



Comparison of Stability^[Cu(C₇H₃NO₄)₂] and Valance / Charge Ratio of Oxygen and Carbon atoms in the Complex by Changing the Vinyl, Acetylene, isopropil

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Abstract

In the complex (bispyridine -2 and 6-dicarboxylate copper II) at position H number 26 with modifications of ligands such as vinyl, acetylene and isopropyl, changes in the valance / charge ratio for oxygen and carbon atoms in these complexes have been investigated by methods Initial calculations (ab initio) have been performed at two levels of HF, DFT. Finally, their stability is compared with the tables and charts resulting from the calculations performed.

Keywords: bispyridine -2 and 6-dicarboxylate copper II.

1. Introduction

In $[Cu(C_7H_3NO_4)_2]$ a six-atom atom composition, corded with two molecules of pyridine -2 and 6-carboxylic or $pydc^{2-}$ anion, each anion is corded with one atom of N of pyridine and two of the O atoms from the carboxylate. The area is slightly diverted from the linear state. Therefore, the geometry obtained from CuN_2O_4 the cordonation can be justified as octahedral occipital deflection. The length of the bonds $Cu1-O1$ and $Cu1-O3$, respectively, [2.2824 (17), 2.3194 (16) Å] are longer than the length of other ligand-metal bonds, which may be due to the Jan-Teller effect. The angle between the two main passages passing through the $pydc^{2-}$ anion determines that these units are perpendicular to each other. In addition, the transversal angles $O1-Cu1-O3[153.33(6)^\circ]$ indicate that the four carboxylate groups of di-anions around the Cu^{II} atom are arranged in a flat tetrahedron position. (2).

2. Computational details

All Computations are performed by means of GAUSSIAN 03 packing [1-6]. 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 Fluoxetine on Fullerene 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 [7-10].

In this report, the desired complex structure was first optimized. Then, the calculation of NBO using the Gaussian 98 software in the base series was calculated from the initial methods of ab initio in both HF and DFT methods, and the Valance / Charge ratio of the complex in different species of this complex With different ligands, they compare and eventually conclude [11-13].

3. Results

The calculations in the base series 6-31 G * are performed using two HF and DFT methods. Charts are also plotted based on the Valance / Charge oxygen and carbon atoms in the complex by changing the vinyl,

acetylene, and propyl vulgar ligands. The results of the calculations are presented below.

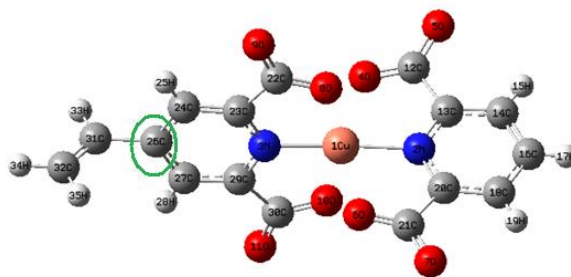


Fig 1. Complex $[Cu(C_7H_3NO_4)_2]$

Table 1 shows the energy level and the Valance / Charge ratio for oxygen and carbon atoms in copper-ASETYLENE, CU-ISOPROPYLE, Cu-VINYLY complexes in the 6-31G base series. Two methods of HF, DFT

	C26		O8				
	valance	charge	valance	charge	energy(hf)	valance/charge(C26)	valance/charge(O8)
Cu-asetylene	1.90386	0.08668	3.46589	-0.47505	-2997.123664	21.96423627	-7.295842543
Cu-isopropyle	1.92863	0.05931	3.12263	-0.13571	-2956.882697	32.51778789	-23.00957925
Cu-vinyle	2.0399	0.0503	3.434	-0.44339	-2955.738651	40.55467197	-7.744874715

	C26		O8				
	valance	charge	valance	charge	energy(B3lyp)	valance/charge(C26)	valance/charge(O8)
Cu-asetylene	1.99989	0.00648	3.29339	-0.30215	-3006.55475	308.625	-10.89985107
Cu-isopropyle	1.95878	0.03237	3.24462	-0.25351	-2966.000774	60.51220266	-12.79878506
Cu-vinyle	1.97798	0.01401	3.327	-0.33569	-2964.74403	141.1834404	-9.910929727

