



Influence of temperature and high pressure on the structural and physical properties in **Fe**-based **C**harge **O**rders systems

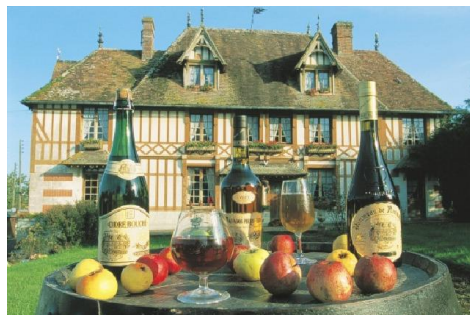
Note: The results from this document can be cited only after the publication
-2015-



Partners



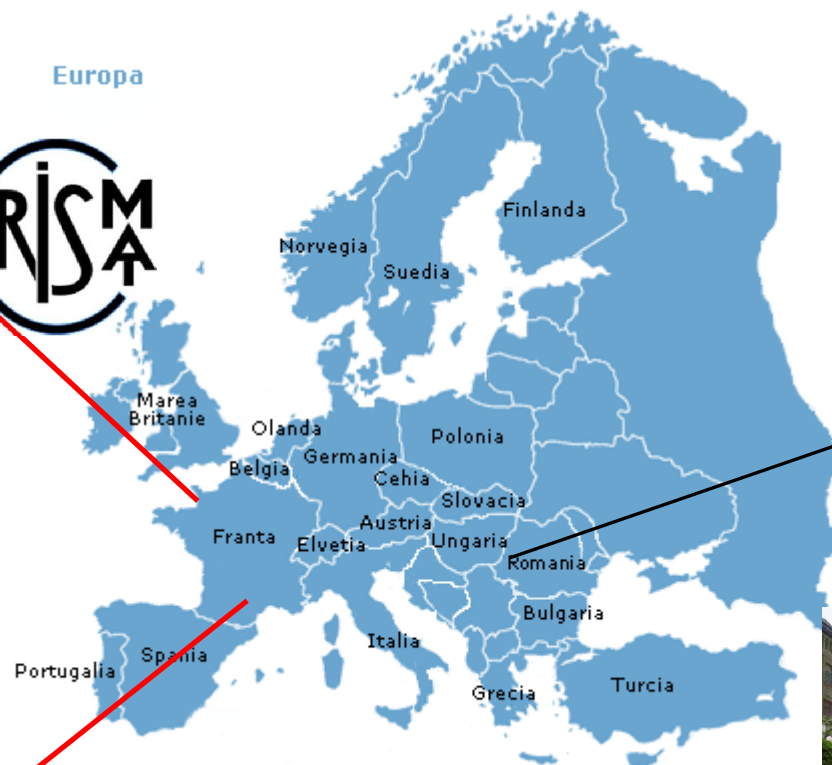
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**Institut Charles Gerhardt
Montpellier**

Europa



Timisoara



Results

➤ Phosphates

- $\text{Fe}_3(\text{PO}_4)_2(\text{OH})_2$ (Barboselite and lipscombite):
Study vs Temperature and Pressure

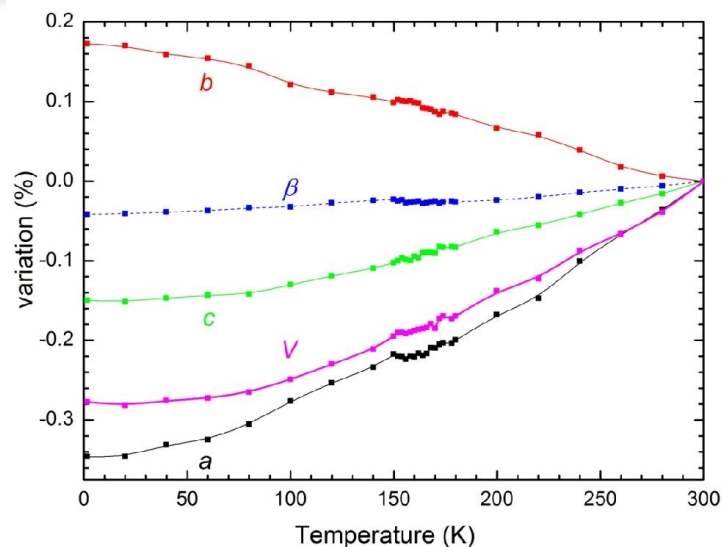
➤ Borates $\text{Fe}_{3-x}\text{Mn}_x\text{BO}_5$ ($0 \leq x \leq 3$)

