Supporting Information

Remarkable Metal-Rich Ternary Chalcogenides $\text{Sc}_{14}\text{M}_3\text{Te}_8$ (M = Ru, Os)

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Table S1. Crystal and structure refinement data for $\text{Sc}_{13.2}\text{Ru}_3\text{Te}_8$.

Empirical formula	$\text{Sc}_{13.2}\text{Ru}_3\text{Te}_8$
Formula weight	1917.49
Temperature	293(2) K
Crystal system	Tetragonal
Space group, Z	$P4/mnc$ (no.128), 2
Unit cell dimensions, Å (Guinier)	
a =	11.3332(4)
b =	11.3332(4)
c =	9.0793(5)
Volume, Å ³	1166.16(9)
Density (calculated)	5.563 Mg/m ³
Absorption coefficient	15.442 mm ⁻¹
F(000)	1684
Crystal size, mm	0.06 x 0.04 x 0.04
Theta range for data collection, deg	2.54 to 24.74
Index ranges	-13 ≤ h ≤ 6, -13 ≤ k ≤ 6, -10 ≤ l ≤ 7
Reflections collected	3534
Independent, obs. reflections(>2σ _I)	539 [R(int) = 0.1104]
Completeness to theta = 24.74°	99.6 %
Absorption correction	SADABS
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	539 / 0 / 37
Goodness-of-fit on F ²	1.034
Final R indices [I > 2σ(I)]	R1 = 0.0275, wR2 = 0.0433
R indices (all data)	R1 = 0.0571, wR2 = 0.0489
Sec. extinc. coefficient	0.00058(7)
Largest diff. peak and hole	1.377 and -1.693 e.Å ⁻³

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Sc}_{13.2}\text{Ru}_3\text{Te}_8$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	Wykoff	x	y	z	U(eq)
Ru(1)	2b	0		0	50009(1)
Te(1)	8h	6421(1)	1043(1)	0	13(1)
Ru(2)	4e	0	0	1619(2)	7(1)
Te(2)	8g	1737(1)	3263(1)	2500	13(1)
Sc(1)	8h	1780(2)	0974(2)	0	9(1)
Sc(2)	16i	5607(2)	3100(2)	1806(2)	14(1)
Sc(3)	4d	0	5000	2500	14(2)

*Occupancy = 0.61(1)

Table S3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10$) for $\text{Sc}_{13.2}\text{Ru}_3\text{Te}_8$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U11	U22	U33	U23	U13	U12
Ru(1)	11(1)	11(1)	5(2)	0	0	0
Te(1)	11(1)	10(1)	18(1)	0	0	0(1)
Ru(2)	9(1)	9(1)	3(1)	0	0	0
Te(2)	14(1)	14(1)	11(1)	-2(1)	-2(1)	-4(1)
Sc(1)	12(2)	10(1)	7(2)	0	0	4(1)
Sc(2)	17(1)	13(1)	11(1)	-2(1)	3(1)	1(1)
Sc(3)	14(3)	14(3)	14(4)	0	0	-1(3)

Table S4. Bond lengths [Å].

Ru(1)-Sc(2)#1	2.793(2)
Ru(1)-Sc(2)#2	2.793(2)
Ru(1)-Sc(2)#3	2.793(2)
Ru(1)-Sc(2)#4	2.793(2)
Ru(1)-Sc(2)#5	2.793(2)
Ru(1)-Sc(2)#6	2.793(2)
Ru(1)-Sc(2)#7	2.793(2)
Ru(1)-Sc(2)#8	2.793(2)
Ru(1)-Ru(2)	3.0698(19)
Ru(1)-Ru(2)#9	3.0698(19)
Te(1)-Sc(2)	2.996(2)
Te(1)-Sc(2)#10	2.996(2)
Te(1)-Sc(3)#11	3.0238(7)
Te(1)-Sc(3)	3.0238(7)
Te(1)-Sc(1)	3.063(3)
Te(1)-Sc(1)#12	3.068(3)
Ru(2)-Sc(2)#8	2.675(2)
Ru(2)-Sc(2)#7	2.675(2)
Ru(2)-Sc(2)#2	2.675(2)
Ru(2)-Sc(2)#4	2.675(2)
Ru(2)-Sc(1)	2.729(3)
Ru(2)-Sc(1)#13	2.729(3)
Ru(2)-Sc(1)#14	2.729(3)
Ru(2)-Sc(1)#12	2.729(3)
Ru(2)-Ru(2)#14	2.940(4)
Te(2)-Sc(3)#11	2.7840(9)
Te(2)-Sc(1)	2.9540(18)
Te(2)-Sc(1)#15	2.9540(18)
Te(2)-Sc(2)#16	3.081(2)
Te(2)-Sc(2)#17	3.081(2)
Te(2)-Sc(2)#18	3.1366(19)
Te(2)-Sc(2)#11	3.1366(19)
Sc(1)-Ru(2)#14	2.729(3)
Sc(1)-Te(2)#10	2.9540(18)