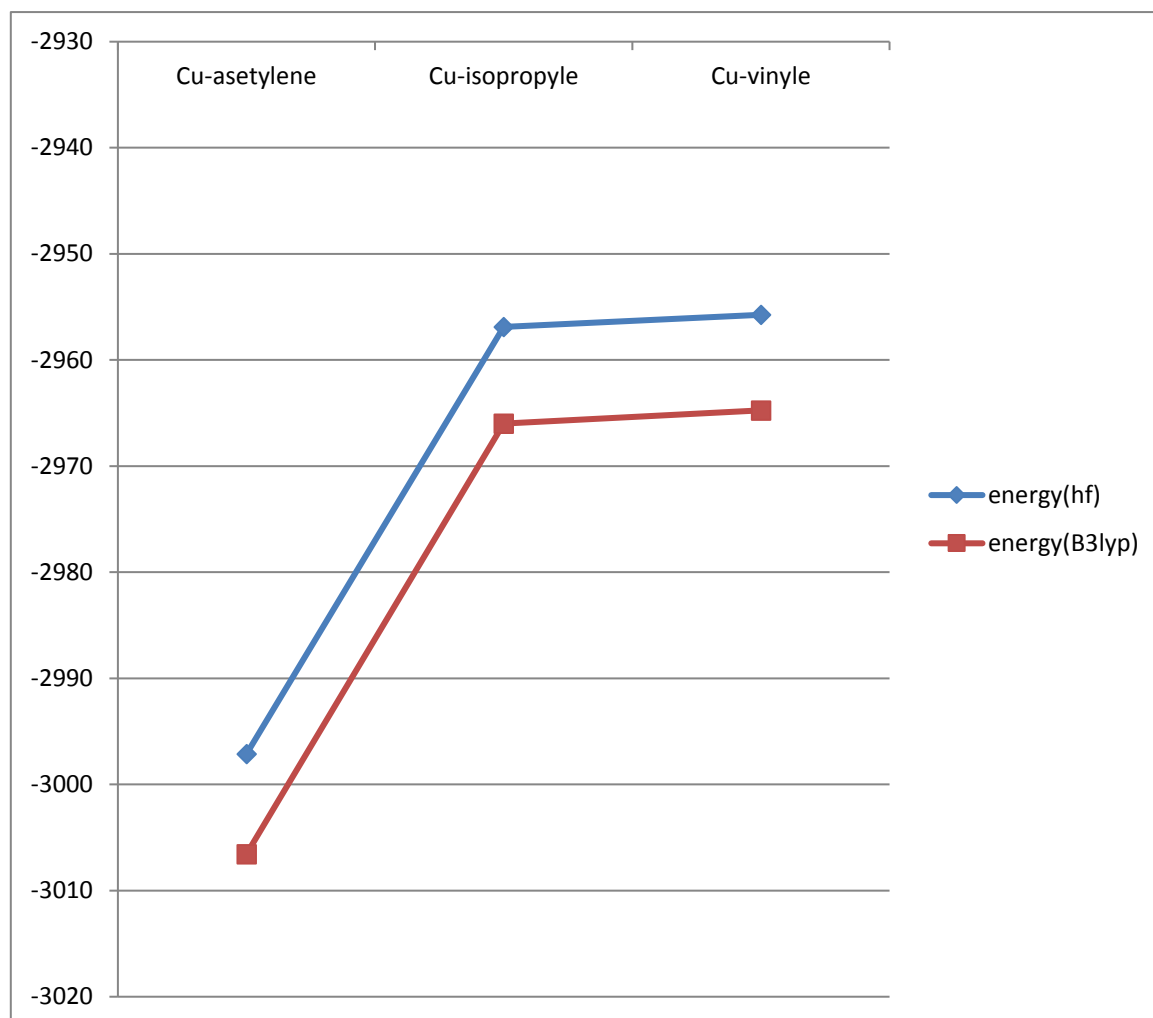


Chart 1 - Chart of Energy Changes in Complexes

Cu-ASETYLENE, CuISOPROPYLE, Cu-VINYLY VINYL in the 6-31G base series * Two methods of HF, DFT

