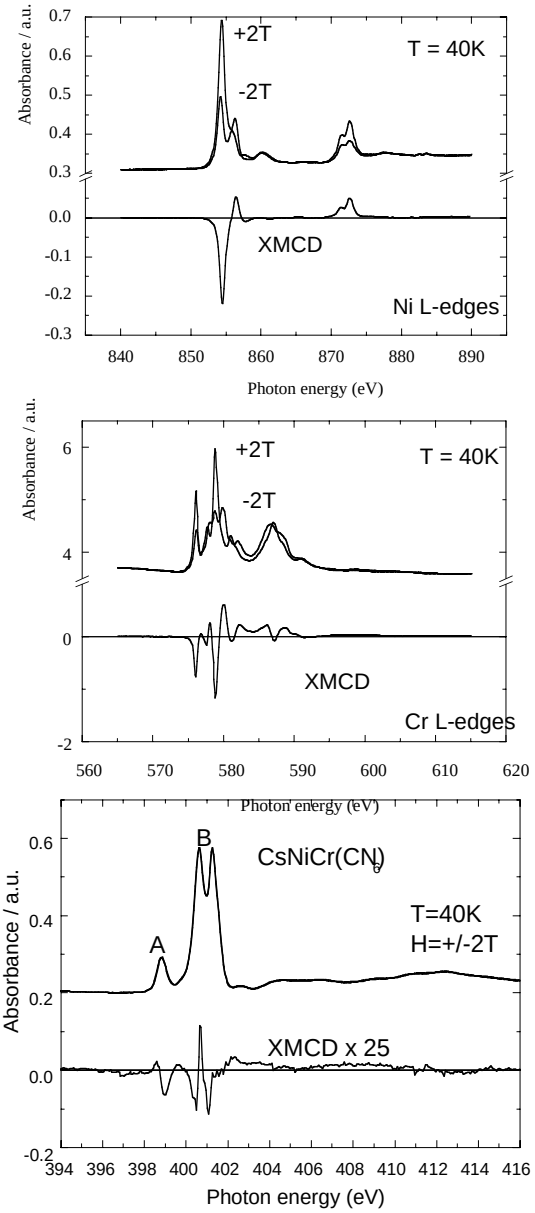
HE-1427: XMCD at Nitrogen K-edge.

We are engaged in the synthesis of new molecule based magnets of formula $Cs^{I}[A^{II}Cr^{III}(CN)_6]$ (A^{II} = transition metal), with a three-dimensional Prussian-Blue structure. The divalent A^{II} and trivalent Cr^{III} ions are coupled through the cyano (CN) bridges. Varying the nature and the stoechiometry of the A^{II} cation, we can control the macroscopic magnetic properties as the nature of the exchange interaction between the cations or the T_C temperature. Since no single crystals are available for this series, we are measuring the local magnetic properties by XMCD to get insight on the magnetic properties and coupling.



For the $Cs^{I}[Ni^{II}Cr^{III}(CN)_6]$ compound (T_C = 90K), we have recorded the XMCD signals at the $L_{2,3}$ edges of chromium nickel transition metal ions and at the nitrogen K edge (H = $\pm$2T, T = 40K) (see Figures). We have checked that the samples are stable under the beam of ID8 and that charging effects could be eliminated by appropriate sample preparation.

We have analysed the $L_{2,3}$ edges of the transition elements and the corresponding dichroic signals through Ligand Field Multiplet calculations. In the calculations, hybridisation has to be taken into account due to the large covalence of the CN bond.

Since the cyano bridge plays such an important role in this series of compounds, the need for measuring the local magnetic properties of nitrogen is obvious. At the nitrogen K edge, a small (1 %) XMCD signal has been measured. It is a very structured signal where feature A could be attributed to hybridisation with the 3d transition ion orbitals and B feature is the antibonding molecular orbital of the cyano bridge. Though it is well known that XMCD at K edges is not a direct measure of local spin polarisation, it has nevertheless been shown that it is related to the magnetic moment carried by the p orbitals and to the spin polarisation of the magnetic neighbours. Quantitative information can only be obtained by *ab initio* calculations. Such calculations developed for a semirelativistic Hamiltonian are in progress.

We have had no shift allocated for this project and these results were obtained thanks to ID8 “in-house” beamtime.