In Ref. 1 the current author presented a physically intuitive set of design criteria in order to identify or design a material in which a ferroelectric (FE) lattice distortion induces weak ferromagnetism (wFM). The criteria target an antiferromagnetic-paraelectric (AFM-PE) structure for which wFM is symmetry-forbidden but symmetry allowed in the FE phase. Said another way, a FE distortion can induce wFM when the phenomenological invariant \( E_{PLM} \sim \mathbf{P} \cdot (\mathbf{L} \times \mathbf{M}) \) is allowed in the energy of the antiferromagnetic-paraelectric (AFM-PE) phase, where \( \mathbf{L} \) is the AFM vector. Here, the polarization \( \mathbf{P} \) and the magnetization \( \mathbf{M} \) are small parameters expanded about \( \mathbf{P} = \mathbf{M} = 0 \).

Using a symmetry analysis, Ref. 1 showed clearly that such an invariant is allowed in paraelectric R3c magnetic A-site ABO\(_3\) materials such as FeTiO\(_3\) but symmetry forbidden in paraelectric R3c magnetic B-site ABO\(_3\) materials such as the most widely studied multiferroic BiFeO\(_3\) (for a more thorough presentation of this comparison see Ederer and Fennie 3). Recently, Ref. 2 have argued that “there is a simple duality between A-site and B-site” R3c ABO\(_3\) materials and that our Letter 1 “breaks this duality by ignoring a non-polar distortion that is directly measured in crystallography 4.” Here we point out that this is not correct. The Comment contains three elementary crystallographic errors:

1. that there is an R3c reference structure for BiFeO\(_3\) with inversion symmetry on Bi rather than on Fe (an error propagated from Kadomtseva et al. 5),
2. that their proposed \( \beta \) distortion: (a) generates this structure (b) is compatible with the translational symmetry of BiFeO\(_3\),
3. that three, not two, fields with different symmetries are required to obtain the R3c structure of BiFeO\(_3\) from the Pm\( \bar{3} \)m phase,

that make the comment fundamentally wrong and unpublishable.

Let us now address each error in some detail:

1. \( \) R3c reference structure.— The authors of the Comment claim that there is another R3c paraelectric reference structure besides the one that we considered in our Letter. This is simply a crystallographic mistake. The authors propagate an error present in the work of Ref. 5. This can be seen by starting, as did Ref. 2 with the 5 atom, cubic perovskite (space group Pm\( \bar{3} \)m), prototype structure of BiFeO\(_3\) where Bi sits in the center of a corner-sharing oxygen octahedra. It should be understood that the experimental ferroelectric R3c structure of BiFeO\(_3\) can be viewed as a slightly distorted version of this prototypical structure, e.g., Fe, not Bi, is approximately octahedrally coordinated as shown in Fig. 3. One can use standard group theoretic methods to show that there is only one distortion (labeled the \( \alpha \) distortion in the Comment) that connects the 5 atom cubic Pm\( \bar{3} \)m BiFeO\(_3\) structure to the 10 atom R3c structure (see Refs. 6 7 8 for details). This distortion removes the inversion center at the 12-fold coordinated site, i.e., the Bi-site, while retaining it at the 6-fold coordinated site, i.e., the Fe-site 8. This paraelectric R3c structure is the one we considered for BiFeO\(_3\) in our Letter in which the Fe-site is now at Wyckoff position 2b and the Bi-site is at Wyckoff position 2a. The second 10 atom R3c paraelectric reference structure proposed by the authors of the Comment follows the work of Kadomtseva et al. 5 who mistakenly switched the Bi and Fe positions in the R3c BiFeO\(_3\) structure. Subsequently, this results in a structure where Bi, rather than Fe, is octahedrally coordinated. This structure is not BiFeO\(_3\)!

2. \( \beta \) distortion.— Since group theory and basic crystallography rules out a second 10-atom R3c reference structure for BiFeO\(_3\) with inversion symmetry on Bi (point 1), the proposed \( \beta \) distortion obviously cannot generate it. In fact, the \( \beta \) distortion proposed by the authors of the Comment generates a distortion that is incompatible with the translational symmetry of BiFeO\(_3\) as we now show. In 10-atom R3c BiFeO\(_3\) structure, there are six translationally inequivalent oxygen atoms, labeled as 1-6 in Figs. 1 and 2 (for example, two atoms both labeled 1 are related by a lattice vector translation). As can be clearly seen, the \( \beta \) distortion does not have the correct translational symmetry, as each pair of atoms marked by the same number move in opposite directions. Further analysis shows that the displacement pattern generated by \( \beta \) has 20 atoms per unit cell and thus does NOT contribute to the R3c (nor the R3c), structure of BiFeO\(_3\).

