

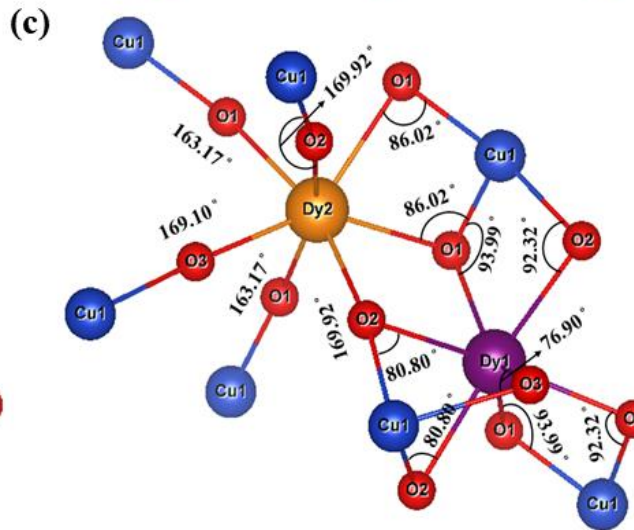
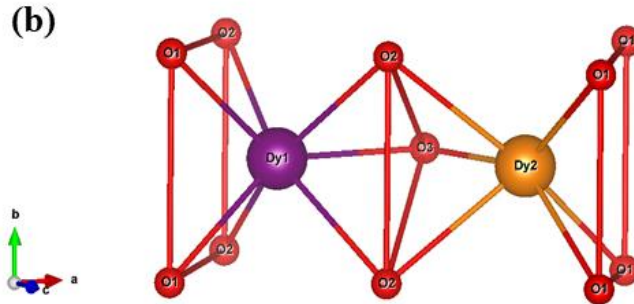
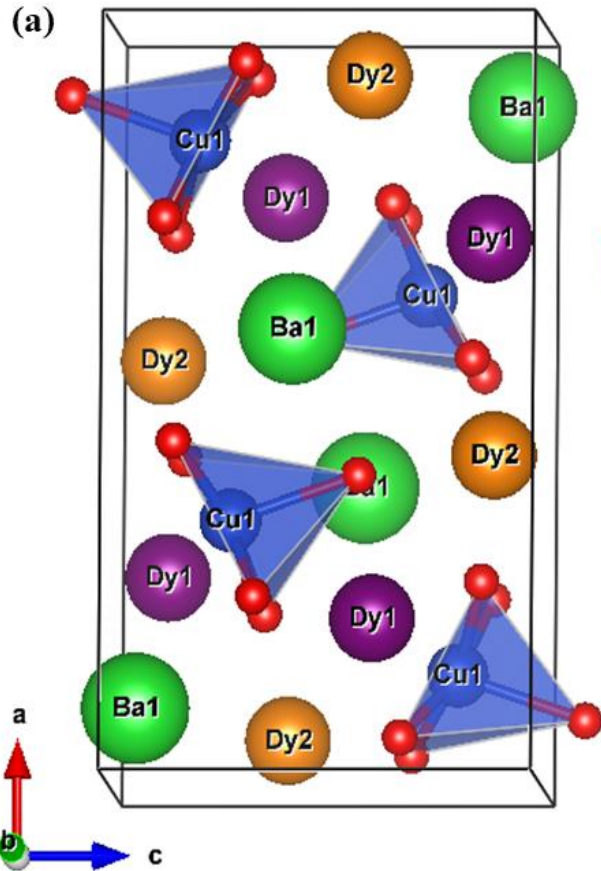
# Green Phases: $R_2BaCuO_5$

Example of  $Ho_2BaCuO_5$ :

**Magnetic-field-induced ferroelectric states in centrosymmetric  $R_2BaCuO_5$  ( $R = Dy$  and  $Ho$ )** P. Yanda, F. Orlandi, P. Manuel, N. Boudjada, J. Rodriguez-Carvajal, and A. Sundaresan.

PHYSICAL REVIEW B **104**, 144401 (2021)

Transparencies summarizing the content of the article.



