Two Manganese-amine complexes incorporated Thioantimonate Exhibiting Diversiform Structure-Directing Actions of Amine-ligands

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Supplementary Information

Table S1. Fractional atomic coordinates and equivalent isotropic displacement parameters (× 10^3 Å^2) for non-hydrogen atoms of compounds **1** and **2**.

Atom	Wyckoff	*x*	*y*	*z*	*U*(eq)[a]
			1		
Mn(1)	2i	0.3064(1)	0.6356(1)	0.6639(1)	25(1)
Sb(1)	2i	0.4440(1)	0.8607(1)	0.5826(1)	31(1)
Sb(2)	2i	0.5954(1)	0.6218(1)	0.5930(1)	20(1)
Sb(3)	2i	0.5401(1)	0.6414(1)	0.3091(1)	23(1)
Sb(4)	2i	0.5817(1)	0.6402(1)	0.217(1)	23(1)
Sb(5)	2i	0.4079(1)	0.8750(1)	0.1689(1)	24(1)
Sb(6)	2i	0.4526(1)	0.8573(1)	0.8776(1)	22(1)
Sb(7)	2i	0.2602(1)	0.7758(1)	0.3494(1)	26(1)
Sb(8)	2i	0.7262(1)	0.5185(1)	0.7774(1)	22(1)
S(1)	2i	0.8693(2)	0.3895(2)	0.7346(2)	33(1)
S(2)	2i	0.5550(2)	0.8448(2)	0.4072(2)	30(1)
S(3)	2i	0.2133(2)	0.8763(2)	0.2353(2)	28(1)
S(4)	2i	0.1773(3)	0.8763(2)	0.5083(2)	44(1)

S(5)	2i	0.7916(2)	0.6354(2)	0.9548(2)	34(1)
S(6)	2i	0.7821(2)	0.6317(2)	0.6769(2)	27(1)
S(7)	2i	0.3157(2)	0.8591(2)	0.7484(2)	26(1)
S(8)	2i	0.3129(2)	0.8714(2)	0.070(2)	26(1)
S(9)	2i	0.6800(2)	0.5930(2)	0.4200(2)	21(1)
S(10)	2i	0.5951(2)	0.8404(2)	0.644(2)	24(1)
S(11)	2i	0.6777(2)	0.6380(2)	0.1824(2)	26(1)
S(12)	2i	0.6075(2)	0.8299(2)	0.6740(2)	23(1)
S(13)	2i	0.4046(2)	0.6724(2)	0.1237(2)	25(1)
S(14)	2i	0.4584(2)	0.6548(2)	0.7986(2)	26(1)
S(15)	2i	0.4018(2)	0.6588(2)	0.5027(2)	21(1)
N(6)	2i	0.1596(7)	0.6220(8)	0.5614(7)	34(2)
N(5)	2i	0.7687(8)	0.9090(8)	0.2657(7)	38(2)
N(4)	2i	0.1697(7)	0.6487(8)	0.7785(8)	37(2)
N(3)	2i	0.9340(7)	0.8476(8)	0.3727(7)	36(2)
N(2)	2i	0.7954(8)	0.8931(8)	0.5415(7)	40(2)
N(1)	2i	0.1778(12)	0.6159(12)	1.0093(12)	85(5)
C(6)	2i	0.9291(9)	0.8052(11)	0.2561(10)	44(3)
C(7)	2i	0.9116(10)	0.7657(10)	0.4199(10)	45(3)
C(4)	2i	0.659(9)	0.6131(14)	0.6161(11)	56(4)
C(8)	2i	0.8848(11)	0.8220(11)	0.5329(10)	46(3)
C(5)	2i	0.8720(11)	0.8869(12)	0.2212(10)	51(3)
C(3)	2i	0.788(10)	0.6804(15)	0.7329(11)	59(4)
C(2)	2i	0.1501(17)	0.5618(16)	0.8145(16)	94(7)
C(1)	2i	0.1019(10)	0.5896(15)	0.9222(10)	58(4)
O(1W)	2i	0.2356(8)	0.1320(8)	0.1033(8)	56(2)
			2		
Sb(2)	2f	1/2	0.2051(1)	1/4	21(1)
Sb(1)	4g	0.1065(1)	0.2224(1)	0.3948(1)	28(1)
Mn(1)	4g	0.1381(1)	0.1157(1)	0.2639(1)	25(1)
Mn(2)	4g	0.2385(1)	0.3042(1)	0.0299(1)	30(1)
S(1)	4g	0.0526(1)	0.0390(1)	0.3191(1)	25(1)
S(2)	4g	0.0233(1)	0.1464(2)	0.4403(1)	45(1)
S(3)	4g	0.2772(1)	0.1922(2)	0.4494(1)	41(1)
S(4)	4g	0.0670(1)	0.4969(2)	0.3636(1)	47(1)

