38734	2.61266
	0.33187	3.16813	0.31058	3.18942
N 31	0.07434	3.42566	0.2506	3.2494
	-0.35305	3.85305	-0.38411	3.88411
N 2	-0.24852	3.74852	-0.24638	3.74638
	-0.3502	3.8502	-0.36572	3.86572
N 3	-0.25555	3.75555	-0.2646	3.7646
	0.09672	0.40328	0.10357	0.39643
H 17	0.1088	0.3912	0.10995	0.39005
	0.10964	0.39036	0.1111	0.3889
H 19	0.11585	0.38415	0.12011	0.37989
	0.1182	0.3818	0.12382	0.37618
H 25	0.12065	0.37935	0.12327	0.37673
	0.1233	0.3767	0.12351	0.37649
H 28	0.12119	0.37881	0.12368	0.37632

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