	Experiment title: NATURAL CIRCULAR DICHROISM IN THE X-RAY REGION	Experiment number: HE-022
Beamline: BL6	**Date of Experiment:** from: 18/9/96 to: 23/9/96	**Date of Report:** 26/02/97
Shifts: 15	**Local contact(s):** J. Goulon, C. Ginet-Goulon, A. Rogalev	*Received at ESRF :* **2 8 FEV. 1997**

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Report:

Natural Circular Dichroism in the X-ray Region
of the two isomers (+) and (-) $Na_3Nd(C_4H_4O_5)_3 2NaBF_4 6H_2O$ single crystals.

From the results obtained during the first allocated beamtime (experiment CH-42) it was necessary to discriminate experimentally between a macroscopic non-enantiomeric differential effect of the order of 10^{-2} shown by the two crystals and a weaker enantiomeric structureless effect of the order of 10^{-3}, which was necessarily overwhelmed by the stronger signal, and at that time could be disentangled only with a normalization procedure; the resulting spectra were shown in the previous report.

In the present continuation (experiment HE-022) of the project on natural circular dichroism (CD) at the L_3 edge of the title compounds we have benefited from the improved experimental conditions achieved for BL6, as of September 1996 in the optics, sample positioning and the detection system which have allowed better statistics and data reproducibility than those obtained in June 1995 for the same chemical compounds.

Moreover a carefully chosen time sequence of the polarization inversion at HELIOS2 allowed the elimination of spurious effects such as time dependent radiation damage decomposition and/or electronic drift that would hamper a data analysis based just on raw data handling.

Exploiting the fact that the automatic data acquisition routine takes spectra at regular intervals of time, we used a simple procedure in order to eliminate the possible spurious signals.

Given that the phase-time sequence is

$(+)1_{st} (-)2_{nd} (-)3_{rd} (+)4_{th}$

and defining D the dichroic signal and S the spurious distortion we can construct the differences in a consecutive range of spectra as:

$(-)2_{nd}-(+)1_{st}=D-S$

$(-)3_{rd}-(+)4_{th}=D+S$

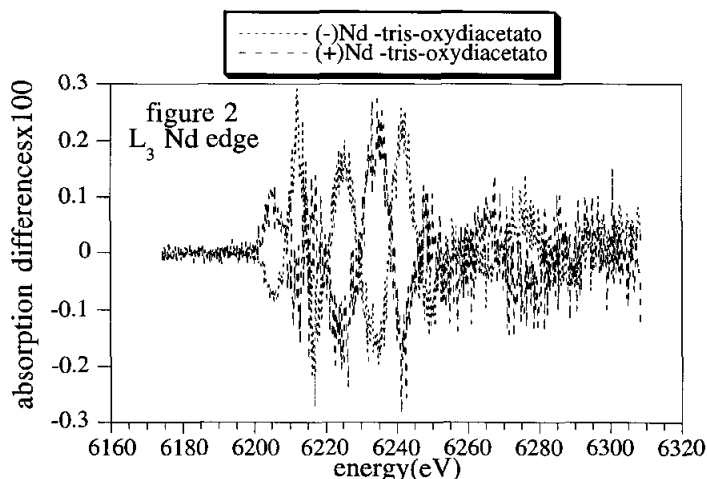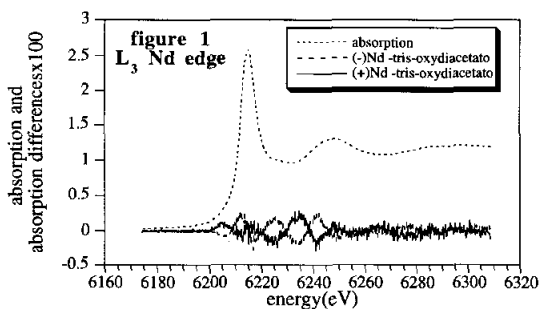according to the convention that the dichroic signal is related to the difference $I_{(-)}-I_{(+)}$.

By taking the apprpriate combination of differences, it is possible to eliminate the parameter S.

In this way we have the possibility to distinguish between the effect due to possible crystal damage or drift (which are phase independent) and the dichroic effect (which is phase dependent).

$[(-)2_{nd}-(+)1_{st}]+[(-)3_{rd}-(+)4_{th}]/2=D$

Thus obtaining the dichroic signal.

Clear enantiomeric spectra, every structure of an isomer being reversed for the other, are obtained as shown in figure 1 and in the enlarged figure 2 when this procedure is applied to the L_3 spectra of the two enantiomers .

figure 1
L_3 Nd edge

.... absorption
- - - - (-)Nd -tris-oxydiacetato
——— (+)Nd -tris-oxydiacetato

.... (-)Nd -tris-oxydiacetato
- - - - (+)Nd -tris-oxydiacetato

figure 2
L_3 Nd edge

More work on the interpretation of the spectra for the preparation of a full paper is under way.