Synthesis, Magnetism and Spectrum Studies of Six Defective Dicubane Tetranuclear $\{M_4O_6\}$ ($M=Ni^{II}$, Co^{II}, Zn^{II}) and Three Trinuclear Cd^{II} Complexes with polydentate Schiff Base Ligands

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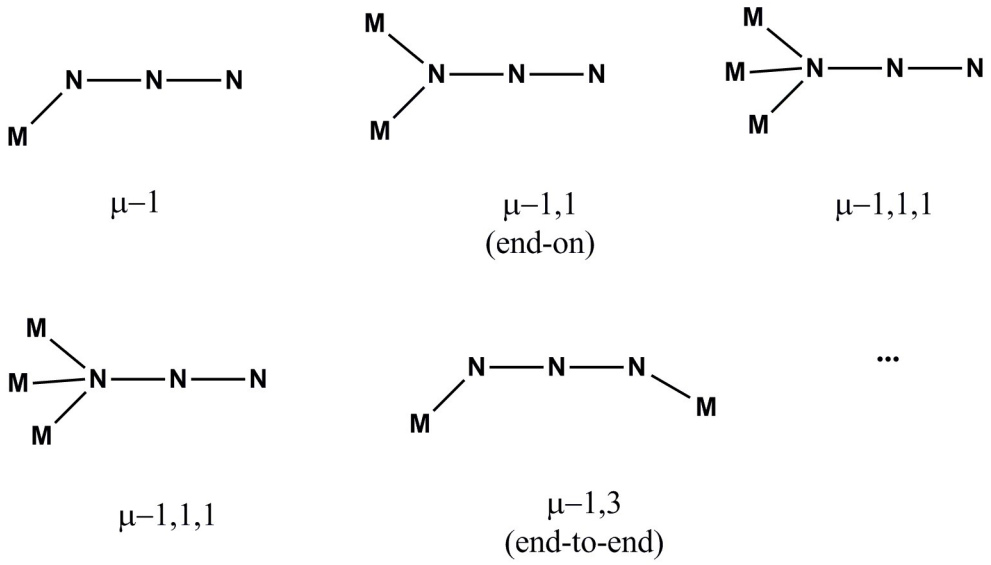
Supplementary Information Contents:



Scheme S1 Azide binding modes.

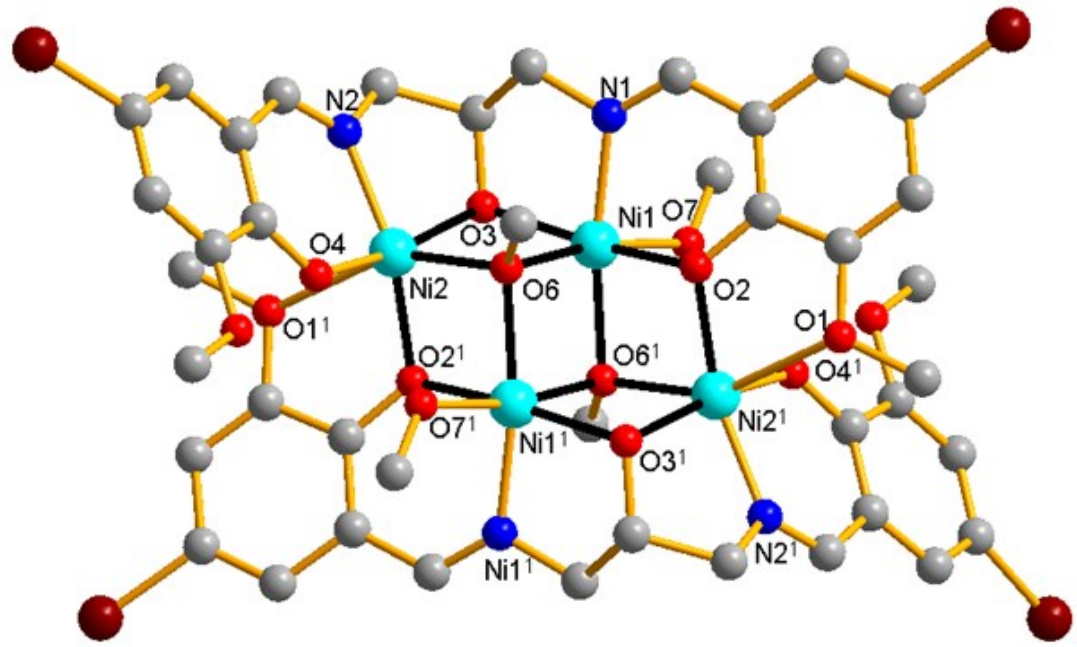


Fig. S2 Molecular structure of $[Ni_4(L^2)_2(\mu_2\text{-}CH_3O)_2(\mu\text{-}CH_3OH)_2](CH_3OH)$ **(3)**. The non-coordinated solvent molecules and H atoms are omitted for clarity.

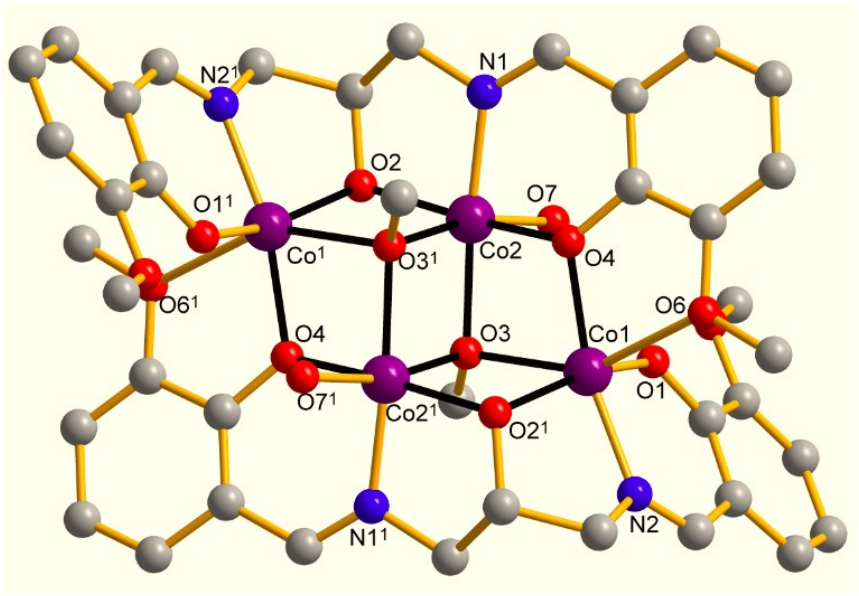


Fig. S3 Molecular structure of $[Co_4\ L^1_2(\mu_2\text{-}CH_3O)_2(\mu\text{-}H_2O)_2](CH_3OH)_2CHCl_3$ **(4).** The non-coordinated solvent molecules and H atoms are omitted for clarity.

