[*C5.* J. Manson] Neutron diffraction study of a molecule-based 2-dimensional magnetic compound $Mn(dca)_2(pym)(H_2O)$: spin density and magnetic phase diagram.

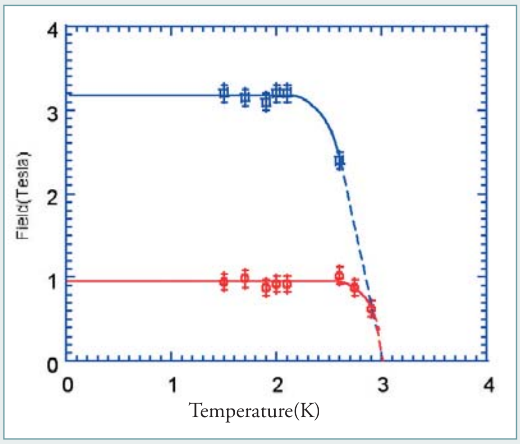

Figure 1. Magnetic phase diagram (H,T) of $Mn(dca)_2(pym)(H_2O)$.

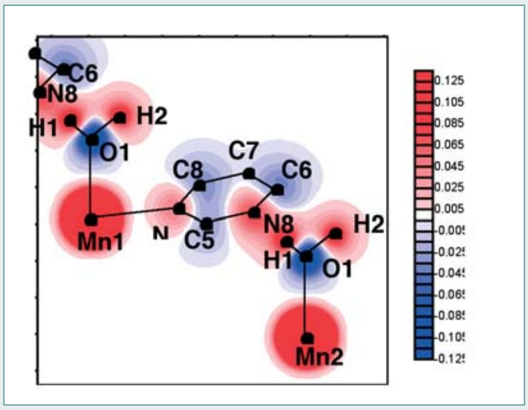

Figure 2. Induced spin density projection along the perpendicular to the O1H1N8 plane at 5 K under 4.5 T

The $Mn^{II}(dca)_2(pym)(H_2O)$ compound (with dca = $N(CN)_2$ and pym = $N_2C_4H_4$) presents a 2-dimensionnal structure formed by layers in which the Mn^{2+} ions are alternately related by single or double (-NC-N-CN-) dicyanamide bridges. These layers, stacked along the *c*-axis, are connected by hydrogen bonds between the coordinated water molecules and N atoms of the pyrimidine rings and of the dicyanamide groups. The magnetic phase diagram established by single-crystal diffraction is reported in Fig. 1. In the AF1 structure, the antiferromagnetic ordered Mn^{2+} layers are AF-coupled to each other, while in the AF2 phase, above the spin flop transition, the layers are ferromagnetically coupled. In order to investigate the magnetic interaction pathways in this compound, particularly between the layers, the induced spin density has been determined by polarised neutron diffraction in the paramagnetic state at 5 K under a field of 4.5 T. The spin density map shown in Fig. 2 clearly evidences a positive spin density on the hydrogen atom of the N8..H1-O1 hydrogen bond, which overlaps with the positive density of the nitrogen atom N8 of the pyrimidine ring. This overlap favors AF coupling between the layers in zero field.

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[*C.6.* A. Goujon] Photoswitchable molecular compounds studied by neutron powder diffraction.

Determining the magnetic structure of photoswitchable magnets is a main goal to understand the mechanism of photo-excitation. Neutron powder diffraction reveals the magnetic structure of compounds and provides an understanding of magnetic and structural correlations (nature, length scale). A dedicated sample holder has been designed to allow photoexcitation measurements to be performed *in situ* on the powder spectrometer G4-1. Ancillary equipments, such as a pulsed laser (Nd:YAG, *Minilite II*) or optical fibers, were also installed on G4-1. The design of the sample holder takes into account the need *(i)* to work with about 1 g of powder, and *(ii)* to illuminate homogeneously the majority of the powder in order to induce sizeable photo-conversion. Photoexcitation of a $[Fe_{0.52}Zn_{0.48}(btr)_2(NCS)_2](H_2O)$ powder was carried out at 15 K using a pulsed laser light (λ = 532 nm). At low temperature, the spin conversion is easily obtained by LIESST (light-induced excited spin state trapping) effect, and accompanied by huge structural changes. Fig. 1 shows a comparison between the low-spin (LS) state spectrum and the photoinduced state obtained after 20 hours. A mixing of the LS and photoinduced HS fractions was evidenced, indicating that 30% of the sample was converted to the HS state. The kinetics of the photoexcitation is shown in Fig. 2. The partial photoconversion is well explained by the strong absorption of the powder. This result is encouraging and further work is underway to increase the yield of photoexcitation.

[A. Goujon, B. Gillon, G. André, A. Gukasov, LLB]

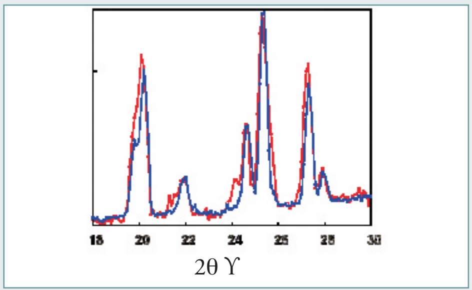

Figure 1. Diffraction pattern of Fe (btr) measured at 2 K (blue): LS state; (red): after 20 hours of photoexcitation.

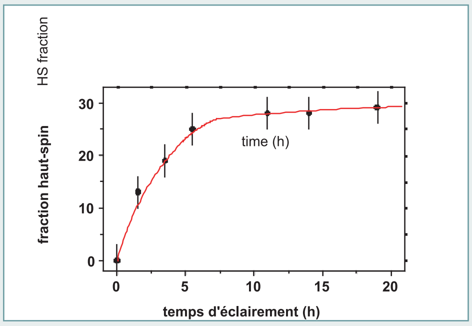

Figure 2. Kinetics of the photoexcitation in In $[Fe_{0.52}Zn_{0.48}(btr)_2(NCS)_2](H^2O)$ at T = 15 K.