Supporting Informations

Four 3D "brick-wall"-like metal-organic frameworks with a flexible ligand of (S,S,R,R)-1,2,3,4-cyclopentanetetracarboxylic acid: crystal structures, luminescent and magnetic properties

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Table S1. Crystal data and structural parameters of complex 1-4

Complex	1	2	3	4
Empirical formula	$C_{42}H_{48}Cu_4N_4O_{24}$	$C_{15}H_{15}Co_2NO_{12}$	$C_{42}H_{36}Cd_4N_4O_{23}$	$C_{14}H_{18}Co_2NO_{12}$
Formula weight	1247.00	519.14	1414.35	510.15
Crystal System	Monoclinic	Triclinic	Monoclinic	Triclinic
Space Group	$P2_1/c$	$P\bar{1}$	C_2/c	$P\bar{1}$
$a/Å$	9.0724(12)	9.1238(12)	30.306(3)	9.0377(14)
$b/Å$	9.1553(12)	9.6201(13)	14.6161(14)	9.7838(15)
$c/Å$	27.683(4)	12.6475(17)	12.0026(11)	11.3709(18)
$\alpha/^o$	90.00	94.475(2)	90.00	88.129(3)
$\beta/^o$	98.481(2)	104.722(2)	107.468(2)	78.639(2)
$\gamma/^o$	90.00	114.437(2)	90.00	65.906(2)
$V/Å^3$	2274.3(5)	956.1(2)	5071.4(8)	898.6(2)
Z	2	2	4	2
$\rho_c/g\ cm^{-3}$	1.821	1.803	1.852	1.885
μ/mm^{-1}	1.943	1.801	1.739	1.915
F(000)	1272	524	2768	518
Crystal size/*mm*	0.32 0.27 0.24	0.30 0.24 0.17	0.30 0.27 0.22	0.30 0.25 0.21
Reflections	11013/4044	4785/3333	12740 / 4520	4464 / 3156
R_{int}	0.0515	0.0192	0.0560	0.0222
T_{max}/T_{min}	0.6528/0.5753	0.7493/0.6140	0.7009/0.6235	0.6893/0.5974
Data/parameters	4044/334	3333 / 294	4520 / 331	3156/291
S	1.013	1.003	1.051	1.066
$R1^a$, wR_2^b[I>2σ(I)]	0.0458, 0.1178	0.0453, 0.1422	0.0411, 0.0769	0.0374, 0.1024
R1, wR_2 (all data)	0.0730, 0.1429	0.0541, 0.1588	0.0600, 0.0847	0.0449, 0.1079
$\Delta\rho_{max}/\Delta\rho_{min}$ /eA^{-3}	0.668/-0.770	0.891/-0.404	0.590/ -0.609	0.716/-0.674

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

Table S2 Selected bond lengths (Å) and bond angles (^{o}) for compound 1-4.

Compound 1			
Cu(1)-O(1)	1.944(3)	O(2)-Cu(1)-O(4)#1	93.61(15)
Cu(1)-O(2)	1.945(3)	O(1)-Cu(1)-N(2)	98.21(17)
Cu(1)-O(4)#1	1.979(3)	O(2)-Cu(1)-N(2)	158.84(16)
Cu(1)-N(2)	1.983(4)	O(4)#1-Cu(1)-N(2)	89.04(16)
Cu(2)-O(8)	1.932(3)	O(8)-Cu(2)-O(9)#2	177.08(14)