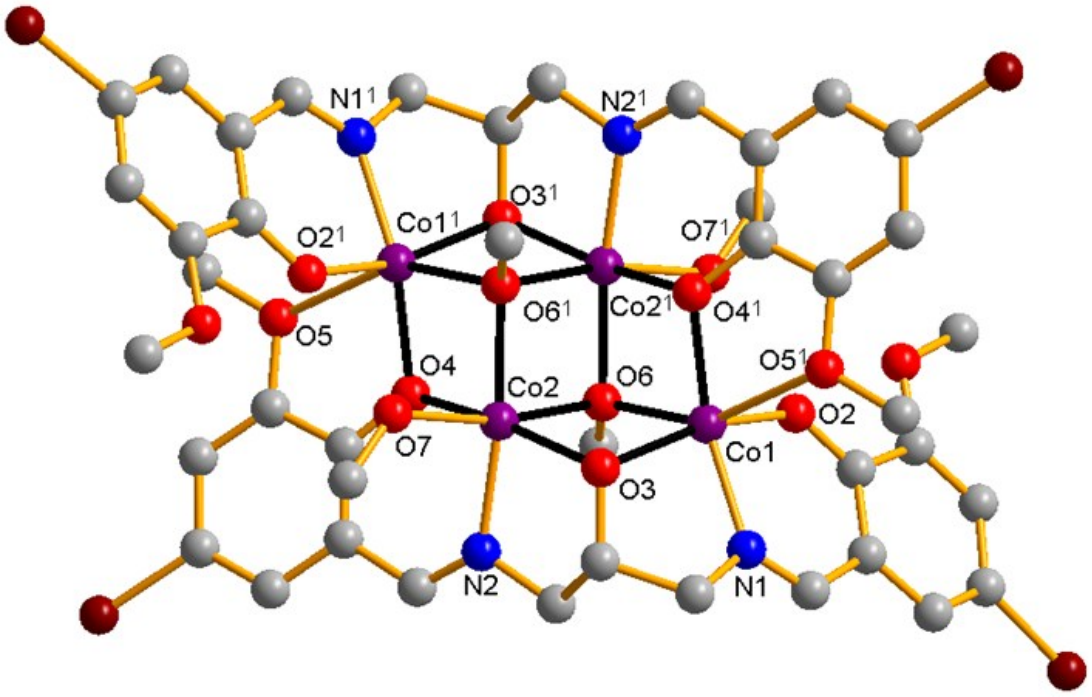


Fig. S4 Molecular structure of $[Co_4(L^2)_2(\mu_2\text{-}CH_3O)_2(\mu\text{-}CH_3OH)_2](CH_3OH)(H_2O)$ **(5).** The non-coordinated solvent molecules and H atoms are omitted for clarity

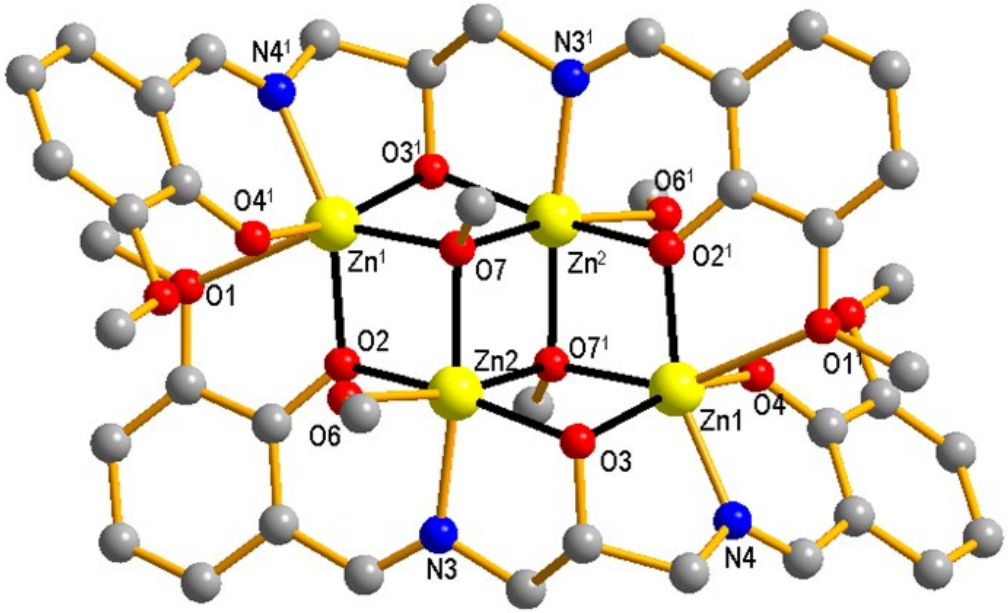


Fig. S5 Molecular structure of $[Zn_4L^1_2(\mu_2\text{-}CH_3O)_2(\mu\text{-}CH_3OH)_2](CH_3OH)_2$ **(6).** The non-coordinated solvent molecules and H atoms are omitted for clarity.

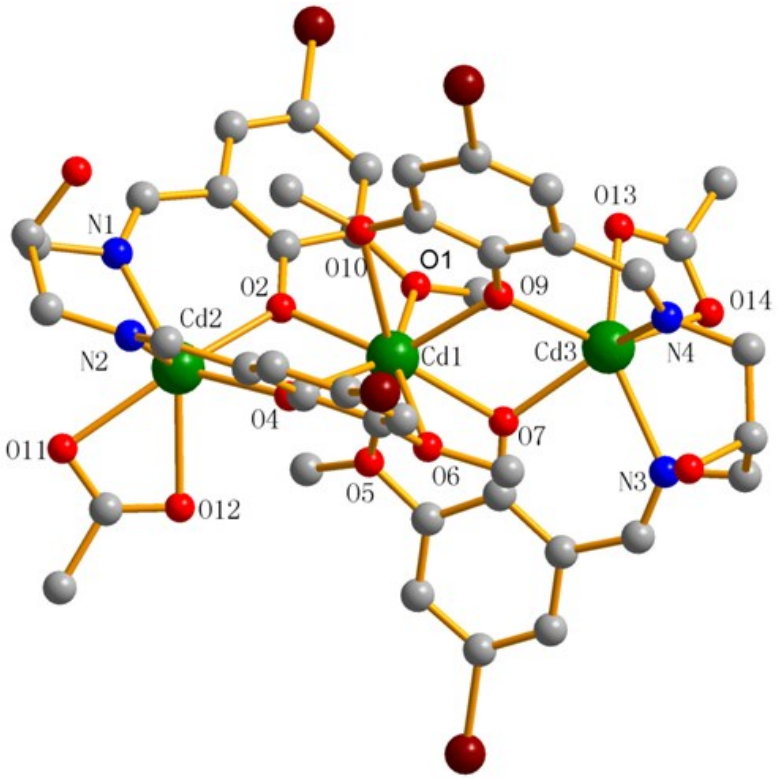


Fig. S6 Molecular structure of $[Cd_3(HL^2)_2(OAc)_2](CH_3OH)_2CH_2Cl_2$ **(9).** The non-coordinated solvent molecules and H atoms are omitted for clarity.

Table S7 Selected bond length (Å) and angles(◦) for compounds **1-4**.

