

MS10 O1

Charge Density Studies of Fe(II) Complexes in Different Spin States Yu Wang^a, J.J. Lee^b, C.F. Sheu^a, T.H. Shih^a, I.J. Hsu^a, ^a*Department of Chemistry, National Taiwan University, Taipei, Taiwan*; ^b*NSRRC, Hsin-Chu, Taiwan*. Email: wangyu@ntu.edu.tw

Keywords: charge density, spin transition, iron complexes

Charge density studies on a few octahedrally coordinated Fe(II) complexes will be presented. The spin state of Fe(II) exhibits either high spin (HS) or low spin (LS) depending upon the ligand field strength of the coordinated ligands. Electron density distribution around the metal should be greatly different for the two spin states, namely a quintet 5T_2 and a singlet 1A_1 states. In order to eliminate any possible experimental differences, we choose a few systems where a HS and a LS state coexist in the same lattice. The comparison of these two spin states are quite clear, it gives a good example for the illustration of the d-orbital distributions of the 3d-transition metal as well as the metal-ligand bond for HS and LS state respectively in Fe(II) complexes. Complimentary x-ray absorption spectroscopy and the IR stretching frequency are also measured to monitor the spin transition. A DFT calculation is studied on one of the isolated molecules, comparable electron density distribution as well as the topological properties associated with the bond critical point with respect to the experimental observations will be discussed.

MS10 O2

Metal-ligand bonds in coordination compounds Miroslav Kohout, *Max Planck Institute for Chemical Physics of Solids, Dresden, Germany*. E-mail: kohout@cpfs.mpg.de

Keywords: electron localization, electron density, pair density

The analysis of chemical bonding in real space can be performed using different position dependent functionals. Recently proposed Electron Localizability Indicator (ELI) is based on integrals over specially designed micro-cells [1]. Loosely speaking, ELI is proportional to the charge that is needed to form a same-spin electron pair. Thus, ELI is connected with the correlation of electronic motion of same-spin electrons [2]. In regions of space, where the bonding occurs, the same-spin electron try to avoid each other. The examination of metal-ligand bonds is complicated by the participation of the inner shell metal orbitals [3]. Some strategies, how to approach this difficult task will be presented.

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MS10 O3

Experimental charge density study and topological properties of Fidarestat El-Eulmi Bendeif^a, Christian Jelsch^a, Benoit Guillot^a, Claude Lecomte^a & Wolfgang Morgenroth^b, ^a*(LCM³B), Université Henri Poincaré, Nancy, France.*, ^b*(HASYLAB), DESY Hamburg, Germany.*

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Keywords: Charge density, Topological analysis, Interaction energy

During the last decade, although a variety of compounds have been observed to inhibit aldose reductase (AR), most drug candidates were not approved for clinical use because of unacceptable side effects and lack of efficacy. Fidarestat (C₁₂H₁₀N₃O₄F) is a new human Aldose Reductase (hAR) Inhibitor. It is a potential candidate therapeutic agent for treatment of diabetic complications because it is currently being tested on human patients [1]. We will present here the accurate crystal structure and the experimental charge density based on high resolution synchrotron diffraction data collected at 100K of this new inhibitor. The density parameters are obtained by least-squares fitting of the model with the software *MoPro* [2], following the Hansen-Coppens formalism [3]. Experimental deformation densities allow a first qualitative view of the non-spherical density and reveal fine details, coherent with the chemistry of the molecule, as for instance lack of electron density in the C—F bond [4-6], and larger density accumulation on imidazole moiety C—N and C—O bonds. The topological analysis of the total electron density performed using the *VMoPro* program [7] will be discussed. As the electrostatic properties are of major importance in numerous biological processes, accurate electrostatic potential and interaction energies calculations of the human aldose reductase complex with fidarestat will also be discussed. This will enable to give useful insight on the specific inhibition activity.

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MS10 O4

Metal-metal bonding in the μ -BMn₂ triangular motif of $[\mu$ -B'Bu (η^5 -C₅H₅)Mn(CO)₂]₂ Ulrike Flierler^a, Michael Burzler^b, Holger Ott^a, Dirk Leusser^a, Julian Henn^a, Holger Braunschweig^b, Dietmar Stalke^a ^a*Institute of Inorganic Chemistry, University of Goettingen.* ^b*Institute of Inorganic Chemistry, University of Wuerzburg.* E-mail: uflierler@chemie.uni-goettingen.de

Keywords: electron density distribution, transition-metal complexes, metal-metal interaction

The nature of the metal-metal bond in polynuclear transition metal complexes is a topic of constant debate. The novel approaches of the quantum mechanic theory of atoms in molecules^[1] may shade some light on that issue^[2-4]. New theoretically and experimentally derived criteria have been introduced to describe these bonds in more detail^[5,6].

We present the borylene complex $[\mu\text{-B}^t\text{Bu}\{\eta^5\text{-C}_5\text{H}_5\}\text{Mn}(\text{CO})_2]_2$ ^[7] which was investigated by a high-resolution low-temperature X-ray diffraction experiment. As the boron bridged Mn–Mn contact is relatively short, it was rather surprising that no bond critical point was found. The analysis of this compound should therefore give further insight in the bonding situation of this supported Mn–Mn bond.

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MS10 O5

Experimental spin density in a piano stool FeIII complex Béatrice Gillon^a, Frédéric Paul^b, Alain Cousson^a,
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Keywords: spin density, Fe(III) complex, molecular electronics

Mononuclear organometallic Fe(III) acetylide complexes featuring one unpaired electron attract currently a strong

interest because of their potential in molecular electronics. These complexes, which are stable under several redox states, can be envisioned as electron or spin reservoirs in larger molecular sized-electronic architectures such as molecular nanowires.[1] Species containing the (dppe)(Cp*)Fe–C≡C– fragment, (dppe = 1,2-bis(diphenylphosphino)ethane, Cp* = C₅Me₅) present a so-called piano stool structure. We have previously shown that the a change in the redox state of the Fe center is readily sensed by the coordination sphere of the metal and can be transmitted to rest of the molecule via the alkynyl group.[2] In order to study the electronic effect of a simpler but isolobal ligand to the acetylide on the electronic structure of the Fe(III) ion (3d⁵ low spin, S=1/2) we have now investigated the electronic structure of the [(dppe)(Cp*)Fe–Cl]⁺ complex where the alkynyl group has been replaced by Cl.[3] The induced spin density in the compound [(dppe)(Cp*)Fe–Cl]⁺, PF₆⁻ was thus determined at 2K under an applied field of 7 Tesla in order to experimentally derive the spin delocalization taking place from the Fe³⁺ ion towards the ligands as well as the nature of the Fe(III) orbitals carrying unpaired spin. The experimental results are reported and compared to DFT (Density Functional Theory) calculations performed on this complex.

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