

MS24-P5 Investigation on the low temperature distorted phase of MgCr₂O₄Shang Gao^{1,2}, Oksana Zaharko¹, Tom Fennell¹, Vladimir Tsurkan^{3,4}, Christian Rueegg^{1,2}

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Despite extensive studies of the spinel ACr₂O₄ systems, some basic questions still remain to be addressed [1-2]. What is the low temperature (LT) nuclear structure? How does this structural distortion influenced the Cr³⁺ spin configuration? And, perhaps the most crucial one for understanding their spin dynamics, what is the exchange strength in the distorted phase? Here, using synchrotron/neutron diffraction and neutron scattering methods, we tried to answer these questions on MgCr₂O₄. Powder synchrotron diffraction shows that the LT structure belongs to the *Fddd* space group, which contradicts previous [4], and space group determined from neutron diffraction but is consistent with the magnetic resonance measurements on the related ZnCr₂O₄ compound [3]. Based on *Fddd* space group, magnetic structure was solved from single crystal neutron diffraction data with both symmetry analysis and simulated annealing methods. Finally, we discussed the spin dynamics in MgCr₂O₄ measured with both hot and cold triple-axis spectrometers.

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Keywords: spinel, spin-lattice coupling, neutron scattering, synchrotron x-ray diffraction

MS24-P6 Mn(H₂O)_{1.5}(C₁₄H₈O₄), a magnetic MOF with a double inorganic sub-networkMichel Francois¹, Romain Sibille²

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Two new magnetic Metal Organic Frameworks (MOFs) were synthesized by solvothermal reaction in the system Mn-C₁₄H₈O₄ (biphenyldicarboxylate = bpdcc)-H₂O. Mn(H₂O)_{1.5}(C₁₄H₈O₄) **1** (SG = C2/c, Z = 8, Dx = 1.67 g/cm³, a = 53.329(2) Å, b = 6.4911(2) Å, c = 7.4036(2) Å, b = 90.59(1)°, V = 2562.8 Å³, R₁ = 8.5%), and Mn₂(OH)₂(C₁₄H₈O₄) **2** (SG = P-1, Z = 1, Dx = 1.927 g/cm³, a = 14.2039(4) Å, b = 6.4785(1) Å, c = 3.4530(3) Å, a = 90.09(1)°, b = 96.84(2)°, g = 91.710(2)°, V = 315.34 Å³, R₁ = 6.8%). The crystal structures of **1** and **2** were solved from synchrotron powder diffraction data using optimization methods in direct space with the FOX program [1], and refined using the Rietveld method. The complexity of **1** needed additional information from IR spectroscopy and thermogravimetric analysis. Compound **1** has a lamellar structure built up from a double inorganic sub-network. It consists of two slabs of metallic ions differing by their hydration: (i) a layer of composition Mn(H₂O)₂, already encountered in Mn(H₂O)₂(C₈H₄O₄) [2], where manganese cations are inside an octahedral environment, and (ii) an original layer with composition Mn(H₂O) where manganese is five-fold O-coordinated in a triangular deformed bi-pyramid. These two slabs are bridged by the benzene biphenyldicarboxylate molecule along the stacking direction corresponding to the long period of 53.32 Å. This original structure influences the magnetic properties. Alternative susceptibility shows two magnetic transitions attributed to the two sub-networks ordering at two different temperatures. Two anomalies at the same temperatures in the heat specific measurement confirm this scenario. Notably, only one magnetic hybrid compound featuring two different inorganic layers was reported before [3]. The layered structure of **2** is isorectangular with that of Cu₂(OH)₂(C₈H₄O₈) [4]. The dicarboxylate molecules bridge the single inorganic slab with composition 'Mn(OH)₂' where Mn atoms are in an octahedral environment.

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