

Erratum: Magnetic structure and high-field magnetization of the distorted kagome lattice antiferromagnet $\text{Cs}_2\text{Cu}_3\text{SnF}_{12}$ [Phys. Rev. B **99, 224404 (2019)]**

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In our original paper the ordered moments of the two crystallographically inequivalent Cu^{2+} sites were placed in two *separate* magnetic phases, so that their magnetic Bragg intensities were added incoherently instead of coherently, as a single $\mathbf{k} = 0$ magnetic structure requires. Refinements with the correct coherent summation favor the coplanar 120° structure of magnetic space group $P2_1/n$ with negative vector chirality and ordered moment $0.52(2)\mu_B$, rather than the all-in-all-out structure of $P2'_1/n'$ with $0.68(3)\mu_B$ reported originally; that identification is therefore withdrawn. The corrected structure reverses the sign of the out-of-plane Dzyaloshinskii-Moriya component, forbids a net out-of-plane moment by symmetry, and agrees with recent nuclear quadrupole resonance (NQR) results [1]. All other results of the original paper are unaffected.

Prompted by a recent NQR study by Grbić *et al.* [1], which finds a spin structure consistent with $P2_1/n$ and negative vector chirality, we reevaluated our previous neutron powder diffraction analysis, and discovered an error. In our paper, the magnetic structure of $\text{Cs}_2\text{Cu}_3\text{SnF}_{12}$ at 10 K was refined against the time-of-flight neutron powder diffraction data measured on SuperHRPD (J-PARC) using the FULLPROF suite. In that analysis, the ordered moments on the two crystallographically inequivalent Cu^{2+} sites, Cu(1) at (0.5, 0.0, 0.5) and Cu(2) at (0.2464, 0.2704, 0.2576), were described by two separate magnetic phases. Since the calculated pattern of a multiphase model is the sum of the intensities of the constituent phases, the magnetic Bragg intensities of the two sublattices were added incoherently, $I(\mathbf{Q}) \propto |\mathbf{F}_\perp^{\text{Cu}(1)}(\mathbf{Q})|^2 + |\mathbf{F}_\perp^{\text{Cu}(2)}(\mathbf{Q})|^2$, where $\mathbf{F}_\perp$ denotes the component of the magnetic structure factor perpendicular to the scattering vector $\mathbf{Q}$. This treatment is incorrect. The two sites order within a single magnetic structure with propagation vector $\mathbf{k} = 0$, and their magnetic structure factors must therefore be summed coherently,

$$I(\mathbf{Q}) \propto |\mathbf{F}_\perp^{\text{Cu}(1)}(\mathbf{Q}) + \mathbf{F}_\perp^{\text{Cu}(2)}(\mathbf{Q})|^2, \quad (1)$$

which differs from the incoherent sum by the interference term $2 \text{Re}[\mathbf{F}_\perp^{\text{Cu}(1)} \cdot \mathbf{F}_\perp^{\text{Cu}(2)*}]$. This term is not negligible: for the all-in-all-out structure it suppresses, for example, the calculated intensity of the (0,1,1) magnetic reflection by a factor of about 5 relative to the incoherent sum.

We have repeated the magnetic structure refinements with the moments on both Cu sites included in a *single* magnetic phase, so that Eq. (1) is satisfied. All other aspects of the analysis are identical to those of the original paper: the same magnetic symmetry operators of the magnetic space groups $P2'_1/n'$ and $P2_1/n$, the same three data banks (backscattering, 90° , and low-angle, weighted 0.2:0.6:0.2), the same fixed ideal 120° moment directions [Figs. 8(a)–8(e) of the original paper], and the magnitude of the ordered moment as the only refined magnetic parameter. The corrected results are summarized in Table I, which replaces Table IV of the original paper. Because the two sublattices now belong to one magnetic phase, a single magnetic R factor per data bank is obtained for each model.