3. Decomposition of R3c structure.— The authors of the Comment claim that three separate distortions of the 5 atom cubic perovskite structure are required to describe the R3c structure of BiFeO\(_3\) and that my Letter ignores one of them. Although we just proved that their proposed third distortion, the \( \beta \) distortion, is not present in BiFeO\(_3\) we feel this point is worth an additional response. To begin with, first-principles calculations of BiFeO\(_3\) in the R3c structure 1 9 account for
all the distortions present in the experimental paper [4] referenced by the authors of the Comment. The claim by the authors of the Comment that we ignored distortions present in the experimental structure of BiFeO$_3$ is not correct (in fact, it is not clear how they came to this conclusion). Additionally, it can easily be shown that the structure of R3c BiFeO$_3$ is completely described by only two fundamental atomic distortions (ignoring strain) of the cubic parent Pm$\bar{3}$m phase [8]. Note, the clearest approach to account for the structural distortions is to use symmetry-adapted lattice modes, i.e., lattice distortions that transform like a particular row of a particular irrep. Using these symmetry-adapted modes and other ideas from group theory one can show that the distortion from $\text{Pm}\bar{3}$m to R3c can be written in terms of two different symmetrized lattice modes (not including strains) (see Ref. [7] for a detailed discussion). The first mode is a polar (i.e., $q=0$) distortion labeled $\Gamma_1^-$. NOTE, this is important: this distortion can be thought of as having two parts, a trivial polar distortion where the atoms move along +/- [111], and a second one that, in the picture of oxygen triangles, causes alternating triangle’s to expand and contract (as shown Fig. [2]), but in either case these distortions transform like the $\Gamma_1^-$ representation, i.e., a polar vector along [111]. The second mode is a non-polar R-point ($q=\pi/a$ 111) distortion (see Fig. [2]), which can be thought of as a rotation characterized by a single angle, which Ref. [2] calls $\alpha$. Using these modes one can account for *all* the structural distortions in both the first-principles and the experimental [4] R3c BiFeO$_3$ structures (again, minus strains). Here is a summary of these two symmeterized lattice modes, shown in Fig. [2] in the language of the experimental reference (see Fig. [3]).

I. Starting with 5-atom $\text{Pm}\bar{3}$m, add just the R-point instability, this doubles the unit cell taking you to 10-atom R3c with (c=d, a=b).

II. Then, starting with R3c, (for illustrative purposes) add only the polar lattice mode at Gamma where all the displacements are in a plane perpendicular to [111]. This basis function contains only oxygen by symmetry and is the one I referred to as the non-trivial component of the FE mode. This takes you to R3c with (c,d,a,b) all different just like in the experiment!

III. For another view, go back to $\text{Pm}\bar{3}$m and add just the non-trivial FE mode. This takes you to R3m (size 1) with c=d, a and b different.

One can understand all this by first realizing that the symmetry adapted R-point mode is really a displacement pattern, not a rigid rotation per se. For example, if we keep in mind the picture of oxygen triangles you can visualize the non-trivial FE mode as one triangle getting bigger and the other getting small (in Kubel this leads to a $c \neq b$). The R-point *displacement pattern*, which translates each oxygen through an equal distance, then effectively rotates the smaller triangle through a larger angle than the larger triangle (thus breaking c=d).

In summary, the Comment of Ref. [2] have argued that “there is a simple duality between A-site and B-site” R3c ABO$_3$ materials and that our Letter [1] “breaks this duality by ignoring a non-polar distortion that is directly measured in crystallography [4].” We have shown that because the structure of BiFeO$_3$ is known to be a network of corner shared Fe-centered oxygen octahedra, then group theoretic analysis and basic crystallography tells us that this is impossible. Additionally we have shown that their proposed $\beta$ distortion breaks translation symmetry of the known BiFeO$_3$ structure and therefore can not contribute to the BiFeO$_3$ structure. Finally we have shown that first-principles calculations account for the distortions present in the experimental structure and that two, rather than three, unique symmetry modes are needed to describe this structure. The authors have not only propagated an error that has appeared in the literature [5], but in trying to reconcile this previous work and our own, have created several new errors as well. Their comment is fundamentally wrong and should not be published.

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FIG. 1: In 10-atom R3c, there are six translationally inequivalent oxygen atoms, labeled as 1-6. Two atoms both labeled by the same number are related by a lattice vector translation. The beta distortion proposed by Ref. 2 does not have the correct translational symmetry, as each pair of atoms marked by the same number move in opposite directions. Note figure taken without permission from Ref. 2 where we added the numbers labeling the six unique oxygen atoms in R3c BiFeO$_3$.

FIG. 2: Using only two properly symmetrized lattice-modes of the parent Pm3m Undistorted structure, i.e., the R-point distortion (the $\alpha$ rotational instability) and the $\Gamma_4$ ferroelectric instability, one can account for all structural distortions in both the first-principles obtained and the experimental [4] R3c BiFeO$_3$ structures (minus strains) (see Ref. 7 for a detailed discussion). Note: here we only show the non-trivial component of the ferroelectric mode (see text for a description).
FIG. 3: Fe-centered, oxygen octahedral in ferroelectric R3c BiFeO$_3$. Note figure is copied without permission from Ref. [4].