We present the borylene complex $[\mu\text{-B}^t\text{Bu}\{(\eta^5\text{-C}_5\text{H}_5)\text{Mn(CO)}_2\}_2]$[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.

[1] R. F. W. Bader, *Atoms in Molecules - A Quantum Theory*, Oxford University Press, New York, 1990.

[2] P. Macchi, D. M. Proserpio, A. Sironi, *J. Am. Chem. Soc.* 1998, *120*, 13429.

[3] R. Bianchi, G. Gervasio, D. Marabello, *Inorg. Chem.* 2000, *39*, 2360.

[4] L. J. Farrugia, P. R. Mallison, B. Stewart, *Acta Crystallogr.* 2003, *B59*, 234.

[5] P. Macchi, A. Sironi, *Coord. Chem. Rev.* 2003, *238-239*, 383.

[6] C. Gatti, D. Lasi, *Faraday Discuss.* 2007, *135*, 55.

[7] H. Braunschweig, C. Burschka, M. Burzler, S. Metz, K. Radacki, *Angew. Chem.* 2006, *118*, 4458; *Angew. Chem. Int. Ed.* 2006, *45*, 4352.

## MS10 O5

## Experimental spin density in a piano stool FeIII complex

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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* = $\text{C}_5\text{Me}_5$) 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 ($3d^5$ low spin, S=1/2) we have now investigated the electronic structure of the $[(\text{dppe})(\text{Cp*})\text{Fe–Cl}]^+$ complex where the alkynyl group has been replaced by Cl.[3] The induced spin density in the compound $[(\text{dppe})(\text{Cp*})\text{Fe–Cl}]^+$, $\text{PF}_6^-$ was thus determined at 2K under an applied field of 7 Tesla in order to experimentally derive the spin delocalization taking place from the $\text{Fe}^{3+}$ 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.

[1] F. Paul, C. Lapinte, Coord. Chem. Rev. ***178-180*** (1998) 427.

[2] F. Paul, L. Toupet, J.-Y. Thépot, K. Costuas, J. F. Halet, C. Lapinte, Organometallics. 2005, *24*, 5464.

[3] F. Paul, G. da Costa, A. Bondon, N. Gauthier, S. Sinbandhit, L. Toupet, K. Costuas, J.-F. Halet, C. Lapinte, Organometallics 2007, *26,* 874.