Sb-based Antiferromagnetic Oxychlorides: $MSb_2O_3(OH)Cl$ (M = Mn, Fe, Co) with 2D Spin-Dimer Structures

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Electronic Supplementary Information

Table S1. Selected important bond lengths (Å) and bond valence sum (BVS) analysis for $MSb_2O_3(OH)Cl$ (M = Mn, Fe, Co).

atoms	bond lengths	bond valence	atoms	bond lengths	bond valence
$MnSb_2O_3Cl(OH)$					
Sb(1)-O(3)	1.990(3)	0.956	Sb(1)-O(1)	2.007(3)	0.912
Sb(1)-O(2)#1	2.048(3)	0.817	Sb(1)-O(4)	2.384(3)	0.329
Sb(2)-O(2)	1.982(3)	0.974	Sb(2)-O(3)	1.996(3)	0.939
Sb(2)-O(1)#2	2.177(3)	0.576	Sb(2)-O(4)	2.189(3)	0.558
Mn(1)-O(2)	2.117(3)	0.413	Mn(1)-O(4)	2.364(4)	0.212
Mn(1)-O(3)#3	2.121(3)	0.409	Mn(1)-O(1)#4	2.373(3)	0.207
Mn(1)-O(1)	2.141(3)	0.387	Mn(1)-Cl(1)#5	2.490(2)	0.381
		BVS			BVS

Sb(1)		3.0	Sb(2)		3.0
Mn(1)		2.0	O(1)		-2.1
O(2)		-2.2	O(3)		-2.3
O(4)		-1.8	Cl(1)		-0.4
$FeSb_2O_3Cl(OH)$					
Sb(1)-O(3)	1.999(2)	0.931	Sb(1)-O(1)	2.015(2)	0.891
Sb(1)-O(2)#1	2.048(2)	0.816	Sb(1)-O(4)	2.355(2)	0.356
Sb(2)-O(2)	1.977(2)	0.990	Sb(2)-O(3)	2.008(2)	0.910
Sb(2)-O(1)#2	2.172(2)	0.584	Sb(2)-O(4)	2.179(2)	0.573
Fe(1)-O(3)#3	2.039(2)	0.438	Fe(1)-O(4)	2.360(3)	0.184
Fe(1)-O(1)	2.044(2)	0.432	Fe(1)-O(1)#4	2.376(2)	0.176
Fe(1)-O(2)	2.064(2)	0.410	Fe(1)-Cl(1)#5	2.4602(15)	0.339
		BVS			BVS
Sb(1)		3.0	Sb(2)		3.1
Fe(1)		2.0	O(1)		-2.1
O(2)		-2.2	O(3)		-2.3
O(4)		-1.9	Cl(1)		-0.3
$CoSb_2O_3Cl(OH)$					
Sb(1)-O(6)	1.996(3)	0.941	Sb(1)-O(1)#2	2.018(3)	0.885
Sb(1)-O(4)#2	2.059(3)	0.793	Sb(1)-O(7)	2.341(3)	0.370

Sb(2)-O(5)	1.984(3)	0.970	Sb(2)-O(2)#3	1.995(3)	0.944
Sb(2)-O(2)#1	2.054(3)	0.804	Sb(2)-O(8)#3	2.386(3)	0.327
Sb(3)-O(3)#3	2.005(3)	0.917	Sb(3)-O(8)#3	2.164(3)	0.596
Sb(3)-O(5)	2.006(3)	0.913	Sb(3)-O(3)#2	2.173(3)	0.583
Sb(4)-O(4)	1.982(3)	0.975	Sb(4)-O(1)	2.147(3)	0.625
Sb(4)-O(6)	2.005(3)	0.918	Sb(4)-O(7)	2.196(3)	0.548
Co(1)-O(4)	2.010(3)	0.423	Co(1)-O(1)#2	2.029(3)	0.402
Co(1)-O(5)	2.056(3)	0.374	Co(1)-O(3)#2	2.279(3)	0.204
Co(1)-O(7)	2.307(3)	0.190	Co(1)-Cl(2)#7	2.4423(14)	0.331
Co(2)-O(2)	2.007(3)	0.427	Co(2)-O(6)	2.036(3)	0.395
Co(2)-O(3)	2.037(3)	0.393	Co(2)-O(8)	2.318(3)	0.353
Co(2)-O(1)	2.394(3)	0.184	Co(2)-Cl(1)#7	2.4185(14)	0.150
		BVS			BVS
Sb(1)		3.0	Sb(2)		3.0
Sb(3)		3.0	Sb(4)		3.1
Co(1)		1.9	Co(2)		1.9
O(1)		-2.1	O(2)		-2.2
O(3)		-2.1	O(4)		-2.2
O(5)		-2.3	O(6)		-2.3
O(7)		-1.9	O(8)		-1.9