S(5)	4g	0.4132(1)	0.0352(2)	0.1743(1)	39(1)
S(6)	4g	0.3919(1)	0.3741(1)	0.2634(1)	43(1)
O(1)	4g	0.0739(3)	0.3050(8)	-0.0288(2)	84(2)
O(2)	4g	0.2410(4)	0.0257(6)	0.0420(2)	75(1)
O(3)	2f	1/2	0.7068(6)	1/4	62(2)
N(8)	4g	0.2682(3)	0.2728(5)	-0.0401(2)	43(1)
N(7)	4g	0.4109(3)	0.3242(5)	0.0702(2)	41(1)
N(6)	4g	0.2078(3)	0.3253(5)	0.1008(2)	40(1)
N(5)	4g	0.2723(3)	0.5772(5)	0.0589(2)	42(1)
N(4)	4g	0.2157(2)	-0.1551(4)	0.2750(1)	24(1)
N(3)	4g	0.1766(3)	0.1119(5)	0.1979(1)	32(1)
N(2)	4g	0.1140(3)	0.3960(4)	0.2614(1)	28(1)
N(1)	4g	0.2945(3)	0.1541(5)	0.3343(2)	32(1)
C(8)	4g	0.2024(5)	0.6245(7)	0.0780(3)	62(2)
C(12)	4g	0.4397(4)	0.5028(8)	0.0822(2)	60(2)
C(11)	4g	0.3753(5)	0.5902(7)	0.1001(2)	59(2)
C(10)	4g	0.3727(4)	0.3031(7)	-0.0240(2)	53(1)
C(9)	4g	0.4392(4)	0.2448(7)	0.0333(2)	52(1)
C(7)	4g	0.2042(4)	0.4987(7)	0.1174(2)	53(1)
C(4)	4g	0.2566(3)	-0.1562(6)	0.2378(2)	35(1)
C(6)	4g	0.2939(3)	-0.1575(6)	0.3322(2)	35(1)
C(5)	4g	0.3570(3)	0.0028(6)	0.3503(2)	40(1)
C(3)	4g	0.1870(3)	-0.0649(7)	0.1853(2)	39(1)
C(2)	4g	0.1887(3)	0.5269(6)	0.2730(2)	44(1)
C(1)	4g	0.1452(3)	-0.2944(5)	0.2637(2)	27(1)

[a] U(eq) is defined as one-third of the trace of the orthogonalized U_{ij} tensor

Table S2. Hydrogen bonds data for compound **1**.

D-H…A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N(6)-H(66A)...S(4)	0.90	2.72	3.618(9)	173.0
N(6)-H(66B)...S(6)#1	0.90	2.84	3.724(9)	165.9
N(5)-H(55A)...S(7)#4	0.89	2.46	3.294(8)	156.1
N(5)-H(55A)...S(10)	0.89	2.85	3.286(8)	111.8
N(5)-H(55B)...S(4)#4	0.89	2.52	3.266(9)	142.2
N(5)-H(55C)...S(11)	0.89	2.50	3.358(9)	161.1
N(4)-H(44)...S(8)#3	0.91	2.80	3.667(9)	160.8
N(3)-H(33A)...S(4)#5	0.90	2.71	3.497(9)	146.5
N(3)-H(33B)...N(5)	0.90	2.35	2.841(11)	113.9
N(3)-H(33B)...N(2)	0.90	2.36	2.830(12)	112.8
N(3)-H(33B)...S(4)#4	0.90	2.81	3.660(9)	157.5
N(2)-H(22A)...S(3)#4	0.89	2.59	3.332(9)	141.0
N(2)-H(22A)...S(12)	0.89	2.81	3.308(8)	116.9
N(2)-H(22B)...S(2)	0.89	2.65	3.429(9)	146.1
N(2)-H(22C)...S(4)#4	0.89	2.44	3.295(9)	161.8
N(1)-H(11A)...S(1)#6	0.89	2.80	3.585(15)	147.4
N(1)-H(11B)...S(8)#3	0.89	2.79	3.660(14)	166.8
N(1)-H(11C)...S(5)#6	0.89	2.76	3.488(13)	139.4
O(1W)-H(1WB)...S(6)#1	0.852(10)	2.56(6)	3.363(9)	158(14)

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

Table S3. Hydrogen bonds data for compound **2**.

D-H…A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1)-H(3)...S(4)#5	0.852(10)	2.69(4)	3.403(5)	143(5)
O(1)-H(4)...S(2)#2	0.860(10)	3.02(4)	3.744(5)	143(5)
O(2)-H(1)...S(5)	0.860(10)	2.56(2)	3.373(4)	159(5)
O(2)-H(2)...S(2)#6	0.859(10)	2.82(4)	3.459(5)	132(5)
O(3)-H(5)...S(6)#1	0.860(10)	2.42(2)	3.248(4)	161(5)
O(3)-H(6)...S(5)#7	0.853(10)	2.578(8)	3.218(4)	132.73(19)
O(3)-H(6)...S(5)#3	0.853(10)	2.578(8)	3.218(4)	132.73(19)
N(8)-H(7)...S(3)#6	0.90	2.87	3.706(4)	154.3
N(8)-H(8)...S(4)#5	0.90	2.63	3.480(4)	158.0
N(7)-H(9)...S(5)	0.91	2.93	3.737(4)	148.2
N(6)-H(10)...S(2)#2	0.90	2.58	3.477(4)	176.1
N(6)-H(11)...S(5)	0.90	2.82	3.634(4)	151.2
N(5)-H(12)...S(3)#5	0.91	2.77	3.653(4)	163.6
N(3)-H(13)...S(2)#2	0.90	2.81	3.618(4)	149.7
N(3)-H(14)...S(6)	0.90	2.71	3.575(4)	162.2
N(2)-H(15)...S(4)#2	0.90	2.46	3.360(4)	176.1
N(2)-H(16)...S(4)	0.90	2.55	3.433(4)	165.7
N(1)-H(17)...S(6)	0.90	2.70	3.530(4)	154.0
N(1)-H(18)...S(3)	0.90	2.57	3.437(4)	161.2