Cu(2)-O(9)#2	1.937(3)	O(8)-Cu(2)-O(10)	92.08(15)
Cu(2)-O(10)	1.981(4)	O(9)#2-Cu(2)-O(10)	86.06(15)
Cu(2)-O(7)	1.996(3)	O(8)-Cu(2)-O(7)	91.63(14)
Cu(2)-N(1)#3	2.191(4)	O(9)#2-Cu(2)-O(7)	91.17(14)
O(4)-Cu(1)#4	1.979(3)	O(10)-Cu(2)-O(7)	145.56(19)
O(9)-Cu(2)#5	1.937(3)	O(8)-Cu(2)-N(1)#3	86.67(15)
N(1)-Cu(2)#6	2.191(4)	O(9)#2-Cu(2)-N(1)#3	92.39(15)
O(1)-Cu(1)-O(2)	90.41(15)	O(10)-Cu(2)-N(1)#3	121.8(2)
O(1)-Cu(1)-O(4)#1	148.59(16)	O(7)-Cu(2)-N(1)#3	92.64(15)
Compound 2			
O(3)-Co(1)#1	2.308(4)	O(6)-Co(1)-O(3)#3	84.56(15)
O(10)-Co(3)	2.126(3)	O(4)#3-Co(1)-O(3)#3	58.40(12)
O(2)-Co(2)	2.069(3)	O(5)-Co(1)-O(3)#3	101.64(14)
O(4)-Co(2)	2.080(3)	O(2)#4-Co(2)-O(2)	180
O(4)-Co(1)#1	2.112(3)	O(2)#4-Co(2)-O(7)#4	89.84(11)
O(8)-Co(1)#2	2.047(3)	O(2)-Co(2)-O(7)#4	90.16(12)
O(7)-Co(2)	2.072(3)	O(2)#4-Co(2)-O(7)	90.16(12)
Co(1)-O(8)#2	2.047(3)	O(2)-Co(2)-O(7)	89.84(11)
Co(1)-N(1)	2.077(3)	O(7)#4-Co(2)-O(7)	180.000(1)
Co(1)-O(6)	2.094(3)	O(2)#4-Co(2)-O(4)	91.43(12)
Co(1)-O(4)#3	2.112(3)	O(2)-Co(2)-O(4)	88.57(12)
Co(1)-O(5)	2.245(3)	O(7)#4-Co(2)-O(4)	84.06(11)
Co(1)-O(3)#3	2.308(4)	O(7)-Co(2)-O(4)	95.94(11)
Co(2)-O(2)#4	2.069(3)	O(2)#4-Co(2)-O(4)#4	88.57(12)
Co(2)-O(7)#4	2.072(3)	O(2)-Co(2)-O(4)#4	91.43(12)
Co(2)-O(4)#4	2.080(3)	O(7)#4-Co(2)-O(4)#4	95.94(11)
Co(3)-O(1)	2.068(3)	O(7)-Co(2)-O(4)#4	84.06(11)
Co(3)-O(1)#5	2.068(3)	O(4)-Co(2)-O(4)#4	180.000(1)
Co(3)-O(9)#5	2.094(4)	O(1)-Co(3)-O(1)#5	180

