

Charge density distribution of high spin and low spin iron atoms on $[\text{Fe}(\text{II})(\text{bpy})_3][\text{Fe}(\text{II})_2(\text{ox})_3]$ complex

Jey Jau Lee*^a Mau-Tsu Tang^a and Yu Wang^b

a, National Synchrotron Radiation Research Center, Hsinchu, Taiwan R.O.C.

b, Department of Chemistry, National Taiwan University, Taipei, Taiwan, R.O.C.

ABSTRACT

Charge density distribution and bond characterization have been investigated on a polymeric 3D complex $[\text{Fe}(\text{II})(\text{bpy})_3][\text{Fe}(\text{II})_2(\text{ox})_3]$, in terms of accurate single crystal diffraction at 100K. The 3D framework is made by iron complex $\text{Fe}(\text{II})_2(\text{ox})_3^{2-}$ in a porous network, which is encapsulated with isolated iron complex of $\text{Fe}(\text{II})(\text{bpy})_3^{2+}$ inside the cage. Each asymmetric unit contains two different spin state Fe^{2+} atoms: a high spin and a low spin states coordinated to six oxygen and six nitrogen atoms respectively.

The experimental approach is based on the multipole model formalism refinement on the diffraction data. The purpose of this work is to compare the charge density distributions at the iron site with a high spin (HS) and a low spin (LS) configuration. The expected differences in the electron density distribution around the iron site will be demonstrated.

There are significant differences at the iron center between HS and LS sites shown in the deformation density maps and in the VSCC derived from the Laplacian. The apparent asphericity in electron density of the LS species is not observed in that of the HS case. The VSCC of the high spin state is approximately spherical; in contrast, the VSCC of the LS case indicates a clear octahedral feature with six local charge concentrations around the iron center. This difference between two spin states can be best illustrated by the isovalue surfaces of Laplacian show as follows.

* Corresponding author: email jjlee@nsrrc.org.tw