Charge Density Studies of Some Iron Nitrosyl Complexes, Yu Wang,* J. J. Lee and I. J. Hsu, *Department of Chemistry, National Taiwan University, Taipei, Taiwan*. E-mail: yuwang@xtal.ch.ntu.edu.tw

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Charge density and bond characterization have been investigated on some Iron-nitrosyl complexes in terms of accurate single crystal diffraction at 100K and an open-shell DFT calculation. The iron atom is four- five-and six-coordinated with sulfur and nitrogen atoms in various geometries. The nitrosyl group (NO) could be linear or bent with Fe-N-O close to or deviate from 180 degree. Since these complexes are related to biological activities, this study may shine some light on how it operates via electron density distribution, especially at the iron site and at the NO group. It is known that NO group could be a radical neutral species or NO^+, a nitrosyl, or NO^-, a nitroxide group. Thus the unpaired electron can be located either at Fe or at the NO group; meanwhile the formal charge of the Fe will be dependent on the charge on the NO group. According to the electron density distribution based on the multipole model and on the DFT calculation, the electronic configuration of iron atom and the charge of NO group can be determined. In addition, the location of the unpaired electron will be confirmed with single crystal EPR and SQUID measurements. The formal charge of Fe will be complimented by the x-ray absorption spectroscopy. Topological analysis on the total electron density will give the bond characterization in terms of topological properties associated with bond critical points. The VSCC of Fe in various coordination geometries, together with the detail descriptions and their correlations to the metal ligand bond will be presented.