Sb-based Antiferromagnetic Oxychlorides: MSb$_2$O$_3$(OH)Cl (M = Mn, Fe, Co) with 2D Spin-Dimer Structures

Lei Geng,*a Qiang Li,*a,b Hongyan Lu,*a Kai Dai,*a P. Shiv Halasyamani*c

Electronic Supplementary Information

Table S1. Selected important bond lengths (Å) and bond valence sum (BVS) analysis for MSb$_2$O$_3$(OH)Cl (M = Mn, Fe, Co).

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<th>bond valence</th>
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FeSb$_2$O$_3$Cl(OH)

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BVS

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CoSb$_2$O$_3$Cl(OH)

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BVS

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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
(Å²) for MSb₂O₃Cl(OH) (M = Mn, Fe, Co). U(eq) is defined as one third of the trace of the orthogonalized Uᵢⱼ tensor.

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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)  
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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)
Figure S1. The experimental powder X-ray diffraction and the simulated patterns from single crystal structure for MnSb$_2$O$_3$(OH)Cl (a), FeSb$_2$O$_3$(OH)Cl (b) and CoSb$_2$O$_3$(OH)Cl (c), respectively (X-ray wavelength $\lambda = 1.5406$ 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$_2$O$_3$(OH)Cl respectively.

**Figure S3.** M-H magnetic hysteresis loop measured at 5 and 300 K for CoSb$_2$O$_3$(OH)Cl respectively.