

	Experiment title: Natural Circular Dichroism in the X-ray Region...	Experiment number: HE-421
Beamline: ID12A	Date of experiment: from: 4 Dec 1998 to: 8 Dec 1998	Date of report: 27 Feb 1999
Shifts: 12	Local contact(s): Andrei Rogalev	<i>Received at ESRF:</i>

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Report:

One is always at the mercy of nature to some extent with regard to the growth of suitable quality enantiomorphic crystals of the correct habit and dimensions for this work. Unfortunately on this occasion we encountered crystal growth problems with some of the originally proposed samples and beam decomposition with the rest. However, the beamtime was used successfully to make two significant series of measurements using backup materials.

(1) Sm L edge XNCD

$\text{Na}_3\text{Sm}(\text{dig})_3 \cdot 2\text{NaBF}_4 \cdot 6\text{H}_2\text{O}$ axial single crystals. XNCD spectra were obtained at the Sm L_1 and $L_{2,3}$ edges. This represents the first XNCD at a rare earth L_1 edge. Data are under analysis using methods developed for our earlier Nd L_3 edge study [1]. This will allow us to examine the anomalous position of the 2p-4f quadrupole excitation at the Sm L_2 edge and to test the L edge XNCD sum rule [2] for the first time with a rare earth photo-absorber.

[1] L Alagna, T Prosperi, S Turchini, J Goulon, A Rogalev, C Goulon-Ginet, C R Natoli, R D Peacock and B Stewart and, *Phys Rev Letters*, **80**, 4799 (1998).

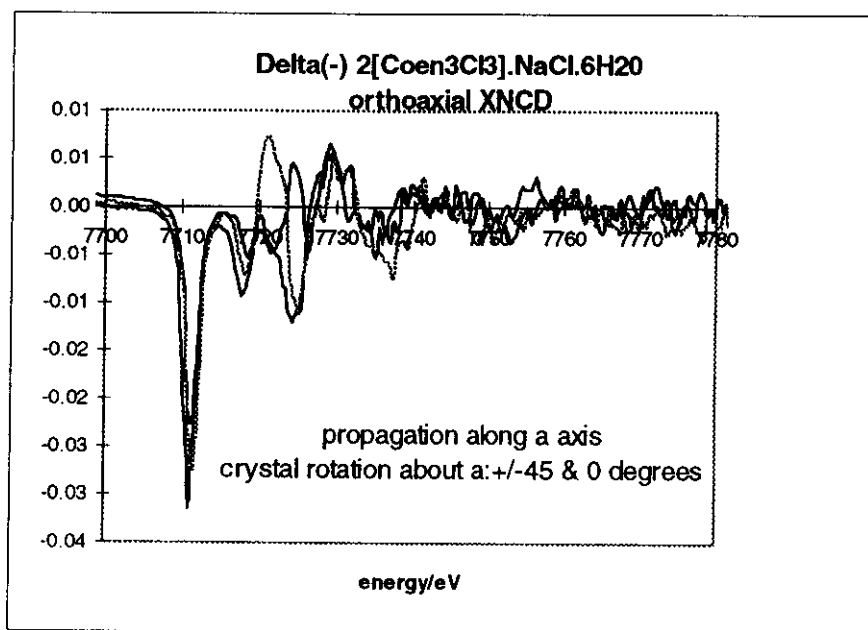
[2] C R Natoli, Ch Brouder, Ph Saintavit, J Goulon, Ch Goulon-Ginet and A Rogalev, *Eur Phys J B*, **4**, 1 (1998)

(2) Co K edge XNCD for biaxial crystal orientation.

$2[\text{Co}(\text{en})_3]\text{Cl}_3 \cdot \text{NaCl} \cdot 6\text{H}_2\text{O}$ single crystals were investigated with beam incident on a biaxial face and as a function of rotation of the crystal around the beam direction (see Figure below).

Comparison with previous measurements on the crystal uniaxial face shows that it is possible to separate linear and circular dichroic effects. The 1s-3d pre-edge feature at ca. 7712eV shows an opposite sign XNCD for uniaxial and biaxial observation directions, consistent with the expectations of the E1-E2 mechanism [3]. There is a weak superimposed angular dependence due to the $\sim 10\%$ dipolar character in this transition as found in a recent ab-initio calculation [4]. In contrast, the crystal rotation reveals strong dipolar transitions in the edge region (7715-7745 eV). These are currently the subject of a polarised xanes calculation. In the xanes region (above 7745 eV) there is again an opposite sign behaviour for axial and orthoaxial spectra and essentially no crystal rotation dependence.

These results are extremely significant with regard to the general possibility of measuring XNCD in optically anisotropic crystal systems. We believe that our observations may be interpretable using the minor linear component of polarisation in the beam and there appears to be no significant interference from linear birefringence and optical rotation effects.



[3] A D Buckingham & M B Dunn, J Chem Soc A, 1988 (1971).

[4] B Stewart, R D Peacock, et al., Nature submitted and unpublished work, 1998-99.