SUPPORTING INFORMATION
Lu₈Te and Lu₇Te. Novel Substitutional Derivatives of Lutetium Metal
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Table S1. Crystal data and structure refinement for Lu₇Te.

Formula weight	1352.39
Temperature	273(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group, Z	<i>Cmcm</i> (No. 63), 4
Unit cell dimensions, Å, Å ³	
<i>a</i>	3.7418(7)
<i>b</i>	12.278(2)
<i>c</i>	19.770(3)
Volume	908.2(3)
Density (calculated)	9.890 Mg/m ³
Absorption coefficient	78.375 mm ⁻¹
F(000)	2196
Crystal size	0.07 × 0.07 × 0.05 mm
Theta range for data collection	2.06 to 28.25°.
Index range	−4 ≤ <i>h</i> ≤ 4, −15 ≤ <i>k</i> ≤ 13, −17 ≤ <i>l</i> ≤ 25
Reflections collected (Obs., [I > 3σ(I)])	2784 (2264)
Independent reflections	626 [R(int) = 0.0381]
Completeness to Θ = 28.25°	94.8 %
Absorption correction	SADABS
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	626 / 0 / 28
Goodness-of-fit on F ²	1.103
Final R indices ^a [I > 2σ(I)]	R1 = 0.0273, wR2 = 0.0652
(all data)	R1 = 0.0309, wR2 = 0.0666
Extinction coefficient	0.00042(4)
Largest diff. peak and hole	4.772 and −2.169 e [−] /Å ^{−3}

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

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) Lu₇Te. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

—		x	y	z	$U(\text{eq})$
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Lu(1)	8 <i>f</i> <i>m</i>	0	200(1)	1090(1)	7(1)
Lu(2)	8 <i>f</i> <i>m</i>	0	2448(1)	6454(1)	6(1)
Lu(3)	8 <i>f</i> <i>m</i>	0	3577(1)	126(1)	7(1)
Lu(4)	4 <i>c</i> <i>m2m</i>	0	4380(1)	2500	7(1)
Te	4 <i>c</i> <i>m2m</i>	0	1480(1)	2500	6(1)

Table S3. Anisotropic displacement parameters ($\times 10^3$) for Lu₇Te. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\text{h}^2 \text{a}^*2\text{U}_{11} + \dots + 2 \text{h k a}^* \text{b}^* \text{U}_{12}]$

	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
Lu(1)	9(1)	6(1)	6(1)	-1(1)	0	0
Lu(2)	8(1)	6(1)	4(1)	-1(1)	0	0
Lu(3)	9(1)	6(1)	5(1)	0(1)	0	0
Lu(4)	7(1)	9(1)	6(1)	0	0	0
Te	5(1)	10(1)	4(1)	0	0	0

Table S4. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for Lu_7Te

Lu(1)-Te	3.1996(10)
Lu(1)-Lu(2)#1	3.3299(11)
Lu(1)-Lu(3)#2	3.3324(8)
Lu(1)-Lu(3)#3	3.3324(8)
Lu(1)-Lu(3)#4	3.3965(8)
Lu(1)-Lu(3)#5	3.3965(8)
Lu(1)-Lu(4)#3	3.5044(7)
Lu(1)-Lu(4)#2	3.5044(7)
Lu(1)-Lu(2)#6	3.5149(9)
Lu(1)-Lu(2)#7	3.5149(9)
Lu(1)-Lu(1)#8	3.7418(7)
Lu(1)-Lu(1)#9	3.7418(7)
Lu(2)-Te #10	3.0837(9)
Lu(2)-Te #11	3.0837(8)
Lu(2)-Lu(1)#12	3.3299(11)
Lu(2)-Lu(3)#13	3.4171(10)
Lu(2)-Lu(3)#14	3.4605(8)
Lu(2)-Lu(3)#15	3.4605(8)
Lu(2)-Lu(1)#15	3.5149(9)
Lu(2)-Lu(1)#14	3.5149(9)
Lu(2)-Lu(4)#11	3.5801(9)
Lu(2)-Lu(4)#10	3.5801(9)
Lu(2)-Lu(2)#8	3.7418(7)
Lu(2)-Lu(2)#9	3.7418(7)
Lu(3)-Lu(3)#4	3.2780(11)
Lu(3)-Lu(3)#5	3.2780(11)
Lu(3)-Lu(1)#16	3.3324(8)
Lu(3)-Lu(1)#17	3.3324(8)

