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Low temperature magnetic structure and lattice anomalies at the commensurate-incommensurate transition of multiferroic YBaCuFeO5

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Ferroelectric materials have been known since almost one century ago [1]. While their potential for applications was rapidly recognized, the possibility of combining ferroelectricity with magnetic order -preferably with ferromagnetism- has resulted in an enormous deal of interest during the last decade. Several new materials combining both types of order have been reported, although their promising multifunctionalities have been obscured by two facts: one one side, most of them are antiferromagnetic. On the other, their transition temperatures are too low for most practical applications (typically below 40K).
The oxygen-defficient double perovskite YBaFeCuO5 constitutes a remarkable exception. Spontaneous electric polarization has been recently reported to exist below an unusually high temperature of TC ≈ 230K [2] coinciding with the occurrence of a commensurate - to - incommensurate reorientation of the Fe3+ and Cu2+ magnetic moments [3,4]. From a more fundamental point of view the observation of incommensurable magnetic order in a tetragonal material at such high temperatures is rather surprising. In particular, the nature of the relevant competing magnetic interactions and its possible link to low dimensionality or geometrical frustration is not understood at present.
Although the existence of the spin reorientation in this material is know since 1995 [3] the low temperature magnetic structure has not yet been solved. Using neutron powder diffraction we have recently been able to propose a spiral model which satisfactorily describes the measured magnetic intensities below TC [4]. Also, investigation of the crystal structure showed the existence of small anomalies in the lattice parameters and some interatomic distances at TC. The relevance of these findings for the magnetoelectric coupling, the direction of the polarization, the modification of the different exchange paths in the structure and the stabilization of the incommensurate magnetic order below TC are discussed.

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