Electronic Supplementary Material (ESI) for Dalton Transactions.

Synthesis and characterization of a series of transition metal oxychlorides: $MBi(SeO_3)_2(H_2O)Cl$ (M = Co, Ni, Cu)

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Electronic Supplementary Information

Table S1. Some selected important bond lengths (Å), bond valences and bond valence sums (BVS) for $MBi(SeO_3)_2(H_2O)Cl$ (M = Co, Ni, Cu).

atoms	bond length	bond valence	atoms	bond length	bond valence
$CoBi(SeO_3)_2(H_2O)Cl$					
Bi(1)-O(5)#1	2.232(2)	0.689		BVS=	4.0
Bi(1)-O(6)	2.275(2)	0.614	Se(2)-O(2)	1.6920(19)	1.379
Bi(1)-O(4)	2.364(2)	0.482	Se(2)-O(6)	1.703(2)	1.337
Bi(1)-O(1)	2.411(2)	0.424	Se(2)-O(4)#2	1.719(2)	1.283
Bi(1)-O(4)#2	2.582(2)	0.268		BVS=	4.0
Bi(1)-O(3)	2.617(2)	0.243	Co(1)-O(7)	2.053(2)	0.377
Bi(1)-Cl(1)	2.9686(7)	0.267	Co(1)-O(3)#3	2.065(2)	0.365
Bi(1)-Cl(1)#8	3.2832(8)	0.114	Co(1)-O(1)	2.071(2)	0.359
	BVS=	3.1	Co(1)-O(2)#4	2.0741(19)	0.356
Se(1)-O(3)	1.685(2)	1.404	Co(1)-O(2)	2.143(2)	0.296
Se(1)-O(5)	1.713(2)	1.305	Co(1)-Cl(1)#3	2.5538(8)	0.245
Se(1)-O(1)	1.717(2)	1.288		BVS=	2.0
$NiBi(SeO_3)_2(H_2O)Cl$					
Bi(1)-O(6)	2.225(2)	0.701		BVS=	4.0
Bi(1)-O(4)	2.267(2)	0.627	Se(2)-O(5)	1.688(2)	1.396
Bi(1)-O(3)#1	2.358(2)	0.490	Se(2)-O(6)#1	1.714(2)	1.300
Bi(1)-O(1)	2.404(2)	0.433	Se(2)-O(1)	1.715(2)	1.297
Bi(1)-O(3)	2.589(2)	0.263		BVS=	4.0
Bi(1)-O(5)	2.607(2)	0.250	Ni(1)-O(7)	2.022(2)	0.369
Bi(1)-Cl(1)	2.9731(8)	0.264	Ni(1)-O(5)#1	2.039(2)	0.353
Bi(1)-Cl(1)#8	3.3341(8)	0.099	Ni(1)-O(1)	2.057(2)	0.337
	BVS=	3.1	Ni(1)-O(2)#6	2.060(2)	0.334
Se(1)-O(2)	1.694(2)	1.372	Ni(1)-O(2)	2.088(2)	0.309
Se(1)-O(4)	1.706(2)	1.329	Ni(1)-Cl(1)#1	2.4848(9)	0.285
Se(1)-O(3)	1.719(2)	1.281		BVS=	2.0
$CuBi(SeO_3)_2(H_2O)Cl$					

Bi(1)-O(5)	2.275(4)	0.613		BVS=	4.0
Bi(1)-O(6)	2.288(4)	0.592	Se(2)-O(2)	1.693(4)	1.378
Bi(1)-O(4)#1	2.310(4)	0.559	Se(2)-O(5)#1	1.711(4)	1.311
Bi(1)-O(3)	2.510(4)	0.325	Se(2)-O(3)	1.714(3)	1.300
Bi(1)-O(4)	2.601(4)	0.254		BVS=	4.0
Bi(1)-O(2)	2.696(4)	0.196	Cu(1)-O(7)	1.958(4)	
Bi(1)-Cl(1)#1	2.8908(13)	0.329	Cu(1)-O(2)#7	1.971(3)	
Bi(1)-Cl(1)	3.0613(13)	0.208	Cu(1)-O(1)	1.971(3)	
	BVS=	3.1	Cu(1)-O(3)#8	1.987(3)	
Se(1)-O(1)	1.688(3)	1.394	Cu(1)-O(1)#8	2.394(4)	
Se(1)-O(6)	1.708(4)	1.322	Cu(1)-Cl(1)#8	2.776(2)	
Se(1)-O(4)	1.725(4)	1.259		BVS=	2.1

Symmetry transformations used to generate equivalent atoms: #1 -x,y-1/2,-z-1/2 #2 -x-1/2,y+1/2,z #3 -x,y+1/2,-z-1/2 #4 -x,-y+1,-z-1 #5 -x-1/2,y-1/2,z #6 -x,-y,-z-1 #7 x,-y+3/2,z+1/2 #8 -x,-y+1,-z

