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The Proof is in the Powder: Revealing Structural Peculiarities in the $Yb_3Rh_4Sn_{13}$ Structure Type

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Supplementary Information

Single-Crystal X-ray Diffraction. Single crystals of $Lu_3Ir_4Ge_{13}$ were cut to the appropriate sizes and then mounted onto separate glass fiber tips using epoxy. These were then attached onto the goniometer head of a Bruker D8 Quest equipped with Mo Kα radiation (λ = 0.71073 A). Absorption correction was done using SADABS 2016/12.[1] Intrinsic methods was used to solve the crystal structure using Bruker SHELXT[2] with the refinement done in SHELXL2014/7.[3]

Powder X-ray Diffraction. Single crystals of $Lu_3Ir_4Ge_{13}$ were ground using a mortar and pestle. The powder was then placed onto a no-background holder and mounted onto a Bruker D8 Advance equipped with a LYNXEYE XE detector and Cu Kα source (λ = 1.54060). Data acquisition was collected using the Bragg-Brentano θ-2θ mode from 10 – 90° with a step size of 0.01 and 2 seconds per count. Rietveld refinement was performed using the Bruker TOPAS software package. The single crystal model was used as a starting model for the refinement.

Table S1. Powder X-ray Diffraction Crystallographic Parameters for $Lu_3Ir_4Ge_{13}$

Crystal System	Tetragonal
Space Group	$I4_1/amd$
a (Å)	17.737(1)
c (Å)	17.784(1)
V (Å^3)	5594.7(6)
Z	16
Temperature (K)	298(2)
R_{wp} [a]	7.85
R_{exp} [b]	2.88
GOF	2.73

[a] $R_{wp} = (\Sigma_i w_i(y_i^{calc} - y_i^{obs})^2/\Sigma_i w_i(y_i^{obs})^2)^{1/2}$. [b] $R_{exp} = (N)/(\Sigma_i w_i(y_i^{obs})^2)^{1/2}$.

Table S2. Powder X-ray Diffraction Atomic Positions for $Lu_3Ir_4Ge_{13}$

Atom	*x*	*y*	*z*	B_{eq} (Å^2)	Occ. (< 1)
Lu1	0.5	0.374912	0.00026	0.370145	
Lu2	0.25127	0.49873	0.125	0.282074	
Lu3	0	0.37479	0.00139	0.236010	
Ir1	0.12521	0.375035	0.124977	0.239670	
Ir2	0.37493	0.37507	0.125	0.159181	
Ir3	0.12524	0.62476	0.125	0.290015	
Ge1A	0.247944	0.75	0.000237	1.315819	0.921
Ge1B	0.240987	0.75	−0.025501	1.316	0.079
Ge2	0	0.332128	0.165995	0.153424	
Ge3	0.250822	0.329944	0.170009	0.224038	
Ge4	0.172778	0.416378	0.000427	0.099813	
Ge5	0	0.660809	0.172972	0.431529	
Ge6	0.124798	0.25	0.068336	1.424429	
Ge7	0.316237	0.385692	0.001707	1.183818	
Ge8	0.070312	0.500892	0.109221	1.32653	
Ge9	0.5	0.348662	0.183120	3.2 (4)	

References

1. Krause, L.; Herbst-Irmer, R.; Sheldrick, G. M.; Stalke, D. *J. Appl. Crystallogr.*, 2015, **48**, 3-10.
2. Sheldrick, G. M. *Acta Crystallogr. Sect. A-Found. Adv.* 2015, **71**, 3-8.
3. Sheldrick, G. M. *Acta Crystallogr. C.*, 2015, **71**, 3-8.