

## ELECTRONIC SUPPLEMENT

# Frustration-driven non-collinear magnetism and AC-conduction mechanism in YBaCuFeO<sub>5</sub> double perovskite

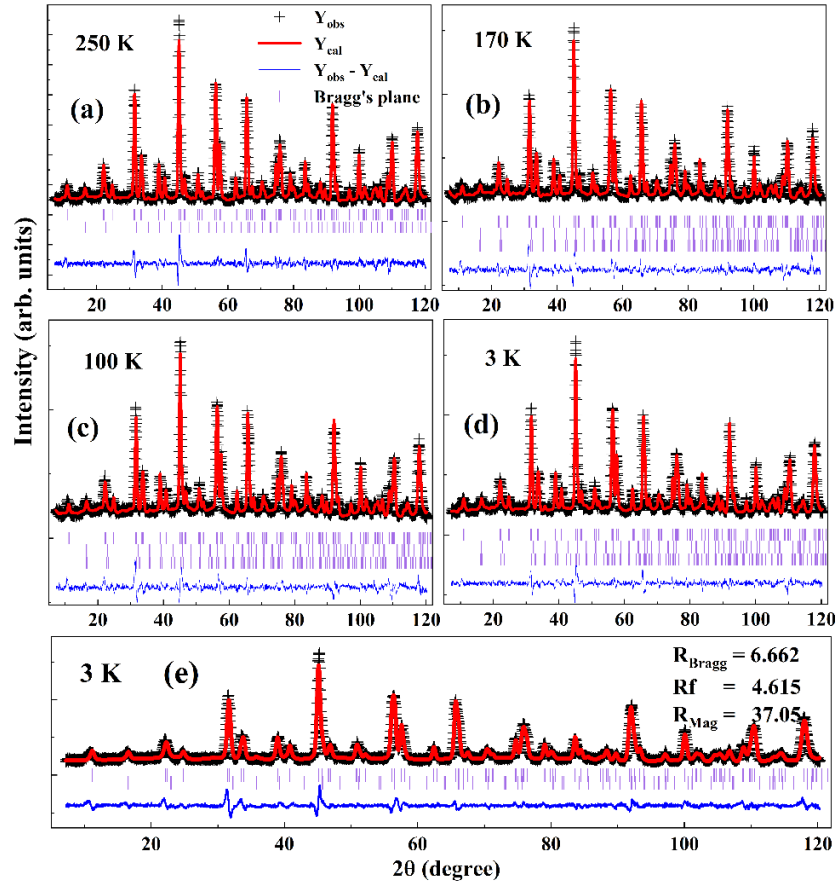
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**FIG S1.** ND refinement of YBCFO at (a) 250 K, (b) 170 K, (c) 100 K and (d) 3 K with B- site cationic disorder. (e) ND refinement of 3 K data with perfect B-site cationic order (and also with only collinear magnetic phase.)

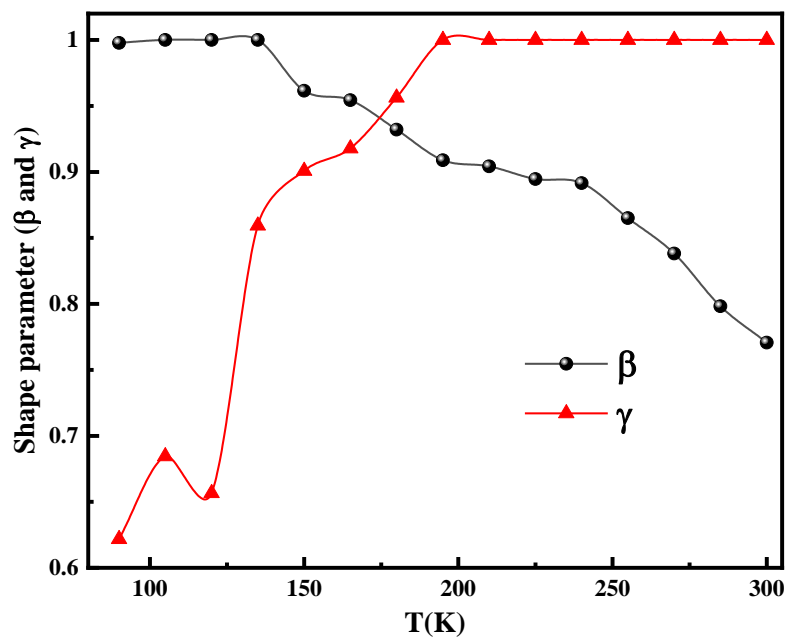
**TABLE S1.** Structural and magnetic parameters of YBCFO at multiple temperatures with  $n_d \approx 0.28$ . CM and ICM in parenthesis stands for commensurate and incommensurate magnetic phases.  $m_f$  and  $m_c$  stands for ordered magnetic moments refined at Fe and Cu rich pyramids respectively. The CM and ICM phase are refined in the model of  $M_l \approx 0$  and  $M_r \approx M_l$  conditions respectively.