- Fe_3BO_5 ($x = 0$)
- $\text{Fe}_{1.5}\text{Mn}_{1.5}\text{BO}_5$ ($x=1.5$)

$\text{Fe}_3(\text{PO}_4)_2(\text{OH})_2$

Barbosalite

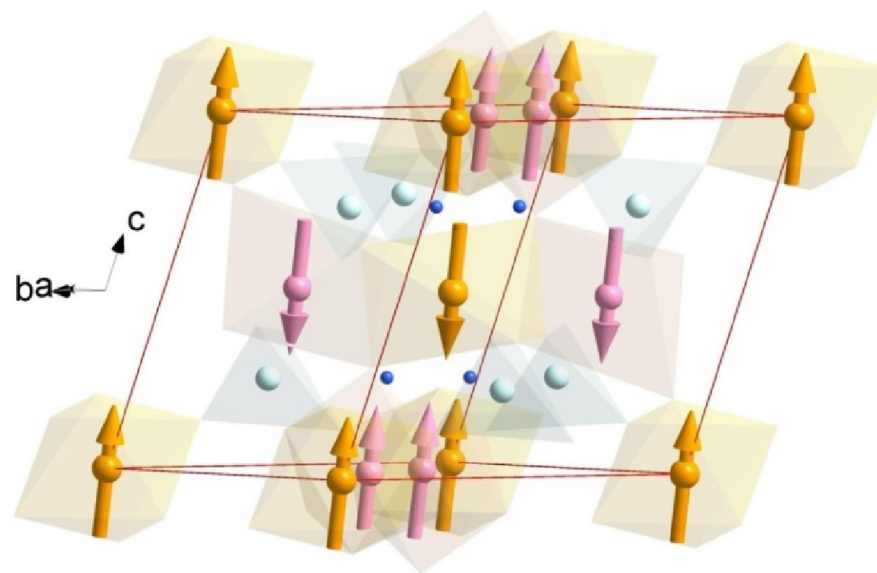
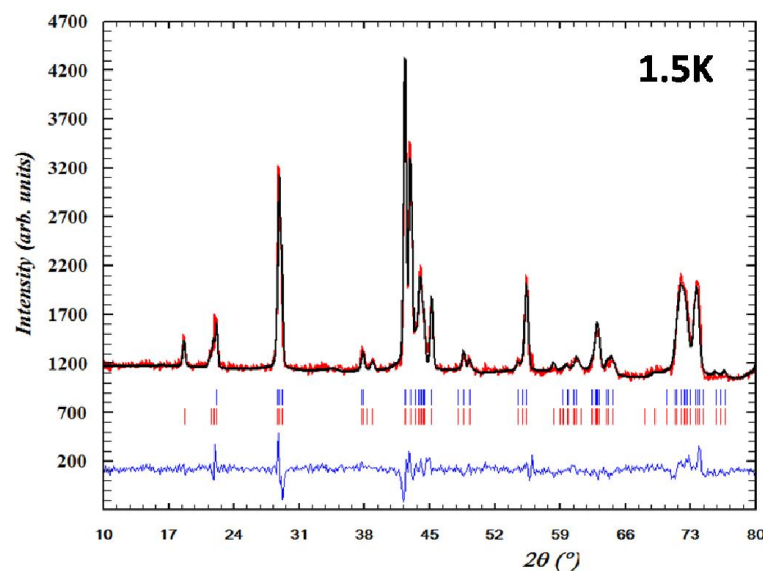
Neutron Powder diffraction- barbosalite : LLB Saclay