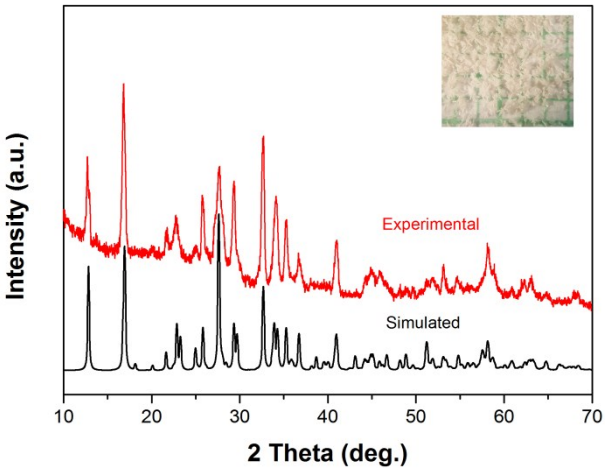
Cl(1)	-0.4	Cl(2)	-0.4

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

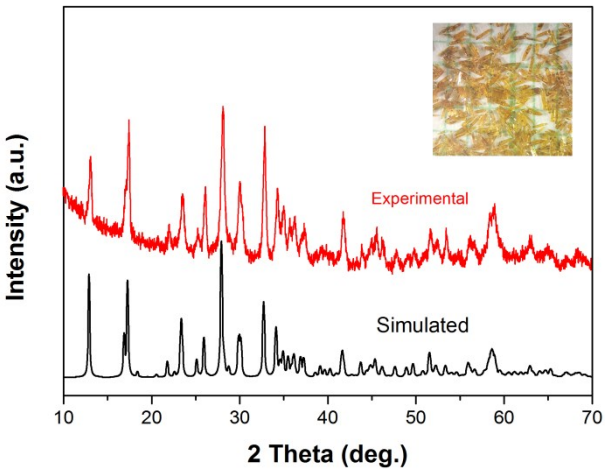
Table S2. The atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for $MSb_2O_3Cl(OH)$ (M = Mn, Fe, Co). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	atoms	x	y	z	U(eq)
$MnSb_2O_3Cl(OH)$	Sb(1)	0.2217(1)	0.0072(1)	0.2777(1)	0.011(1)
	Sb(2)	0.2327(1)	0.4184(1)	0.2606(1)	0.011(1)
	Mn(1)	0.0032(1)	0.2111(1)	0.0072(1)	0.012(1)
	Cl(1)	0.3515(2)	0.7494(2)	0.0508(1)	0.029(1)
	O(1)	0.0002(4)	0.0110(3)	0.1374(2)	0.013(1)
	O(2)	-0.0001(4)	0.4122(3)	0.1328(2)	0.013(1)
	O(3)	0.1579(4)	0.2200(3)	0.3531(3)	0.013(1)
	O(4)	0.3039(5)	0.2176(4)	0.1373(3)	0.016(1)
$FeSb_2O_3Cl(OH)$	Sb(1)	0.2169(1)	0.0033(1)	0.2808(1)	0.011(1)
	Sb(2)	0.2410(1)	0.4167(1)	0.2612(1)	0.011(1)
	Fe(1)	0.0103(1)	0.2059(1)	0.0105(1)	0.011(1)
	Cl(1)	0.3398(1)	0.7557(1)	0.0522(1)	0.026(1)
	O(1)	-0.0044(3)	0.0163(3)	0.1387(2)	0.013(1)
	O(2)	0.0116(3)	0.4079(3)	0.1310(2)	0.013(1)
	O(3)	0.1563(3)	0.2199(3)	0.3581(2)	0.012(1)
	O(4)	0.3111(4)	0.2100(3)	0.1404(2)	0.014(1)
$CoSb_2O_3Cl(OH)$	Sb(1)	0.2211(1)	0.5326(1)	0.2661(1)	0.011(1)
	Sb(2)	0.2241(1)	0.0428(1)	0.0148(1)	0.012(1)
	Sb(3)	0.2350(1)	0.4585(1)	0.0082(1)	0.011(1)