Lu(3)-Lu(1)#4	3.3965(8)
Lu(3)-Lu(1)#5	3.3965(8)
Lu(3)-Lu(2)#13	3.4171(10)
Lu(3)-Lu(2)#6	3.4605(8)

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Lu(3)-Lu(2)#7	3.4605(8)
Lu(3)-Lu(3)#18	3.5292(14)
Lu(3)-Lu(3)#8	3.7418(7)
Lu(3)-Lu(3)#9	3.7418(7)
Lu(4)-Te #16	3.1857(14)
Lu(4)-Te #17	3.1857(14)
Lu(4)-Lu(1)#17	3.5044(7)
Lu(4)-Lu(1)#19	3.5044(7)
Lu(4)-Lu(1)#16	3.5044(7)
Lu(4)-Lu(1)#20	3.5044(7)
Lu(4)-Te	3.5604(18)
Lu(4)-Lu(2)#7	3.5801(9)
Lu(4)-Lu(2)#6	3.5801(9)
Lu(4)-Lu(2)#11	3.5801(9)
Lu(4)-Lu(2)#10	3.5801(9)
Lu(4)-Lu(4)#8	3.7418(7)
Te-Lu(2)#7	3.0837(9)
Te-Lu(2)#10	3.0837(9)
Te-Lu(2)#6	3.0837(9)
Te-Lu(2)#11	3.0837(9)
Te-Lu(4)#2	3.1857(14)
Te-Lu(4)#3	3.1857(14)
Te-Lu(1)#13	3.1996(10)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,z-1/2 #2 x-1/2,y-1/2,z #3 x+1/2,y-1/2,z
 #4 -x-1/2,-y+1/2,-z #5 -x+1/2,-y+1/2,-z #6 -x+1/2,-y+1/2,z-1/2
 #7 -x-1/2,-y+1/2,z-1/2 #8 x+1,y,z #9 x-1,y,z

#10 -x+1/2,-y+1/2,-z+1 #11 -x-1/2,-y+1/2,-z+1
 #12 -x,-y,z+1/2 #13 x,y,-z+1/2 #14 -x-1/2,-y+1/2,z+1/2
 #15 -x+1/2,-y+1/2,z+1/2 #16 x+1/2,y+1/2,z #17 x-1/2,y+1/2,z
 #18 -x,-y+1,-z #19 x+1/2,y+1/2,-z+1/2 #20 x-1/2,y+1/2,-z+1/2

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Table S5. Crystal data and structure refinement for Lu₈Te.

Formula weight	1527.36
Temperature	273(2) K
Wavelength	0.71073 Å
Crystal system	Hexagonal
Space group, Z	$P\bar{6}2m$ (No. 189), 1
Unit cell dimensions	a = 9.000(3) Å b = 9.000(3) Å c = 3.687(2) Å V = 258.61(9) Å ³
Density (calculated)	9.807 Mg/m ³
Absorption coefficient	78.250 mm ⁻¹
F(000)	620
Crystal size (mm)	0.09 × 0.07 × 0.03
Theta range for data collection	2.61 to 28.21°.
Index ranges	-9 ≤ h ≤ 11, -11 ≤ k ≤ 11, -4 ≤ l ≤ 4
Reflections collected (Obs. [I > 3σ(I)])	1473 (1205)
Independent reflections	262 [R(int) = 0.0816]
Completeness to theta = 28.21°	99.4 %
Absorption correction	SADABS
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	262 / 0 / 14
Goodness-of-fit on F ²	1.060
Final R indices ^a [I > 2σ(I)]	R1 = 0.0328, wR2 = 0.0648
R indices (all data)	R1 = 0.0367, wR2 = 0.0656
Absolute structure parameter	0.47(9)
Extinction coefficient	0.0010(4)
Largest diff. peak and hole	1.892 and -2.650 e ⁻ /Å ⁻³