# The Green-Phases

Space group: *Pnma*

Cell parameters  $a \approx 12.32 \text{ \AA}$ ,  
 $b \approx 5.72 \text{ \AA}$ ,  $c \approx 7.23 \text{ \AA}$

Approximate coordinates of  
magnetic atoms

**R1** (4c): 0.288  $\frac{1}{4}$  0.115

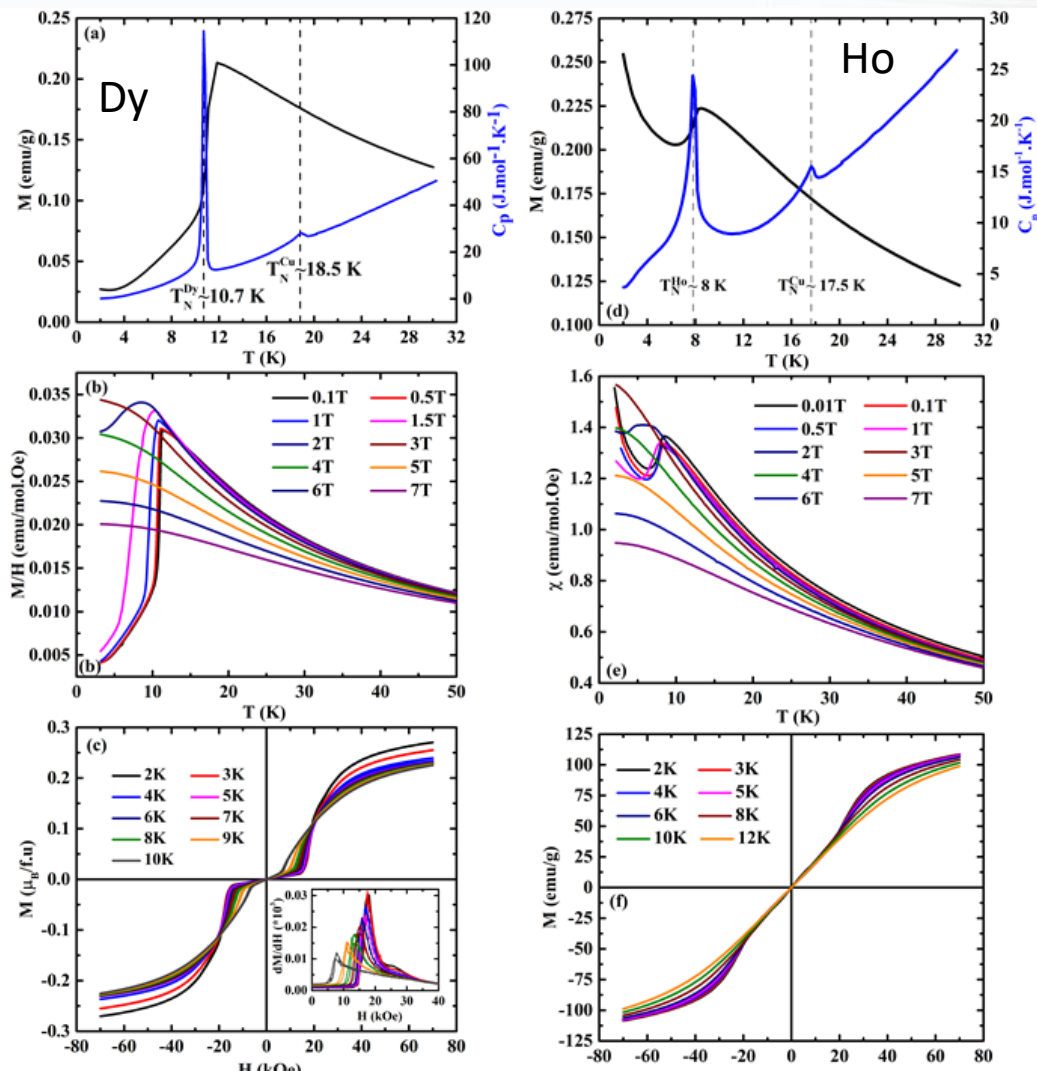
**R2** (4c): 0.074  $\frac{1}{4}$  0.395

