

# Experimental report

15/03/2017

**Proposal:** 5-31-2267

**Council:** 10/2012

**Title:** Crystal and magnetic structures of the  $\text{CaFe}_{2+n}\text{O}_{4+n}$  family members

**Research area:** Materials

**This proposal is a new proposal**

**Main proposer:** Yohann BREARD

**Experimental team:** Denis PELLOQUIN  
Charlene DELACOTTE  
Yohann BREARD

**Local contacts:** Emmanuelle SUARD

**Samples:**  $\text{CaFe}_5\text{O}_7$

Instrument	Requested days	Allocated days	From	To
D2B	3	3	22/02/2013	25/02/2013

## Abstract:

we have revisited the Ca-Fe-O system, focusing our attention on the family  $\text{CaFe}_{2+n}\text{O}_{4+n}$ . Terms  $n = 1, 2$  and  $3$  have been isolated as single phase bulk ceramics-the syntheses are reproducible. Firstly, we have shown by building of the reciprocal spaces (E.D.) at room temperature that the real symmetry of compounds is not orthorhombic (as it was reported) but monoclinic (S.G. P21). Moreover, X-ray Le bail refinements Vs temperature, reveal that oxides go through a structural transition TS ( $TS = 350\text{K}$  for  $n = 3$ ,  $TS = 330\text{K}$  for  $n = 2$  and  $TS = 300\text{K}$  for  $n = 1$ ). This has been clearly confirmed by E.D. observations for which extra dots are detected at  $T < TS$ . Adding to that, the thermal dependences of the magnetic susceptibility and electronic conductivity show transitions at  $T = TS$  indicating an electro-magneto-structural coupling which has never been reported. we ask for 3 days of beam time on the D2b diffractometer which would allow us to perform structural and magnetic characterizations

Magnetodielectric effect in crystals of the non centrosymmetric CaOFeS at low temperature  
by C. Delacotte, O. Pérez, A. Pautrat, D. Berthebaud, S. Hébert, E. Suard\*, D. Pelloquin and A. Maignan. Published in **Inorganic Chemistry** Vol: 54, Issue: 13, P: 6560-6565 ( JUL 2015)

Nearly pure powder sample and single crystals of the stoichiometric iron calcium CaOFeS oxysulfide have been synthesized by solid state reaction. The structural analysis of CaOFeS at room temperature by combining single crystal diffraction, neutron diffraction data and transmission electron microscopy leads to a stoichiometric hexagonal non centrosymmetric  $P6_3mc$  layered structure