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

Table S6. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Lu_8Te . $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

			x	y	z	U(eq)
Lu(1)	$3f$	$m2m$	2770(2)	0	0	6.6(4)
Lu(2)	$3g$	$m2m$	6135(2)	0	5000	6.8(4)
Lu(3)	$2c$	$\bar{6}..$	3333	6667	0	6.3(4)
Te	$1b$	$\bar{6}2m$	0	0	5000	7.0(8)

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Table S7. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Lu_8Te . The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Lu(1)	6.9(6)	8.5(8)	5.1(7)	0	0	4.3(4)
Lu(2)	7.7(6)	7.9(8)	5.0(6)	0	0	3.9(4)
Lu(3)	6.5(6)	6.5(6)	5.9(9)	0	0	3.3(3)
Te	8(1)	8(1)	4(2)	0	0	4.1(5)

Table S8. Bond lengths [$\text{\AA}$] for Lu₈Te..

Lu(1)-Te#1	3.1004(15)
Lu(1)-Te	3.1004(15)
Lu(1)-Lu(3)#2	3.2829(15)
Lu(1)-Lu(3)#3	3.2829(15)
Lu(1)-Lu(2)	3.545(2)
Lu(1)-Lu(2)#1	3.545(2)
Lu(1)-Lu(2)#4	3.6114(15)
Lu(1)-Lu(2)#5	3.6114(15)
Lu(1)-Lu(2)#6	3.6114(15)
Lu(1)-Lu(2)#7	3.6114(15)
Lu(1)-Lu(1)#1	3.6869(19)
Lu(1)-Lu(1)#8	3.6869(19)
Lu(2)-Lu(3)#9	3.3452(11)
Lu(2)-Lu(3)#2	3.3452(11)
Lu(2)-Lu(3)#3	3.3452(11)
Lu(2)-Lu(3)#10	3.3452(11)
Lu(2)-Te #11	3.479(2)
Lu(2)-Lu(1)#8	3.545(2)
Lu(2)-Lu(1)#12	3.6114(15)
Lu(2)-Lu(1)#13	3.6114(15)
Lu(2)-Lu(1)#14	3.6114(15)
Lu(2)-Lu(1)#15	3.6114(15)
Lu(2)-Lu(2)#1	3.6869(19)
Lu(3)-Lu(1)#16	3.2829(15)
Lu(3)-Lu(1)#17	3.2829(15)
Lu(3)-Lu(1)#5	3.2829(15)
Lu(3)-Lu(2)#18	3.3452(11)

Lu(3)-Lu(2)#16	3.3452(11)
Lu(3)-Lu(2)#17	3.3452(11)
Lu(3)-Lu(2)#19	3.3452(11)
Lu(3)-Lu(2)#7	3.3452(11)
Lu(3)-Lu(2)#5	3.3452(11)
Lu(3)-Lu(3)#8	3.6869(19)
Lu(3)-Lu(3)#1	3.6869(19)
Te-Lu(1)#20	3.1004(15)

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Te-Lu(1)#21	3.1004(15)
Te-Lu(1)#8	3.1004(15)
Te-Lu(1)#22	3.1004(15)
Te-Lu(1)#17	3.1004(15)
Te-Lu(2)#5	3.479(2)
Te-Lu(2)#23	3.479(2)
Te-Lu(2)#6	3.479(2)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z-1 #2 x,y-1,z #3 y,x,-z #4 -y,x-y-1,z-1
 #5 -x+y+1,-x+1,z #6 -y,x-y-1,z #7 -x+y+1,-x+1,z-1
 #8 x,y,z+1 #9 y,x,-z+1 #10 x,y-1,z+1 #11 x+1,y,z
 #12 -y+1,x-y,z+1 #13 -x+y+1,-x,z #14 -y+1,x-y,z
 #15 -x+y+1,-x,z+1 #16 x,y+1,z #17 -y,x-y,z
 #18 -y,x-y,z-1 #19 x,y+1,z-1 #20 -x+y,-x,z
 #21 -y,x-y,z+1 #22 -x+y,-x,z+1 #23 x-1,y,z

Figure S1. Coordination environments (Lu–pink, Te–black) in Lu_7Te . In *a–c*, the polyhedra are viewed along $[100]$.