Symmetry transformations used to generate equivalent atoms: #1 -x+1, y, -z+1/2; #2 -x, y, -z+1/2; #3 x, y+1, z; #4 x, y-1, z; #5 x, -y+1, z-1/2; #6 x, -y, z-1/2; #7 -x+1, y+1, -z+1/2.

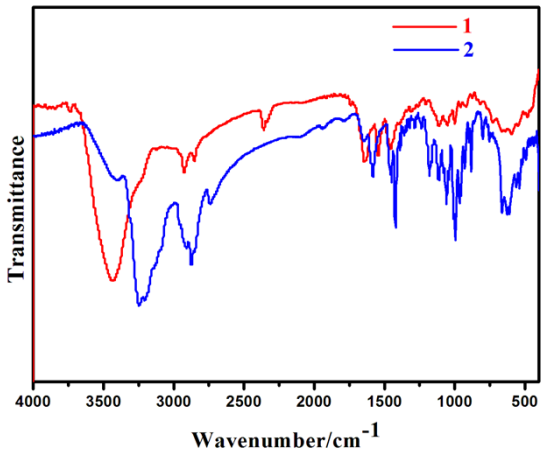
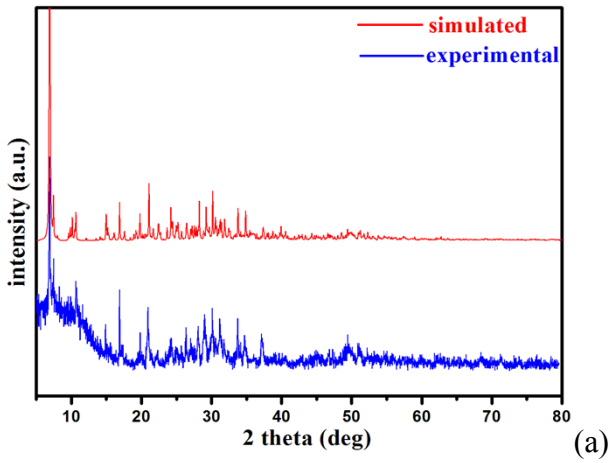
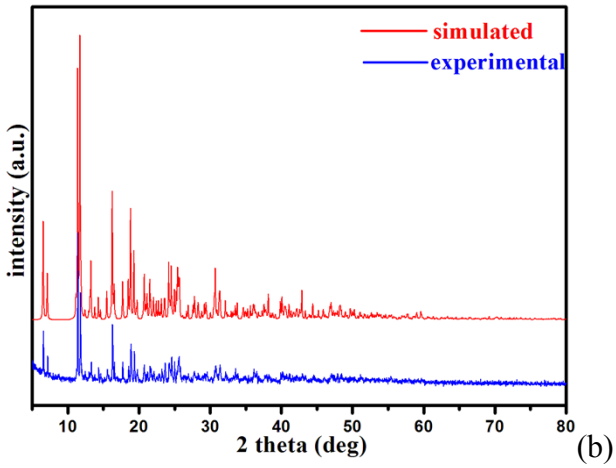


Fig. S1 The IR spectrum of compounds **1** and **2**.



(a)



(b)

Fig. S2. Experimental and simulated XRD powder pattern for compounds **1** (a) and **2** (b).

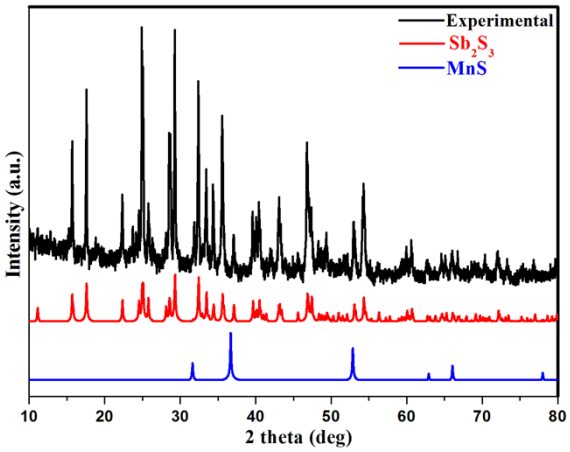


Fig. S3. The PXRD pattern of the TGA residue of **1** (600 ºC).