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

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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].