- a): Lu1–Lu2, 3.51 Å ($\times 2$), 3.33 Å (coplanar); Lu1–Lu3, 3.33 Å ($\times 2$), 3.40 Å ($\times 2$); Lu1–Lu4, 3.50 Å ($\times 2$); Lu1–Te, 3.20 Å. Coplanar interactions: Lu2–Lu3, 3.42 Å, Lu3–Lu3, 3.53 Å, Lu3–Lu4, 4.80 Å, Lu2–Lu4, 4.21 Å.
- b): Lu2–Lu1, 3.51 Å ($\times 2$), 3.33 Å (coplanar); Lu2–Lu3, 3.46 Å ($\times 2$), 3.42 Å (coplanar); Lu2–Lu4, 3.58 Å ($\times 2$); Lu2–Te, 3.08 Å. Coplanar interactions: Lu1–Lu3, 4.56 Å, Lu3–Lu4, 4.80 Å, Lu4–Te, 3.56 Å, Lu1–Te, 3.20 Å.
- c): Lu3–Lu1, 3.40 Å ($\times 2$), 3.33 Å ($\times 2$); Lu3–Lu3, 3.28 Å ($\times 2$), 3.53 Å (coplanar); Lu3–Lu2, 3.46 Å ($\times 2$), 3.42 Å (coplanar). Coplanar interactions: Lu1–Lu1, 4.34 Å, Lu1–Lu3, 4.56 Å, Lu3–Lu2, 3.42 Å, Lu2–Lu1, 3.33 Å.
- d): Lu4–Lu1, 3.50 Å ($\times 4$); Lu4–Lu2, 3.58 Å ($\times 4$); Lu4–Te, 3.19 Å ($\times 2$), 3.56 Å (coplanar). Coplanar interactions: Lu1–Lu2, 3.33 Å, Lu2–Lu2, 4.14 Å, Lu1–Te, 3.20 Å.
- e): Te–Lu2, 3.08 Å

Fig. S2 Coordination polyhedra in Lu_8Te . The dark circle is Te1, all the numbered blue or light blue circles represent the corresponding Lu atoms. a, c and d, the Lu1, Lu3 and Te1 polyhedra are viewed down [001] direction.

a): Lu1-Lu2, $3.55\text{\AA}(\times 2)$, $3.61\text{\AA}(\times 4)$; Lu1-Lu3, $3.28\text{\AA}(\times 2)$; Lu1-Te, $3.10(\times 2)\text{\AA}$. coplane interactions: Lu2-Lu2, $4.83\text{\AA}$, Lu2-Te2, $3.48\text{\AA}$.

b): Lu2-Lu1, $3.55\text{\AA}(\times 2)$, $3.61\text{\AA}(\times 4)$; Lu2-Lu3, $3.35\text{\AA}(\times 4)$; Lu2-Te1, $3.48\text{\AA}$. coplane interactions: Lu1-Lu1, $4.31\text{\AA}$, Lu1-Lu3, $3.28\text{\AA}$.

c): Lu3-Lu1, $3.28\text{\AA}(\times 3)$; Lu3-Lu2, $3.35\text{\AA}(\times 6)$. coplane interactions: Lu2-Lu2, $4.83\text{\AA}$.

d): Te1-Lu1, $3.10\text{\AA}(\times 6)$; Te-Lu2, $3.48\text{\AA}(\times 3)$. coplane interactions: Lu1-Lu1, $4.32\text{\AA}$.