



HAL
open science

X-ray optical activity in achiral crystals of coordination complexes

Elen Duverger-Nédellec, Elisabeth A. Hillard, Patrick Rosa, Ph. Saintavit,
Marie-Anne Arrio, Fabrice Wilhelm, Andrei Rogalev

► **To cite this version:**

Elen Duverger-Nédellec, Elisabeth A. Hillard, Patrick Rosa, Ph. Saintavit, Marie-Anne Arrio, et al.. X-ray optical activity in achiral crystals of coordination complexes. 1st French-German Young Crystallographers' Meeting, DKG - German Society for Crystallography; AFC - French Crystallography Association, Sep 2023, Strasbourg, France. hal-04630918

HAL Id: hal-04630918

<https://hal.science/hal-04630918v1>

Submitted on 1 Jul 2024

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

ABSTRACTS - PHYSICS

P06

X-ray optical activity in achiral crystals of coordination complexes

Elen Duverger-Nédellec,¹ Elizabeth A. Hillard,¹ Patrick Rosa,¹ Philippe Saintavit,² Marie-Anne Arrio,² Fabrice Wilhelm,³ Andrei Rogalev³

¹ Univ. Bordeaux, CNRS, Bordeaux INP, ICMCB, UMR 5026, F-33600 Pessac, France; ² IMPMC, CNRS, Sorbonne Université, Muséum National d'Histoire Naturelle, UMR 7590, 75252 Paris, France; ³ European Synchrotron Radiation Facility (ESRF), 38043 Grenoble, France

Natural Circular Dichroism (NCD), the differential absorption of right- and left-circularly polarized light, is an efficient technique, widely used in pharmacology, for absolute configuration determination of chiral 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 reported in the literature have been performed using synchrotron sources, especially the ESRF ID12 beamline at the K-edge of light transition metals² or at the L_{2,3}-edge of heavier atoms, such as lanthanides.³

XIMTEX project (Experimental investigation of microscopic theory of Natural Circular Dichroism using X-rays) aims to explore XNCD signal produced by coordination complexes, understand the influence of the metal, the ligands and the symmetry on the shape and intensity of the signal and experimentally verify the XNCD theoretical angular dependencies predicted by Natoli et al.⁴ using model compounds. Investigations were performed at the ID12 beamline on the model compounds [FeCl₄][PPh₄] and [CuCl₄][TEA][TMA] crystallizing in the achiral tetragonal space groups *I*-4 and *P*-4₂*m*, respectively. For the first time, it was proved that achiral systems can generate XNCD. The polar and azimuthal dependences of these crystal systems were fully characterized, supporting theoretical predictions.⁴

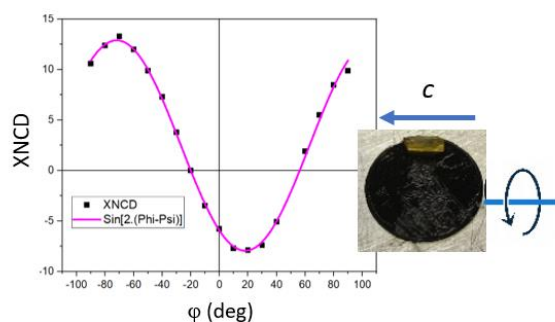


Figure 1: Angular (azimuthal) dependence of the XNCD intensity of an achiral iron coordination complex.

References:

- (1) Goulon, J.; Rogalev, A.; Brouder, C. X-Ray Detected Optical Activity. In *Comprehensive Chiroptical Spectroscopy*; John Wiley & Sons, Ltd, 2011; pp 457–491. <https://doi.org/10.1002/9781118120187.ch17>.
- (2) Srinivasan, A.; Cortijo, M.; Bulicanu, V.; Naim, A.; Clerac, R.; Saintavit, P.; Rogalev, A.; Wilhelm, F.; Rosa, P.; Hillard, E. A. Enantiomeric Resolution and X-Ray Optical Activity of a Tricobalt Extended Metal Atom Chain. *Chem. Sci.* 2018, 9 (5), 1136–1143. <https://doi.org/10.1039/c7sc04131d>.
- (3) Mitcov, D.; Platonov, M.; Buch, C. D.; Reinholdt, A.; Døssing, A. R.; Wilhelm, F.; Rogalev, A.; Piligkos, S. Hard X-Ray Magnetochiral Dichroism in a Paramagnetic Molecular 4f Complex. *Chem. Sci.* 2020, 11 (31), 8306–8311. <https://doi.org/10.1039/D0SC02709J>.
- (4) Natoli, C. R.; Brouder, C.; Saintavit, Ph.; Goulon, J.; Goulon-Ginet, C.; Rogalev, A. Calculation of X-Ray Natural Circular Dichroism. *Eur. Phys. J. B* 1998, 4 (1), 1–11. <https://doi.org/10.1007/s100510050344>.

