

Supplemental Information for Magnetism and Fermiology of Kagome Magnet $\text{YMn}_6\text{Sn}_4\text{Ge}_2$

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Supplementary Table 1 : Calculated total energy for $\text{YMn}_6\text{Sn}_5\text{Ge}$.

Position of Ge substitution	Energy (eV)
2e	-85.75591
2d	-85.89259
2c	-86.24354

Supplementary Note 1: Neutron Diffraction. The magnetic structure was modeled using irreducible representations and the program SARAh¹ was used to perform the calculations of representational analysis. Only irreducible representation Γ_5 can produce a flat spiral and the basis vectors for the two Mn sites are shown in Supplementary Table 2. Only two free parameters were needed to refine the data: the magnitude of the spins, which we fix to be constant for all Mn atoms, and the phase of the Mn atoms at Site 2. The constraints to ensure all moments are equal and aligned ferromagnetically within a plane are as follows for the site 1 (μ_1) and site 2 (μ_2) Mn atoms:

$$\mu_1 = -c_1\psi_1 + c_1\psi_2 + i(-c_1\psi_3 + c_1\psi_4) \quad (1)$$

$$\mu_2 = -\frac{3}{2}c_1\psi_1 + \frac{\sqrt{3}}{2}c_1\psi_2 + i\left(-\frac{3}{2}c_1\psi_3 + \frac{\sqrt{3}}{2}c_1\psi_4\right) \quad (2)$$

Here, c_1 is the refined variable and the phase, α , for the Mn site 2 moments was refined via the refinement program FULLPROF². The refined values are $c_1 = 0.73 \pm 0.01$, corresponding to a moment of $\mu = 2.19\mu_B \pm 0.03\mu_B$ and $\alpha = 7.9^\circ \pm 0.7^\circ$.

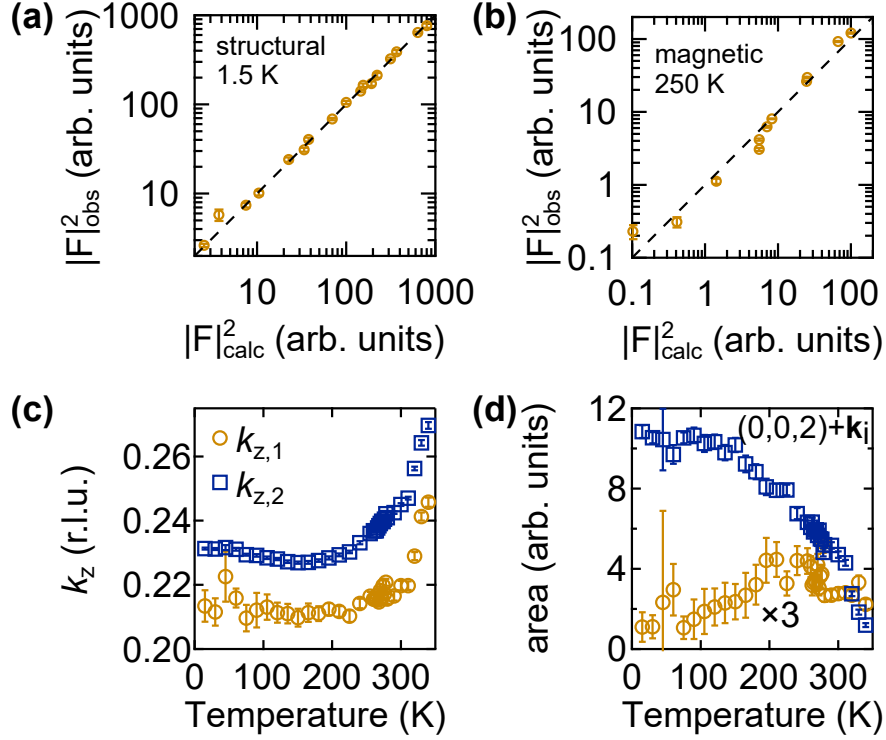
The parameters $\mathbf{k}$, α , and β are shown in Supplementary Table 3 for YMn_6Sn_6 and $\text{YMn}_6\text{Sn}_4\text{Ge}_2$. The angle α is the change in angle between the first layer of Mn moments within a unit cell and the second layer of Mn moments in that unit cell. The angle β is the angle of rotation between the second layer of Mn atoms in a unit cell and the Mn moments in the layer above.