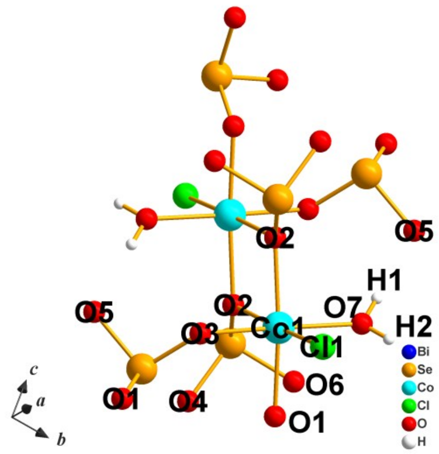
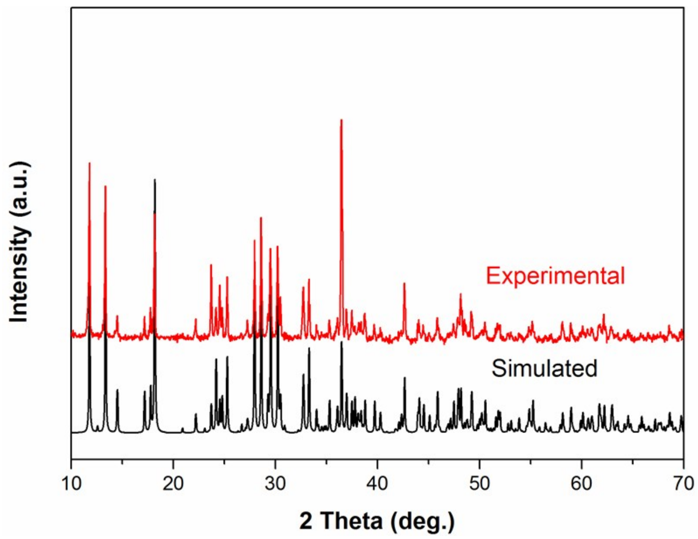
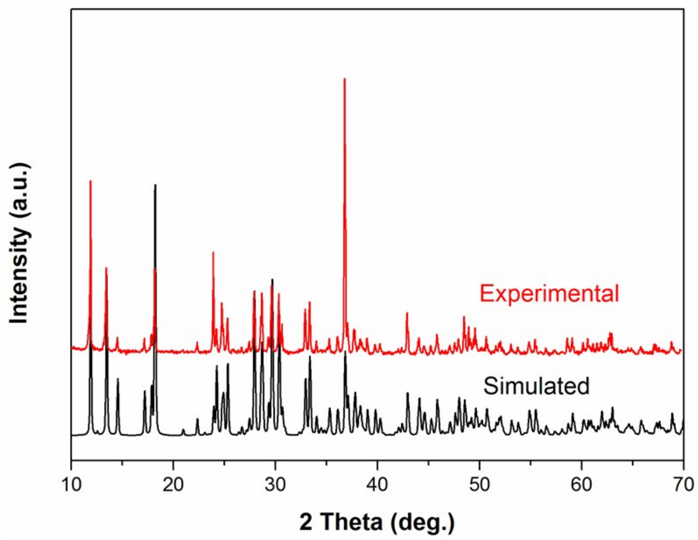


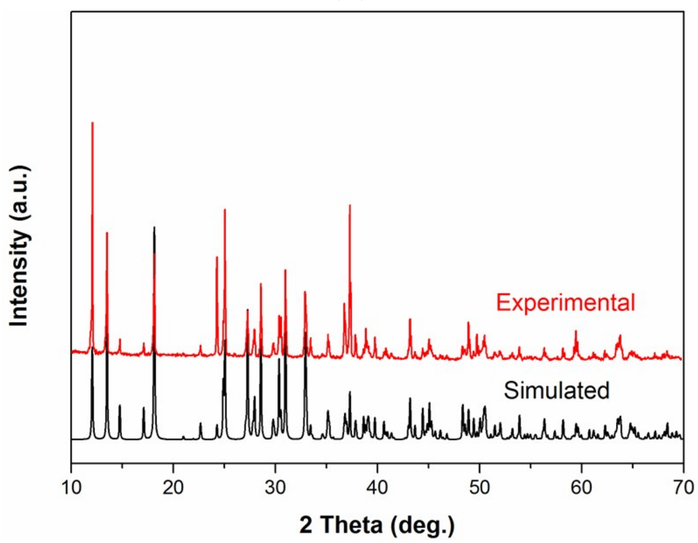
Fig. S1 The structural geometry of hydrogen atoms for $CoBi(SeO_3)_2(H_2O)Cl$.



(a)



(b)



(c)

Fig. S2 The experimental and simulated powder x-ray diffraction patterns for Co (a), Ni (b), and Cu (c) , respectively (λ = 1.5406 Å).

