

CHEMISTRY OF MATERIALS

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Table S1a. Crystal data for Yb₁₄MnSb₁₁

Empirical formula	Yb ₁₄ MnSb ₁₁
Formula weight	3816.75
Crystal size	0.20 x 0.02 x 0.02 mm
Crystal habit	needle
Crystal color	silver
Crystal system	Tetragonal
Space group	I4(1)/acd
Unit cell dimensions	a = 16.615(2) Å b = 16.615(2) Å c = 21.948(4) Å
Volume	6059(2) Å ³
Z	8
Density (calculated)	8.368 g cm ⁻³
Absorption coefficient	52.711 mm ⁻¹
F(000)	12528
Absorption correction(1)	psi scans
Max. and min. trans. coeff.	0.339 and 0.262
Temperature	143(2) K
Scan type	ω
Index ranges	0 ≤ h ≤ 21, 0 ≤ k ≤ 21, -28 ≤ l ≤ 28
Reflections collected	6669
Independent reflections	1743 (R(int) = 0.0750)
Data/ restraints/ parameters	1743 / 0 / 62
Final R indices (1) [I>2σ(I)]	R1 = 0.0299, wR2 = 0.0479
Reflections observed	1372
R indices (all data)	R1 = 0.0481, wR2 = 0.0528
Goodness-of-fit (2) on F ²	0.973
Extinction coefficient	0.000095(2)
Largest diff. peak and hole	1.706 and -1.807 eÅ ⁻³

Table S1b. Crystal data for Yb₁₄MnBi₁₁

Empirical formula	Yb ₁₄ MnBi ₁₁
Formula weight	4776.28
Crystal size	0.28 x 0.22 x 0.18 mm
Crystal habit	plate
Crystal color	silver
Crystal system	Tetragonal
Space group, Z	I4(1)/acd, 8
Unit cell dimensions	a = 17.000(3) Å, b = 17.000(3) Å, c = 22.259(6) Å
Volume	6433(2) Å ³
Density (calculated)	9.863 g cm ⁻³
Absorption coefficient	100.512 mm ⁻¹
F(000)	15344
Absorption correction(3)	Xabs2
Max. and min. trans. coeff.	0.35 and 0.27
Temperature	143(2) K
Scan type	ω
Index ranges	0 ≤ h ≤ 11, 0 ≤ k ≤ 16, 0 ≤ l ≤ 21
Reflections collected	1111
Independent reflections	753 (R(int) = 0.0706)
Data/ restraints/ parameters	753 / 0 / 62
Final R indices (1) [I>2σ(I)]	R1 = 0.0631, wR2 = 0.1335
Reflections observed	515
R indices (all data)	R1 = 0.1290, wR2 = 0.1504
Goodness-of-fit (2) on F ²	1.071
Extinction coefficient	0.000007(2)
Largest diff. peak and hole	4.443 and -3.714 eÅ ⁻³

1) $R1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}$; $wR2 = \frac{[\sum [w(F_o^2 - F_c^2)^2]}{\sum [w(F_o^2)^2]}^{(1/2)}$

2) Goodness-of-Fit = $[\sum [w(F_o^2 - F_c^2)^2] / (M - N)]^{(1/2)}$ where M is the number of reflections and N is the number of parameters refined.

3) Parkin, S. R., Moezzi, B., Hope, H. (1995). J. Appl. Cryst., 28, 53-56.
XABS2: an empirical absorption correction program.

Table S2.Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for $\text{Yb}_{14}\text{MnSb}_{11}$ and $\text{Yb}_{14}\text{MnBi}_{11}$ **$\text{Yb}_{14}\text{MnSb}_{11}$**

	U11	U22	U33	U23	U13	U12
Sb(1)	5(1)	5(1)	7(1)	0(1)	0(1)	0(1)
Sb(2)	6(1)	6(1)	9(1)	-1(1)	2(1)	0(1)
Sb(3)	10(1)	6(1)	6(1)	1(1)	0(1)	2(1)
Sb(4)	6(1)	6(1)	9(1)	0	0	2(1)
Yb(1)	6(1)	6(1)	9(1)	0(1)	1(1)	0(1)
Yb(2)	7(1)	8(1)	11(1)	2(1)	0(1)	2(1)
Yb(3)	6(1)	6(1)	7(1)	0(1)	0	0
Yb(4)	6(1)	12(1)	7(1)	-3(1)	-1(1)	1(1)
Mn(1)	7(1)	7(1)	9(2)	0	0	0

 $\text{Yb}_{14}\text{MnBi}_{11}$

	U11	U22	U33	U23	U13	U12
Bi(1)	5(2)	5(2)	9(3)	0(2)	0(2)	-2(2)
Bi(2)	9(3)	9(3)	10(2)	-3(2)	2(2)	2(2)
Bi(3)	9(3)	11(3)	5(2)	1(2)	2(2)	2(2)
Bi(4)	9(3)	9(3)	11(4)	0	0	-2(4)
Yb(1)	12(3)	12(3)	6(3)	-1(2)	-1(2)	0(2)
Yb(2)	21(3)	8(3)	10(3)	0(2)	-2(2)	1(2)
Yb(3)	6(4)	13(4)	6(4)	1(3)	0	0
Yb(4)	10(3)	18(3)	8(3)	0(2)	-2(2)	1(2)
Mn(1)	29(13)	29(13)	4(17)	0	0	0

The anisotropic displacement factor exponent takes the form:

$$-2(\pi)^2 [(ha^*)^2 U(11) + \dots + 2hka^*b^*U(12)]$$