<Electronic Supplementary Information>

Subtle metal(II) effects on SCSC guest exchange of 2D coordination networks

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Electronic Supplementary Information (ESI) available: Experimental details and crystal-structure determination. Crystallographic data, Bond length (Å) and angle (°), IR spectra, TGA and DSC curves, Bond length and geometry including the bite angle of nitrate, Two kinds of intra-channels of 2D sheet, ^{1}H NMR spectra, PXRD patterns.

Table S1 Crystallographic data

	$5C_4H_8O$@ $[Co(NO_3)_2L]$	$4C_4H_8O_2$@ $[Ni(NO_3)_2L]$	$5C_4H_8O$@ $[Cu(NO_3)_2L]$	$4C_4H_8O_2$@ $[Zn(NO_3)_2L]$	$4.5C_4H_8O_2$@ $[Co(NO_3)_2L]$	$4C_4H_8O_2$@ $[Cu(NO_3)_2L]$
Formula	$C_{56}H_{61}CoN_5O_{17}$	$C_{52}H_{53}N_5NiO_{20}$	$C_{56}H_{61}CuN_5O_{17}$	$C_{52}H_{53}N_5O_{20}Zn$	$C_{54}H_{57}CoN_5O_{21}$	$C_{52}H_{53}CuN_5O_{20}$
M_w	1135.02	1126.70	1139.63	1133.36	1171.97	1131.53
Cryst. sys.	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/n$
a (Å)	20.773(4)	20.708(4)	20.469(2)	20.963(4)	20.952(4)	20.698(4)
b (Å)	12.132(2)	12.244(2)	12.089(1)	12.279(3)	12.383(3)	12.339(3)
c (Å)	22.870(5)	22.873(4)	22.945(2)	22.875(5)	23.012(5)	22.916(5)
β (°)	114.95(3)	115.467(2)	114.455(1)	115.26(3)	115.30(3)	114.74(3)
V (Å^3)	5226(2)	5236(2)	5168.5(9)	5325(2)	5398(2)	5316(2)
Z	4	4	4	4	4	4
ρ (g cm^{-3})	1.443	1.429	1.465	1.414	1.442	1.414
μ (mm^{-1})	0.390	0.454	0.504	0.521	0.479	0.588
R_{int}	0.0577	0.1626	0.0587	0.0675	0.0658	0.0761
GoF on F^2	1.073	1.021	1.008	0.959	1.154	0.921
R_1 [$I>2\sigma(I)$][a]	0.0735	0.0923	0.0675	0.0910	0.1024	0.0789
wR_2 (all data)[b]	0.2408	0.3080	0.2174	0.3204	0.3424	0.2694

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, [b] $wR_2 = (\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2])^{1/2}$

Table S2 Bond lengths (Å) and angles (°)

