

## **Yb<sub>14</sub>MgBi<sub>11</sub>: Structure, Thermoelectric Properties and the Effect of Structure on Low Lattice Thermal Conductivity**

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### **Supporting Information**

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<b>STable 1</b>	Measured thermal diffusivity, calculated density, calculated specific heat and thermal conductivity of Yb <sub>14</sub> MgBi <sub>11</sub> and Yb <sub>14</sub> MnBi <sub>11</sub> .
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**Stable 1.** Measured Thermal Diffusivity, Calculated Density, Calculated Specific Heat and Thermal Conductivity of Yb<sub>14</sub>MgBi<sub>11</sub> and Yb<sub>14</sub>MnBi<sub>11</sub>.

Temperature (K)	Diffusivity (mm <sup>2</sup> /s)	Density (g*cm <sup>-3</sup> ) <sup>a</sup>	Specific Heat (J*K <sup>-1</sup> *g <sup>-1</sup> ) <sup>b</sup>	Thermal conductivity (W*m <sup>-1</sup> *K <sup>-1</sup> )
Yb <sub>14</sub> MgBi <sub>11</sub>				
300.5	1.163	9.559	0.1263	1.40
372.8	1.264	9.522	0.1286	1.55
472.7	1.350	9.470	0.1318	1.69
573.7	1.409	9.419	0.1351	1.79
672.7	1.428	9.369	0.1383	1.85
773.7	1.416	9.319	0.1415	1.87
873.4	1.417	9.269	0.1447	1.90
Yb <sub>14</sub> MnBi <sub>11</sub>				
298.2	1.042	9.727	0.1254	1.27
372.9	1.152	9.688	0.1278	1.43
471.5	1.256	9.637	0.1309	1.58
575.5	1.344	9.583	0.1343	1.73
676.1	1.389	9.531	0.1375	1.82
775.0	1.393	9.481	0.1406	1.86
874.3	1.426	9.431	0.1438	1.93

a. Density is calculated using the room temperature density and thermal expansion data from Ref[45]. The equation used in calculation is:

$$Density = \frac{Room\ temperature\ density}{[1 + 0.000018 * (Temperature - 300)]^3}$$

0.000018 is the thermal expansion ratio per K for Yb<sub>14</sub>MnSb<sub>11</sub> and 300 K is the room temperature.

b. Specific heat is calculated using data from Ref[36], adjusted by molecular masses of compounds.

$$Specific\ heat = \frac{Molecular\ mass\ of\ Yb_{14}MnSb_{11}}{Molecular\ mass\ of\ sample} \times Specific\ Heat\ of\ Yb_{14}MnSb_{11}$$

$$Specific\ Heat\ of\ Yb_{14}MnSb_{11} = 0.145 + 0.00004 \times Temperature$$