1.7 K-300K, $\lambda=2.458 \text{ \AA}$

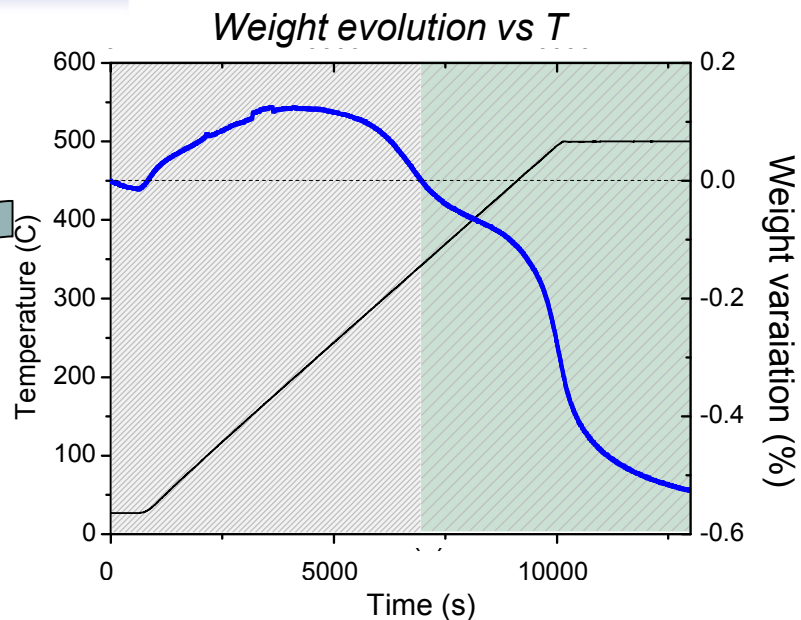
Temperature evolution of the lattice parameters in $P2_1/n$ space group

Magnetic structure model

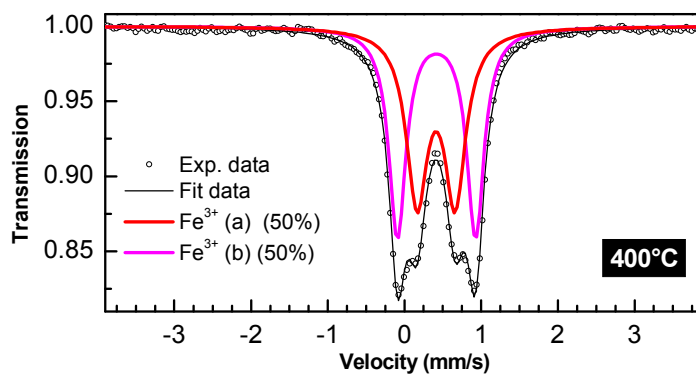


$\text{Fe}_3(\text{PO}_4)_2(\text{OH})_2$

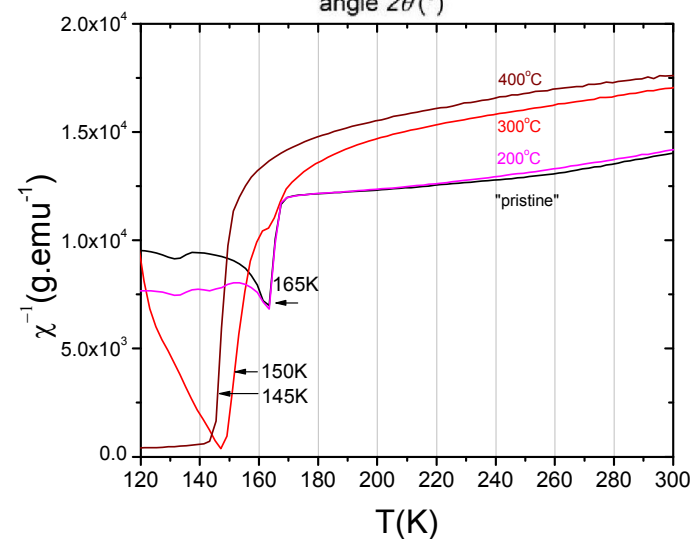
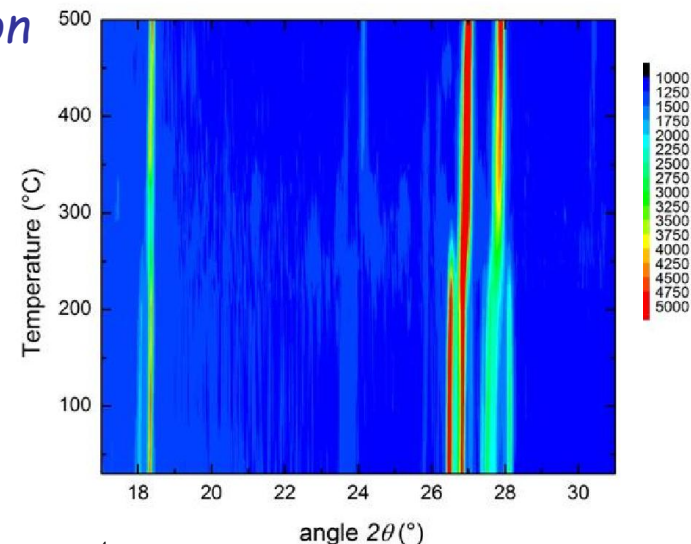
Barbosalite *Barbosalite to lipscombite transition*