The ordered moment is revised accordingly. If the all-in-all-out structure ($P2'_1/n'$ with positive vector chirality) is imposed, the coherent refinement yields $0.60(2)\mu_B$ with the global $\chi^2 = 5.56$, instead of $0.68(3)\mu_B$ with the global $\chi^2 = 5.84$ reported in the original paper; for the best-fitting structure (see below) the ordered moment is $0.52(2)\mu_B$. The moment reduction from the expected $1\mu_B$ for the $S = 1/2$ spin is therefore 40%–48%, rather than the 32% quoted originally.

The correction also reverses the model preference expressed by the neutron data. In the original (incoherent) analysis the refinements based on $P2'_1/n'$ gave distinctly smaller magnetic R factors (6%–8%) than those based on $P2_1/n$ (11%–13%), which was the basis for identifying the all-in-all-out structure. Under the correct coherent treatment the best fit is instead obtained for $P2_1/n$ with *negative vector chirality* [Fig. 8(e) of the original paper], with the magnetic R factor 5.2% (QA bank) and the global $\chi^2 = 5.21$, compared with 14.9% and 5.56 for the all-in-all-out structure (Table I); the negative-chirality $P2_1/n$ structure gives the smaller magnetic R factor in each of the three data banks, so this preference is unchanged under any reweighting of them. The preference has a transparent origin. For $P2_1/n$ the magnetic intensity of the (0,2,0) reflection vanishes identically: at (0, k , 0) the a and c^* moment components of the screw-related sublattices cancel exactly, and the surviving b component is parallel to the scattering vector. For $P2'_1/n'$, by contrast, (0,2,0) is among the strongest calculated magnetic reflections. The 10 K data show essentially no magnetic intensity at (0,2,0) beyond the nuclear peak, and the intensity distribution over the (1,1,0), (0,0,2), (1,1,2), and (2,0,0) reflections likewise follows the $P2_1/n$ negative-chirality pattern. The two fits are compared directly for these reflections in Fig. 1: the original refinement predicts a magnetic peak at (0,2,0) that the data do not show [Fig. 1(a)]

TABLE I. Corrected refinement results for the four coplanar 120° spin structures, replacing Table IV of the original paper. The two Cu sublattices are now included in a single magnetic phase [Eq. (1)], with the common moment magnitude $|M|$ as the only refined magnetic parameter. The magnetic R factor (R_{mag} , integrated-intensity Bragg R factor of the magnetic phase) is listed for each of the three data banks: backscattering (BS), 90° (QA, given the most weight in the refinement), and low-angle (LA); the global χ^2 (Bragg contribution) is for the three data banks refined together. All values were obtained with FULLPROF.2K version 7.95 (2023), whereas version 6.20 (2018) was used in the original paper. With version 7.95 the *original* (incoherent) two-phase all-in-all-out model yields the global $\chi^2 = 5.45$; global χ^2 values should therefore be compared only within a single program version. Boldface highlights the best-fitting structure and its magnetic space group.

Magnetic space group	Vector chirality	$ M $ (μ_B)	R_{mag} (%)			global χ^2
			BS	QA	LA	
$P2'_1/n'$	Positive	0.60(2)	14.5	14.9	42.5	5.56
	Negative	0.48(2)	24.4	11.5	32.5	5.57
$P2_1/n$	Positive	0.40(1)	20.2	14.4	28.1	5.41
	Negative	0.52(2)	4.9	5.2	29.1	5.21

and it underestimates the observed intensity at (2,0,0) and around (0,0,2) [Figs. 1(b) and 1(c)], whereas the corrected refinement accounts for all of them. The weak in-plane ferromagnetism reported in the original paper does not by itself discriminate between the two magnetic space groups: all four candidate structures are fully compensated (zero net moment), and a symmetry-allowed in-plane canting exists for *both* magnetic space groups, with mutually orthogonal in-plane directions (Fig. 9 of the original

† I_{obs} (10 K) --- original: $P2'_1/n'$, positive chirality (incoherent) — corrected: $P2_1/n$, negative chirality (coherent)

