

A series of new hybrid chalcogenogermanates: the rare examples of chalcogenogermanates combined with trivalent vanadium complexes

Hai-Ying Luo, Jian Zhou and Shumei Cao

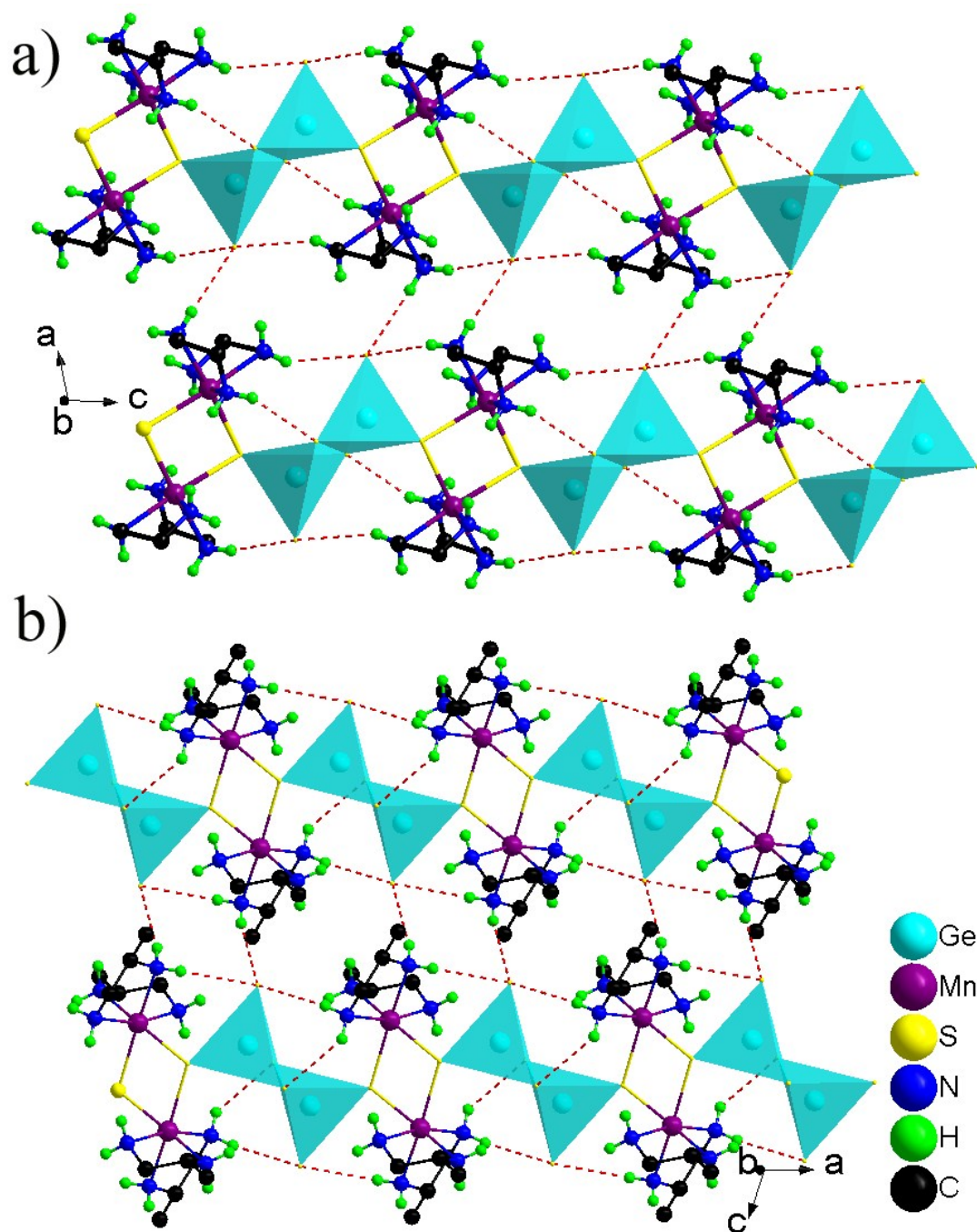


Fig. S1 The formation of 2-D layers constructed from N-H...S H-bonds in 1 (a) and 2 (b).