$5C_4H_8O@[Co(NO_3)_2L]$		$4C_4H_8O_2@[Ni(NO_3)_2L]$		$5C_4H_8O@[Cu(NO_3)_2L]$	
Co(1)-O(11)	2.090(3)	Ni(1)-O(10)	2.039(5)	N(2)-Cu(1)$^{\#1}$	2.016(4)
Co(1)-N(1)	2.112(3)	Ni(1)-N(1)	2.053(5)	N(3)-Cu(1)$^{\#2}$	2.053(4)
Co(1)-N(3)$^{\#1}$	2.140(3)	Ni(1)-N(2)$^{\#1}$	2.079(5)	O(7)-Cu(1)	2.008(5)
Co(1)-N(2)$^{\#2}$	2.146(3)	Ni(1)-N(3)$^{\#2}$	2.084(5)	O(11)-Cu(1)	2.212(5)
Co(1)-O(8)	2.160(3)	Ni(1)-O(7)	2.104(5)	O(10')-Cu(1)	2.21(6)
Co(1)-O(9)	2.205(3)	Ni(1)-O(8)	2.153(5)	Cu(1)-N(1)	2.020(4)
O(11)-Co(1)-N(1)	90.2(1)	O(10)-Ni(1)-N(1)	91.0(2)		
O(11)-Co(1)-N(3)$^{\#1}$	90.9(1)	O(10)-Ni(1)-N(2)$^{\#1}$	85.7(2)		
N(1)-Co(1)-N(3)$^{\#1}$	88.1(1)	N(1)-Ni(1)-N(2)$^{\#1}$	93.7(2)	O(7')-Cu(1)-N(1)	91.8(9)
O(11)-Co(1)-N(2)$^{\#2}$	84.8(1)	O(10)-Ni(1)-N(3)$^{\#2}$	92.0(2)	O(7)-Cu(1)-N(1)	88.2(2)
N(1)-Co(1)-N(2)$^{\#2}$	93.4(1)	N(1)-Ni(1)-N(3)$^{\#2}$	86.6(2)	N(2)$^{\#3}$-Cu(1)-N(1)	176.8(2)
N(3)$^{\#1}$-Co(1)-N(2)$^{\#2}$	175.5(1)	N(2)$^{\#1}$-Ni(1)-N(3)$^{\#2}$	177.6(2)	N(2)$^{\#3}$-Cu(1)-N(3)$^{\#2}$	87.6(2)
O(11)-Co(1)-O(8)	174.0(1)	O(10)-Ni(1)-O(7)	170.7(2)	N(1)-Cu(1)-N(3)$^{\#2}$	93.3(2)
N(1)-Co(1)-O(8)	94.0(1)	N(1)-Ni(1)-O(7)	96.9(2)		
N(3)$^{\#1}$-Co(1)-O(8)	93.5(1)	N(2)$^{\#1}$-Ni(1)-O(7)	89.1(2)		
N(2)$^{\#2}$-Co(1)-O(8)	90.7(1)	N(3)$^{\#2}$-Ni(1)-O(7)	93.2(2)		
O(11)-Co(1)-O(9)	117.3(1)	O(10)-Ni(1)-O(8)	111.4(2)		
N(1)-Co(1)-O(9)	152.1(1)	N(1)-Ni(1)-O(8)	157.5(2)		
N(3)$^{\#1}$-Co(1)-O(9)	95.1(1)	N(2)$^{\#1}$-Ni(1)-O(8)	86.1(2)		
N(2)$^{\#2}$-Co(1)-O(9)	85.6(1)	N(3)$^{\#2}$-Ni(1)-O(8)	94.5(2)		

