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Supporting Information

Synthesis, Structure and Bonding of Sc_6MTe_2 (M=Ag, Cu, Cd): Heterometal Induced Polymerization of Metal Chains in Sc_2Te

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Table S1. Single crystal X-ray data collection and structure refinement parameters for Sc_6MTe_2 (M = Ag, Cu)

formula, Z	Sc_6AgTe_2	$Sc_6Cu_{0.80(2)}Te_{2.20(2)}$
temperature	293(2) K	293(2) K
crystal system, space group, Z	orthorhombic, *Pnma* , 4	orthorhombic, *Pnma* , 4
lattice parameters[a] (Å, Å^3)	a = 20.094 (9)	a = 19.853 (4)
	b = 3.913 (1)	b = 3.914 (1)
	c = 10.688 (2)	c = 10.644 (2)
	V = 840.4 (5)	V = 827.1 (3)
d_{calc} , (g/cm^3)	5.002	4.726
crystal size (mm)	0.11 x 0.1 x 0.04	0.08 x 0.08 x 0.04
diffractometer	SMART CCD	SMART CCD
absorption coefficient (mm^{-1})	13.537	13.957
index range	$-12 \le h \le 26$, $-5 \le k \le 2$, $-12 \le l \le 12$	$-11 \le h \le 25$, $-2 \le k \le 5$, $-14 \le l \le 8$
reflections collected	3241	3149
independent reflections	1042 [R(int) = 0.0273]	1120 [R(int) = 0.0506]
absorption correction	SADABS	SADABS
goodness -of-fit on F^2	1.123	1.016
$R1$, w$R2$[b] for $I > 2\sigma$ (F_o^2)	$R1$ = 0.0239, Rw = 0.0574	$R1$ = 0.0276, Rw = 0.0623
$R1$, w$R2$ for all data	$R1$ = 0.0265, Rw = 0.0583	$R1$ = 0.0345, Rw = 0.0643
largest diff. peak and hole	0.977 and -1.875 e/Å^3	1.633 and -0.997 e/Å^3

[a] Guinier data.

[b] $R1 = \Sigma \, || F_o| - |F_c || \, / \, \Sigma \, |F_o|$; $wR2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$.
in Sc_6AgTe_2: $w^{-1} = [\sigma^2(F_o^2) + (0.0327p)^2 + 1.3898p]$, where $p = (F_o^2 + 2F_c^2)/3$
in $Sc_6Cu_{0.80(2)}Te_{2.20(2)}$: $w^{-1} = [\sigma^2(F_o^2) + (0.0310p)^2]$, where $p = (F_o^2 + 2F_c^2)/3$.

Table S2. Anisotropic displacement parameters (Å2 x 103) for Sc_6AgTe_2 and $Sc_6Cu_{0.80(2)}Te_{2.20(2)}$. The anisotropic displacement factor exponent takes the form: $-2p^2[$ h2 a*2U11 + ... + 2 h k a* b* U12]

Sc_6AgTe_2	U11	U22	U33	U23	U13	U12
Ag1	12(1)	10(1)	11(1)	0	2(1)	0
Te2	12(1)	10(1)	10(1)	0	1(1)	0
Te3	12(1)	9(1)	11(1)	0	0(1)	0
Sc1	12(1)	20(1)	13(1)	0	2(1)	0
Sc2	14(1)	16(1)	9(1)	0	0(1)	0
Sc3	13(1)	12(1)	10(1)	0	0(1)	0
Sc4	16(1)	15(1)	15(1)	0	-4(1)	0
Sc5	17(1)	10(1)	11(1)	0	0(1)	0
Sc6	13(1)	23(1)	15(1)	0	1(1)	0

$Sc_6Cu_{0.80(2)}Te_{2.20(2)}$	U11	U22	U33	U23	U13	U12
Cu1	11(1)	9(1)	10(1)	0	3(1)	0
Te2	12(1)	11(1)	8(1)	0	1(1)	0
Te3	11(1)	9(1)	10(1)	0	0(1)	0
Sc1	10(1)	24(1)	12(1)	0	1(1)	0
Sc2	14(1)	26(1)	8(1)	0	0(1)	0
Sc3	13(1)	13(1)	10(1)	0	0(1)	0
Sc4	17(1)	23(1)	16(1)	0	6(1)	0
Sc5	13(1)	10(1)	10(1)	0	0(1)	0
Sc6	12(1)	18(1)	15(1)	0	2(1)	0