**Cu** (4c): 0.906  $\frac{1}{4}$  0.711

Site **R1** surrounded by 3  
**Cu<sup>2+</sup>** ions

Site **R2** surrounded by 6  
**Cu<sup>2+</sup>** ions

# Physical Properties of $\text{Dy}_2\text{BaCuO}_5$ and $\text{Ho}_2\text{BaCuO}_5$ .



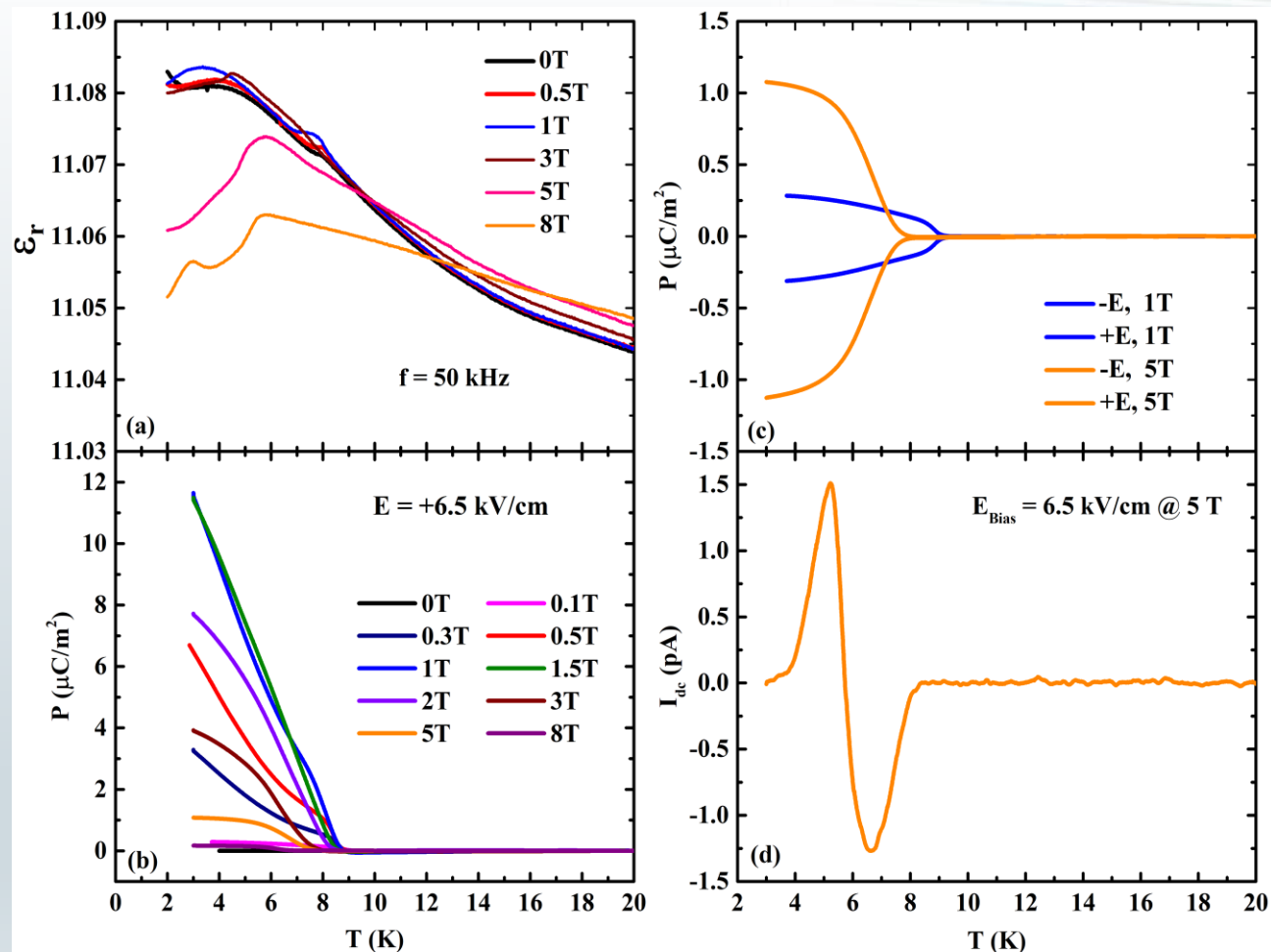
(a & d) Left axis. Temperature dependent DC magnetization measured under 100 Oe in field cooled condition, Right axis. Specific heat measured under zero magnetic field.

(b & e) DC magnetization measured under different magnetic fields.