$^{\#1}$ -x+1/2,y-1/2,-z+3/2
$^{\#2}$ -x+1,-y+1,-z+1

$^{\#1}$ -x+1,-y+1,-z+1
$^{\#2}$ -x+3/2,y+1/2,-z+1/2

$^{\#1}$ x-1/2,-y+1/2,z+1/2
$^{\#2}$ -x+1,-y+1,-z+1
$^{\#3}$ x+1/2,-y+1/2,z-1/2

$4C_4H_8O_2@[Zn(NO_3)_2L]$		$4.5C_4H_8O_2@[Co(NO_3)_2L]$		$4C_4H_8O_2@[Cu(NO_3)_2L]$	
Zn(1)-O(11')	2.02(1)	N(2)-Co(1)$^{\#2}$	2.149(3)	Cu(1)-O(7)	1.996(5)
Zn(1)-N(1)	2.120(3)	N(3)-Co(1)$^{\#3}$	2.139(3)	Cu(1)-O(8')	2.00(1)
Zn(1)-N(3)$^{\#1}$	2.139(3)	O(7)-Co(1)	2.16(3)	Cu(1)-N(1)	2.016(3)
Zn(1)-N(2)$^{\#2}$	2.153(3)	O(7')-Co(1)	2.15(2)	Cu(1)-N(2)$^{\#1}$	2.029(3)
Zn(1)-O(9)	2.162(6)	O(9')-Co(1)	2.151(9)	Cu(1)-N(3)$^{\#2}$	2.096(3)
Zn(1)-O(10)	2.20(2)	O(10)-Co(1)	2.094(4)	Cu-O(10)	2.206(4)
Zn(1)-O(7)	2.20(1)	Co(1)-N(1)	2.131(3)		
Zn(1)-O(10')	2.24(5)			O(7)-Cu(1)-N(1)	92.9(2)
Zn(1)-O(7')	2.35(3)	N(4)-O(7)-Co(1)	85(2)	O(8')-Cu(1)-N(1)	92.0(4)
Zn(1)-N(5')	2.45(2)	N(4')-O(7')-Co(1)	101(1)	N(1)-Cu(1)-N(2)$^{\#1}$	178.3(1)
O(11')-Zn(1)-N(1)	152.7(4)	N(4')-O(9')-Co(1)	91.3(8)	O(7)-Cu(1)-N(3)$^{\#2}$	154.8(2)
O(11')-Zn(1)-N(3)$^{\#1}$	86.4(3)	N(5)-O(10)-Co(1)	111.9(4)	O(8')-Cu(1)-N(3)$^{\#2}$	95.9(4)
N(1)-Zn(1)-N(3)$^{\#1}$	86.4(1)	O(10)-Co(1)-N(1)	89.7(1)	N(1)-Cu(1)-N(3)$^{\#2}$	86.2(1)
N(1)-Zn(1)-N(2)$^{\#2}$	93.5(1)	O(10)-Co(1)-N(3)$^{\#4}$	91.93(1)	N(2)$^{\#1}$-Cu(1)-N(3)$^{\#2}$	93.7(1)
N(3)$^{\#1}$-Zn(1)-N(2)$^{\#2}$	177.2(1)	N(1)-Co(1)-N(3)$^{\#4}$	87.22(1)	O(7)-Cu(1)-O(10)	113.2(2)
N(1)-Zn(1)-O(9)	150.7(2)	O(10)-Co(1)-O(7')	175.5(6)	O(8')-Cu(1)-O(10)	170.2(4)
N(3)$^{\#1}$-Zn(1)-O(9)	96.3(2)	N(1)-Co(1)-O(7')	94.4(6)	N(1)-Cu(1)-O(10)	94.4(1)
N(2)$^{\#2}$-Zn(1)-O(9)	85.2(2)	N(3)$^{\#4}$-Co(1)-O(7')	90.0(5)	N(2)$^{\#1}$-Cu(1)-O(10)	87.9(1)
N(1)-Zn(1)-O(10)	93.8(4)	O(10)-Co(1)-N(2)$^{\#2}$	84.7(1)	N(3)$^{\#2}$-Cu(1)-O(10)	92.0(1)
N(3)$^{\#1}$-Zn(1)-O(10)	93.6(6)	N(1)-Co(1)-N(2)$^{\#2}$	93.2(1)		
N(2)$^{\#2}$-Zn(1)-O(10)	83.6(6)	N(3)$^{\#4}$-Co(1)-N(2)$^{\#2}$	176.6(1)		
O(9)-Zn(1)-O(10)	115.0(4)	O(10)-Co(1)-O(9')	115.2(4)		
N(1)-Zn(1)-O(7)	94.3(2)	N(1)-Co(1)-O(9')	154.7(4)		
N(3)$^{\#1}$-Zn(1)-O(7)	93.0(3)	N(3)$^{\#4}$-Co(1)-O(9')	95.5(3)		
N(2)$^{\#2}$-Zn(1)-O(7)	89.8(3)				
O(9)-Zn(1)-O(7)	56.5(2)				
O(10)-Zn(1)-O(7)	169.9(5)				

$^{\#1}$ -x+1/2,y-1/2,-z+3/2
$^{\#2}$ -x+1,-y+1,-z+1

$^{\#2}$ -x+1,-y+1,-z+1
$^{\#3}$ -x+1/2,y+1/2,-z+3/2
$^{\#4}$ -x+1/2,y-1/2,-z+3/2

