Metal-Rich Chalcogenides. Synthesis, Structure, and Bonding of the Layered $\text{Lu}_{11}\text{Te}_4$. Comparison with the Similar Sc_8Te_3 and $\text{Ti}_{11}\text{Se}_4$.

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Table S1. Crystal and Structure Refinement Data for $\text{Lu}_{11}\text{Te}_4$

formula weight	2435.07
temperature	293(2) K
wavelength	0.71073 Å
crystal system, space group	Monoclinic, $C2/m$
unit cell dimensions (Å, deg. Å ³) ^a	
<i>a</i>	30.412(3)
<i>b</i>	3.9504(4)
<i>c</i>	21.073(2)
β	102.960(2)
<i>V</i>	2467.2(4)
<i>Z</i> , <i>d</i> _{calc} (Mg/m ³)	6, 9.833
abs. coeff., mm ⁻¹	72.236
<i>F</i> (000)	5934
crystal size, mm.	0.89 × 0.41 × 0.14
θ range	0.99 to 25.98 deg.
limiting indices	−32 ≤ <i>h</i> ≤ 36, −4 ≤ <i>k</i> ≤ 4, −25 ≤ <i>l</i> ≤ 21
reflections collected / unique	7036 / 2760 [<i>R</i> (int) = 0.0719]
completeness to θ = 25.98	99.1 %
absorption correction	SADABS
max., min. transm.	0.6614, 0.1227
refinement method	full-matrix least-squares on <i>F</i> ²
data / restraints / parameters	2760 / 0 / 138
goodness-of-fit on <i>F</i> ²	0.920
<i>R</i> 1, <i>wR</i> 2 [<i>I</i> > 2σ (<i>I</i>)]	0.0388, 0.0785
(all data)	0.0598, 0.0832
extinction coefficient	0.000149(6)
largest diff. peak and hole, e ⁻ /Å ³	5.526, −6.188

^a CCD data.

Table S2. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Lu_{11}Te . The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$. $U_{12} = U_{23} = 0$.

	U11	U22	U33	U13
Lu(1)	8(1)	12(1)	9(1)	0(1)
Lu(2)	7(1)	18(1)	8(1)	-1(1)
Lu(3)	11(1)	12(1)	16(1)	4(1)
Lu(4)	8(1)	28(1)	6(1)	-2(1)
Lu(5)	11(1)	11(1)	19(1)	6(1)
Lu(6)	6(1)	39(1)	10(1)	-1(1)
Lu(7)	23(1)	29(1)	67(1)	31(1)
Lu(8)	11(1)	13(1)	15(1)	3(1)
Lu(9)	6(1)	12(1)	9(1)	0(1)
Lu(10)	7(1)	12(1)	11(1)	-2(1)
Lu(11)	7(1)	13(1)	7(1)	-2(1)
Lu(12)	7(1)	12(1)	9(1)	-1(1)
Lu(13)	10(1)	18(1)	10(1)	1(1)
Lu(14)	8(1)	29(1)	13(1)	-3(1)
Lu(15)	8(1)	14(1)	12(1)	0(1)
Lu(16)	8(1)	14(1)	13(1)	1(1)
Lu(17)	30(1)	18(1)	15(1)	-3(1)
Te(1)	9(1)	9(1)	9(1)	0(1)
Te(2)	12(1)	12(1)	11(1)	-1(1)
Te(3)	7(1)	11(1)	10(1)	0(1)
Te(4)	9(1)	13(1)	9(1)	0(1)
Te(5)	13(1)	12(1)	18(1)	7(1)
Te(6)	6(1)	10(1)	8(1)	-1(1)

Table S3. Charge iterated (CI) values for H_{ii} for three phases (eV). (CI means interaction is consistent charge.)

	s	p	d
Lu	-6.925	-4.16	-5.27
Te	-20.09	-10.89	

Lu₈Te (CI, Lu vs Te)Crystal data from: Ling Chen and John D. Corbett, *J. Am. Chem. Soc.* **2003**, *125*, 7794–7795.

Ti	-6.722	-3.83	-7.28
Se	-20.55	-12.82	

Ti₂Se (CI, Ti vs Se)Crystal data from Weirich, T. E.; Pöttgen, R.; Simon, A. *Z. Kristallog.* **1996**, *211*, 928–928.

Sc	-6.75	-3.38	-6.12
Te	-21.2	-12.0	

Sc₂Te (CI, Sc vs Te)Data from: Maggard, P. A.; Corbett, J. D. *Inorg. Chem.* **1998**, *37*, 814–820.

Table S4 Bond order in $\text{Lu}_{11}\text{Te}_4$ vs Sc_8Te_3 comparison, Figure 5(a).

Num	Bond	Bond	Num	Bond	Num	Bond	Num	Bond	Num	Bond	Num	Bond	Num	Bond	Bond
1	Lu1-Lu2	Sc1-Sc2	7	Lu4-Lu6	Sc4-Sc6	13	Lu9-Lu9	Sc9-Sc9	19	Lu11-Lu14	Sc11-Sc14				
2	Lu2-Lu2	Sc2-Sc2	8	Lu4-Lu7	Sc4-Sc7	14	Lu9-Lu10	Sc9-Sc10	20	Lu12-Lu13	Sc12-Sc13				
3	Lu2-Lu3	Sc2-Sc3	9	Lu6-Lu7	Sc6-Sc7	15	Lu9-Lu11	Sc9-Sc11	21	Lu13-Lu14	Sc13-Sc14				
4	Lu3-Lu4	Sc3-Sc4	10	Lu7-Lu8	Sc7-Sc8	16	Lu10-Lu11	Sc10-Sc11	22	Lu14-Lu15	Sc14-Sc15				
5	Lu4-Lu5	Sc4-Sc5	11	Lu7-Lu8	Sc7-Sc8	17	Lu10-Lu12	Sc10-Sc12							
6	Lu5-Lu6	Sc5-Sc6	12	Lu7-Lu7	Sc7-Sc7	18	Lu11-Lu12	Sc11-Sc12							

Bond Ordering in M_{11}Ch_4 , Figure 5(b).

Num	Bond	Bond	Num	Bond	Num	Bond	Num	Bond	Num	Bond	Num	Bond	Bond
1	Lu1-Lu2	Ti1-Ti2	8	Lu4-Lu7	Ti4-Ti7	15	Lu9-Lu11	Ti9-Ti11	22	Lu14-Lu15		Ti14-Ti15	
2	Lu2-Lu2	Ti2-Ti2	9	Lu6-Lu7	Ti6-Ti7	16	Lu10-Lu11	Ti10-Ti15	23	Lu15-Lu16		Ti15-Ti16	
3	Lu2-Lu3	Ti2-Ti3	10	Lu7-Lu8	Ti7-Ti8	17	Lu10-Lu12	Ti10-Ti12	24	Lu14-Lu17		Ti14-Ti17	
4	Lu3-Lu4	Ti3-Ti4	11	Lu7-Lu8	Ti7-Ti8	18	Lu11-Lu12	Ti15-Ti12	25	Lu13-Lu16		Ti13-Ti16	
5	Lu4-Lu5	Ti4-Ti5	12	Lu7-Lu7	Ti7-Ti7	19	Lu11-Lu14	Ti11-Ti14	26	Lu16-Lu17		Ti16-Ti17	
6	Lu5-Lu6	Ti5-Ti6	13	Lu9-Lu9	Ti9-Ti9	20	Lu12-Lu13	Ti9-Ti12					
7	Lu4-Lu6	Ti4-Ti6	14	Lu9-Lu10	Ti10-Ti16	21	Lu13-Lu14	Ti13-Ti14					