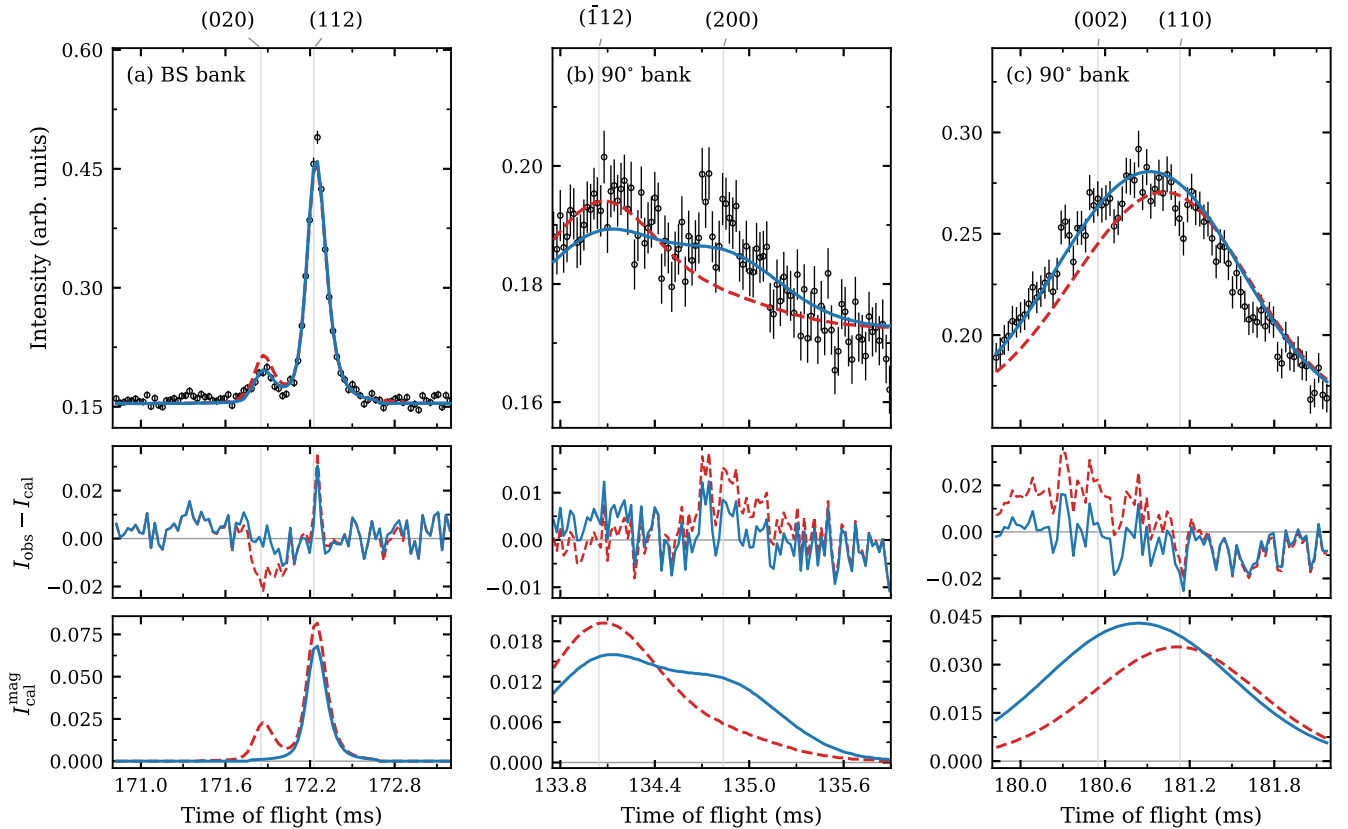


FIG. 1. Original and corrected fits to the 10 K neutron powder diffraction data, shown for the magnetic reflections discussed in the text. (a) Backscattering bank, where (0,2,0) and (1,1,2) are resolved; (b),(c) 90° bank around $(\bar{1}, 1, 2)/(2, 0, 0)$ and $(0, 0, 2)/(1, 1, 0)$. Vertical gray lines mark the calculated reflection positions. Top row: observed intensity (circles, with statistical error bars) together with the calculated profile of the original refinement (red dashed; all-in-all-out structure of $P2'_1/n'$; the two Cu sublattices in separate magnetic phases and therefore added incoherently) and of the corrected refinement (blue solid; $P2_1/n$ with negative vector chirality; both sublattices in a single magnetic phase and added coherently). Middle row: the corresponding difference curves $I_{\text{obs}} - I_{\text{cal}}$, plotted on a common vertical scale within each panel. Bottom row: the calculated magnetic contribution alone for the two models. The original model places substantial magnetic intensity at (0,2,0), where the data show none, and too little at (2,0,0) and (0,0,2); the corrected model removes both discrepancies.

paper); the in-plane direction of the canted moment relative to the crystallographic axes was not determined. The out-of-plane magnetization, however, does bear on the model choice, as discussed below.

The corrected best-fit structure—the coplanar 120° structure of $P2_1/n$ (irreducible representation Γ_1 of the original paper) with negative vector chirality—has two physical implications. First, it implies a sign change of the component of the Dzyaloshinskii-Moriya (DM) vector perpendicular to the kagome plane, D_z . As discussed in the original paper, the ordered state of the kagome antiferromagnet is selected by the DM interaction, and the sign of D_z determines the vector chirality of the $\mathbf{k} = 0$ 120° structure: one sign stabilizes the positive-chirality (all-in-all-out) state and the opposite sign the negative-chirality state [2,3]. The revision of the refined structure from positive to negative vector chirality therefore reverses the sign of D_z inferred for $\text{Cs}_2\text{Cu}_3\text{SnF}_{12}$; in particular, the sign is now opposite to that in jarosite, where D_z selects the positive-chirality all-in-all-out structure [3,4]. Second, the negative-chirality structure does not allow out-of-plane canted moments. Whereas for positive vector chirality the in-plane