1		2		3		4	
Ni2-O3[1]	2.026(3)	Ni1-O1	2.384(3)	O2-Ni2[1]	1.988(3)	Co1-O3	2.139(4)
Ni2-O4	2.006(3)	Ni1-O2	1.992(3)	Ni1-O6[1]	2.056(3)	Co1-O4	2.016(4)
Ni2-N2	1.996(3)	Ni1-O3[1]	2.110(3)	Ni1-O6	2.051(3)	Co1-O1	1.968(3)
Ni2-N3[1]	2.107(3)	Ni1-O4	2.062(3)	Ni1-N1	1.991(4)	Co1-O2[1]	2.089(3)
Ni2-N3	2.095(3)	Ni1-O6	2.006(3)	Ni1-O3	2.049(4)	Co1-O6	2.400(4)
Ni2-O6	2.097(3)	Ni1-N2	1.988(3)	Ni1-O2	2.001(4)	Co1-N2	2.016(4)
Ni1-O3	2.067(3)	Ni2-O2	2.000(3)	Ni1-O7	2.107(4)	Co2-O3	2.040(4)
Ni1-O4	1.993(3)	Ni2-O3	2.075(3)	Ni2-O6	2.041(3)	Co2-O3[1]	2.017(4)
Ni1-O5	2.338(3)	Ni2-O4[1]	2.061(3)	Ni2-O4	2.002(3)	Co2-O4	1.942(4)
Ni1-O2	2.010(3)	Ni2-O4	2.080(3)	Ni2-O1[1]	2.410(3)	Co2-O2	1.974(4)
Ni1-N1	1.981(3)	Ni2-O5	2.135(3)	Ni2-O3	2.082(3)	Co2-N1	1.959(4)
Ni1-N3	2.118(3)	Ni2-N1	1.994(3)	Ni2-O2[1]	1.988(3)	Co2-O7	2.027(4)
O3-Ni1[1]	2.026(3)	O2-Ni1-O1	71.49(11)	Ni2-N2	1.982(4)	O3-Co2[1]	2.018(4)
N3-Ni1[1]	2.107(3)	O3[1]-Ni1-O1	104.15(11)	O6-Ni1[1]	2.056(3)	O2-Co1[1]	2.089(3)
O3[1]-Ni2-N3[1]	81.85(11)	O3[1]-Ni1-O2	97.62(11)	O1-Ni2[1]	2.410(3)	O3-Co1-O6	149.26(14)
O3[1]-Ni2-N3	106.42(11)	O4-Ni1-O1	151.85(10)	O6-Ni1-O61	84.77(13)	O4-Co1-O3	78.38(14)
O3[1]-Ni2-O6	98.65(11)	O4-Ni1-O2	80.47(10)	O61-Ni1-O7	85.74(14)	O4-Co1-O2[1]	96.82(14)
O4-Ni2-O3[1]	168.46(10)	O4-Ni1-O3[1]	81.69(10)	O6-Ni1-O7	170.51(14)	O4-Co1-O6	70.96(14)
O4-Ni2-N3[1]	89.08(11)	O6-Ni1-O1	85.87(12)	N1-Ni1-O6	95.97(15)	O1-Co1-O3	89.91(15)
O4-Ni2-N3	79.63(11)	O6-Ni1-O2	91.70(11)	N1-Ni1-O6[1]	169.09(16)	O1-Co1-O4	95.63(14)
O4-Ni2-O6	91.61(12)	O6-Ni1-O3[1]	168.05(11)	N1-Ni1-O3	84.38(16)	O1-Co1-O2[1]	160.34(16)
N2-Ni2-O3[1]	85.47(12)	O6-Ni1-O4	92.55(11)	N1-Ni1-O2	88.52(16)	O1-Co1-O6	95.14(15)
N2-Ni2-O4	88.21(12)	N2-Ni1-O1	91.86(13)	N1-Ni1-O7	93.39(16)	O1-Co1-N2	91.43(16)
N2-Ni2-N3	167.83(12)	N2-Ni1-O2	162.84(13)	O3-Ni1-O6[1]	106.48(13)	O2[1]-Co1-O3	77.81(14)
N2-Ni2-N31	94.75(12)	N2-Ni1-O3[1]	82.09(12)	O3-Ni1-O6	82.14(14)	O2[1]-Co1-O6	103.27(14)
N2-Ni2-O6	96.09(12)	N2-Ni1-O4	116.28(12)	O3-Ni1-O7	100.38(15)	N2-Co1-O3	120.31(17)
N3-Ni2-N3[1]	84.64(12)	N2-Ni1-O6	91.21(13)	O2-Ni1-O6	90.26(14)	N2-Co1-O4	160.10(17)
N3-Ni2-O6	84.84(11)	O3-Ni2-O2	170.06(11)	O2-Ni1-O61	80.58(13)	N2-Co1-O2[1]	81.88(16)
O6-Ni2-N3[1]	169.15(11)	O4[1]-Ni2-O2	90.71(11)	O2-Ni1-O3	168.99(14)	N2-Co1-O6	89.92(16)
O3-Ni1-O5	103.14(10)	O4-Ni2-O2	79.85(10)	O2-Ni1-O7	88.42(15)	O3[1]-Co2-O3	79.06(16)
O3-Ni1-N3	80.63(11)	O4[1]-Ni2-O3	82.58(10)	O6-Ni2-O11	152.01(12)	O3[1]-Co2-O7	167.5(2)
O4-Ni1-O3	97.77(10)	O4-Ni2-O3	106.64(10)	O6-Ni2-O3	81.59(13)	O4-Co2-O3[1]	87.82(15)
O4-Ni1-O5	72.47(10)	O5-Ni2-O2	85.98(11)	O4-Ni2-O6	92.45(14)	O4-Co2-O3	82.56(16)
O4-Ni1-O2	90.78(11)	O5-Ni2-O3	101.53(11)	O4-Ni2-O1[1]	83.80(14)	O4-Co2-O2	168.86(15)
O4-Ni1-N3	79.35(11)	O5-Ni2-O4[1]	172.42(10)	O4-Ni2-O3	167.90(13)	O4-Co2-N1	89.84(17)
O2-Ni1-O3	168.41(10)	O5-Ni2-O4	88.26(10)	O3-Ni2-O11	106.38(13)	O4-Co2-O7	90.46(18)
O2-Ni1-O5	86.85(11)	N1-Ni2-O2	89.26(12)	O21-Ni2-O6	81.27(13)	O2-Co2-O3	102.41(16)
O2-Ni1-N3	93.36(11)	N1-Ni2-O3	84.28(12)	O21-Ni2-O4	92.50(14)	O2-Co2-O3[1]	83.42(15)
N1-Ni1-O3	82.62(12)	N1-Ni2-O4[1]	96.69(12)	O21-Ni2-O11	71.24(13)	O2-Co2-O7	99.57(17)
N1-Ni1-O4	165.19(12)	N1-Ni2-O4	169.07(12)	O21-Ni2-O3	96.96(14)	N1-Co2-O3	172.02(17)
N1-Ni1-O5	92.97(11)	N1-Ni2-O5	90.09(12)	N2-Ni2-O6	118.06(15)	N1-Co2-O31	98.30(16)

N1-Ni1-O2	91.12(13)	Ni2-O2-Ni1	101.88(11)	N2-Ni2-O4	91.30(16)	N1-Co2-O2	84.65(17)
N1-Ni1-N3	115.19(12)	Ni2-O3-Ni1[1]	96.08(11)	N2-Ni2-O11	89.81(14)	N1-Co2-O7	94.1(2)
N3-Ni1-O5	151.82(10)	Ni2-O4-Ni1	96.89(10)	N2-Ni2-O3	82.36(15)	O7-Co2-O3	88.4(2)
Ni21-O3-Ni1	99.91(11)	Ni2[1]-O4-Ni1	98.03(11)	N2-Ni2-O2[1]	160.12(16)	Co2[1]-O3-Co1	97.39(15)
Ni1-O4-Ni2	103.70(12)			Ni1-O6-Ni1[1]	95.23(13)	Co2-O3-Co1	95.10(17)
Ni2-N3-Ni2[1]	95.36(12)			Ni2-O6-Ni[1]	97.94(14)	Co2[1]-O3-Co2	100.94(16)
Ni2[1]-N3-Ni1	95.72(11)			Ni2-O6-Ni1[1]	96.77(13)	Co2-O4-Co1	102.36(16)
Ni2-N3-Ni1	96.57(12)			Ni1-O3-Ni2	96.69(14)	Co2-O2-Co1[1]	100.45(14)
				Ni21-O2-Ni1	100.36(14)		
[1]-X,-Y,-Z		[1]-X,-Y,-1-Z		[1]1-X,1-Y,1-Z		[1]1-X,1-Y,1-Z	