$^{\#1}$ x-1/2,-y+1/2,z+1/2
$^{\#2}$ -x+1/2,y-1/2,-z+1/2

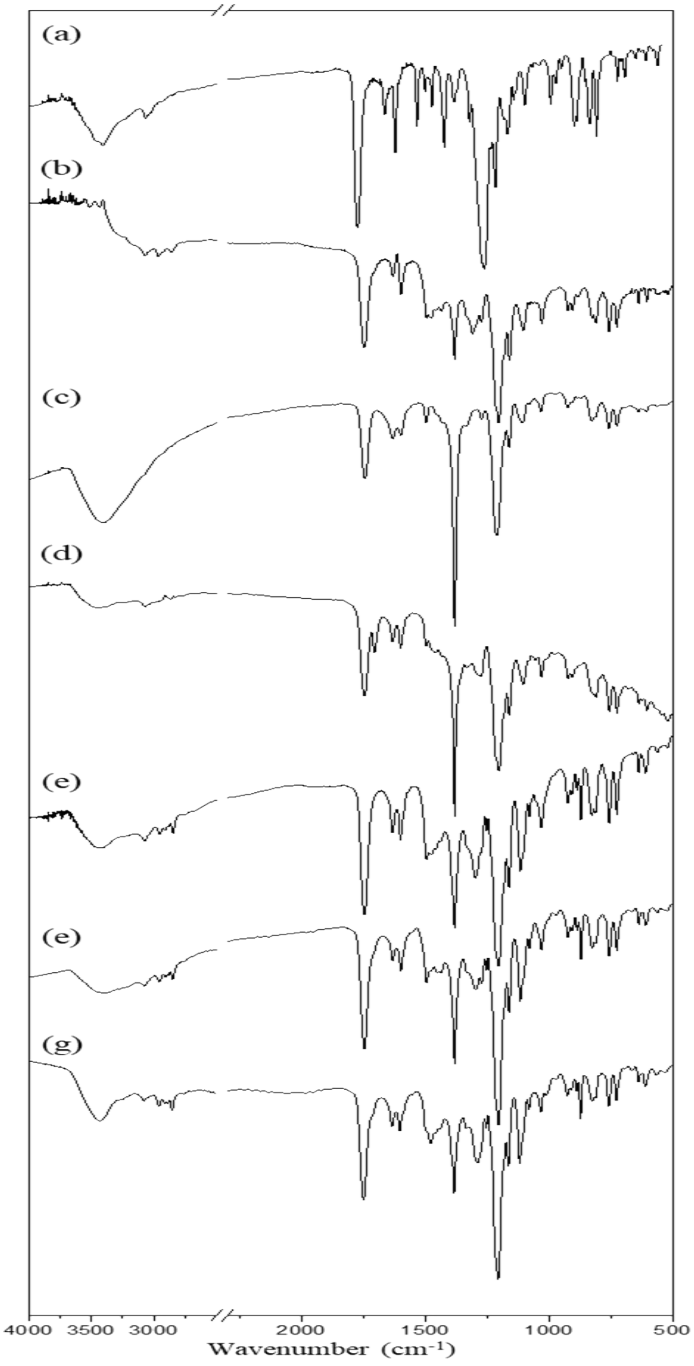

Fig. S1 IR Spectra of Ligand (a), $5C_4H_8O@[Co(NO_3)_2L]$ (b), $4C_4H_8O_2@[Ni(NO_3)_2L]$ (c), $5C_4H_8O@[Cu(NO_3)_2L]$ (d), $4C_4H_8O_2@[Zn(NO_3)_2L]$ (e), $4.5C_4H_8O_2@[Co(NO_3)_2L]$ (f), and $4C_4H_8O_2@[Cu(NO_3)_2L]$ (g).

