Supporting Information

R₆TT' ₂, New Variants of the Fe₂P Structure Type. Sc₆TTe₂ (T= Ru, Os, Rh, Ir), Lu₆MoSb₂, and the Anti-Typic Sc₆Te_{0.80}Bi_{1.68}

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Table S1. Some structure determination and refinement data.

empirical formula	Sc ₆ RhTe ₂	Sc ₆ OsTe ₂	Sc ₆ Te _{0.797(5)} Bi _{1.682(8)}	Lu ₆ MoSb ₂
f.w.	627.87	715.16	722.9	1389.26
crystal system	Hexagonal	Hexagonal	Hexagonal	Hexagonal
space group, Z	<i>P</i> 6 ₂ <i>m</i> (No. 189), 1	<i>P</i> 6 ₂ <i>m</i> (No. 189), 1	<i>P</i> 6 ₂ <i>m</i> (No. 189), 1	<i>P</i> 6 ₂ <i>m</i> (No. 189), 1
<i>a</i> Å	7.718(10)	7.627(2)	7.6821(3)	7.935(1)
<i>c</i> Å	3.8379(7)	3.864(1)	4.0815(4)	4.2630(9)
<i>V</i> Å ³	197.98(5)	194.67(9)	208.60(2)	232.43(7)
abs. coeff, mm ⁻¹	13.976	28.397	49.914	69.973
<i>d</i> _{calc} , Mg/m ₃	5.266	6.1	5.76	9.925
crystal size, mm	0.09 x 0.08 x 0.07	0.07 x 0.04 x 0.03	0.10 x 0.07 x 0.07	0.05 x 0.03 x 0.01
reflects. collec. (>3σ)	2177 (2138)	547 (540)	1966 (1931)	1426 (1354)
indep. obs. refl. (2σ _i)	210 [R(int) = 0.0197]	172 [R(int) = 0.0241]	213 [R(int) = 0.0244]	236 [R(int) = 0.0366]
absorp. corr.	SADABS	SADABS	SADABS	SADABS
R1, wR2 [I>2σ(I)]	0.0139, 0.0333	0.0166, 0.0489	0.0105, 0.0240	0.0176, 0.0391
R1, wR2 (all data)	0.0139, 0.0333	0.0167, 0.0490	0.0105, 0.0240	0.0176, 0.0391
Abs. struct. parameter	0.05(9)	0.00(4)	0.00(2)	0.01(3)
twin Law	none	-1 0 0 0 -1 0 0 0 -1	-1 0 0 0 -1 0 0 0 -1	none
BASF	none	0.1801	0.1848	none
largest diff. peak, e ⁻ Å ⁻³	0.388 (1.52 Å from Sc2), -0.629 (0.85 Å from Rh)	1.562 (0.82 Å from Os), 0.967 (1.93 Å from Te)	0.709 (0.88 Å from Bi), -0.827 (2.07 Å from Sc2)	1.412 (1.01 Å from Mo), -1.714 (0.36 Å from Mo)

Table S2 Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$).

Sc_6RhTe_2 . 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}
Sc(1)	12(1)	10(1)	18(1)	0	0	5(1)
Sc(2)	16(1)	20(1)	13(1)	0	0	10(1)
Te	11(1)	11(1)	13(1)	0	0	6(1)
Rh	31(1)	31(1)	11(1)	0	0	15(1)

Sc_6OsTe_2 . 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}
Sc(1)	5(1)	3(1)	13(1)	0	0	2(1)
Sc(2)	9(1)	6(1)	8(1)	0	0	3(1)
Te	5(1)	5(1)	6(1)	0	0	3(1)
Os	21(1)	21(1)	6(1)	0	0	10(1)

$\text{Sc}_6\text{Te}_{0.797(5)}\text{Bi}_{1.680(8)}$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sc(1)	7(1)	7(1)	16(1)	0	0	4(1)
Sc(2)	10(1)	9(1)	9(1)	0	0	5(1)
Bi	8(1)	8(1)	11(1)	0	0	4(1)
Te	10(1)	10(1)	9(1)	0	0	5(1)

Lu_6MoSb_2 . 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)	7(1)	7(1)	8(1)	0	0	3(1)
Lu(2)	9(1)	9(1)	7(1)	0	0	5(1)
Sb	7(1)	7(1)	10(1)	0	0	4(1)
Mo	11(1)	11(1)	7(1)	0	0	5(1)

Table S3 Parameters used in EH calculations

atoms	orbital	$H_i(\text{ev})$	α_1	c_1	α_2	c_2
Sc	4s	-6.74	1.3			
	4p	-3.38	1.3			
	3d	-6.12	4.4	0.4228	1.700	0.7276
Te	5s	-21.20	2.5			
	5p	-12.00	2.2			
Os	6s	-7.79	2.5			
	6p	-4.04	2.4			
	5d	-6.41	5.6	0.6372	2.416	0.5598
Ru	5s	-4.33	2.1			
	5p	-2.08	2			
	4d	-6.52	5.4	0.5340	2.300	0.6365
Fe	4s	-5.26				
	4p	-2.25				
	3d	-6.47	5.4	0.5505	2.0	0.626
Mo	5s	-5.78	2			
	5p	-2.86	1.9			
	4d	-6.66	4.5	0.6097	1.90	0.6097
Bi	6s	-9.05	2.6			
	6p	-7.54	2			
Sb	5s	-18.80	2.3			
	5p	-11.70	2			
Lu	6s	-7.46	1.7			
	6p	-4.62	1.7			
	5d	-6.00	2.8	0.7044	1.21	0.488