Mossbauer spectra for the sample at 400°C



Echantillon	IS (mm/s)	QS (mm/s)	LW (mm/s)	%
MP127 400°C	0.41(2)	0.50(2)	0.33(2)	49.9(2)
	0.42(1)	1.02(1)	0.27(2)	50.1(2)
				Fe ³⁺ (a)
				Fe ³⁺ (b)

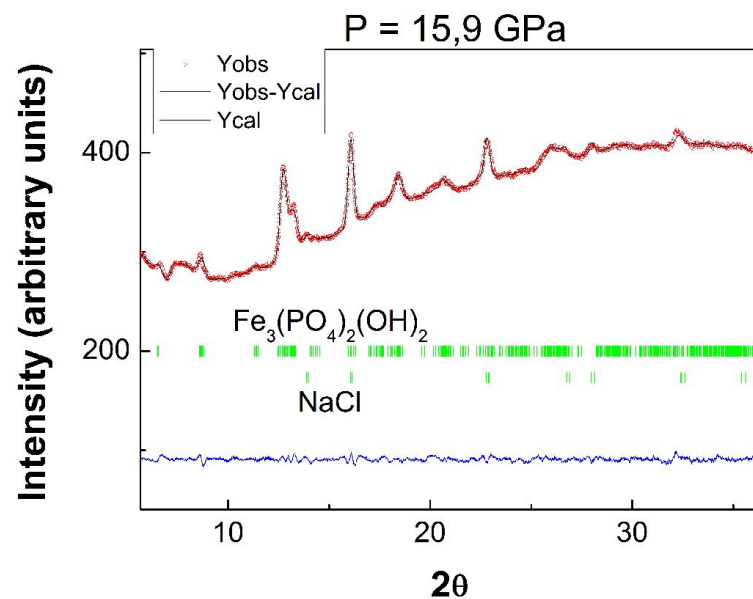


$\text{Fe}_3(\text{PO}_4)_2(\text{OH})_2$

