Ultra-Low Thermal Conductivity and Promising Thermoelectric Performance in the Structurally Complex Zintl Phase: $Eu_{14}GaAs_{11}$

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Table S1. Crystallographic Sites, Fractions, and Multiplicity Determined through Rietveld Refinement of X-ray Powder Diffraction‡

Name	Type	*x*	*y*	*z*	Frac	Uiso	Multiplicity
As1	As	0.1335(4)	0.3835(4)	0.12500	1	0.0085	16
As2	As	0.0035(4)	0.1166(5)	0.81054(24)	1	0.0088	32
As3	As	0.8700(4)	0.9745(4)	0.95306(28)	1	0.0103	32
As4	As	0.0077(15)	0.2577(15)	0.12500	0.5	0.017	16
Ga1	Ga	0.00000	0.25000	0.87500	1	0.0081	8
Eu1	Eu	-0.04406(23)	-0.07193(24)	0.82889(18)	1	0.0089	32
Eu2	Eu	-0.02207(21)	0.12327(26)	0.00287(18)	1	0.0111	32
Eu3	Eu	0.3540(3)	0.00000	0.25000	1	0.0079	16
Eu4	Eu	0.18009(21)	0.40577(26)	0.84381(19)	1	0.011	32

‡It is important to acknowledge that a degree of uncertainty is inherent in these values due to the complex nature of the polycrystalline sample's structure.

Table S2. Chemical Analysis from Energy Dispersive Spectroscopy (EDS)‡

Eu nominal %	Eu at.% from EDS	Ga nominal %	Ga at.% from EDS	As nominal %	As at.% from EDS
53.85	50.91(2)	3.85	2.49(2)	42.31	46.63(2)

‡Based on 10 data points of a $Eu_{14}GaAs_{11}$ pellet with an FEI Scios DualBeam FIB/SEM instrument equipped with an Oxford Instruments X-Max 50 mm^2 Si drift detector.

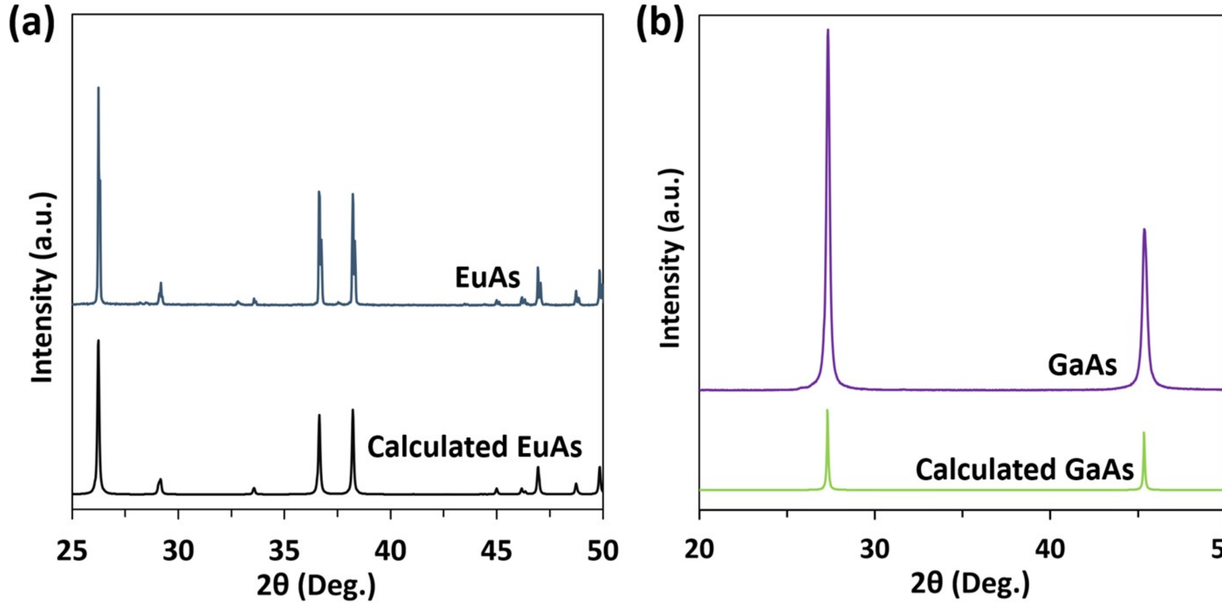

Fig. S1. PXRD patterns of binary precursors compared to calculated patterns of (a) EuAs, and (b) GaAs.