Sc(1)-Te(1)#13	3.068(3)
Sc(1)-Sc(1)#12	3.252(4)
Sc(1)-Sc(1)#13	3.252(4)
Sc(1)-Sc(2)#2	3.358(2)
Sc(1)-Sc(2)#16	3.358(2)
Sc(1)-Sc(2)#4	3.411(3)
Sc(1)-Sc(2)#18	3.411(3)
Sc(2)-Ru(2)#19	2.675(2)
Sc(2)-Ru(1)#19	2.793(2)
Sc(2)-Te(2)#12	3.081(2)
Sc(2)-Te(2)#11	3.1366(19)
Sc(2)-Sc(2)#20	3.197(3)
Sc(2)-Sc(2)#21	3.197(3)
Sc(2)-Sc(2)#10	3.280(4)
Sc(2)-Sc(1)#19	3.358(2)
Sc(2)-Sc(1)#4	3.411(3)
Sc(2)-Sc(3)	3.635(2)
Sc(3)-Te(2)#10	2.7840(9)
Sc(3)-Te(2)#11	2.7840(9)
Sc(3)-Te(1)#4	3.0238(7)
Sc(3)-Te(1)#11	3.0238(7)
Sc(3)-Te(1)#22	3.0238(7)
Sc(3)-Sc(2)#4	3.635(2)
Sc(3)-Sc(2)#23	3.635(2)
Sc(3)-Sc(2)#24	3.635(2)

Symmetry transformations used to generate equivalent atoms:

#1 $x+1/2, -y+1/2, z+1/2$ #2 $-x+3/2, y-1/2, -z+1/2$
#3 $-y+3/2, -x+1/2, z+1/2$ #4 $y+1/2, x-1/2, -z+1/2$
#5 $-x+3/2, y-1/2, z+1/2$ #6 $y+1/2, x-1/2, z+1/2$ #7 $-y+3/2, -x+1/2, -z+1/2$
#8 $x+1/2, -y+1/2, -z+1/2$ #9 $-x+2, -y, -z+1$ #10 $x, y, -z$
#11 $-x+1, -y, -z$ #12 $y+1, -x+1, -z$ #13 $-y+1, x-1, z$
#14 $-x+2, -y, -z$ #15 $-y+1/2, -x+1/2, z-1/2$ #16 $-x+3/2, y-1/2, z-1/2$
#17 $-y+1, x-1, -z$ #18 $y+1/2, x-1/2, z-1/2$ #19 $-x+3/2, y+1/2, -z+1/2$
#20 $-y+1, x, z$ #21 $y, -x+1, z$ #22 $-y+1/2, -x+1/2, z+1/2$
#23 $-x+1, -y, z$ #24 $-y+1/2, -x+1/2, -z+1/2$

Empirical formula	Sc ₁₄ Os ₃ Te ₈
Formula weight	2220.84
Temperature	293(2) K
Crystal system	Tetragonal
Space group, <i>Z</i>	<i>P4/mnc</i> (No. 128), 2
Unit cell dimensions (Guinier) Å	<i>a</i> = 11.4008(9) <i>b</i> = 11.4008(9) <i>c</i> = 9.0745(10)
Volume, Å ³	1179.49(19)
Density (calculated)	6.253 Mg/m ³
Absorption coefficient	29.491 mm ⁻¹
<i>F</i> (000)	1876
Crystal size, mm	0.072 × 0.04 × 0.03
Theta range for data collection, deg	2.53 to 23.47
Index ranges	-11 ≤ <i>h</i> ≤ 12, -11 ≤ <i>k</i> ≤ 12, -10 ≤ <i>l</i> ≤ 2
Reflections collected	3244
Independent obs. refl. (>2σ _{<i>I</i>})	430 [<i>R</i> (int) = 0.0429]
Completeness to theta = 23.47°	90.5 %
Absorption correction	SADAM
Max. and min. transmission	0.3065, 0.1798
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameters	430 / 0 / 37
Goodness-of-fit on <i>F</i> ²	0.992
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0169, <i>wR</i> 2 = 0.0369
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0184, <i>wR</i> 2 = 0.0375
Extinction coefficient	0.0029(1)
Largest diff. peak and hole	0.615 and -0.589 e ⁻ /Å ⁻³

