## Structural and magnetic transformations from CuCl to $Cu_2Cl(OH)_3$ induced by $H_2O$ and $CuCl_2$

 $D. P. Pimentel^{1)}$ 

Institute of Physics Gleb Wataghin (IFGW), University of Campinas (UNICAMP), 13083-859 Campinas, Sao Paulo, Brazil
Federal Institute of Maranhão, IFMA-PPGEM, Avenida Getúlio Vargas, 4, CEP 65030-005 Sao Luis, MA, Brazil
PPGCM-Materials Science and Engineering Graduate Program, UFPI-Federal University of Piaui, 64049-550 Teresina, PI, Brazil

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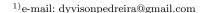
Introduction. This study investigates the oxidation dynamics of "pure" CuCl during prolonged environmental exposure using X-ray diffraction and temperature-dependent magnetization measurements. Traditionally considered diamagnetic [1,2], CuCl reveals an antiferromagnetic transition at 4.7 K, potentially induced by the integration of water molecules into the CuCl matrix [3]. The hydration process initiates oxidation reactions that transform CuCl into Cu<sub>2</sub>Cl(OH)<sub>3</sub>, as confirmed by X-ray analysis and magnetization measurements, which show magnetic transitions at 6.4 and 16 K.

**Experimental techniques.** CuCl powder samples with 99.9 % purity were analyzed using a SQUID magnetometer (MPMS-7) and a high-precision X-ray diffractometer (D2 PHASER).

## Results and discussions.

X-ray diffraction (XRD) analysis. Time-resolved X-ray diffraction analysis revealed that after 24 h of air exposure, incipient secondary phases become detectable, with their intensities increasing over time. After six weeks, the characteristic peaks of CuCl disappear, indicating a complete conversion to Cu<sub>2</sub>Cl(OH)<sub>3</sub>. This transformation is driven by atmospheric moisture, confirming the total phase transition of CuCl. The proposed reaction is:  $6\text{CuCl} + 3\text{H}_2\text{O} + 3/2\text{O}_2 \rightarrow 2\text{Cu}_2\text{Cl}(O\text{H})_3 + 2\text{CuCl}_2$ . The resulting CuCl<sub>2</sub> may further react with water as follows:  $4\text{CuCl}_2 + 6\text{H}_2\text{O} + \text{O}_2 \rightarrow 4\text{Cu}_2\text{Cl}(O\text{H})_3 + 2\text{CuCl}_2$  [4]. Eventually yielding Cu<sub>2</sub>Cl(OH)<sub>3</sub> as the predominant phase.

Magnetic analysis. Magnetization measurements under Zero-Field Cooling (ZFC) and Field Cooling (FC) conditions revealed magnetic transitions at approximately 16 and 6.4 K. Significant negative magnetiza-



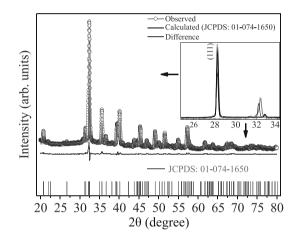


Fig. 1. (Color online) Rietveld diffractogram for CuCl after 6 weeks of exposure to the environment, showing the total transformation of CuCl into Cu<sub>2</sub>Cl(OH)<sub>3</sub>, as noted on the card: JCPDS: 01-074-1650. The appearance of the peak at  $2\theta = 32.22^{\circ}$ , corresponding to the (11-2) plane reflection of Cu<sub>2</sub>Cl(OH)<sub>3</sub>, and the decrease in intensity at  $2\theta = 28.49^{\circ}$  corresponding to the (111) plane reflection of CuCl, insertion of the figure

tion under ZFC conditions is attributed to intense spin interactions between copper ions and intercalated water molecules. A notable increase in magnetization with prolonged environmental exposure is observed. Magnetic hysteresis curves confirm the coexistence of ferromagnetism and antiferromagnetism in oxidized CuCl. The presence of horizontal and vertical shifts in the hysteresis curves suggests an exchange bias phenomenon [5–7], indicating interactions between ferromagnetic and antiferromagnetic phases. Exposure of CuCl to the environment for eight weeks revealed signatures of antiferromagnetic transitions at 6.4 and 16 K, with divergent behavior between ZFC and FC curves. Oscillatory patterns in magnetization indicate possible spin reorientations, potentially due to the exchange bias effect [8–10].

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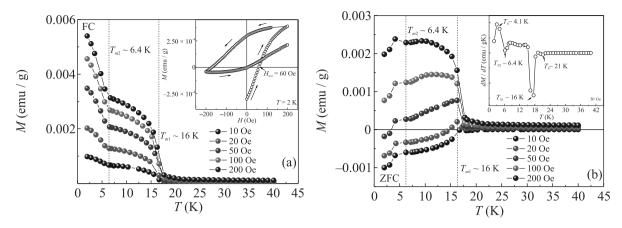


Fig. 2. (Color online) ZFC-FC magnetization of CuCl after 2 weeks of oxidation, measured under various magnetic fields. The inset of (a) displays the hysteresis loop at  $2 \, \mathrm{K}$ . (b) – The inset shows the derivative of magnetization as a function of temperature for the ZFC curve measured at  $50 \, \mathrm{Oe}$ 

Conclusion. The study demonstrates that prolonged exposure of CuCl to the environment leads to its complete transformation into Cu<sub>2</sub>Cl(OH)<sub>3</sub> due to water absorption, resulting in complex and intriguing magnetic behaviors, including ferromagnetism and antiferromagnetism. These findings offer new perspectives for exploring the magnetic properties of Cu<sub>2</sub>Cl(OH)<sub>3</sub> and their potential applications in advanced materials.

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Conflict of interest. The author declares no conflict of interest.

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