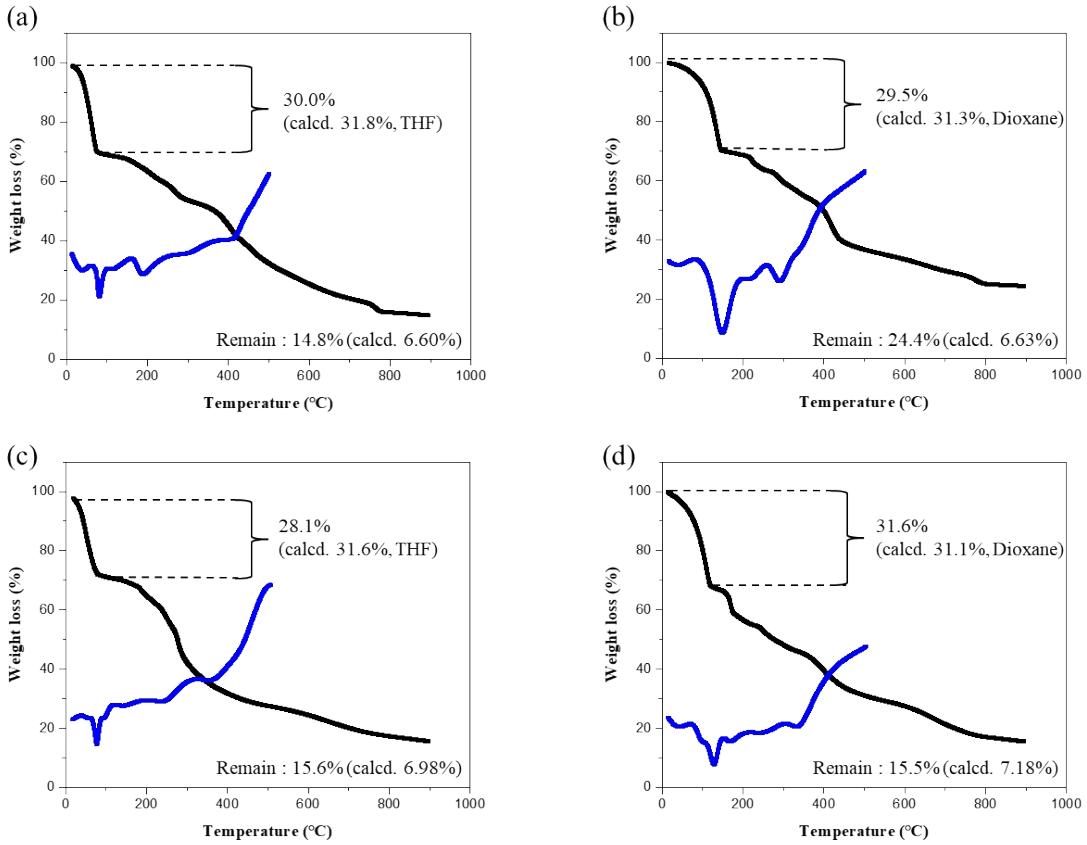

Fig. S2 TGA and DSC curves for $5C_4H_8O@[Co(NO_3)_2L]$ (a), $4C_4H_8O_2@[Ni(NO_3)_2L]$ (b), $5C_4H_8O@[Cu(NO_3)_2L]$ (c), and $4C_4H_8O_2@[Zn(NO_3)_2L]$ (d).