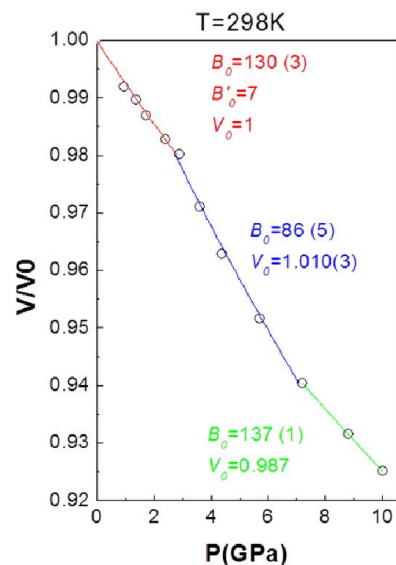
Barbosalite

Barbosalite vs P

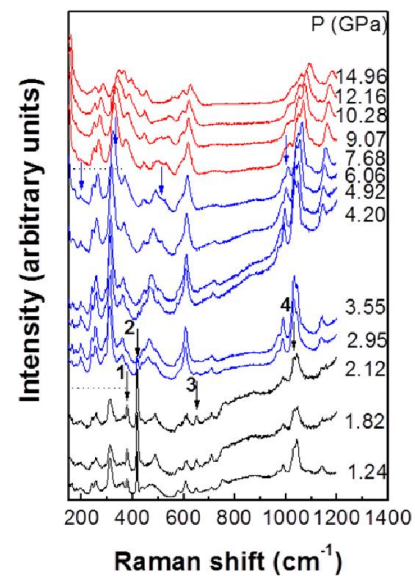
X-Ray diffraction vs P



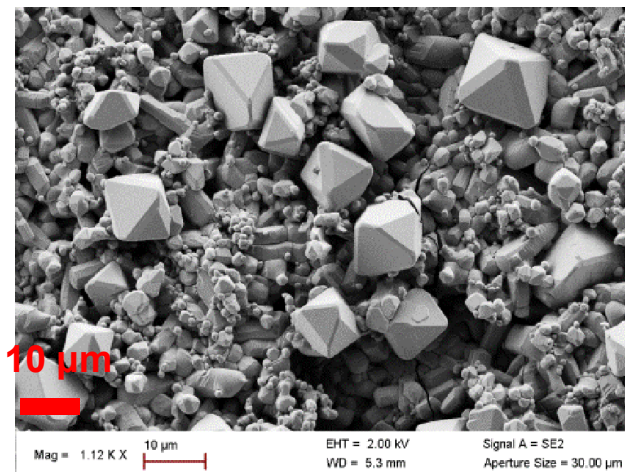
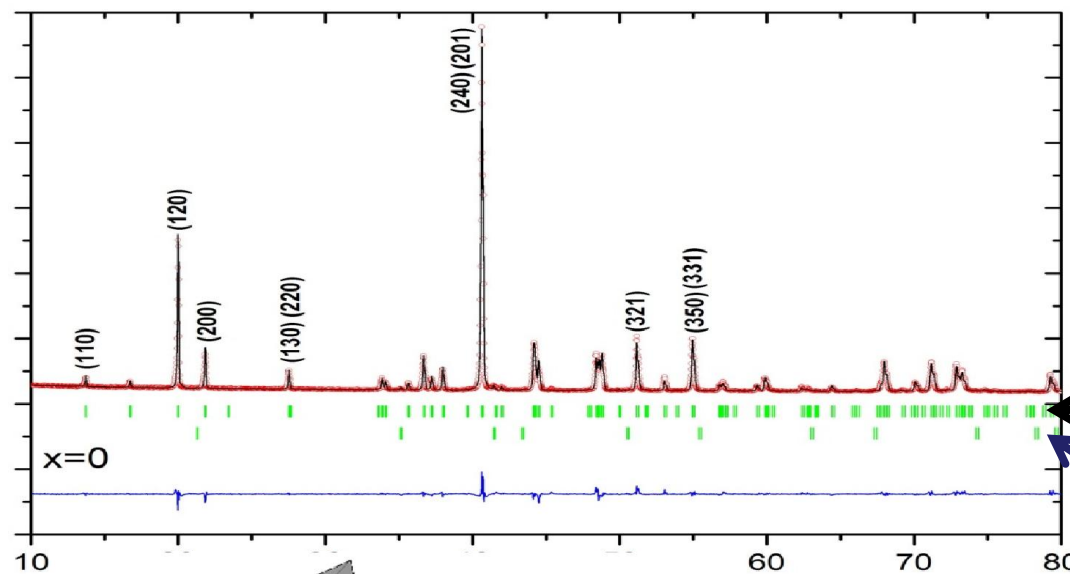
Raman Spectroscopy vs P