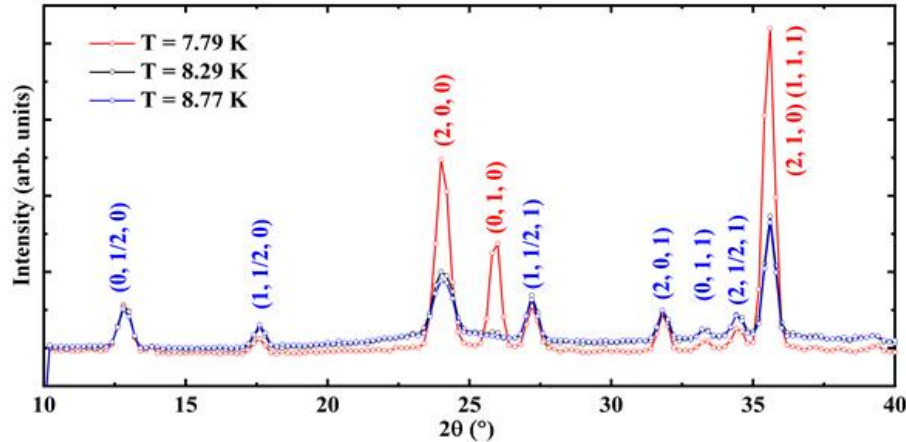
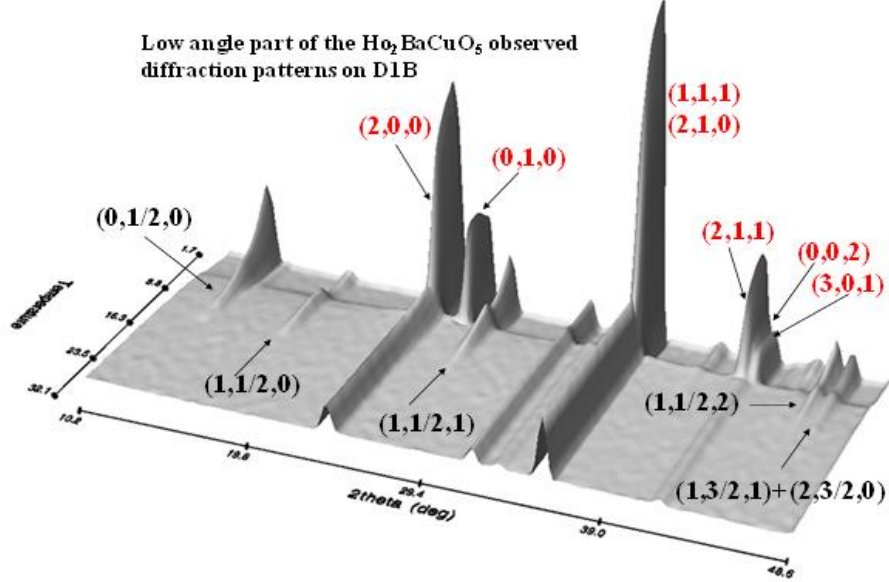
(c & f) Isothermal  $M(H)$  curves; for  $\text{Dy}_2\text{BaCuO}_5$  and  $\text{Ho}_2\text{BaCuO}_5$  respectively.

# Electrical Properties of $\text{Ho}_2\text{BaCuO}_5$ .

- (a) Dielectric constant against temperature measured with frequency  $f = 50$  kHz under different magnetic fields.
- (b)  $T$ - $H$  dependent polarization.
- (c & d) Switching of polarization and dc bias signal.



Low angle part of the  $\text{Ho}_2\text{BaCuO}_5$  observed diffraction patterns on D1B

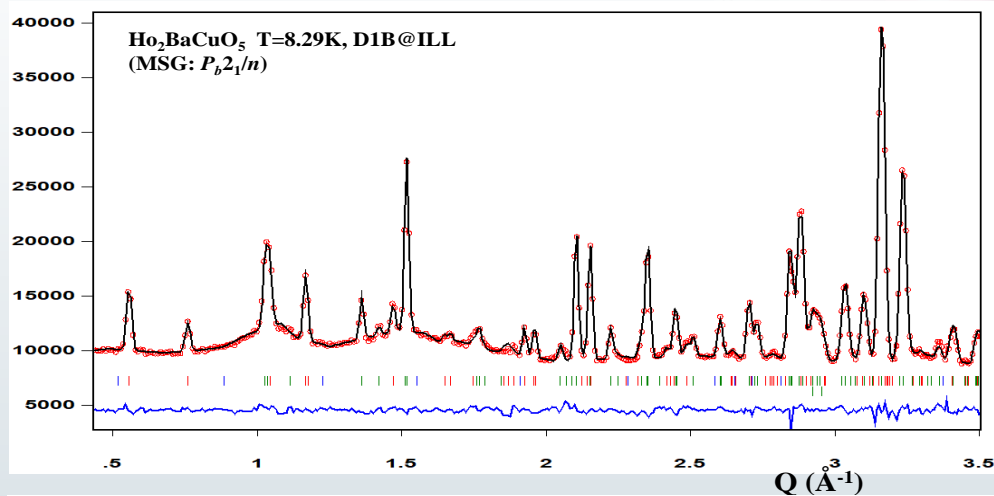


# Neutron diffraction of $\text{Ho}_2\text{BaCuO}_5$ .

(Upper panel) 3D visualization of the low angle part of diffraction patterns taken on D1B ( $\lambda=2.52$  Å). The abrupt change of background and the simultaneous appearance of the  $\mathbf{k}_2 = (0, 0, 0)$  magnetic peaks indicates a first-order magnetic phase transition.