Co(3)-O(9)	2.094(4)	O(1)-Co(3)-O(9)#5	86.93(15)
Co(3)-O(10)#5	2.126(3)	O(1)#5-Co(3)-O(9)#5	93.07(15)
O(8)#2-Co(1)-N(1)	96.07(14)	O(1)-Co(3)-O(9)	93.07(15)
O(8)#2-Co(1)-O(6)	96.69(14)	O(1)#5-Co(3)-O(9)	86.93(15)
N(1)-Co(1)-O(6)	153.48(14)	O(9)#5-Co(3)-O(9)	180.00(15)
O(8)#2-Co(1)-O(4)#3	99.71(12)	O(1)-Co(3)-O(10)	99.37(13)
N(1)-Co(1)-O(4)#3	95.06(13)	O(1)#5-Co(3)-O(10)	80.63(13)
O(6)-Co(1)-O(4)#3	105.54(13)	O(9)#5-Co(3)-O(10)	90.83(15)
O(8)#2-Co(1)-O(5)	98.57(14)	O(9)-Co(3)-O(10)	89.17(15)
N(1)-Co(1)-O(5)	95.31(13)	O(1)-Co(3)-O(10)#5	80.63(12)
O(6)-Co(1)-O(5)	59.82(13)	O(1)#5-Co(3)-O(10)#5	99.37(13)
Compound 3			
Cd(1)-O(3)	2.309(4)	O(6)#1-Cd(1)-O(2)#2	89.70(14)
Cd(1)-N(1)	2.312(5)	O(5)#1-Cd(1)-O(2)#2	96.18(14)
Cd(1)-O(6)#1	2.352(4)	O(1)#2-Cd(1)-O(2)#2	53.34(14)
Cd(1)-O(5)#1	2.356(4)	O(3)-Cd(1)-O(4)	53.47(13)
Cd(1)-O(1)#2	2.393(4)	N(1)-Cd(1)-O(4)	88.54(15)
Cd(1)-O(2)#2	2.465(4)	O(6)#1-Cd(1)-O(4)	85.80(13)
Cd(1)-O(4)	2.549(4)	O(5)#1-Cd(1)-O(4)	87.83(13)
Cd(1)-O(3)	2.309(4)	O(1)#2-Cd(1)-O(4)	135.58(14)
Cd(2)-O(7)#1	2.208(4)	O(2)#2-Cd(1)-O(4)	170.81(14)
Cd(2)-O(5)	2.229(4)	O(7)#1-Cd(2)-O(5)	85.62(15)
Cd(2)-N(2)	2.263(5)	O(7)#1-Cd(2)-N(2)	104.16(19)
Cd(2)-O(4)	2.328(4)	O(5)-Cd(2)-N(2)	166.74(17)
Cd(2)-O(12)	2.386(4)	O(7)#1-Cd(2)-O(4)	87.54(14)
Cd(2)-O(9)	2.417(4)	O(5)-Cd(2)-O(4)	83.87(14)
O(1)-Cd(1)#4	2.393(4)	N(2)-Cd(2)-O(4)	87.59(17)
O(2)-Cd(1)#4	2.465(4)	O(7)#1-Cd(2)-O(12)	155.64(16)
O(5)-Cd(1)#1	2.356(4)	O(5)-Cd(2)-O(12)	83.10(16)

O(6)-Cd(1)#1	2.352(4)	N(2)-Cd(2)-O(12)	90.87(19)
O(7)-Cd(2)#1	2.208(4)	O(4)-Cd(2)-O(12)	112.51(14)
O(3)-Cd(1)-N(1)	100.96(15)	O(7)#1-Cd(2)-O(9)	81.24(14)
O(3)-Cd(1)-O(6)#1	136.94(14)	O(5)-Cd(2)-O(9)	105.85(15)
N(1)-Cd(1)-O(6)#1	90.07(15)	N(2)-Cd(2)-O(9)	84.75(17)
O(3)-Cd(1)-O(5)#1	104.42(14)	O(4)-Cd(2)-O(9)	164.43(14)
N(1)-Cd(1)-O(5)#1	145.25(15)	O(12)-Cd(2)-O(9)	81.19(14)
O(6)#1-Cd(1)-O(5)#1	55.21(13)	O(6)#1-Cd(1)-O(2)#2	89.70(14)
O(3)-Cd(1)-O(1)#2	86.75(14)	O(6)#1-Cd(1)-O(1)#2	122.48(14)
N(1)-Cd(1)-O(1)#2	121.34(16)	O(5)#1-Cd(1)-O(1)#2	83.69(14)
O(3)-Cd(1)-O(2)#2	132.61(14)	N(1)-Cd(1)-O(2)#2	83.44(15)
Compound 4			
Co(1)-O(9)	2.045(2)	O(12)-Co(1)-O(2)	100.14(9)
Co(1)-N(1)	2.079(3)	O(1)#1-Co(2)-O(1)	180.00(14)
Co(1)-O(1)	2.109(2)	O(1)#1-Co(2)-O(4)	88.32(9)
Co(1)-O(8)	2.130(2)	O(1)-Co(2)-O(4)	91.68(9)
Co(1)-O(12)	2.172(2)	O(1)#1-Co(2)-O(4)#1	91.68(9)
Co(1)-O(2)	2.291(3)	O(1)-Co(2)-O(4)#1	88.32(9)
Co(2)-O(1)#1	2.067(2)	O(4)-Co(2)-O(4)#1	180.000(1)
Co(2)-O(1)	2.067(2)	O(1)#1-Co(2)-O(3)#1	95.33(9)
Co(2)-O(4)	2.075(2)	O(1)-Co(2)-O(3)#1	84.67(9)
Co(2)-O(4)#1	2.075(2)	O(4)-Co(2)-O(3)#1	90.02(9)
Co(2)-O(3)#1	2.078(2)	O(4)#1-Co(2)-O(3)#1	89.98(9)
Co(2)-O(3)	2.078(2)	O(1)#1-Co(2)-O(3)	84.67(9)
Co(3)-O(5)	2.077(2)	O(1)-Co(2)-O(3)	95.33(9)
Co(3)-O(5)#2	2.077(2)	O(4)-Co(2)-O(3)	89.98(9)
Co(3)-O(6)#2	2.079(3)	O(4)#1-Co(2)-O(3)	90.02(9)
Co(3)-O(6)	2.079(3)	O(3)#1-Co(2)-O(3)	180.00(16)
Co(3)-O(7)#2	2.146(3)	O(5)-Co(3)-O(5)#2	180.00(13)