Supplementary Table 2 : Basis vectors for the space group $P6/mmm$ with $\mathbf{k} = (0, 0, 0.233)$ and the irreducible representation Γ_5 . The single Mn Wyckoff site in the crystal structure is split into two orbits with positions $(0.5, 0, z)$ (site 1, left five columns of table) and $(0, 0.5, 1 - z)$ (site 2, right five columns of table) where $z \approx 0.23$. The atoms of the nonprimitive basis for site 1 are defined according to 1: $(0.5, 0, z)$, 2: $(0.5, 0.5, z)$, 3: $(0, 0.5, z)$. The atoms of the nonprimitive basis for site 2 are defined according to 1: $(0, 0.5, 1 - z)$, 2: $(0.5, 0, 1 - z)$, 3: $(0.5, 0.5, 1 - z)$.

Mn site 1 (0.5, 0, z)		BV components			Mn site 2 (0, 0.5, 1 - z)		BV components		
BV	Atom	$m_{\parallel}a$	$m_{\parallel}b$	$m_{\parallel}c$	BV	Atom	$m_{\parallel}a$	$m_{\parallel}b$	$m_{\parallel}c$
ψ_1	1	1	0	0	ψ_1	1	0	-2	0
	2	-1	-1	0		2	1	0	0
	3	0	-2	0		3	-1	-1	0
ψ_2	1	1	3	0	ψ_2	1	0	0	0
	2	-1	2	0		2	$\sqrt{3}$	$2\sqrt{3}$	0
	3	0	1	0		3	$-\sqrt{3}$	$\sqrt{3}$	0
ψ_3	1	$-\sqrt{3}$	0	0	ψ_3	1	0	0	0
	2	$-\sqrt{3}$	$-\sqrt{3}$	0		2	$-\sqrt{3}$	0	0
	3	0	0	0		3	$-\sqrt{3}$	$-\sqrt{3}$	0
ψ_4	1	$\sqrt{3}$	$\sqrt{3}$	0	ψ_4	1	4	2	0
	2	$\sqrt{3}$	0	0		2	1	2	0
	3	$2\sqrt{3}$	$\sqrt{3}$	0		3	1	-1	0

Supplementary Table 3 : Comparison of the Mn moment angles between YMn_6Sn_6 ($T = 4$ K)³, and $\text{YMn}_6\text{Sn}_4\text{Ge}_2$ ($T = 1.5$ K).

$\text{YMn}_6\text{Sn}_{6-x}\text{Ge}_x$	$\mathbf{k}$	α	β
x			
0	(0, 0, 0.26)	-5°	99°
2	(0, 0, 0.23)	8°	76°



Supplementary Figure 1 : Rietveld refinement results from the HB-3 single crystal neutron diffraction experiment. Error bars displayed in the plot represent plus and minus one standard deviation. (a) Data show the observed versus calculated structure factors for the $\text{YMn}_6\text{Sn}_4\text{Ge}_2$ nuclear structure at 1.5 K (R_F -factor = 2.65). **(b)** Data show the observed versus calculated structure factors for the $\text{YMn}_6\text{Sn}_4\text{Ge}_2$ magnetic structure at 250 K (R_F -factor = 10.6). The black dashed lines denote $|F|_{\text{calc}}^2 = |F|_{\text{obs}}^2$. Temperature dependence of the **(c)** wavevector, $\mathbf{k}_i = (0, 0, k_{z,i})$, and **(d)** area for the magnetic structures related to $i = 1$ (orange open circles) and $i = 2$ (blue open squares). The $(0, 0, 2) + \mathbf{k}_1$ area in **(d)** is multiplied by three for clarity.

Supplementary References

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