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ABSTRACTS - PHYSICS

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X-ray optical activity in achiral crystals of coordination complexes

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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

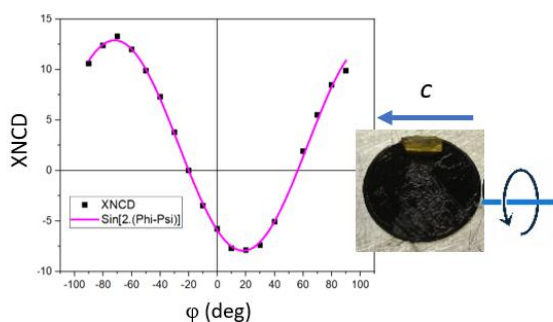


Figure 1: Angular (azimuthal) dependence of the XNCD intensity of an achiral iron coordination complex.

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