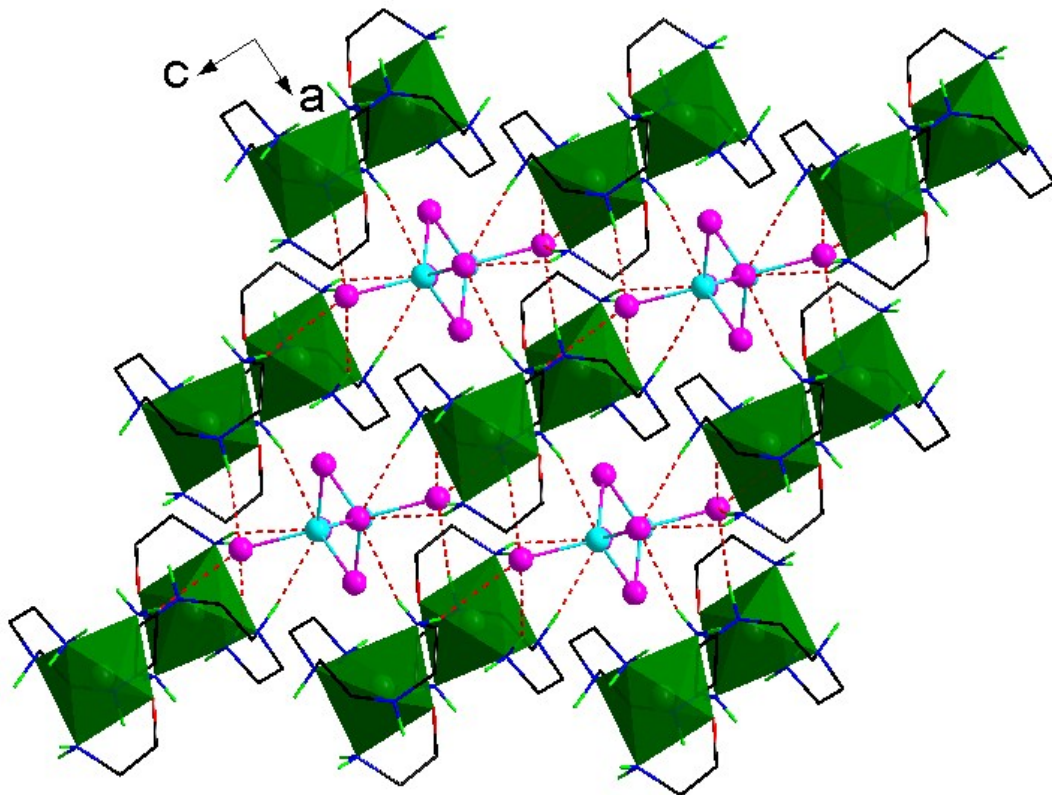


Fig. S2 3-D H-bonding network structure in **5**. All H bonded to C atoms are omitted for clarity.

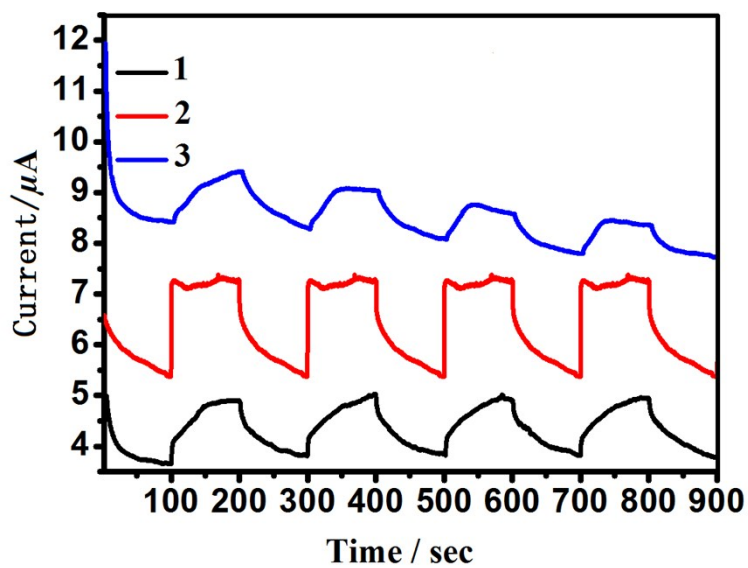
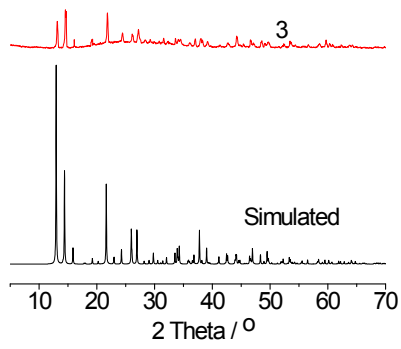
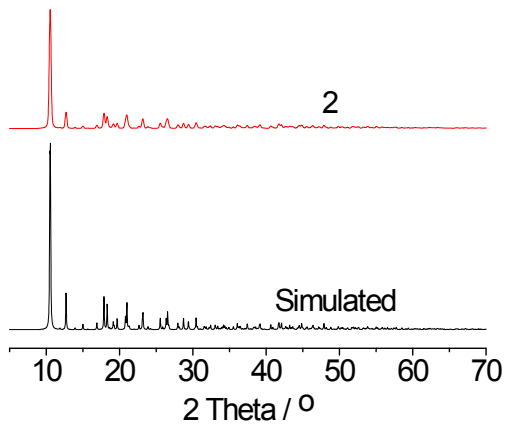
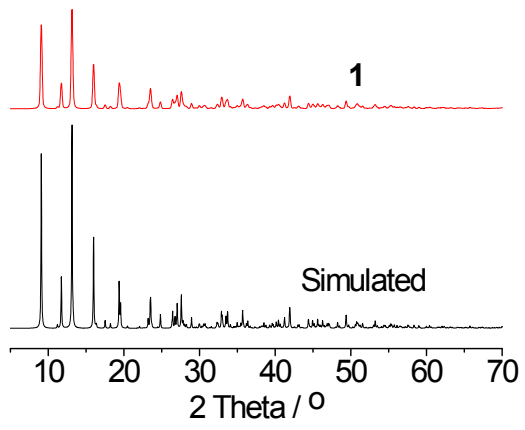


