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X-ray optical activity in crystals of coordination complexes

Elen Duverger-Nédellec,¹ Elizabeth A. Hillard,¹ Patrick Rosa,¹ Philippe Saintavit,² James Ablett,³ Fabrice Wilhelm,⁴ Andrei Rogalev⁴

¹Univ. Bordeaux, CNRS, Bordeaux INP, ICMCB, UMR 5026, F-33600 Pessac, France

²IMPMC, CNRS, Sorbonne Université, Muséum National d'Histoire Naturelle, UMR 7590, 75252 Paris, France

³Synchrotron SOLEIL, L'Orme des Merisiers, BP 48, 91192 Saint Aubin, France

⁴European Synchrotron Radiation Facility (ESRF), 38043 Grenoble, France

E-mail: elizabeth.hillard@icmcb.cnrs.fr

Natural Circular Dichroism (NCD), the differential absorption of right- and left-circularly polarized light, is a workhorse technique for the stereochemical characterization of molecules and macromolecules. While this technique is most often applied in the UV-visible energy range, core-level optical activity using X-rays demonstrates some unique features such as element specificity and orbital selectivity, but is limited to single crystal measurements.¹ The majority of X-ray Natural Circular Dichroism (XNCD) studies have been performed using synchrotron sources, especially the ESRF ID12 at the K-edge of light transition metals² or at the L_{2,3}-edge of heavier atoms, such as lanthanides.³

Our work is devoted to extending X-ray optical activity to new techniques and molecular crystals, especially those based on coordination complexes. To this end, we have recently observed the first example of Resonant Inelastic X-ray Scattering – NCD (RIXS-NCD) at the GALAXIES beamline at the SOLEIL synchrotron. We have also recently investigated at the ID12 optically active but non-chiral systems and fully characterized the polar and azimuthal dependence of a tetragonal crystal system, thus supporting theoretical predictions.⁴

These new results will be presented in conjunction with a presentation of our approach to the conception and synthesis of model systems.

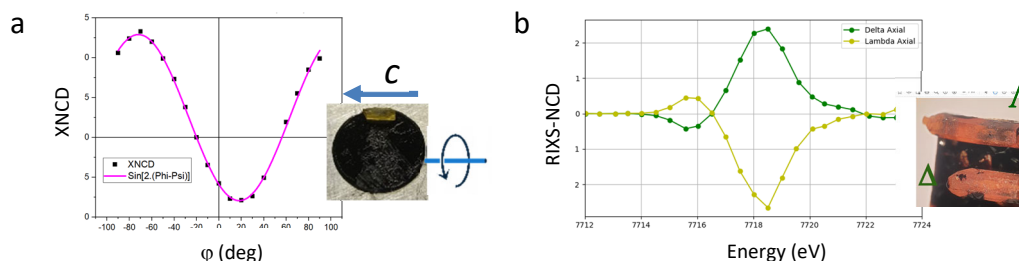


Figure a) Angular (azimuthal) dependence of the XNCD intensity of an achiral iron coordination complex; b) RIXS-NCD of enantiomers of a chiral cobalt complex.

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