Erratum: Interplay of $4f - 3d$ interactions and spin-induced ferroelectricity in the green phase Gd_2BaCuO_5 [Phys. Rev. Research 2, 023271 (2020)]

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In this article, we found two errors thanks to our colleague J. M. Perez-Mato to check and scrutinize this paper before uploading the results in the magnetic database MAGNDATA [1,2] in the Bilbao Crystallographic Server [3]. The first error is that the Supplemental Material tables contained the wrong atom positions imported from the paper [4]. In this paper, the authors used a nonconventional origin (0,1/2,0), and the atomic positions of Gd1 and Gd2 were interchanged. After correcting this, the differences in the atomic positions obtained between 1.3 K [4] and 300 K are 0.106 Å for Gd1, 0.477 Å for Gd2, and 0.437 Å for Cu. These differences are too high and are not possible because there is no structural phase transition (except a small change associated with the magnetic ordering) in the temperature range of 1.3–300 K. The second error is that there exists another superspace group of higher symmetry, resulting from the mixing of two irreducible representations than that of $Pm1'(\alpha, 0, g)ss$ which has fewer degrees of freedom and provides a similar goodness of fit. The higher symmetry group is $P2_1ma1'(0, 0, g)0s0s$, and it does not appear directly in ISODISTORT [5] unless the mixing of representations is selected from the beginning.

We have reanalyzed the magnetic structure with the proper atom coordinates (those obtained at room temperature) for all temperatures and rewritten the Supplemental Material. The use of the right coordinates changes the orientation of the magnetic moments slightly. The refined neutron-diffraction pattern and the magnetic structure at 1.3 K are shown in Fig. 3. The content of the main text remains nearly unchanged except the following phrases that are correctly written as:

P. 1 (abstract): the polar magnetic space-groups $Pm1'(\alpha, 0, g)ss$ and P_aca2_1 should be replaced by $P2_1ma1'(0, 0, g)0s0s$ and P_c2_1ca, respectively.

P. 2 (first line): Replace "$m1'$" by "$2mm1'$".

P. 4 (bottom left): Paragraph starting with "Going down in symmetry …" and finishing just before "The superspace groups …" should be replaced by

Another option is that mixing the representations $mLD2$ and $mLD3$, we obtain another orthorhombic polar group, $P2_1ma1'(0, 0, g)0s0s$, which gives similar results as those provided by the lowest symmetry monoclinic group $Pm1'(a, 0, g)ss$ but with half the number of free parameters.

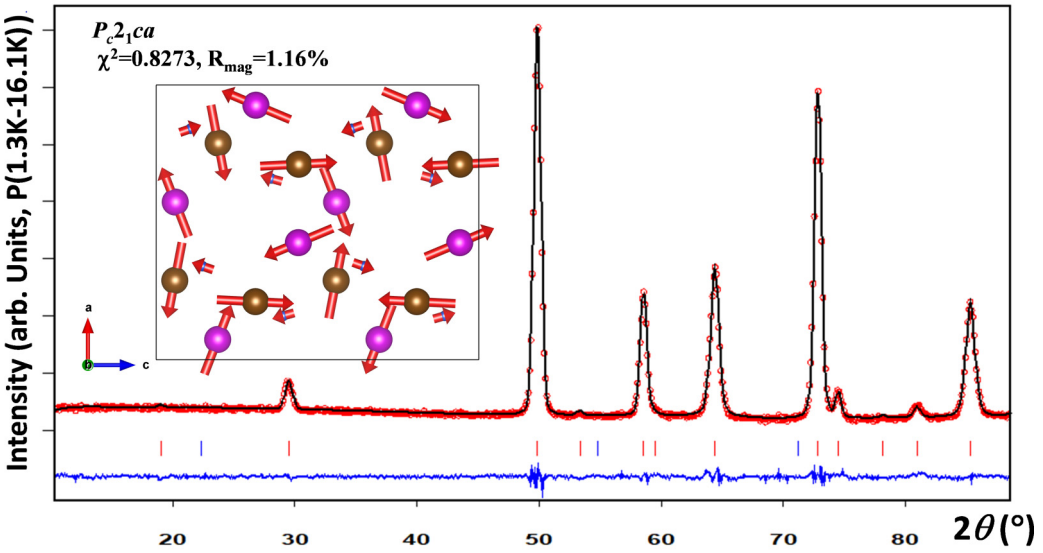

FIG. 3. Refined neutron-diffraction data recorded at 1.3 K. The inset shows the noncollinear commensurate magnetic structure of Gd_2BaCuO_5 at 1.3 K in the magnetic unit cell. (Gd1, purple; Gd2, orange; Cu, blue).

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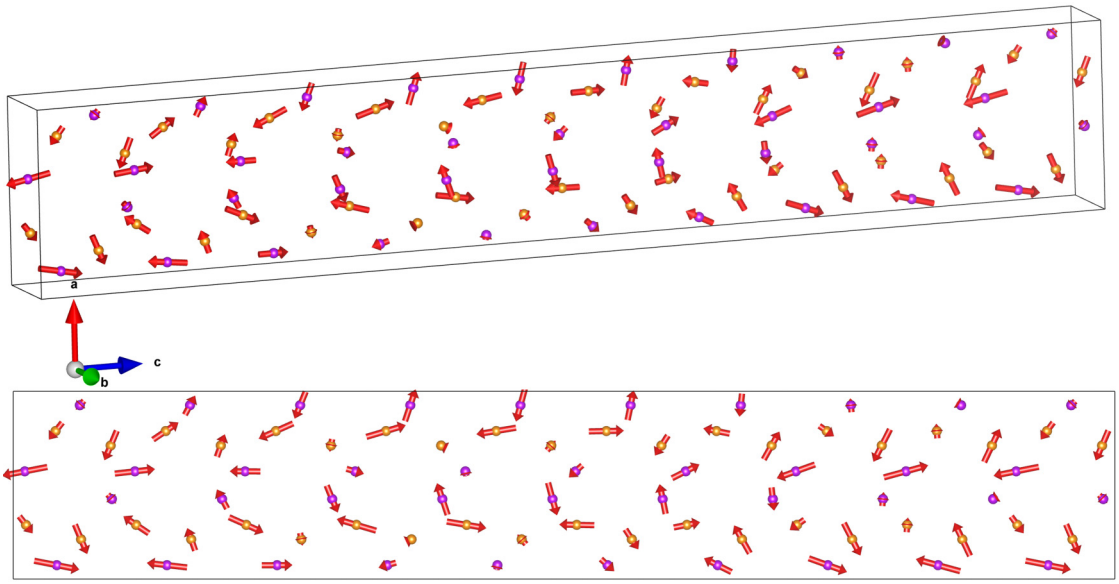

FIG. 4. Magnetic structure of Gd_2BaCuO_5 at 9.8 K viewed along the *b* axis (bottom) and a general orientation (upper part) described in $P2_1ma1'(0, 0, g)0s0s$. The magnetic structure shown here is constituted by $1\times1\times10$ unit cells of the paramagnetic structure. The nonmagnetic atoms as well as the Cu atoms have been removed for the sake of clarity. (Gd1, purple; Gd2, orange).

P. 4 (middle right): Phrase starting with "The deduced …" should be replaced by

The deduced magnetic structure (see Fig. 4) is polar $P2_1ma1'(0, 0, g)0s0s$ (point group $2mm1'$, allowing polarization along the *a* axis, such as in the low-temperature phase).

In the same paragraph, Fig. S11 is replaced by Fig. S14.

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