X-ray Charge Density of a New Magnetic Metal Organic Framework, $Mn_3(C_8O_4H_4)_3(C_5H_{11}ON)_2$

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A new magnetic metal organic framework material has been synthesized, $Mn_3(C_8O_4H_4)_3(C_5H_{11}ON)_2$.[1] Magnetic susceptibility measurements from 2 to 400 K reveal anti-ferromagnetic ordering at ~4 K and a total magnetic moment of 6.0 μ_B. The magnetic phase transition is confirmed by heat capacity data (2 - 300 K). The crystal structure is studied by conventional single crystal X-ray diffraction data at 300, 275, 250, 225, 200, 175, 150, 125 and 100 K, and synchrotron data at 20 K. The electron distributions around the two unique Mn centers are different, and both have substantial anisotropy. Orbital population analysis reveals large electron donation (1.7 e) to each Mn atom and the maximum possible number of un-paired electrons is 3.2 for both Mn sites. Thus, there is a considerable orbital component to the magnetic moment. Bader topological analysis shows an absence of Mn-Mn bonding and the magnetic ordering is via super-exchange through the oxygen bridges. Formal electron counting suggests mixed valence Mn sites, but this is not supported by the Bader atomic charges, Mn(1)=+0.11, Mn(2)= +0.17. The topological measures show the dominant metal-ligand interactions to be electrostatic, and a simple exponential correlation is derived between Mn-O bond lengths and the values of $\nabla^2\rho$ at the bond critical points.

[1] Poulsen R. D., Bentien A., Chevalier M., Iversen, B. B., *J. Am. Chem. Soc.*, 2005, *submitted*. [2] Poulsen R. D., Bentien, A., Graber T., Iversen B. B., *Acta Cryst.*, 2004, **A60**, 382.

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