DM component cants the spins out of the kagome plane into the umbrella (all-in-all-out) configuration, for negative vector chirality it induces no out-of-plane canting and the spins remain strictly coplanar [2]; equivalently, in the magnetic space group $P2_1/n$ the only symmetry-allowed uniform magnetization is along the b axis, which lies in the kagome plane, so that a net out-of-plane moment is forbidden. (In $P2'_1/n'$, by contrast, a net out-of-plane component is symmetry allowed, and the original paper noted that it could not be excluded by the neutron data.) This is in agreement with the magnetization data reported in the original paper: at low field a spontaneous in-plane moment of $2.4 \times 10^{-3} \mu_B$ per Cu^{2+} was observed, while no spontaneous moment was detected perpendicular to the kagome plane. The absence of an out-of-plane spontaneous moment, which within $P2'_1/n'$ would require the symmetry-allowed out-of-plane canting to be accidentally small, follows by symmetry in the corrected structure, providing independent support for it.

Consequently, the identification of the all-in-all-out structure ($P2'_1/n'$ with positive vector chirality) as the magnetic structure of $\text{Cs}_2\text{Cu}_3\text{SnF}_{12}$ must be withdrawn. Although the magnetic Bragg reflections are weak and, because $\mathbf{k} = 0$, coincide with nuclear reflections, the pronounced differences in the magnetic R factors identify the coplanar 120° structure of magnetic space group $P2_1/n$ with negative vector chirality, with ordered moment $0.52(2)\mu_B$, as the correct magnetic model. This determination is corroborated by the absence of an out-of-plane spontaneous moment in the magnetization data, as discussed above, and is in full agreement with the recent NQR findings [1]. All results concerning the crystal structure, the structural and magnetic transition temperatures, the symmetry analysis of the allowed canting, and the magnetization and high-field measurements are unaffected.

An artificial intelligence assistant (Claude Fable, Anthropic) was used to reanalyze the neutron powder diffraction data, including the identification of the incoherent-summation error, the corrected coherent FULLPROF refinements, and the symmetry analysis reported here, and to prepare this Erratum. All of the material has been reviewed and its correctness confirmed by the authors, who take full responsibility for the content.

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