Table S8 Selected bond length (Å) and angles(◦) for compounds **5-7**

5		6		7	
Co2-O4	2.046(2)	Zn1-O3	2.0544(16)	Cd2-Cl1	2.4581(10)
Co2-O3	2.052(2)	Zn1-O2	2.0794(16)	Cd2-O4	2.249(2)
Co2-O6	2.112(2)	Zn1-O6	2.2020(17)	Cd2-O2	2.251(3)
Co2-O6[1]	2.066(2)	Zn1-O7[1]	2.1636(16)	Cd2-N1	2.256(3)
Co2-O7	2.148(3)	Zn1-O7	2.0225(15)	Cd2-N2	2.272(3)
Co2-N2	2.040(3)	Zn1-N3	2.0451(19)	Cd1-O1	2.599(2)
Co1-O4[1]	2.027(2)	Zn2-O3	2.1654(16)	Cd1-O1[1]	2.599(2)
Co1-O3	2.112(2)	Zn2-O2[1]	2.0013(16)	Cd1-O5[1]	2.508(2)
Co1-O6	2.098(2)	Zn2-O4	2.0122(17)	Cd1-O5	2.508(2)
Co1-O2	2.009(2)	Zn2-O7[1]	2.0650(16)	Cd1-O4	2.284(2)
Co1-N1	2.029(3)	Zn2-N4	2.0202(19)	Cd1-O4[1]	2.284(2)
O3-Co2-O4	165.65(9)	O2-Zn1-O3	166.44(6)	Cd1-O2[1]	2.310(2)
O6-Co2-O4	88.59(9)	O6-Zn1-O3	103.99(6)	Cd1-O2	2.310(2)
O6[1]-Co2-O4	81.89(9)	O6-Zn1-O2	86.16(6)	O4-Cd2-Cl1	123.56(6)
O6[1]-Co2-O3	107.48(9)	O7-Zn1-O3	106.49(6)	O4-Cd2-O2	74.65(8)
O6-Co2-O3	81.78(9)	O7[1]-Zn1-O3	83.63(6)	O4-Cd2-N1	132.35(9)
O7-Co2-O4	89.14(10)	O7-Zn1-O2	82.21(6)	O4-Cd2-N2	82.16(10)
O7-Co2-O3	102.25(10)	O7[1]-Zn1-O2	87.42(6)	O2-Cd2-Cl1	117.05(7)
O7-Co2-O6	169.14(9)	O7-Zn1-O6	89.56(6)	O2-Cd2-N1	84.63(10)
O7-Co2-O6[1]	85.20(9)	O7[1]-Zn1-O6	170.02(6)	O2-Cd2-N2	140.29(10)
N2-Co2-O4	87.30(10)	N3-Zn1-O3	83.39(7)	N1-Cd2-Cl1	104.09(8)

N2-Co2-O3	83.06(10)	N3-Zn1-O2	87.05(7)	N1-Cd2-N2	87.91(12)
N2-Co2-O6	95.43(10)	N3-Zn1-O6	93.66(7)	N2-Cd2-Cl1	102.60(9)
N2-Co2-O6[1]	169.18(11)	N3-Zn1-O7	168.55(7)	O1[1]-Cd1-O1	92.98(11)
N2-Co2-O7	95.08(11)	N3-Zn1-O7[1]	93.63(7)	O5[1]-Cd1-O1	95.72(8)
O3-Co1-O4[1]	98.34(9)	O2[1]-Zn2-O3	99.03(6)	O5-Cd1-O1[1]	95.72(8)
O6-Co1-O4[1]	81.55(9)	O4-Zn2-O3	163.70(6)	O5-Cd1-O1	158.04(8)
O6-Co1-O3	80.71(9)	O4-Zn2-O2[1]	95.47(7)	O5[1]-Cd1-O1[1]	158.04(8)
O2-Co1-O4[1]	95.71(10)	O7[1]-Zn2-O3	83.33(6)	O5-Cd1-O5[1]	83.52(11)
O2-Co1-O3	162.59(9)	O7[1]-Zn2-O21	83.08(6)	O4-Cd1-O1	136.18(8)
O2-Co1-O6	91.28(9)	O7[1]-Zn2-O4	91.10(6)	O4-Cd1-O11	78.18(8)
N1-Co1-O4[1]	158.78(11)	N4-Zn2-O3	80.32(7)	O4[1]-Cd1-O1[1]	136.18(8)
N1-Co1-O3	80.34(10)	N4-Zn2-O21	152.57(7)	O4[1]-Cd1-O1	78.18(8)
N1-Co1-O6	118.76(10)	N4-Zn2-O4	90.21(7)	O4-Cd1-O5[1]	81.60(8)
N1-Co1-O2	90.21(11)	N4-Zn2-O7[1]	123.70(7)	O4-Cd1-O5	65.56(8)
Co1[1]-O4-Co2	99.14(10)	Zn2-O3-Zn1	95.79(6)	O4[1]-Cd1-O5[1]	65.56(8)
C18-O4-Co2	124.9(2)	Zn2[1]-O2-Zn1	96.86(6)	O4[1]-Cd1-O5	81.60(8)
C18-O4-Co1[1]	122.7(2)	Zn2[1]-O7-Zn1	96.66(6)	O4-Cd1-O4[1]	135.92(11)
Co1-O3-Co2	98.31(10)	Zn2[1]-O7-Zn1[1]	95.53(6)	O4[1]-Cd1-O2	131.15(9)
C10-O3-Co2	111.85(19)			O4-Cd1-O2[1]	131.15(9)
C10-O3-Co1	110.78(19)			O4[1]-Cd1-O2[1]	72.85(8)
Co1-O6-Co2[1]	96.22(9)			O4-Cd1-O2	72.85(8)
Co1-O6-Co2	96.87(9)			O2[1]-Cd1-O1	77.42(8)
				O2-Cd1-O1[1]	77.42(8)
				O2-Cd1-O1	63.34(8)
				O2[1]-Cd1-O1[1]	63.34(8)
				O2-Cd1-O5	138.35(8)
				O2[1]-Cd1-O5	88.56(8)
				O2-Cd1-O5[1]	88.56(8)
				O2[1]-Cd1-O5[1]	138.35(8)
				O2[1]-Cd1-O2	122.11(12)
[1]1/2-X,3/2-Y,1/2-Z		[1]2-X,1-Y,1-Z		1-X,+Y,1/2-Z	

Table S9 Selected bond length (Å) and angles(◦) for compounds **8-9.**

8				9			
Cd1-O2	2.274(2)	N1-Cd2-N2	89.59(12)	Cd1-O10	2.623(3)	O4-Cd2-O2	84.38(13)
Cd1-O4	2.267(2)	N1-Cd2-O11	89.83(12)	Cd1-O2	2.259(3)	O4-Cd2-O12	126.93(14)
Cd1-O1	2.624(2)	O9-Cd3-O7	73.97(9)	Cd1-O4	2.277(3)	O4-Cd2-O11	81.71(12)
Cd1-O9	2.273(2)	O9-Cd3-N3	82.86(11)	Cd1-O6	2.549(3)	O4-Cd2-N2	135.24(12)
Cd1-O6	2.533(2)	O9-Cd3-O13	127.12(10)	Cd1-O7	2.260(3)	O4-Cd2-N1	107.10(16)
Cd1-O5	2.571(2)	O9-Cd3-N4	139.63(11)	Cd1-O5	2.610(3)	O4-Cd2-C39	27.16(17)
Cd1-O7	2.263(2)	O9-Cd3-O14	87.28(10)	Cd1-O9	2.263(3)	O12-Cd2-C39	55.51(15)
Cd2-O2	2.264(2)	O9-Cd3-C41	108.24(11)	Cd1-O1	2.532(3)	O11-Cd2-O12	28.46(19)
Cd2-O4	2.241(2)	O7-Cd3-N3	125.13(10)	Cd2-O2	2.277(3)	O11-Cd2-C39	115.56(14)
Cd2-O12	2.279(3)	O7-Cd3-O13	145.41(10)	Cd2-O4	2.256(3)	N2-Cd2-O12	86.07(18)
Cd2-N2	2.281(3)	O7-Cd3-O14	107.19(10)	Cd2-O12	2.389(4)	N2-Cd2-O11	86.06(13)
Cd2-O11	2.549(3)	O7-Cd3-C41	129.16(11)	Cd2-O11	2.369(5)	N2-Cd2-N1	103.7(2)
Cd2-N1	2.245(3)	N3-Cd3-O13	87.44(11)	Cd2-N2	2.289(4)	N2-Cd2-C39	138.87(14)
Cd3-O9	2.229(2)	N4-Cd3-C41	120.80(12)	Cd2-N1	2.292(4)	N1-Cd2-O12	94.67(15)
Cd3-O7	2.288(2)	O14-Cd3-O13	105.09(12)	Cd2-C39	2.712(6)	N1-Cd2-O11	117.63(17)
Cd3-N3	2.293(3)			Cd3-O7	2.249(3)	N1-Cd2-C39	73.12(11)
Cd3-O13	2.433(3)			Cd3-O9	2.269(3)	O7-Cd3-O9	118.33(15)
Cd3-N4	2.270(3)			Cd3-O14	2.417(4)	O7-Cd3-O14	113.47(14)
Cd3-O14	2.346(3)			Cd3-O13	2.295(4)	O7-Cd3-O13	80.54(12)
O2-Cd1-O1	63.28(8)			Cd3-N3	2.295(4)	O7-Cd3-N3	120.24(14)
O2-Cd1-O6	93.23(9)			Cd3-N4	2.240(4)	O7-Cd3-C41	140.62(13)
O2-Cd1-O5	136.52(8)			O2-Cd1-O10	76.99(10)	O9-Cd3-O14	86.94(14)

