3P062 Electronic Structure of Molecular-Scale Logic-gate

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§1. Introduction

It has been known that some Cu complexes change dynamically their structure with outer perturbations (light, redox reaction, etc.). For example, in this conference for molecular structures held in the last year, we presented our study for an inorganic photochromic complex $[Cu^{II}(dieten)_2]^{2+}$ (dieten = N,N'-diethyl ethylenediamine) and showed that $[Cu^{II}(dieten)_2]^{2+}$ changes the planar structure in the electronic ground state into tetragonal one in the first excited states [1]. The origin of the dynamic motion of Cu complex comes from the difference of preferred ligand fields of Cu^{+} and Cu^{2+}. By using such a dynamic motion of the Cu complex, it may be possible that we can construct molecular–scale logic gate. In this poster session, we'll focus on a Cu complex which was synthesized by Livoreil *et al.* (see Fig. 1) [2]. Livoreil *et al.* revealed that the complex rotates as shown in the Fig. 1 by using a spectroscopic technique. The object of this study is to understand the molecular motion of this complex from a theoretical point of view.

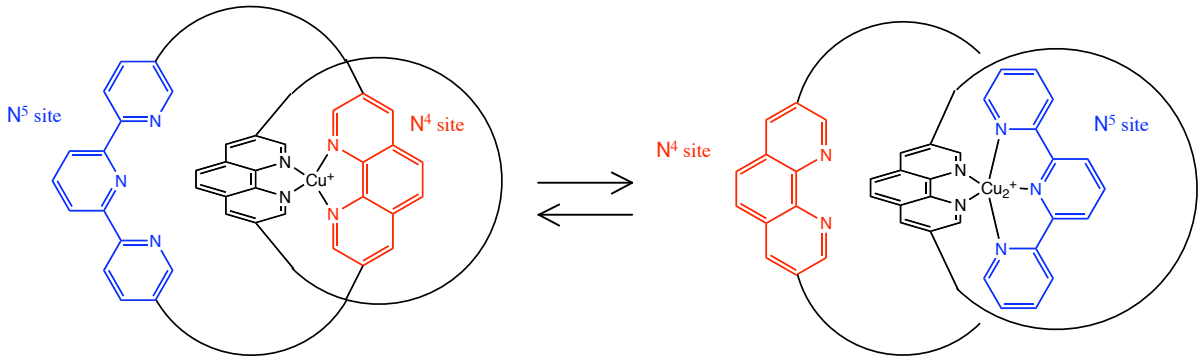

Fig. 1 Molecular logic gate introduced by Livoreil *et al.*

§2. Computational details

Geometry optimizations were performed using the B3LYP flavor of density functional theory with 6-31G(d,p) basis sets. Frequency analyses were also performed to check whether the optimized geometries were those of energy minimum or not. All the calculations were performed using the package program of GAUSSIAN'03.

§3. Results and discussion

The HOMO of the N^4-site Cu^+ ion complex (see Fig. 1) is shown in the Fig. 2. The orbital is clearly Cu's 3d e_γ orbital. If the complex is oxidized to form 2+ ion complex, the configuration of Cu ion becomes $(3d)^9$. Thus, It is well understood that the coordination structure of the complex can be modulated by using redox reaction easily. Results of the total system calculations will be discussed at poster session.

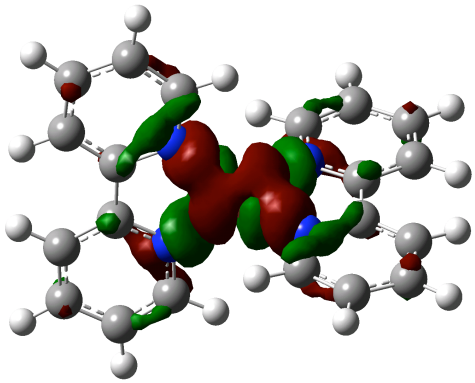

Fig. 2 HOMO of $[Cu(2,2'\text{-bipyridine})]^+$ (N_4 site complex)

References

[1] H. Mori, K. Ishii, and E. Miyoshi, *J. Theo. Comput. Chem.* submitted (2005).

[2]Aude Livoreil *et al. J. Am. Chem. Soc.* **119**, 12114 (1997).