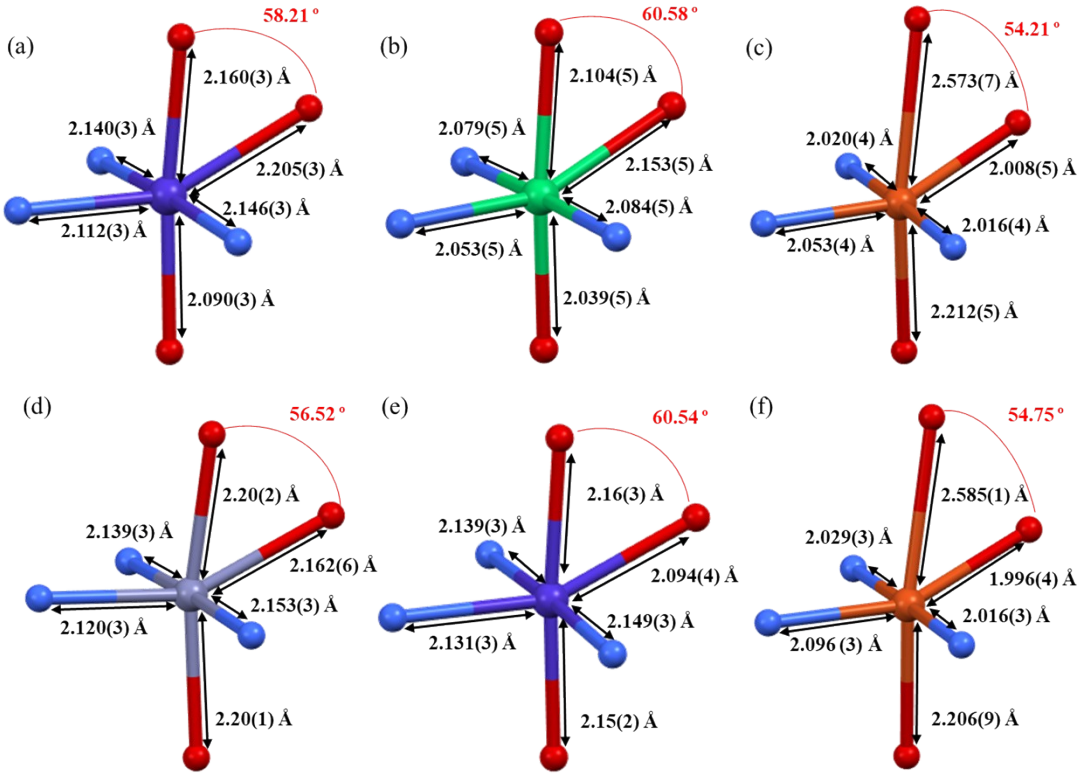

Fig. S3 Bond length and geometry including the bite angle of nitrate of $5C_4H_8O@[Co(NO_3)_2L]$ (a), $4C_4H_8O_2@[Ni(NO_3)_2L]$ (b), $5C_4H_8O@[Cu(NO_3)_2L]$ (c), $4C_4H_8O_2@[Zn(NO_3)_2L]$ (d), $4.5C_4H_8O_2@[Co(NO_3)_2L]$ (e), and $4C_4H_8O_2@[Cu(NO_3)_2L]$ (f).

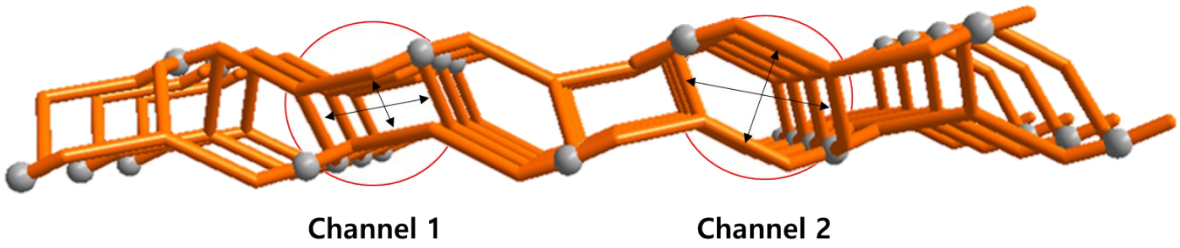

Fig. S4 Two kinds of intra-channels of 2D sheet.