O4-Cd1-O2	72.98(8)	O2-Cd1-O4	74.10(10)	O9-Cd3-O13	130.91(13)
O4-Cd1-O1	135.77(8)	O2-Cd1-O6	79.55(10)	O9-Cd3-N3	113.60(16)
O4-Cd1-O9	131.07(9)	O2-Cd1-O7	135.78(11)	O9-Cd3-C41	27.06(16)
O4-Cd1-O6	82.24(8)	O2-Cd1-O5	137.24(10)	O14-Cd3-C41	53.69(15)
O4-Cd1-O5	64.39(8)	O2-Cd1-O9	131.29(11)	O13-Cd3-O14	26.67(15)
O9-Cd1-O2	116.12(9)	O2-Cd1-O1	65.27(10)	O13-Cd3-C41	88.36(15)
O9-Cd1-O1	77.45(8)	O4-Cd1-O10	75.93(10)	N3-Cd3-O14	142.00(15)
O9-Cd1-O6	139.51(8)	O4-Cd1-O6	95.77(11)	N3-Cd3-O13	115.42(17)
O9-Cd1-O5	98.64(8)	O4-Cd1-O5	63.22(10)	N3-Cd3-C41	135.95(15)
O6-Cd1-O1	93.55(8)	O4-Cd1-O1	139.23(10)	N4-Cd3-O7	83.31(14)
O6-Cd1-O5	73.56(9)	O6-Cd1-O10	156.45(9)	N4-Cd3-O9	103.61(18)
O5-Cd1-O1	155.48(8)	O6-Cd1-O5	101.43(10)	N4-Cd3-O14	101.52(17)
O7-Cd1-O2	134.71(9)	O7-Cd1-O10	136.34(10)	N4-Cd3-O13	88.18(15)
O7-Cd1-O4	136.29(9)	O7-Cd1-O4	132.33(11)	N4-Cd3-N3	103.11(17)
O7-Cd1-O1	77.77(8)	O7-Cd1-O6	64.95(10)		
O7-Cd1-O9	73.64(9)	O7-Cd1-O5	77.84(10)		
O7-Cd1-O6	65.87(8)	O7-Cd1-O9	73.02(11)		
O7-Cd1-O5	77.92(8)	O7-Cd1-O1	79.82(10)		
O2-Cd2-O12	89.78(10)	O5-Cd1-O10	94.45(10)		
O2-Cd2-N2	134.32(10)	O9-Cd1-O10	63.47(10)		
O2-Cd2-O11	139.39(10)	O9-Cd1-O4	118.69(11)		
O4-Cd2-O2	73.66(8)	O9-Cd1-O6	137.33(11)		
O4-Cd2-O12	112.20(10)	O9-Cd1-O5	75.82(10)		
O4-Cd2-N2	81.53(10)	O9-Cd1-O1	91.81(11)		

O4-Cd2-O11	131.64(11)	O1-Cd1-O10	97.43(10)
O4-Cd2-N1	136.03(11)	O1-Cd1-O6	74.28(11)
O12-Cd2-N2	135.49(11)	O1-Cd1-O5	156.81(10)
O12-Cd2-O11	53.38(10)	O2-Cd2-O12	108.40(13)
N2-Cd2-O11	85.23(10)	O2-Cd2-O11	145.52(17)
N1-Cd2-O2	82.92(10)	O2-Cd2-N2	126.83(12)
N1-Cd2-O12	104.21(12)	O2-Cd2-N1	79.55(12)
		O2-Cd2-C39	128.4(2)

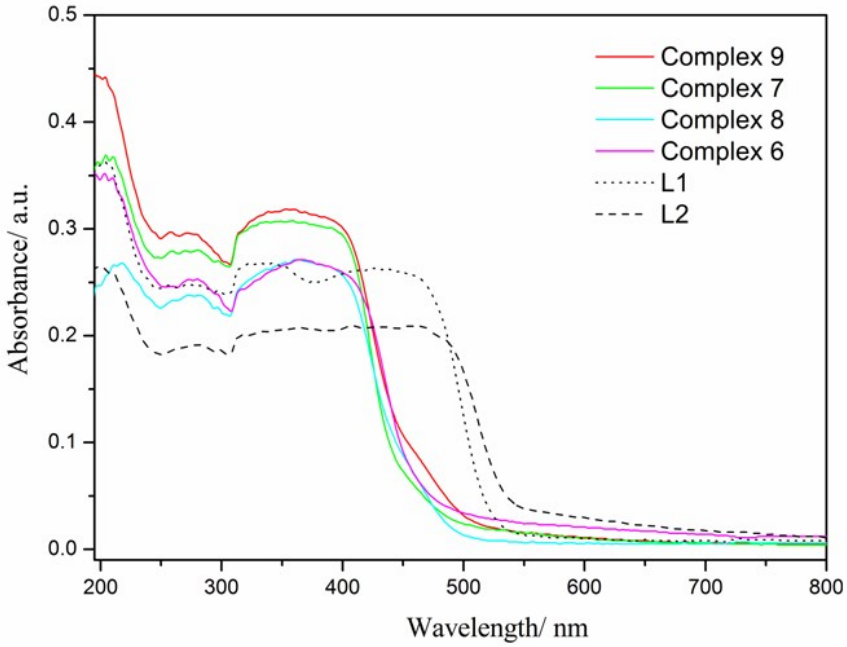
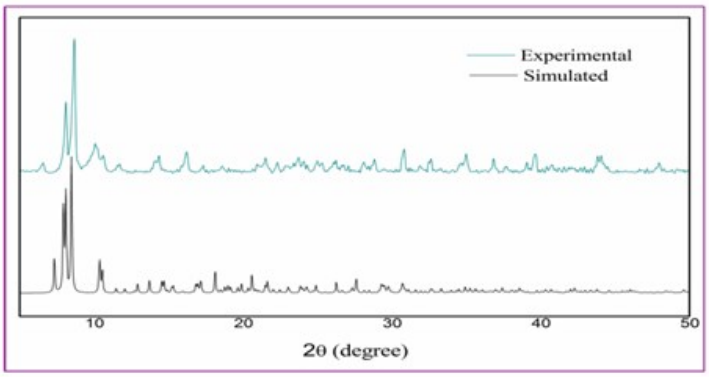
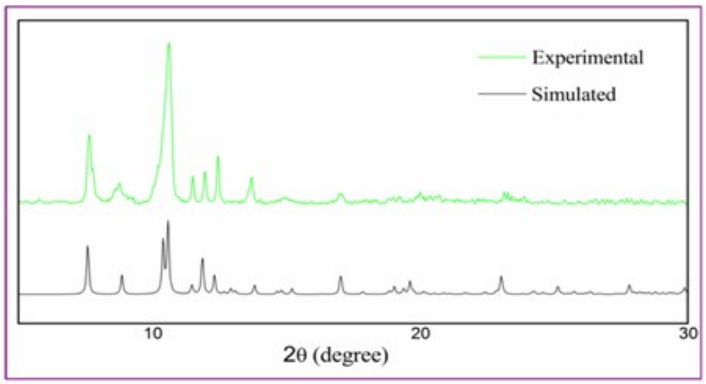


Fig. **S10** UV–Vis reflectance spectra of **6-9** in $BaSO_4$ after Kubelka–Munk transformation.

