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Experiment Report Form

	Experiment title: Solid state and solution X-ray Natural, Magneto-Circular and Magneto-Chiral dichroism of the nonanuclear Mn(III) chiral single molecule magnet, Mn9.	**Experiment number**: CH-5357
Beamline: ID12	**Date of experiment**: from: 6/6-2018 to: 12/6-2018	**Date of report**: 12.09.2022
Shifts: 18	**Local contact(s)**: Andrei Rogalev, Fabrice Wilhelm	*Received at ESRF:*

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Report:

This beamtime was allocated to continue the measurements on $[Mn_9O_4(Me\text{-}sao)_6(LipO)_3(MeO)_3(MeOH)_3](Cl)$ (Mn_9), Me-saoH_2 = methylsalicylaldoxime, LipOH = lipoic acid (see the previous experimental report CH-5014). This time the measurements should be carried out on single crystals of Mn_9, in order to observe the XNCD and XMChiD of Mn_9. However, the crystals grown were not of a size suitable for measuring XNCD or XMChiD. Therefore, measurements were performed on back-up samples of $Na_5[Ho(ODA)_3](BF_4)_2\cdot 6(H_2O)$ where ODA^{2-} = oxydiacetate.

The results of the measurements on $Na_5[Ho(ODA)_3](BF_4)_2\cdot 6(H_2O)$ have been published (***Chem. Sci.***, 2020,**11**, 8306-8311) and were highlighted by the ESRF (https://www.esrf.fr/Apache_files/Highlights/2020/119-ESRF-Highlights-2020.html#/page/118). Since the results are published we simply put the abstract of the paper here and otherwise refer to the full paper in Chemical Science for further information.

Abstract of published paper

Magnetochiral dichroism (MXD) originates in the coupling of local electric fields and magnetic moments in systems where a simultaneous break of space parity and time-reversal symmetries occurs. This magnetoelectric coupling, displayed by chiral magnetic materials, can be exploited to manipulate the magnetic moment of

molecular materials at the single molecule level. We demonstrate herein the first experimental observation of X-ray magnetochiral dichroism in enantiopure chiral trigonal single crystals of a chiral mononuclear paramagnetic lanthanide coordination complex, namely, holmium oxydiacetate, at the Ho L_3-edge. The observed magnetochiral effect is opposite for the two enantiomers and is rationalised on the basis of a multipolar expansion of the matter–radiation interaction. These results demonstrate that 4f–5d hybridization in chiral lanthanoid coordination complexes is at the origin of magnetochiral dichroism, an effect that could be exploited for addressing of their magnetic moment at the single molecule level.