| <i>P4mm</i>                                    | 300 K     | 250 K      | 170 K     | 100 K     | 50 K      | 3 K       |
|--|-----------|------------|-----------|-----------|-----------|-----------|
| <b>a = b (Å)</b>                               | 3.8750(7) | 3.8680(7)  | 3.8633(5) | 3.8644(8) | 3.8645(9) | 3.8610(6) |
| <b>c (Å)</b>                                   | 7.6725(2) | 7.6538(3)  | 7.6419(3) | 7.6387(2) | 7.6359(4) | 7.6288(4) |
| <b>V (Å<sup>3</sup>)</b>                       | 115.21(4) | 114.51(4)  | 114.06(3) | 114.07(5) | 114.04(5) | 113.72(4) |
| <b>Y [1a]<br/>(0 0 z)</b>                      | 0.5049(7) | 0.5096(10) | 0.5049(4) | 0.5066(2) | 0.5058(3) | 0.5033(2) |
| <b>Ba [1a]<br/>(0 0 z)</b>                     | 0         | 0          | 0         | 0         | 0         | 0         |
| <b>Cu1 [1b]<br/>(0.5 0.5 z)</b>                | 0.2833(4) | 0.2812(4)  | 0.2749(4) | 0.2775(7) | 0.2823(2) | 0.2823(6) |
| <b>Fe1 [1b]<br/>(0.5 0.5 z)</b>                | 0.2400(1) | 0.2516(6)  | 0.2540(2) | 0.2494(1) | 0.2462(5) | 0.2521(4) |
| <b>Cu2 [1b]<br/>(0.5 0.5 z)</b>                | 0.7013(2) | 0.7175(3)  | 0.7256(2) | 0.7240(1) | 0.7204(6) | 0.7209(2) |
| <b>Fe2 [1b]<br/>(0.5 0.5 z)</b>                | 0.7506(5) | 0.7515(6)  | 0.7483(8) | 0.7484(4) | 0.7494(7) | 0.7481(1) |
| <b>O1 [1b]<br/>(0.5 0.5 z)</b>                 | 0.0358(6) | 0.0321(7)  | 0.0245(1) | 0.0272(5) | 0.0259(2) | 0.0287(6) |
| <b>O2 [1b]<br/>(0.5 0 z)</b>                   | 0.3236(2) | 0.3262(4)  | 0.3237(5) | 0.323(4)  | 0.3233(5) | 0.3231(5) |
| <b>O3 [1b]<br/>(0.5 0 z)</b>                   | 0.6938(3) | 0.6935(4)  | 0.6920(5) | 0.6915(5) | 0.6916(5) | 0.6914(2) |
| <b>m<sub>f</sub> (μ<sub>B</sub>)<br/>(CM)</b>  | 3.38 (4)  | 3.72 (3)   | 3.52 (2)  | 3.38 (6)  | 3.43 (7)  | 3.45 (1)  |
| <b>m<sub>c</sub> (μ<sub>B</sub>)<br/>(CM)</b>  | 1.70 (2)  | 2.05 (5)   | 1.83 (4)  | 1.88 (2)  | 1.55 (3)  | 1.61 (2)  |
| <b>m<sub>f</sub> (μ<sub>B</sub>)<br/>(ICM)</b> | -         | -          | 3.72 (5)  | 3.54 (3)  | 3.43 (3)  | 3.19 (3)  |
| <b>m<sub>c</sub> (μ<sub>B</sub>)<br/>(ICM)</b> | -         | -          | 1.91 (5)  | 1.42 (1)  | 1.55 (3)  | 1.21 (2)  |
| <b>R<sub>Bragg</sub></b>                       | 6.097     | 5.581      | 4.904     | 6.045     | 5.092     | 4.079     |

|                           |       |       |       |       |       |       |
|---------------------------|-------|-------|-------|-------|-------|-------|
| $R_F$                     | 3.579 | 4.257 | 3.263 | 4.306 | 3.327 | 2.707 |
| $R_{\text{mag}}$<br>(CM)  | 6.742 | 21.47 | 12.60 | 12.27 | 10.49 | 9.659 |
| $R_{\text{mag}}$<br>(ICM) | -     | -     | 18.97 | 16.78 | 13.91 | 23.08 |