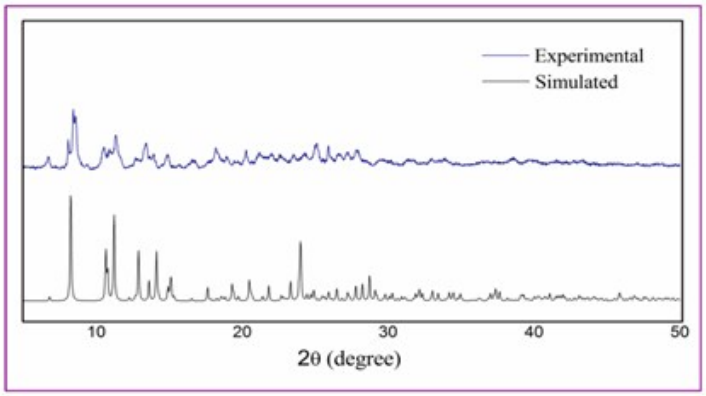
(a)


Experimental
Simulated
10
20
30
40
50
2θ (degree)

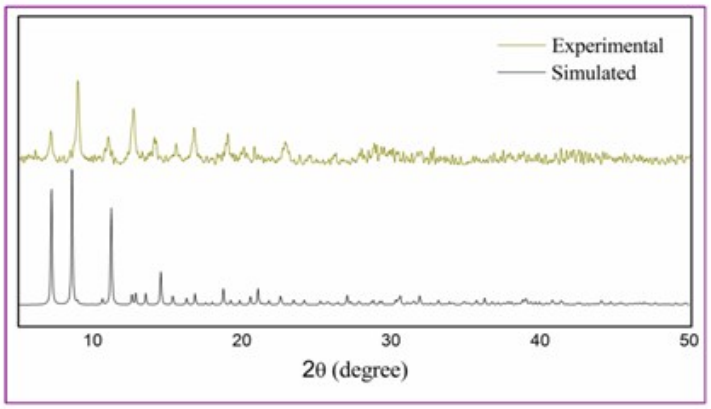
(b)


Experimental
Simulated
10
20
30
2θ (degree)

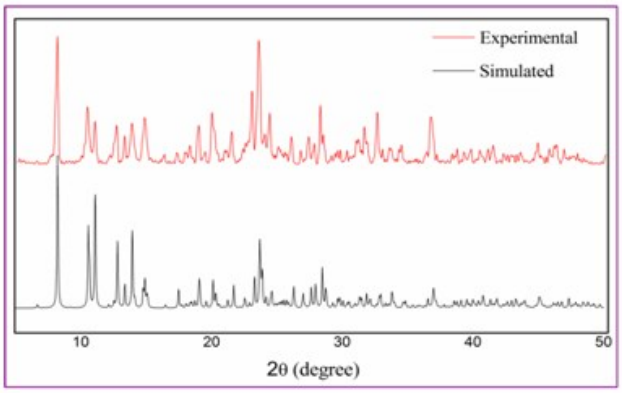
(c)


Experimental
Simulated
10
20
30
40
50
2θ (degree)

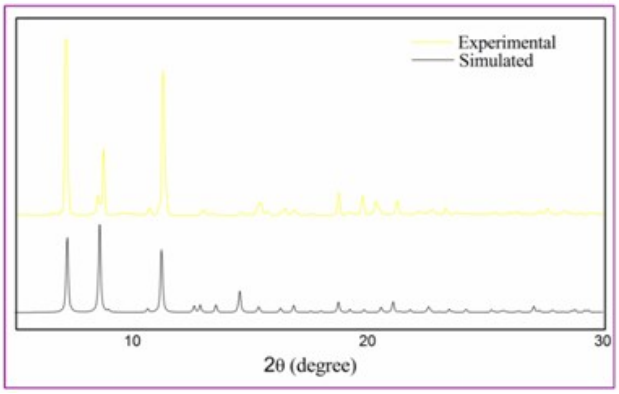
(d)


Experimental
Simulated
10
20
30
40
50
2θ (degree)

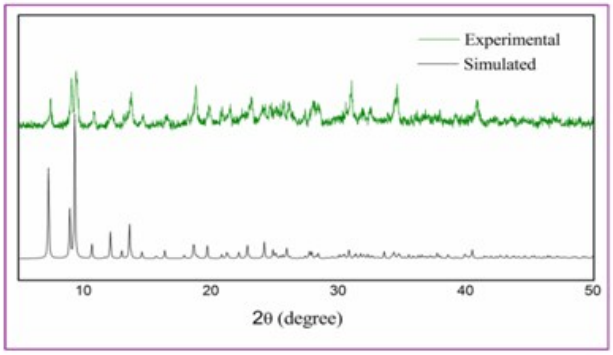
(e)


Experimental
Simulated
10
20
30
40
50
2θ (degree)

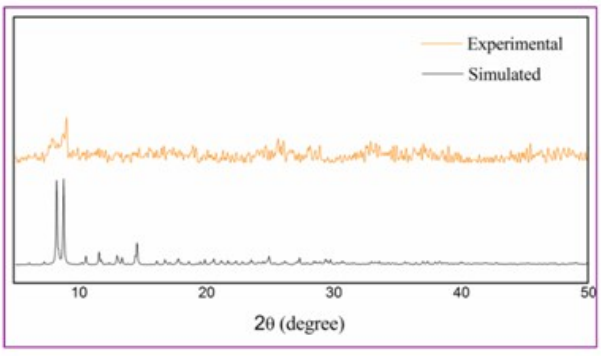
(f)


Experimental
Simulated
10
20
30
2θ (degree)

(g)


Experimental
Simulated
10
20
30
40
50
2θ (degree)

(h)


Experimental
Simulated
10
20
30
40
50
2θ (degree)

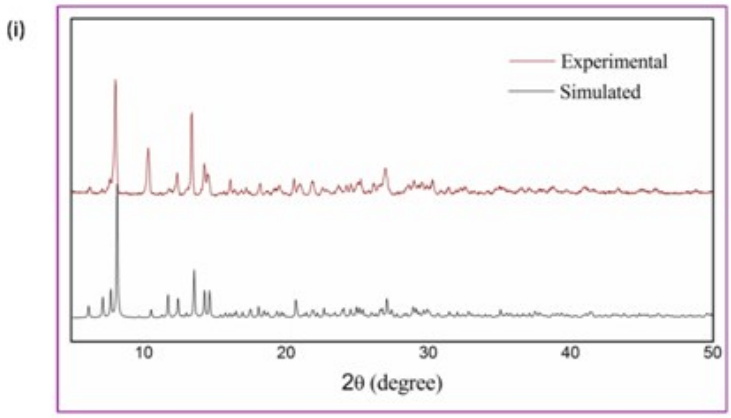


Fig. S11 PXRD patterns for **1**(a), **2**(b), **3**(c), **4**(d), **5**(e), **6**(f), **7**(g), **8**(h), **9**(i).

Table S12 Geometry analysis by using shape 2.0 software

1	HP-6	PPY-6	OC-6	TPR-6	JPPY-6
Ni1	29.781	23.941	1.195	11.736	26.832
Ni2	29.691	18.567	3.265	9.57	21.864
2					
Ni1	29.928	18.427	3.496	8.922	21.689
Ni2	27.321	23.624	1.176	12.98	26.188
3					
Ni1	28.668	23.583	1.167	12.284	26.385
Ni2	29.61	17.89	3.8	8.156	21.081
4					
Co1	31.129	16.229	4.576	8.32	19.729
Co2	28.678	23.523	1.038	12.366	26.433
5					
Co1	30.149	16.429	4.626	7.132	19.594
Co2	29.067	22.757	1.337	12.043	25.637
6					
Zn1	28.383	23.775	1.179	13.615	26.536
Zn2	30.675	16.26	5.158	7.171	19.48
7					
	PP-5	vOC-5	TBPY-5	SPY-5	JTBPY-5
Cd1	28.676	5.653	5.323	1.704	9.351
	OP-8	HBPY-8	TDD-8	BTPR-8	TT-8
Cd2	33.68	15.235	2.111	3.55	13.787
8					
	OP-8	HBPY-8	TDD-8	BTPR-8	TT-8
Cd1	32.514	14.913	3.528	4.06	13.807