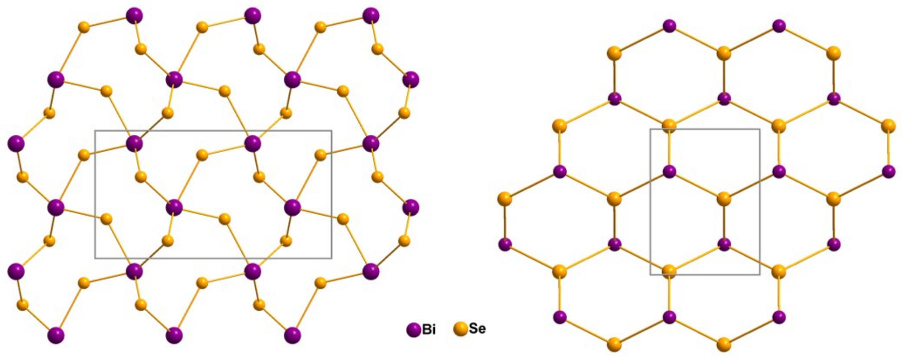
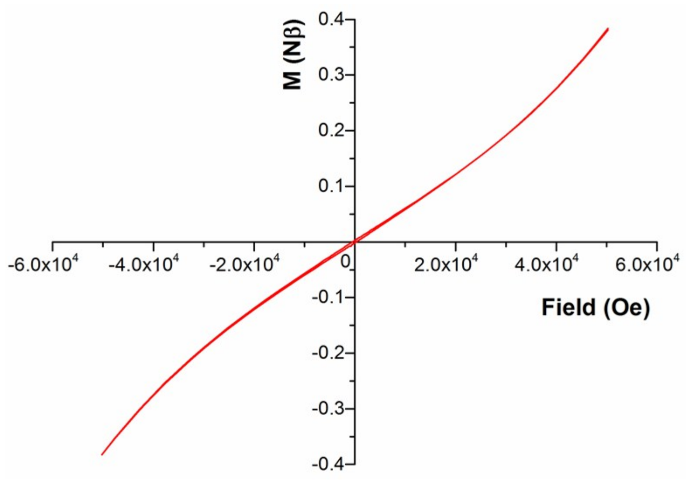
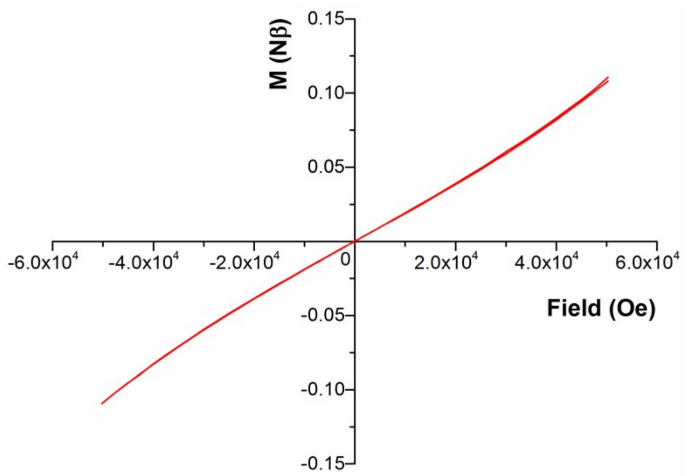


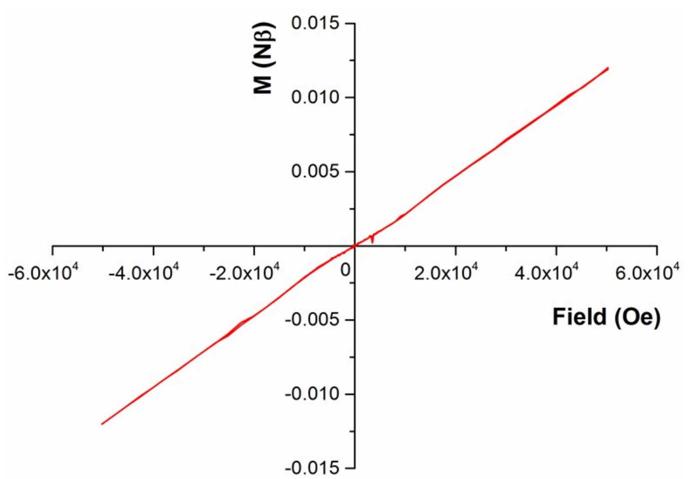
Fig. S3 The comparison of 2D $[Bi(SeO_3)_2]_\infty$ layer (left) in $CoBi(SeO_3)_2(H_2O)Cl$ with the 2D $[BiSeO_3]\infty$ layer (right) in γ-$BiSeO_3Cl$. Oxygen atoms are omitted for clarity.



(a)



(b)



(c)

Fig.S4 The magnetization vs. magnetizing field for coumpound $CoBi(SeO_3)_2(H_2O)Cl$ (a), $NiBi(SeO_3)_2(H_2O)Cl$ (b) and $CuBi(SeO_3)_2(H_2O)Cl$ (c).