**TABLE S2.** Inputs for energy minimization calculation.

| T (K) | $d_{\text{FM}}$ (Å) | $d_{\text{AFM}}$ (Å) | q (r.l.u)  | C (Å)     |
|-------|---------------------|----------------------|------------|-----------|
| 300   | 4.0872(3)           | 3.5853(1)            | 0          | 7.6725(2) |
| 250   | 4.0542(3)           | 3.5995(9)            | 0          | 7.6538(3) |
| 170   | 4.0243(1)           | 3.6176(1)            | 0.022(28)  | 7.6419(3) |
| 100   | 4.0415(9)           | 3.5971(7)            | 0.0419(19) | 7.6387(2) |
| 50    | 4.0692(2)           | 3.5667(7)            | 0.051(17)  | 7.6359(4) |
| 3     | 4.0751(6)           | 3.5536(5)            | 0.059(23)  | 7.6288(4) |



**FIG S2.** Variation of symmetric ( $\beta$ ) and asymmetric ( $\gamma$ ) parameters with temperature.

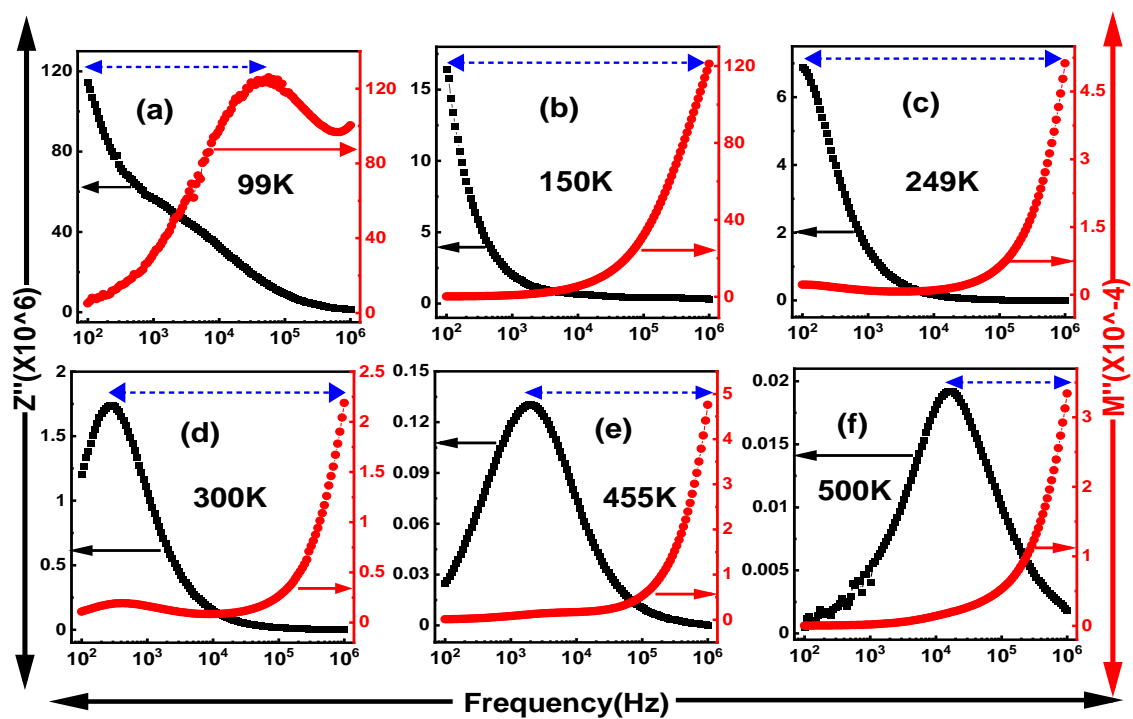


FIG S3. (a-f) Frequency dependent  $Z''$  and  $M''$  at different temperatures.