	HP-6	PPY-6	OC-6	TPR-6	JPPY-6
Cd2	25.56	17.669	15.289	15.915	20.74
Cd3	29.573	10.538	16.268	2.805	14.276

9

	OP-8	HBPY-8	TDD-8	BTPR-8	TT-8
Cd1	32.28	15.519	2.941	3.961	14.366
	HP-6	PPY-6	OC-6	TPR-6	JPPY-6
Cd3	32.649	9.763	12.208	7.124	13.541
Cd2	28.184	10.178	18.584	2.834	13.643

HP-6	1	D6h	Hexagon
PPY-6	2	C5v	Pentagonal pyramid
OC-6	3	Oh	Octahedron
TPR-6	4	D3h	Trigonal prism
JPPY-6	5	C5v	Johnson pentagonal pyramid J2
OP-8	1	D8h	Octagon
TDD-8	6	D2d	Triangular dodecahedron
BTPR-8	10	C2v	Biaugmented trigonal prism
TT-8	12	Td	Triakis tetrahedron
HBPY-8	3	D6h	Hexagonal bipyramid
SPY-5	4	C4v	Spherical square pyramid

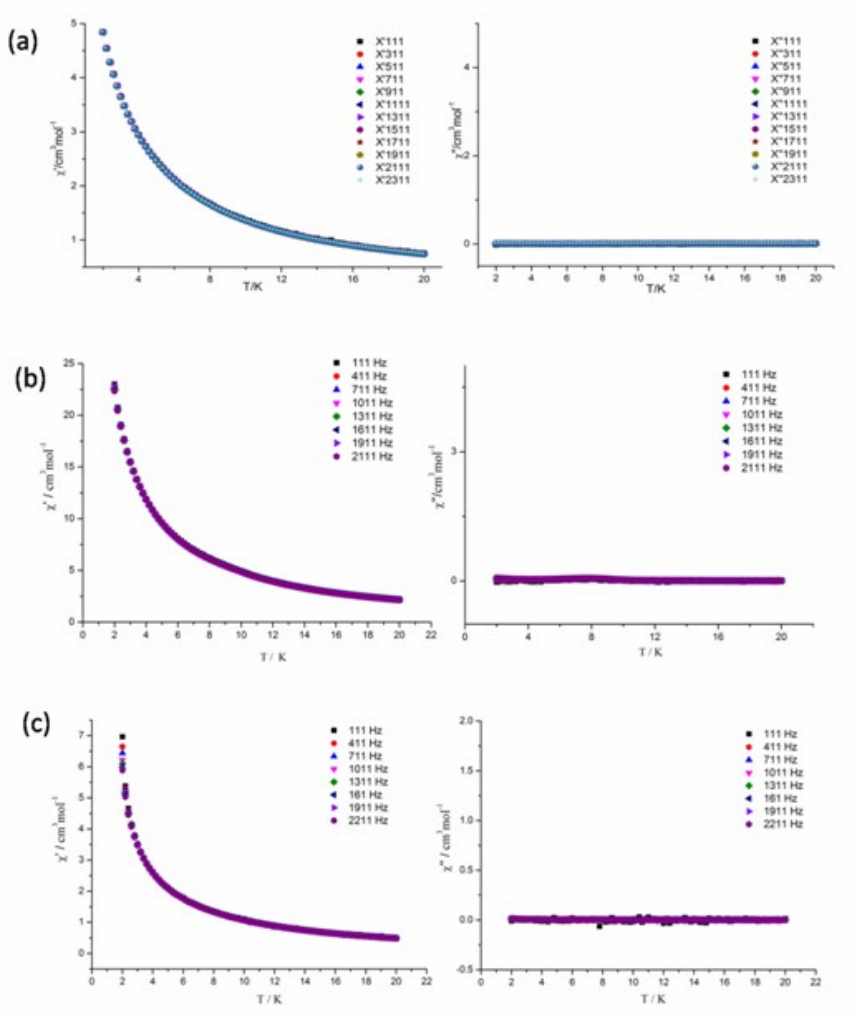


Fig. S13 plot of temperature dependence of the in-phase (χ') and out-of phase(χ'') AC susceptibility signals for compound **1** (a), **2** (b) and **3** (c) under zero dc field at the indicated frequencies.

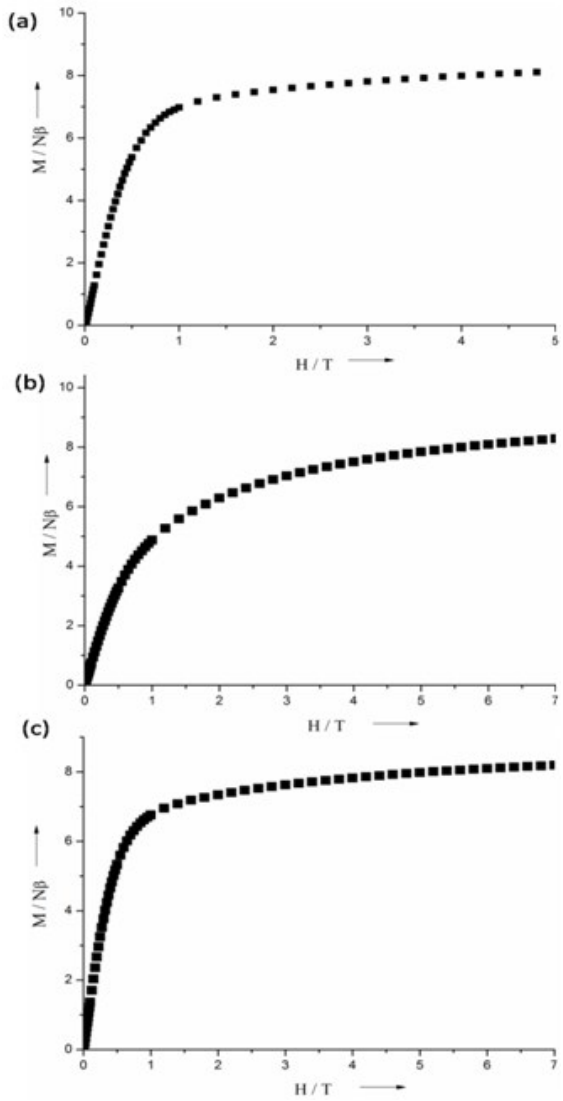
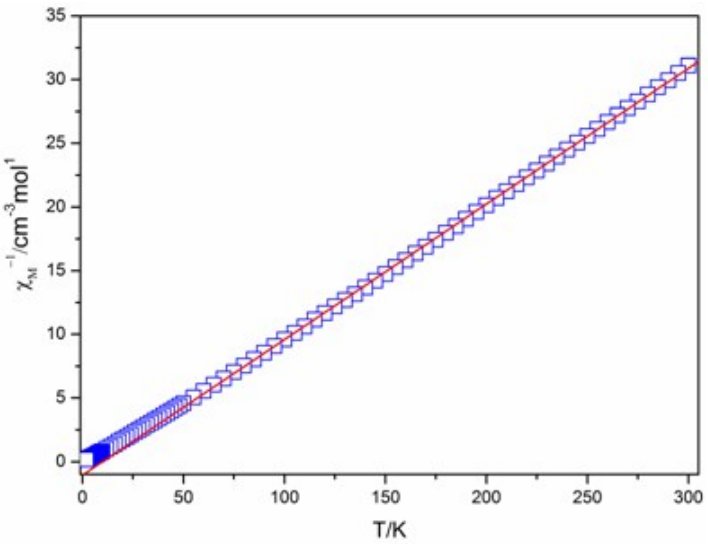


Fig. **S14**. M versus H/T plot for complexes **1** (a), **2** (b) and **3** (c). the blue solid line represents the curve generated from Brillouin function.

