

# Structure resolution of the new $\text{Ca}_2\text{MnO}_3\text{X}$ ( $\text{X} = \text{Cl}, \text{Br}$ ) oxyhalides

Christophe LEPOITTEVIN (Institut Néel, CNRS and Université Grenoble Alpes, Grenoble)

Fabio DENIS ROMERO (Institut Néel, CNRS and Université Grenoble Alpes, Grenoble)

Stéphanie KODJIKIAN (Institut Néel, CNRS and Université Grenoble Alpes, Grenoble)

Claire V. COLIN (Institut Néel, CNRS and Université Grenoble Alpes, Grenoble)

## Abstract

Mixed anion oxyhalides with the general formula

$\text{Ca}_2\text{MnO}_3\text{X}$  ( $\text{X} = \text{Cl}, \text{Br}$ ) were synthesized using solid-state reaction

methods. These two materials crystallize in a novel structure type

due to the small ionic radius of  $\text{Ca}^{2+}$  and the strong Jahn-Teller

effect of  $\text{Mn}^{3+}$ . The structure model was obtained using combination of 3D Electron Diffraction and STEM HAADF

imaging, and refined against X-ray powder diffraction data. The resulting structure (space group  $\text{Cmcm}$ ) consists on one-

dimensional chains of  $\text{MnO}_4$  square planes, with an

angle of  $\sim 120^\circ$  between neighboring planes. At low temperatures,

the two materials adopt magnetic arrangements, with ferromagnetic

chains coupled antiferromagnetically.