Co(3)-O(7)	2.146(3)	O(5)-Co(3)-O(6)#2	86.74(12)
O(9)-Co(1)-N(1)	95.46(11)	O(5)#2-Co(3)-O(6)#2	93.26(12)
O(9)-Co(1)-O(1)	99.47(9)	O(5)-Co(3)-O(6)	93.26(12)
N(1)-Co(1)-O(1)	94.43(10)	O(5)#2-Co(3)-O(6)	86.74(12)
O(9)-Co(1)-O(8)	96.33(10)	O(6)#2-Co(3)-O(6)	180.0(2)
N(1)-Co(1)-O(8)	157.60(11)	O(5)-Co(3)-O(7)#2	80.67(9)
O(1)-Co(1)-O(8)	102.31(9)	O(5)#2-Co(3)-O(7)#2	99.33(9)
O(9)-Co(1)-O(12)	99.92(10)	O(6)#2-Co(3)-O(7)#2	89.73(11)
N(1)-Co(1)-O(12)	98.53(10)	O(6)-Co(3)-O(7)#2	90.27(11)
O(1)-Co(1)-O(12)	155.47(10)	O(5)-Co(3)-O(7)	99.33(9)
O(8)-Co(1)-O(12)	60.67(9)	O(5)#2-Co(3)-O(7)	80.67(9)
O(9)-Co(1)-O(2)	157.49(9)	O(6)#2-Co(3)-O(7)	90.27(11)
N(1)-Co(1)-O(2)	91.56(11)	O(6)-Co(3)-O(7)	89.73(11)
O(1)-Co(1)-O(2)	58.59(8)	O(7)#2-Co(3)-O(7)	180.00(14)
O(8)-Co(1)-O(2)	84.72(10)		

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

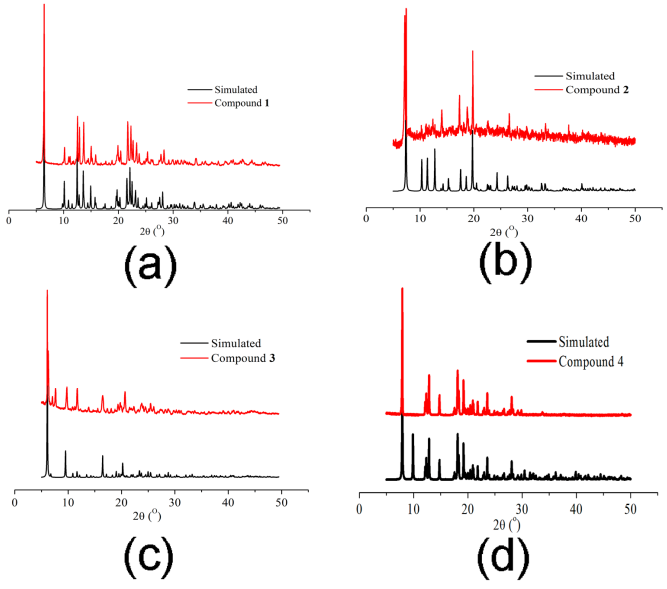

Fig. S1 The Powder X-ray diffraction (PXRD) patterns of **1**(a), **2**(b), **3**(c), **4**(d).