-Two structural transition observed in function of P



Fe₃BO₅



Pbam
9.465 Å
12.310 Å
3.077 Å

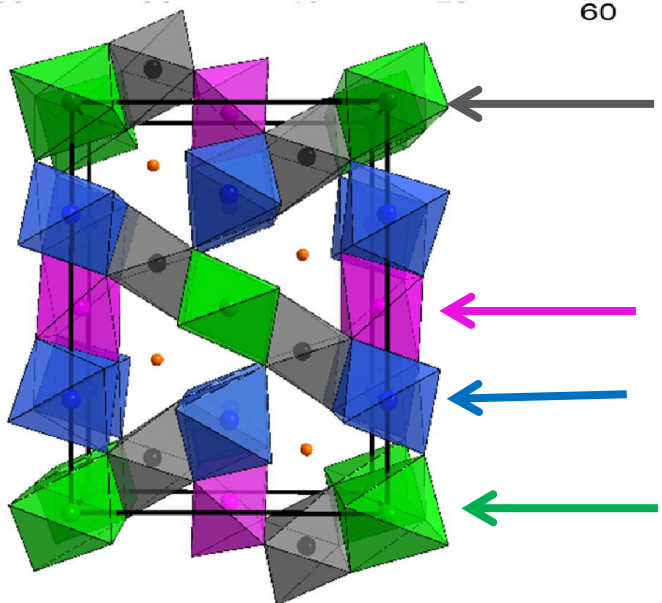
Fe₃O₄

Fe4 (4h): 0.7444 0.3875 ½

Fe2 (2d) : ½ 0 ½

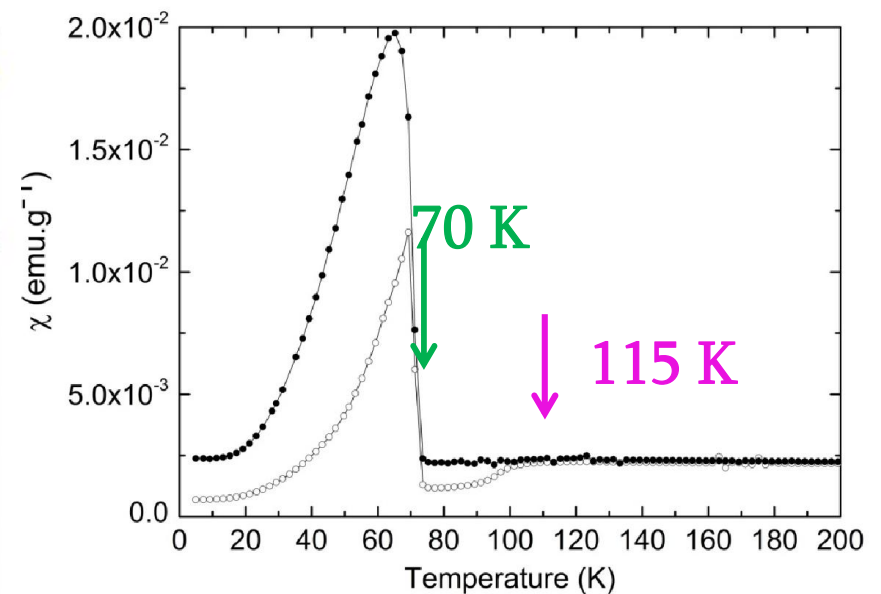
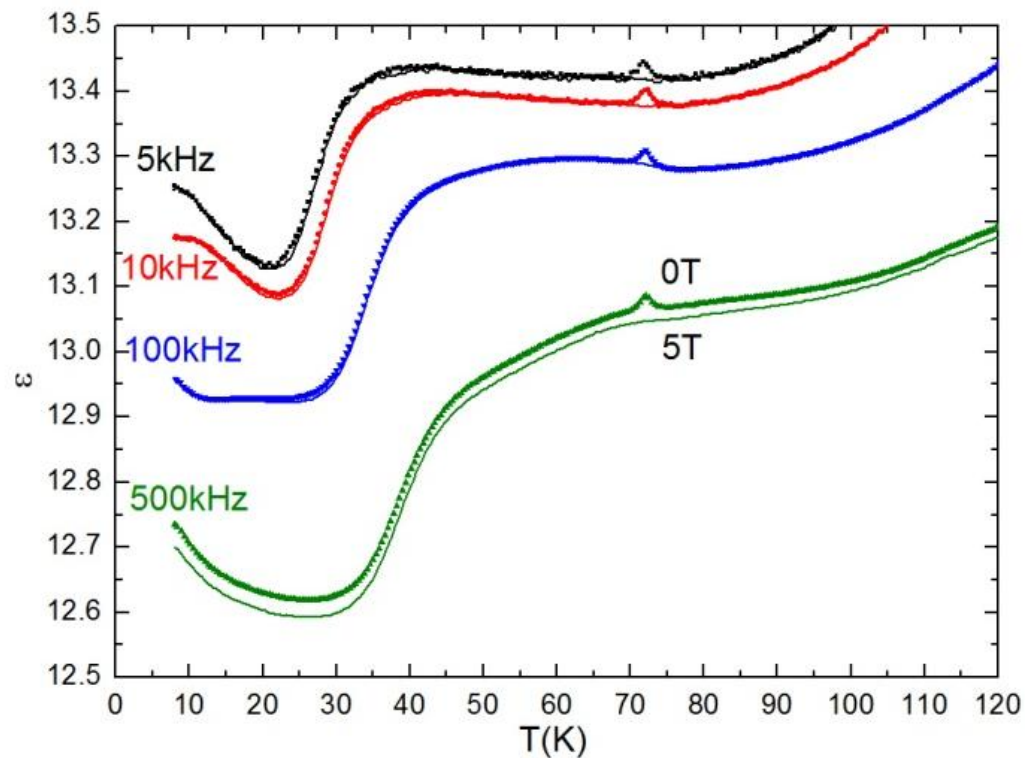
Fe3 (4g): 0.0003 0.2743 0