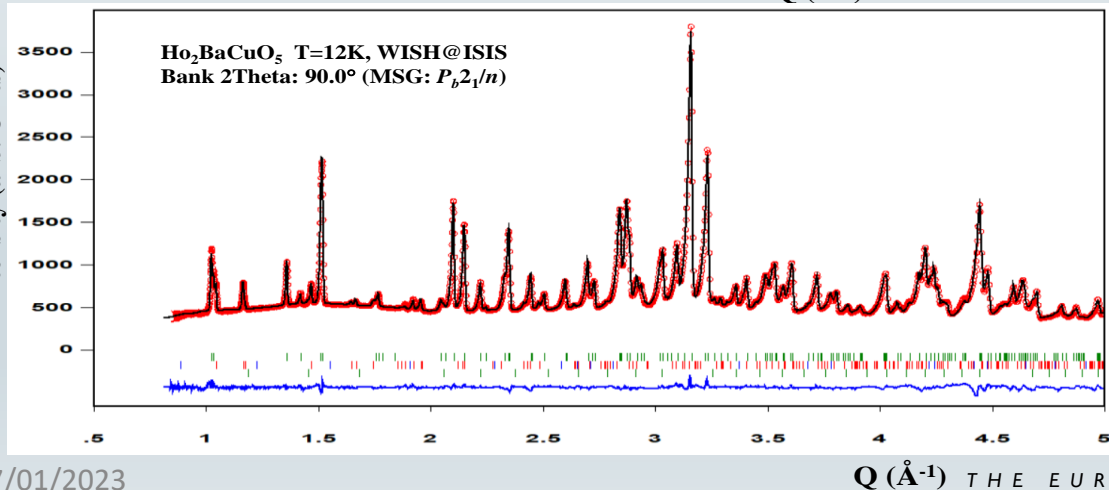
(Bottom panel) Details of the evolution of diffraction patterns of  $\text{Ho}_2\text{BaCuO}_5$  around the transition at  $T_N^{\text{Ho}} \approx 8$  K. The indexing of peaks (blue for  $\mathbf{k}_1 = (0, \frac{1}{2}, 0)$ , red for  $\mathbf{k}_2 = (0, 0, 0)$ ) is given with respect to the paramagnetic unit cell.

Intensity (arb. Units)



Rietveld refinement of  
D1B data @ 8.3K

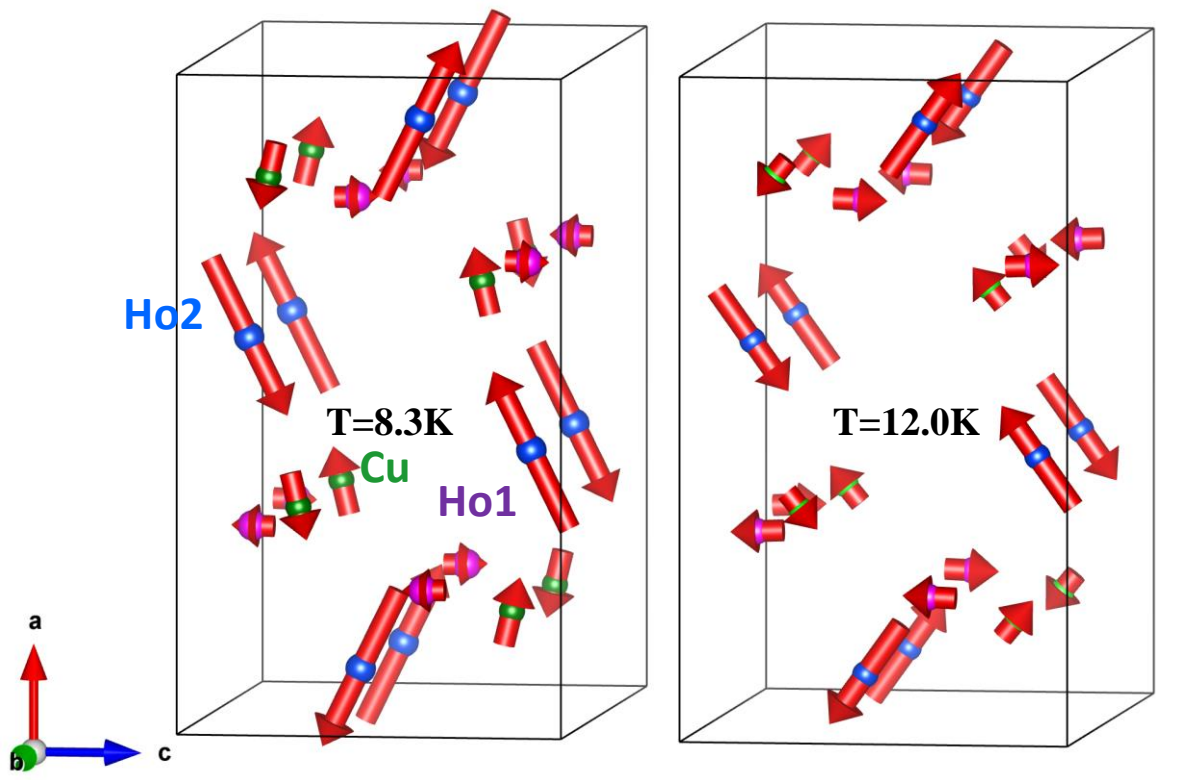
Intensity (arb. Units)