(a)



(b)

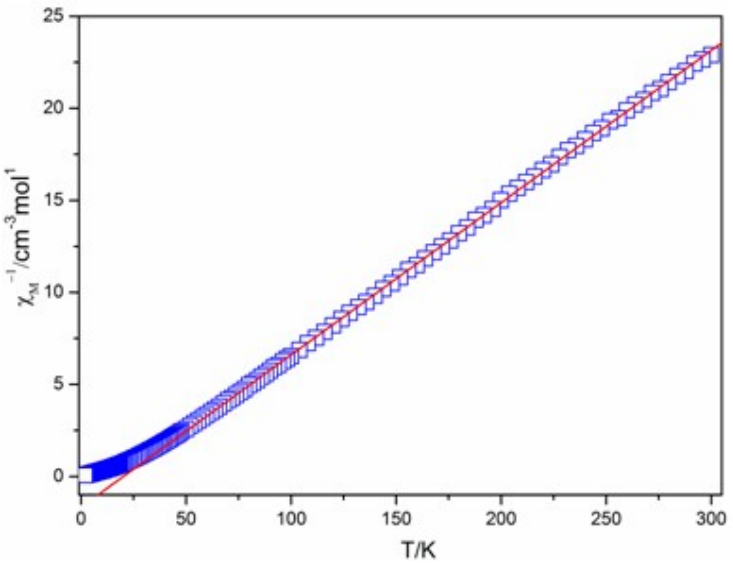


Fig. S15 the best fitting of the Curie-Weiss law for **4** and **5** in the 50-300 K range.

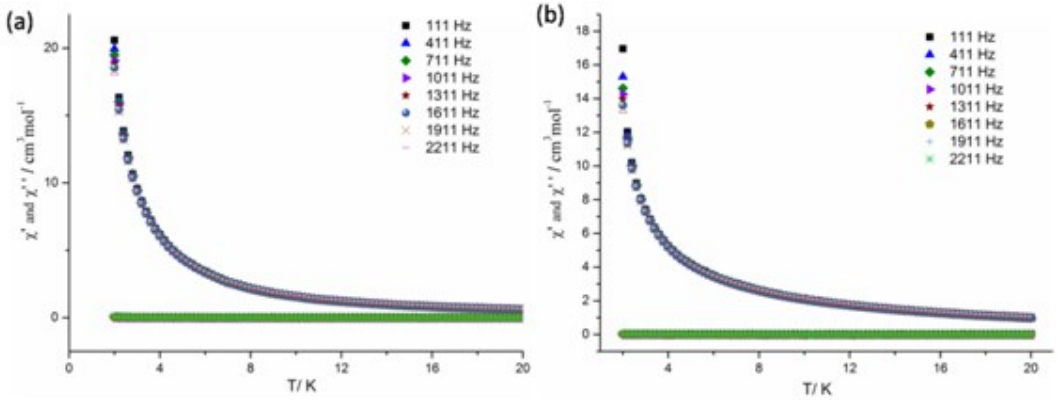


Fig. S16 plot of temperature dependence of the in-phase (χ') and out-of phase(χ'') AC susceptibility signals for compound **4** (a) and **5** (b) under zero dc field at the indicated frequencies.

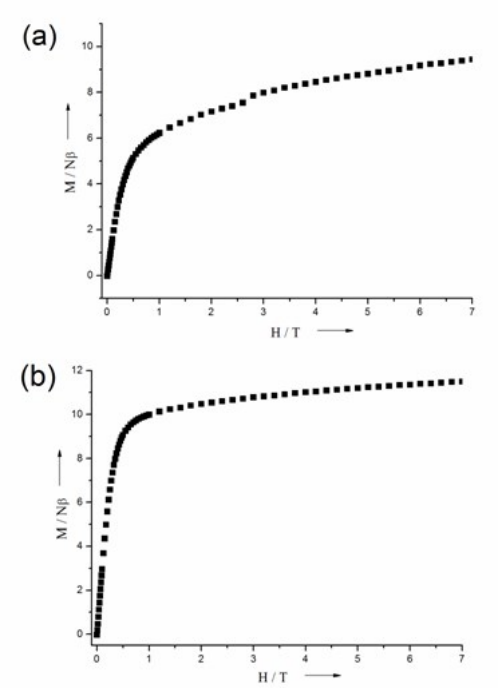


Fig. S**17**. magnetization M versus H/T plot for complexes **4** (a) and **5** (b).

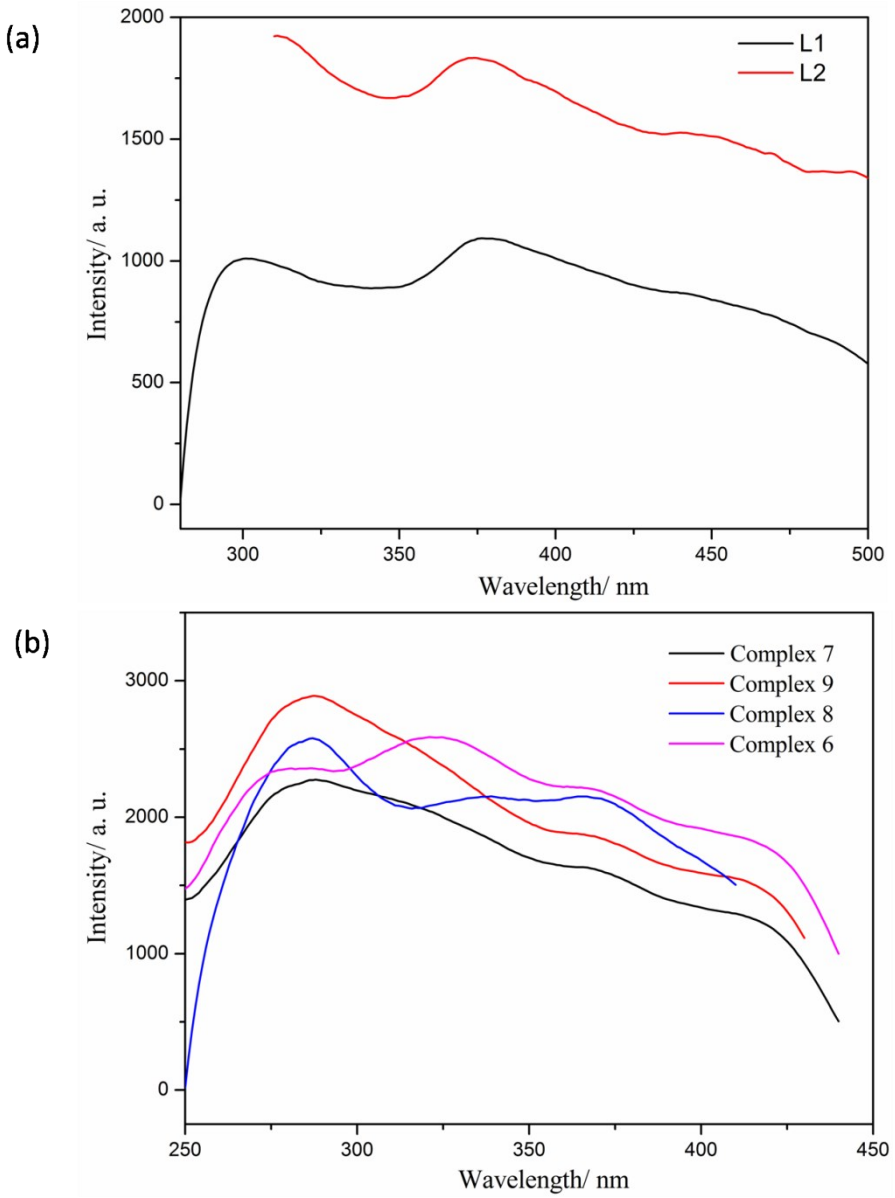


Fig. S18 Excitation spectra of two ligands and complexes **6-9** in solid state at room temperature. (a): λ_{em}= 537 nm for H_3L_1, λ_{em}= 548 nm for H_3L_2; (b): λ_{em}= 462 nm for **6**, λ_{em}= 463 nm for **7**, λ_{em}= 448 nm for **8**, λ_{em}= 451 nm for **9**.