Fig. S3 Photocurrent density versus time of **1-3** at 0.6 V potential.



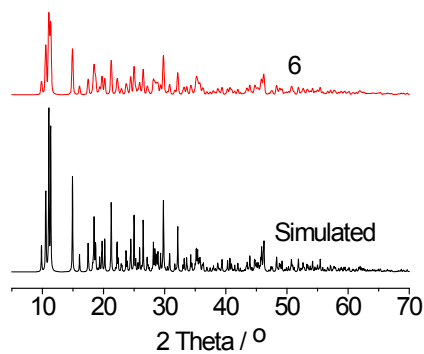
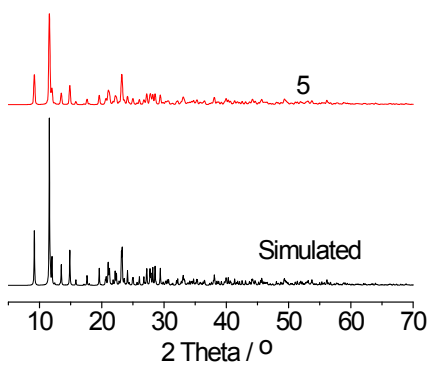
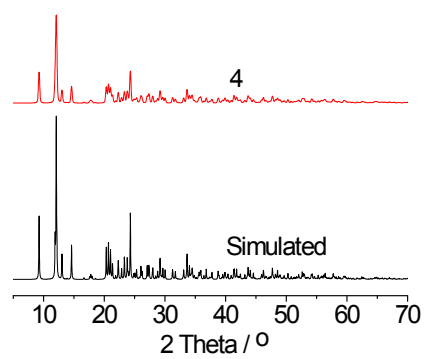


Fig. S5 Simulated, experimental powder XRD patterns of polycrystalline samples of **1-6**.

Table S1 Hydrogen bonds for **1** [Å and deg].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N(1)-H(1A)···S(3)#1	0.90	2.64	3.542(3)	175.2
N(1)-H(1B)···S(3)	0.90	2.60	3.474(3)	163.0
N(2)-H(2A)···S(2)#2	0.90	2.87	3.658(3)	147.4
N(2)-H(2B)···S(2)#3	0.90	2.61	3.437(3)	153.4

N(3)-H(3A)···S(3)#1	0.90	2.85	3.733(4)	165.6
N(3)-H(3B)···S(3)#3	0.90	2.75	3.557(3)	149.2

Symmetry transformations used to generate equivalent atoms: (#1) $-x+2, -y, -z+2$; (#2) $x, -y+1/2, z+1/2$; (#3) $x, y, z+1$.

Table S2 Hydrogen bonds for **2** [Å and deg].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N(4)-H(4AA)···S(2)#1	0.90	2.69	3.355(3)	132.0
N(4)-H(4AB)···S(3)#1	0.90	2.61	3.497(3)	167.4
N(4)-H(4AB)···S(3)#1	0.90	2.61	3.497(3)	167.4
N(4)-H(4AA)···S(2)#1	0.90	2.69	3.355(3)	132.0
N(3)-H(3BC)···S(3)#3	0.90	2.65	3.514(3)	160.6
N(3)-H(3BD)···S(3)#2	0.90	2.70	3.561(3)	159.8
N(3)-H(3BC)···S(3)#3	0.90	2.65	3.514(3)	160.6
N(3)-H(3BD)···S(3)#2	0.90	2.70	3.561(3)	159.8
N(1)-H(1BD)···S(2)	0.90	2.91	3.797(4)	167.1
N(1)-H(1BD)···S(2)	0.90	2.91	3.797(4)	167.1

Symmetry transformations used to generate equivalent atoms: (#1) $-x+1, -y+1, -z-1$; (#2) $-x, -y+1, -z+1$; (#3) $x, y, z+1$.