Rietveld refinement of  
WISH data @ 12K



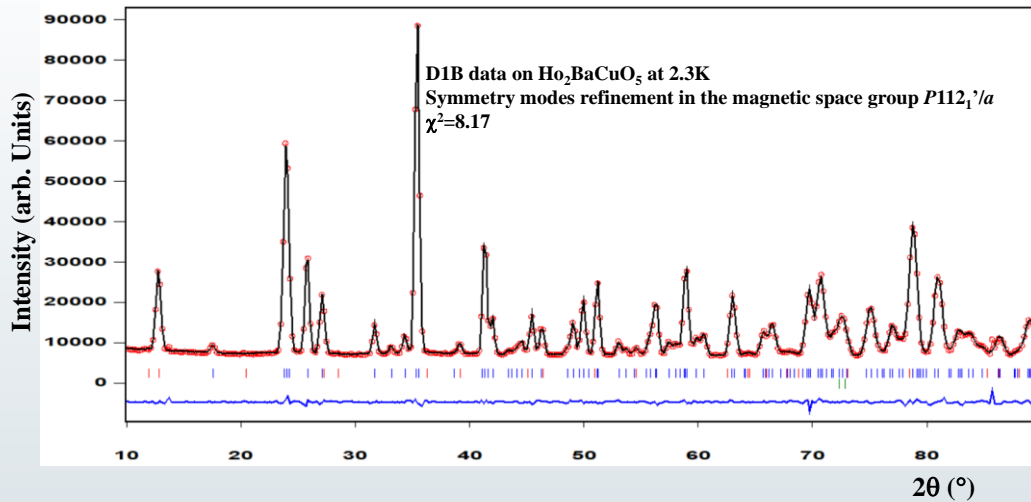
# Magnetic structure of $\text{Ho}_2\text{BaCuO}_5$ ( $T > 8\text{K}$ )



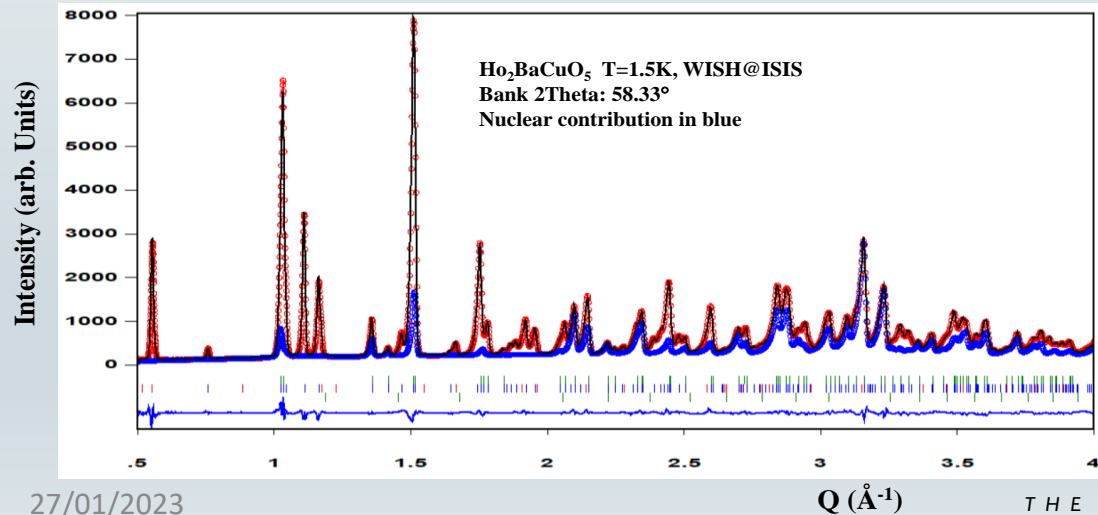
Magnetic structure of  $\text{Ho}_2\text{BaCuO}_5$ . Only the magnetic atoms are represented and the refinement was done by nullifying the components along  $\mathbf{b}$  for all atoms.  $\text{Ho}_1$  atoms bring a quite weak magnetic moment ( $\approx 0.42(3) \mu_B$ ) at  $T = 8.3\text{ K}$  (D1B), similar to  $T = 12.0\text{ K}$  ( $\approx 0.49(1) \mu_B$ ) (WISH). The relative scale of magnetic moments is respected between the two temperatures except the moments of  $\text{Ho}_1$  and  $\text{Cu}$  atoms that have been multiplied by 2 for displaying purposes.