Fe1 (2a): 0 0 0



Fe_3BO_5

Coupling between magnetic and dielectric properties.
& Effect of applied magnetic field on ϵ .

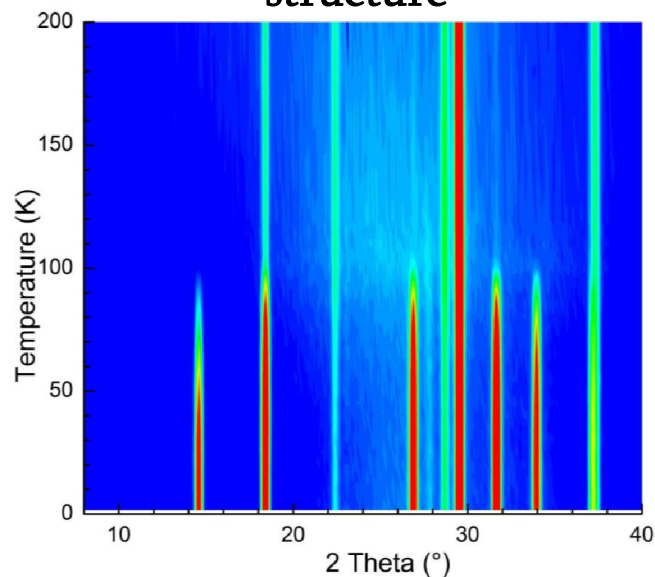


Magnetic ordering of the
Fe3-Fe1-Fe3 ladders

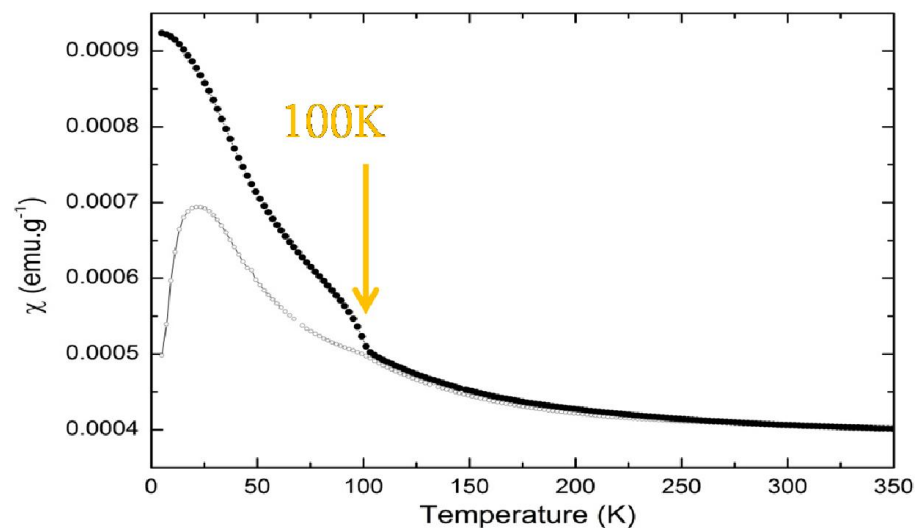
Magnetic ordering of the Fe4-**Fe2**-Fe4
ladders

$\text{Mn}_{1.5}\text{Fe}_{1.5}\text{BO}_5$

NPD : Mn/Fe distribution & magnetic structure



Macroscopic magnetic behavior



M4-M2-M4 AFM trimers ($\uparrow \downarrow \uparrow$)
with F coupling along c

M3-M1-M3 FM coupling in the bc plane
with AF coupling a

+ ED for SG determination