Table S3 Hydrogen bonds for **3** [Å and deg].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N(2)-H(2A)···S(1)#1	0.90	2.78	3.646(5)	161.7
N(1)-H(1A)···S(2)#2	0.89	2.35	3.234(4)	174.4
N(1)-H(1C)···S(2)#3	0.89	2.72	3.578(4)	163.1
N(1)-H(1B)···S(1)#3	0.89	2.88	3.379(4)	116.9

Symmetry transformations used to generate equivalent atoms: (#1) $x, y, z+1$; (#2) $-x+1/2, y-1/2, -z+3$; (#3) $-x+1, -y, z+1$.

Table S4 Hydrogen bonds for **4** [Å and deg].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...Se(1)#2	0.90	2.91	3.674(7)	144.3
N(1)-H(1B)...Se(3)	0.90	3.05	3.802(7)	142.6
N(2)-H(2A)...Se(3)#2	0.90	2.77	3.634(7)	161.6
N(3)-H(3A)...Se(1)#3	0.90	2.72	3.569(7)	157.5
N(3)-H(3B)...Se(3)	0.90	2.89	3.720(7)	153.8
N(4)-H(4A)...Se(3)#3	0.90	3.06	3.863(7)	150.1
N(4)-H(4B)...O(1)#4	0.90	1.94	2.836(9)	177.0
N(5)-H(5A)...Se(1)#1	0.90	2.60	3.438(7)	154.7
N(5)-H(5B)...Se(3)	0.90	2.60	3.485(7)	168.6

Symmetry transformations used to generate equivalent atoms: (#1) $-x,-y,-z+2$; (#2) $x-1/2,-y+1/2,z+1/2$; (#3) $x+1/2,-y+1/2,z+1/2$; (#4) $-x,-y,-z+3$.

Table S5 Hydrogen bonds for **5** [Å and deg].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...Se(3)	0.90	2.81	3.628(6)	151.0
N(1)-H(1B)...Se(1)#1	0.90	2.62	3.460(6)	155.1
N(2)-H(2A)...Se(1)#2	0.90	2.88	3.569(6)	134.7
N(2)-H(2B)...Se(3)#3	0.90	2.85	3.653(6)	149.5
N(3)-H(3C)...Se(1)#4	0.91	2.60	3.452(6)	156.4
N(4)-H(4C)...Se(3)	0.91	2.64	3.511(6)	159.5
N(5)-H(5A)...O(1)#5	0.90	2.06	2.942(7)	167.1
N(5)-H(5B)...Se(1)#1	0.90	2.82	3.605(6)	147.2

Symmetry transformations used to generate equivalent atoms: (#1) $-x+1,-y+1,-z+2$; (#2) $x,y,z-1$; (#3) $x-1/2,-y+3/2,z-1/2$; (#4) $x+1/2,-y+3/2,z-1/2$; (#5) $-x+1,-y+1,-z+1$.

Table S6 Hydrogen bonds for **6** [Å and deg].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
---------	--------	----------	----------	--------

N(1)-H(1A)...Se(3)#3	0.90	2.79	3.666(3)	164.7
N(1)-H(1B)...Se(1)#4	0.90	2.84	3.623(3)	145.7
N(2)-H(2A)...Se(1)#5	0.90	2.88	3.647(3)	143.8
N(2)-H(2B)...Se(3)	0.90	2.88	3.590(3)	136.7
N(3)-H(3B)...Se(1)	0.90	2.92	3.790(3)	163.1
N(4)-H(4A)...Se(1)#5	0.90	2.86	3.752(3)	169.2
N(4)-H(4B)...N(6)#2	0.90	2.21	3.020(5)	148.9
N(5)-H(5A)...Se(3)#3	0.90	2.66	3.363(3)	135.4
N(5)-H(5A)...N(6)	0.90	2.43	2.893(4)	112.4
N(5)-H(5B)...Se(3)	0.90	2.63	3.517(3)	169.0
N(6)-H(6D)...Se(2)#6	0.886(10)	2.83(2)	3.607(3)	147(4)
N(6)-H(6C)...Se(3)#3	0.891(10)	2.80(2)	3.651(4)	160(4)

Symmetry transformations used to generate equivalent atoms: (#1) $-x+1,-y+1,-z+2$;
 (#2) $-x+1,-y+2,-z+1$; (#3) $-x+1,-y+2,-z+2$; (#4) $x,y+1,z$; (#5) $-x,-y+1,-z+1$; (#6)
 $x+1,y+1,z$.