

# Spin state of $\text{Co}^{3+}$ in $\text{Co}_3\text{BO}_5$ : experimental and theoretical investigations

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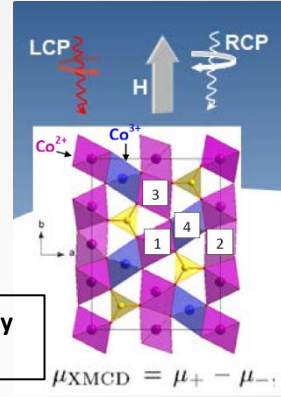
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T= 5 K  
 H= ±17 T  
 EMD

ferrimagnetically ordered phase

$$\frac{\text{XMCD}(\text{Co}_2\text{Co})}{\text{XMCD}(\text{Co}_2\text{Fe})} = \frac{2}{3} \cdot \left(1 + \frac{\text{XMCD}(\text{Co}^{3+})}{2 \cdot \text{XMCD}(\text{Co}^{2+})}\right)$$

$$\frac{\text{XMCD}(\text{Co}_2\text{Co})}{\text{XMCD}(\text{Co}_2\text{Fe})} = 0.70(0.03)$$

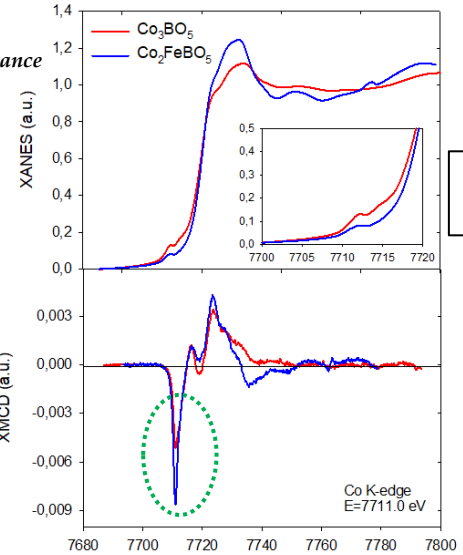
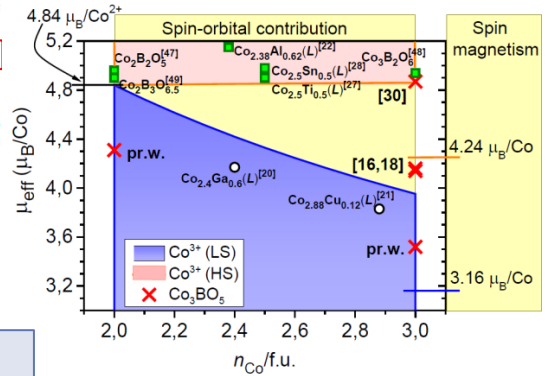
rather small net  $\text{Co}^{3+}$  magnetization, a strong experimental support for the LS  $\text{Co}^{3+}$  scenario

TABLE I. Magnetic moments of the ludwigite  $\text{Co}_3\text{O}_2\text{BO}_3$  at 2 K for each direction in  $\mu_B$  units.  $M$  represents the modulus of the magnetic moment vector.  $R_p = 14.5\%$ ,  $R_{wp} = 13.2\%$ ,  $R_{\text{exp}} = 2.05\%$ ,  $\chi^2 = 41.4\%$ ,  $R_{\text{Bragg}} = 8.0\%$ ,  $R_{\text{mag}} = 8.6\%$ .

Atom (Wyckoff positions)	$M_x$	$M_y$	$M_z$	$M$
Co4 (4h)	-0.5(1)	-0.1(1)	0	0.5
Co3 (4g)	1.7(1)	3.38(8)	0	3.8
Co2 (2d)	0.4(2)	3.06(9)	0	3.1
Co1 (2a)	1.2(1)	-3.4(1)	0	3.6

D.C. Freitas PRB (2016)

LS  $\text{Co}^{3+}$  at 4 site?



## Conclusions

- paramagnetic susceptibility (100-250 K): two HS  $\text{Co}^{2+}$  ions and some orbital contribution
- lattice parameters: anomalies at 500 and 700 K
- octahedral environment and oxidation state of Co4 site are strongly affected by T
- DSC:  $\text{Co}_3\text{BO}_5\text{C}$  is thermally stable (300-800 K)
- GGA+U calculations: at low-temperatures the system is insulator ( $E_g=1.4$  eV), HS  $\text{Co}^{2+}$  and LS  $\text{Co}^{3+}$  at high temperatures ( $T>700$  K), charge ordering disappears, system becomes metallic with all Co ions in  $3d^7$  high-spin state.

## Single-crystal X-ray diffraction vs T