Sb(4)	0.2372(1)	0.1175(1)	0.2562(1)	0.011(1)
Co(1)	0.0086(1)	0.3286(1)	0.1317(1)	0.011(1)
Co(2)	0.0094(1)	0.2471(1)	0.3814(1)	0.011(1)
Cl(1)	0.6652(2)	0.2843(1)	0.3494(1)	0.023(1)
Cl(2)	0.6614(2)	0.2867(2)	0.1001(1)	0.025(1)
O(1)	0.0024(4)	0.0216(3)	0.3057(1)	0.013(1)
O(2)	0.0042(4)	0.4374(3)	0.4438(1)	0.014(1)
O(3)	0.0045(4)	0.0444(3)	0.4399(1)	0.011(1)
O(4)	0.0079(4)	0.1281(3)	0.1894(1)	0.012(1)
O(5)	0.1590(4)	0.2553(3)	0.0552(1)	0.012(1)
O(6)	0.1602(4)	0.3163(3)	0.3056(1)	0.013(1)
O(7)	0.3063(4)	0.3262(4)	0.1944(1)	0.016(1)
O(8)	0.3082(4)	0.2398(4)	0.4445(1)	0.016(1)



(a)



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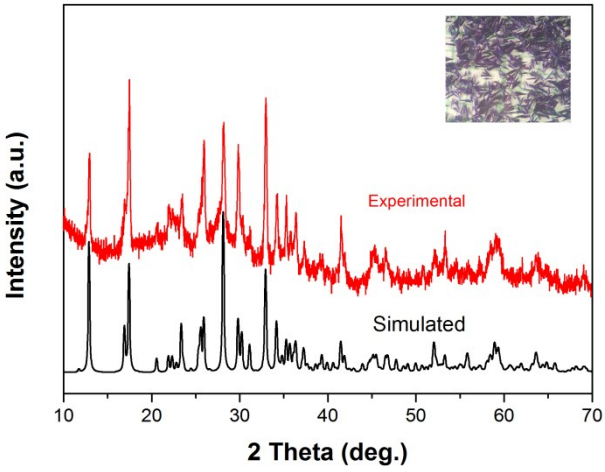

(c)

Figure S1. The experimental powder X-ray diffraction and the simulated patterns from single crystal structure for $MnSb_2O_3(OH)Cl$ (a), $FeSb_2O_3(OH)Cl$ (b) and $CoSb_2O_3(OH)Cl$ (c), respectively (X-ray wavelength λ = 1.5406 Å). Inserts are crystal pictures of the compounds under optical microscope.

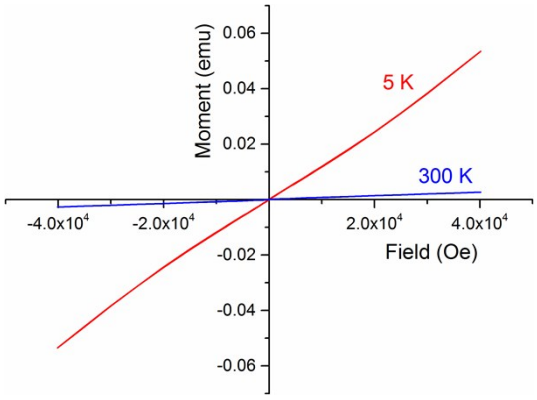

Figure S2. M-H magnetic hysteresis loop measured at 5 and 300 K for $MnSb_2O_3(OH)Cl$ respectively.

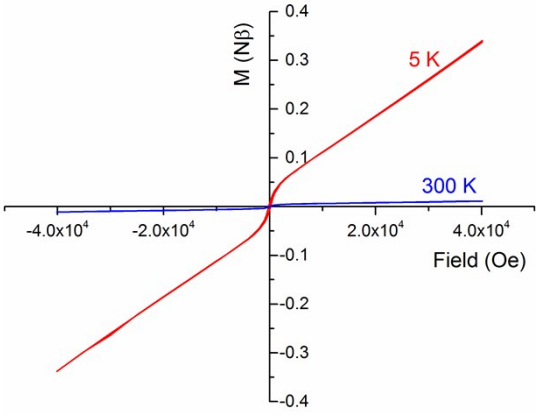

Figure S3. M-H magnetic hysteresis loop measured at 5 and 300 K for $CoSb_2O_3(OH)Cl$ respectively.