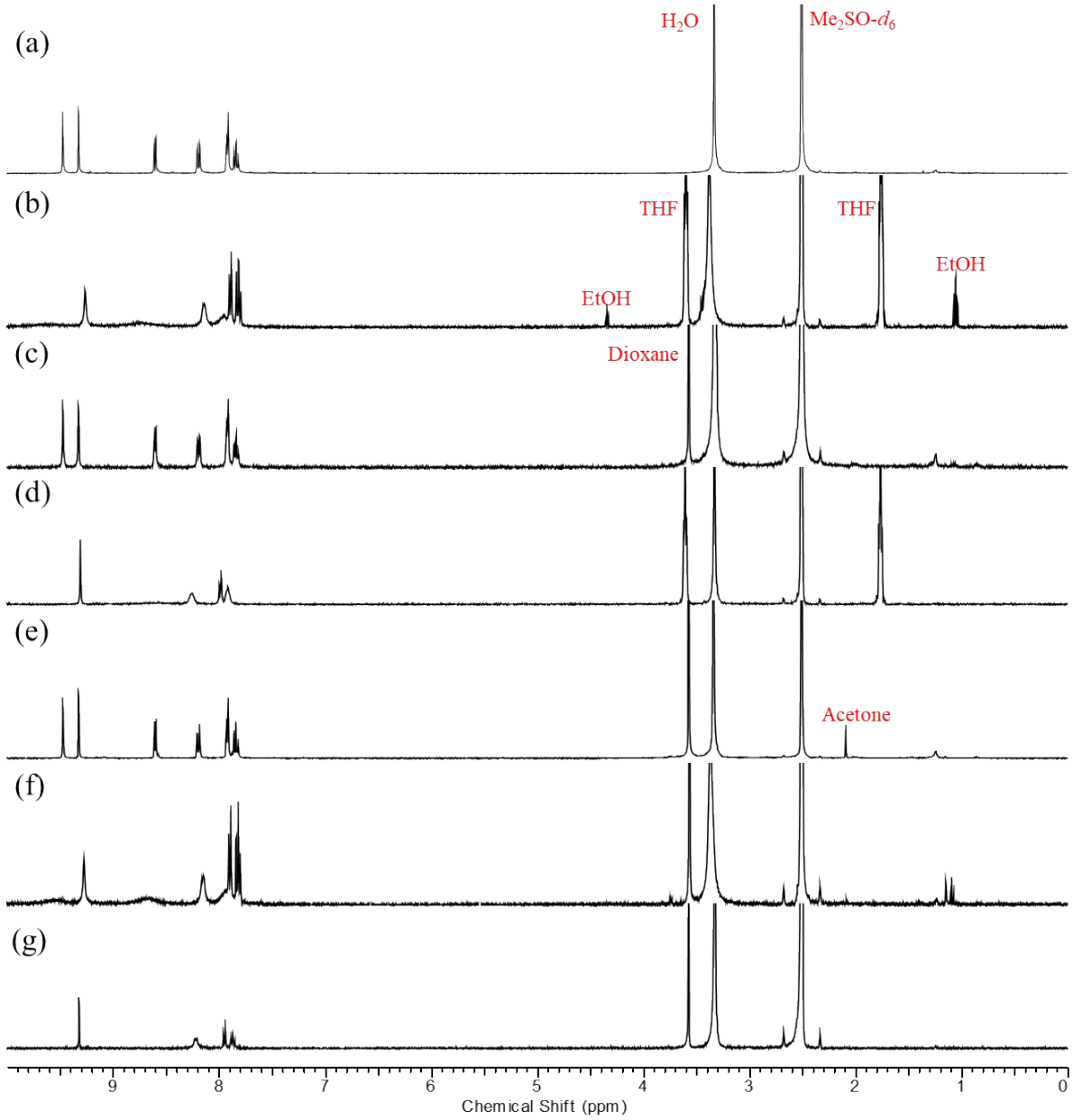

Fig. S5 ^{1}H NMR Spectra of Ligand (a), $5C_4H_8O@[Co(NO_3)_2L]$ (b), $4C_4H_8O_2@[Ni(NO_3)_2L]$ (c), $5C_4H_8O@[Cu(NO_3)_2L]$ (d), $4C_4H_8O_2@[Zn(NO_3)_2L]$ (e), $4.5C_4H_8O_2@[Co(NO_3)_2L]$ (f), and $4C_4H_8O_2@[Cu(NO_3)_2L]$ (g).