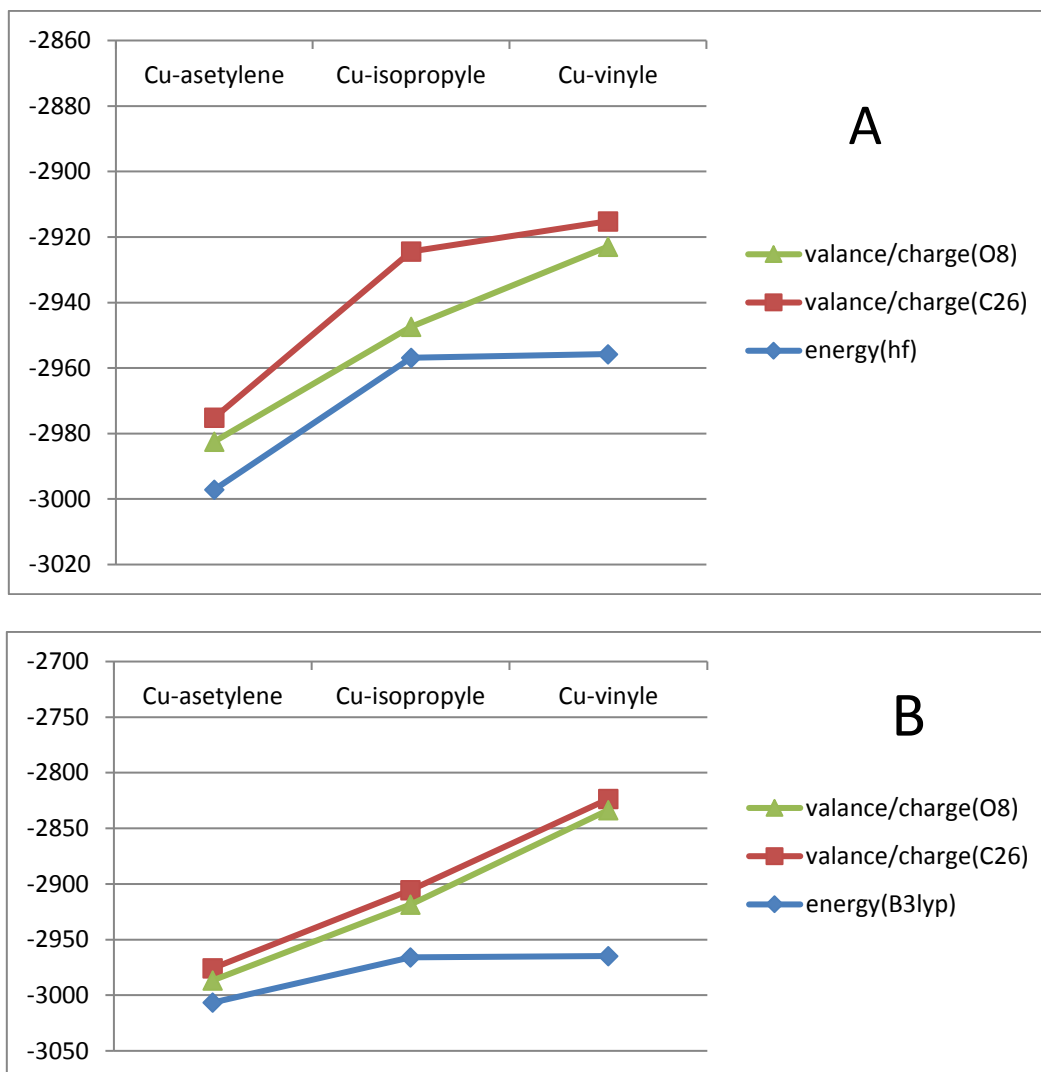


Diagram 2: Comparison of Energy Changes and Valance / Charge Ratios for Oxygen (O8) and Carbon (C26) atoms in Cu-ASETYLENE, Cu- ISOPROPYLE, Cu-VINYLY Complexes at 6-31G Base * by Method A) HF B) DFT

Conclusion

Investigating the electron capability of atoms relative to the atomic charge and its dependence on the stability of the complexes has been considered. The graph of the ratio of the Valence electrons to the charge charge has shown that in all the complexes the process has been the same and in the negative direction of growth is more consistent, which indicates the stability of the above complexes. The smaller the electrons in the atom in question, the more stimulating and affecting the valence layer electrons, will cause the line gradient to increase and the curve becomes sharper (sharper). Totally, due to the presence of large electrons in the copper layer, no significant change was observed with the change of the ligand on the copper complex. This data has a similar trend at both levels of HF, DFT.

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