Magnetic space group  $P_b 112_1/n$

Propagation vector  $\mathbf{k}_1 = (0, \frac{1}{2}, 0)$



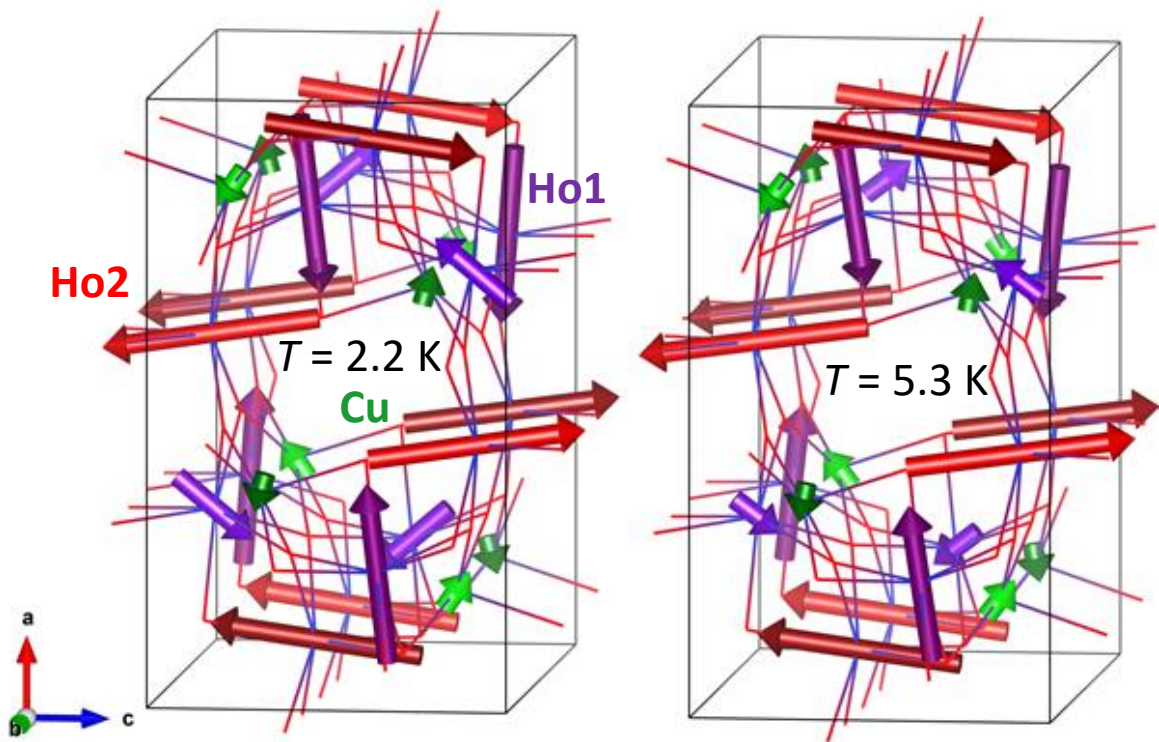
Rietveld refinement of the  
D1B data @ 2.3K