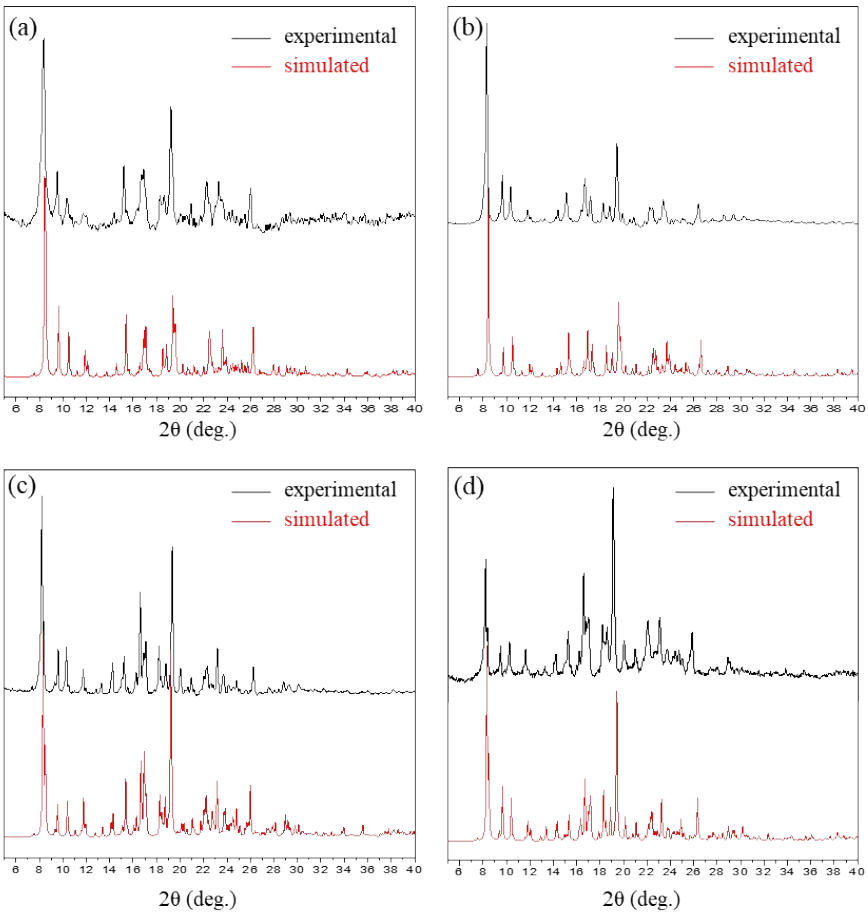

Fig. S6 PXRD patterns of $5C_4H_8O@[Co(NO_3)_2L]$ (a), $5C_4H_8O@[Cu(NO_3)_2L]$ (b), $4.5C_4H_8O_2@[Co(NO_3)_2L]$ (c), and $4C_4H_8O_2@[Cu(NO_3)_2L]$ (d).

	$5C_4H_8O@[Co(NO_3)_2L]$	$4C_4H_8O_2@[Ni(NO_3)_2L]$	$5C_4H_8O@[Cu(NO_3)_2L]$	$4C_4H_8O_2@[Zn(NO_3)_2L]$
anisole	O	O	O	O
trans-decalin	O	△	△	△
cis-decalin	O	△	X	△
1,3-dimethyladamantane	O	△	X	△

Fig. S7 Guest exchange condition of several solvent for 4 days (O is completely exchanged, X is not exchanged and △ is partially exchanged).