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Revisiting the antiferromagnetic structure of $Tb_{14}Ag_{51}$. The importance of distinguishing alternative symmetries for a multidimensional order parameter

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We revisit the antiferromagnetic structure of $Tb_{14}Ag_{51}$ with the propagation vector [1/3,1/3,0] and parent space group P6/m using both magnetic symmetry and irreducible representation arguments. We have found a new magnetic structure under the hexagonal Shubnikov magnetic space group P-6′, which fits much better the experimental data. This new solution was obtained by constraining the spin arrangement to one of the three possible magnetic space groups of maximal symmetry that can be realised by a magnetic ordering transforming according to the 4-dimensional physically irreducible representation that is known to be relevant in this magnetic phase. The refined model, parameterised under P-6′, implicitly includes the presence of a third harmonic with the propagation vector at the gamma point [0, 0, 0], which has an important weight in the final result. The structure consists of 13 symmetry-independent Tb magnetic moments with the same size of 8.48(2)μB, propagating cycloidally in the ab-plane. The modulation has a substantial deviation from being purely sinusoidal due to the contribution of the mentioned third harmonic.

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