Rietveld refinement of the  
WISH data @ 1.5K



# Magnetic structure of $\text{Ho}_2\text{BaCuO}_5$ ( $T < 8\text{K}$ )



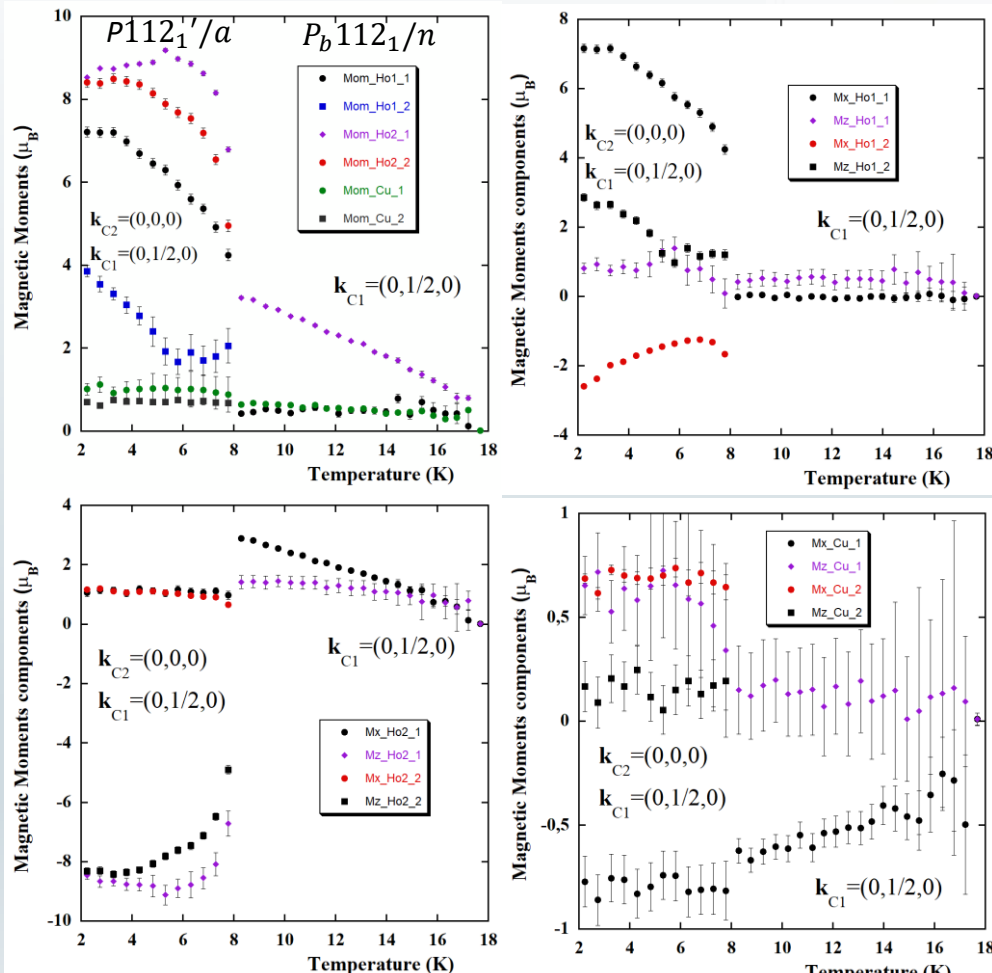
Wireframe schemes of the low-temperature magnetic structure of  $\text{Ho}_2\text{BaCuO}_5$  at  $T = 2.2\text{ K}$  and  $T = 5.3\text{ K}$ .

Both figures correspond to the magnetic space group  $P112_1'/a$ . The relative scale of magnetic moments is respected between the two temperatures except for the moments of Cu atoms that have been multiplied by 2 for display purposes.

Magnetic space group  $P112_1'/a$

Propagation vectors  $\mathbf{k}_1 = (0, \frac{1}{2}, 0) + \mathbf{k}_2 = (0, 0, 0)$

# Magnetic Moments of $\text{Ho}_2\text{BaCuO}_5$ as a function of Temperature



Magnetic moments and their components for atoms Ho1, Ho2 and Cu as a function of temperature for  $\text{Ho}_2\text{BaCuO}_5$ . The refinements have been performed with no contribution of  $m\text{GM}_3^-$  (no y-components). In the region of  $k_{C1}$  ( $T > 8\text{K}$ ) there are single sites (Ho1\_1, Ho2\_1 and Cu\_1) and in the region of two propagation vectors  $k_{C1} + k_{C2}$  ( $T < 8\text{K}$ ) the sites of magnetic atoms are split (Ho1\_1, Ho1\_2, Ho2\_1, Ho2\_2, Cu\_1, Cu\_2).

# Magnetic structures of $\text{Ho}_2\text{BaCuO}_5$

The magnetic structures of  $\text{Ho}_2\text{BaCuO}_5$  are unusual and complicated.

The presence of two magnetic sublattices formed by  $\text{Cu}^{2+}$  and  $\text{R}^{3+}$  ions and two different sites for rare earth are responsible for the peculiar behavior of the magnetic ordering.

At  $T_N^{\text{Cu}}$ , spin ordering occurs with  $\mathbf{k}_1 = (0, \frac{1}{2}, 0)$  under the influence of copper-copper exchange interaction in both compounds.

The rare earth magnetic moments become weakly polarized below  $T_N^{\text{Cu}}$ .

Below  $T_N^{\text{Ho}}$ , the reorientation of the copper and rare earth spin structure with two propagation vectors:  $\mathbf{k}_1 = (0, \frac{1}{2}, 0)$  and  $\mathbf{k}_2 = (0, 0, 0)$  occurs under the influence of  $4f$ - $3d$  interaction.