

Supplementary data

Table I. Single crystal and powder X-ray diffraction data of Lu₂PdSi₃.

Crystal Data	SCXRD	PXRD
Chemical formula	Lu ₂ PdSi ₃	
Formula weight / g mol ⁻¹	540.61	
Crystal system	hexagonal	
Space group	<i>P6/mmm</i> (Nr. 191)	
Unit cell dimensions		
<i>a</i> / Å	4.0217(4)	4.02672(5)
<i>b</i> / Å	4.0217(4)	4.02672(5)
<i>c</i> / Å	3.9180(6)	3.92175(7)
α / °	90	90
β / °	90	90
γ / °	120	120
Cell volume / Å ³	54.880(11)	55.070(2)
<i>Z</i>	1	1
Calculated density / g cm ⁻³	8.179	
Radiation type / Å	Mo K α	Mo K α_1
Temperature / K	296(2)	293
Crystal form, color	prism, metallic	
Data Collection		
Diffractometer	Bruker Kappa Apex II Single crystal X-ray diffractomet er with CCD detector	STOE Stadi P Powder X- ray diffractome ter with Dectris Mythen 1K

Data collection method	Rotating method data acquisition using ω and φ scans	Transmission
Range of h, k, l	$-7 \leq h \leq 7, -7 \leq k \leq 7, -7 \leq l \leq 7$	
Absorption coefficient / μm^{-1}	49.280	
$F(000)$	115	
Range of Data Collection	5.20° to 44.82°	$5^\circ \leq 2\theta \leq 50^\circ$
d (min), d (max) for cell determination / Å		0.8330, 8.1306
Reflections collected/unique	3941/118	
Completeness to $\theta = 44.82^\circ$	1.000	
Refinement method	Full-matrix least-squares against F^2	Rietveld
Data/parameters/restraints	118/7/0	
Goodness of fit on F^2	1.113	1.4
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0111,$ $wR_2 = 0.0272$	
R indices all data	$R_1 = 0.0111,$ $wR_2 = 0.0272$	$R_p = 0.0696,$ $R_{wp} = 0.0894$
Largest diff. peak and hole / $e/\text{Å}^3$	1.037, -1.555	

Table II. Atomic positions, occupancy, and isotropic temperature parameters for Lu₂PdSi₃.

Atom	Multiplicity and Wyckoff letter	x	y	z	Isotropic temperature parameters [\AA^2]	Occupancy
Lu	<i>1a</i>	0	0	0	0.92	0.04167
Pd	<i>2d</i>	0.33333	0.66667	0.5	0.47	0.01970
Si	<i>2d</i>	0.33333	0.66667	0.5	0.89	0.06293