Table S6. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Sc}_{14}\text{Os}_3\text{Te}_8$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Os(1)	0	0	0	8(1)
Os(2)	0	0	3386(1)	7(1)
Te(1)	1412(1)	3948(1)	0	12(1)
Te(2)	3237(1)	1763(1)	2500	12(1)
Sc(2)	591(1)	1886(1)	1791(1)	12(1)
Sc(1)	1767(2)	961(2)	5000	9(1)
Sc(3)*	0	5000	2500	14(1)

*Occupancy = 0.91(1)

Table S7. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Sc}_{14}\text{Os}_3\text{Te}_8$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12} \dots]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Os(1)	9(1)	9(1)	8(1)	0	0	0
Os(2)	7(1)	7(1)	8(1)	0	0	0
Te(1)	11(1)	9(1)	15(1)	0	0	-1(1)
Te(2)	11(1)	11(1)	14(1)	2(1)	2(1)	0(1)
Sc(2)	13(1)	10(1)	12(1)	2(1)	1(1)	-2(1)
Sc(1)	8(1)	10(1)	10(1)	0	0	-1(1)
Sc(3)	10(2)	10(2)	23(2)	0	0	-2(1)

Table S8. Bond lengths [$\text{\AA}$] for $\text{Sc}_{14}\text{Os}_3\text{Te}_8$.

Os(1)-Sc(2)	2.7780(14)
Os(1)-Sc(2)#1	2.7780(14)
Os(1)-Sc(2)#2	2.7780(14)
Os(1)-Sc(2)#3	2.7780(14)
Os(1)-Sc(2)#4	2.7780(14)
Os(1)-Sc(2)#5	2.7780(14)
Os(1)-Sc(2)#6	2.7780(14)
Os(1)-Sc(2)#7	2.7780(14)
Os(1)-Os(2)#1	3.0724(6)
Os(1)-Os(2)	3.0724(6)
Os(2)-Sc(2)#6	2.6781(14)
Os(2)-Sc(2)#2	2.6781(14)
Os(2)-Sc(2)#7	2.6781(14)
Os(2)-Sc(2)	2.6781(14)
Os(2)-Sc(1)	2.7211(17)
Os(2)-Sc(1)#7	2.7211(17)
Os(2)-Sc(1)#8	2.7211(17)
Os(2)-Sc(1)#9	2.7211(17)
Os(2)-Os(2)#8	2.9297(10)
Te(1)-Sc(2)#3	3.0077(15)
Te(1)-Sc(2)	3.0077(15)
Te(1)-Sc(3)#10	3.0294(5)
Te(1)-Sc(3)	3.0294(5)
Te(1)-Sc(1)#11	3.093(2)
Te(1)-Sc(1)#12	3.104(2)
Te(2)-Sc(3)#13	2.8427(7)
Te(2)-Sc(1)	2.9650(13)
Te(2)-Sc(1)#12	2.9650(13)
Te(2)-Sc(2)	3.0872(16)
Te(2)-Sc(2)#14	3.0872(16)

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Te(2)-Sc(2)#2	3.1610(15)
Te(2)-Sc(2)#15	3.1610(15)

Sc(2)-Te(2)#7	3.1610(15)
Sc(2)-Sc(2)#7	3.187(2)
Sc(2)-Sc(2)#2	3.187(2)
Sc(2)-Sc(2)#3	3.250(3)
Sc(2)-Sc(1)	3.3751(17)
Sc(2)-Sc(1)#7	3.4103(17)
Sc(2)-Sc(3)	3.6707(14)
Sc(1)-Os(2)#8	2.7211(17)
Sc(1)-Te(2)#16	2.9650(13)
Sc(1)-Te(1)#17	3.093(2)
Sc(1)-Te(1)#18	3.104(2)
Sc(1)-Sc(1)#9	3.243(3)
Sc(1)-Sc(1)#7	3.243(3)
Sc(1)-Sc(2)#16	3.3751(17)
Sc(1)-Sc(2)#2	3.4103(17)
Sc(1)-Sc(2)#9	3.4103(17)
Sc(3)-Te(2)#19	2.8427(7)
Sc(3)-Te(2)#7	2.8427(7)
Sc(3)-Te(1)#20	3.0294(5)
Sc(3)-Te(1)#10	3.0294(5)
Sc(3)-Te(1)#18	3.0294(5)
Sc(3)-Sc(2)#21	3.6707(14)
Sc(3)-Sc(2)#14	3.6707(14)
Sc(3)-Sc(2)#20	3.6707(14)

Symmetry transformations used to generate equivalent atoms:

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

Fig. S1 χ_M of $\text{Sc}_{13.2}\text{Ru}_3\text{Te}_8$

Fig. S2 Resistivity of $\text{Sc}_{13.2}\text{Ru}_3\text{Te}_8$.