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► **To cite this version:**

Elisabeth A. Hillard, Elen Duverger-Nédellec, Patrick Rosa, Ph. Saintavit, Marie-Anne Arrio, et al..  
X-ray natural optical activity beyond chirality. Congrès de l'Association Française de Cristallographie  
- AFC 2024, AFC, Jul 2024, Montpellier, France. hal-04752203

**HAL Id: hal-04752203**

**<https://hal.science/hal-04752203v1>**

Submitted on 24 Oct 2024

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# X-ray Natural Optical Activity beyond Chirality

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## Abstract

While optical activity in achiral space groups was predicted by Gibbs as long ago as 1882 [1], linear and circular birefringence effects hamper the measurement of circular dichroism in the UV-vis energy ranges [2]. We have used tender X-rays at the ESRF beamline ID12 to examine Natural Circular Dichroism (XNCD) [3] at the K-edges of copper and iron coordination salts respectively belonging to the achiral, but optically active, point groups  $D_2d$  and  $S_4$ . The angular dependence of the XNCD signals was revealed with respect to the polar axis, theta, as well as the azimuthal axis, phi, by careful orientation of millimetric-sized crystals in the X-ray beam. In the case of  $D_2d$ , the XNCD followed the expected angular dependence in theta and phi [3]. However, for  $S_4$ , an offset of about  $27^\circ$  in phi was observed and the more complicated angular dependence was ostensibly not respected. This result was subsequently confirmed using Resonant Inelastic X-ray Scattering-NCD at the SOLEIL synchrotron, in the first example of this RIXS-NCD technique, and can be rationalized using symmetry arguments.

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[2] a) R. Gautier, J. M. Klingsporn, R. P. Van Duyne and K. R. Poeppelmeier, Nature Mater, 2016, 15, 591–592; b) B. Kahr, A. T. Martin and K.-H. Ernst, Chirality, 2018, 30, 378–382; c) L.-L. Xu, H.-F. Zhang, M. Li, S. W. Ng, J.-H. Feng, J.-G. Mao and D. Li, J. Am. Chem. Soc., 2018, 140, 11569–11572; d) Y. Li, X. Ma, X. Xu, Y. Ye and B. Wang, Chem. Eur. J., 2023, 29, e202203534.

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Acknowledgments: We thank the French Agence National de la Recherche for funding via the XIMTEX (PCR ANR-21-CE29-0032) project.