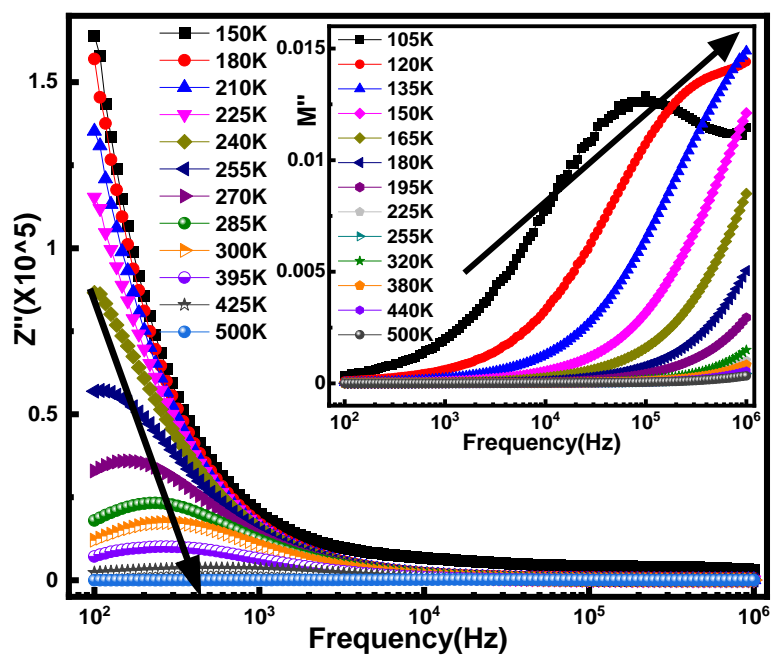
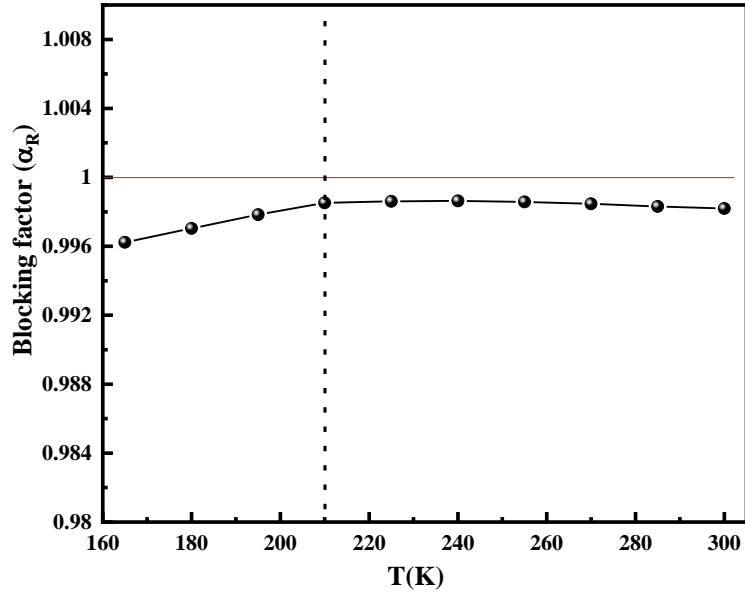
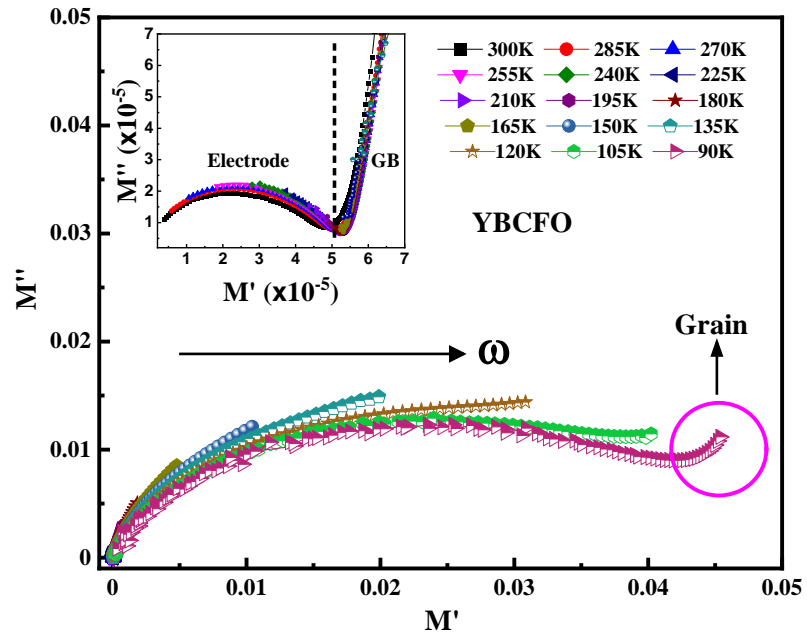


FIG S4.  $Z''$  vs frequency at selected temperatures starting from 150K-500K. (Inset:  $M''$  vs frequency)



**FIG S5.** Blocking factor changes with T.



**FIG S6.** Modulus Cole-Cole plot of in the temperature range of 90-300 K range. **Inset:** Zoomed image of plot in the low frequency zone separating electrode and grain boundary effects.