Electronic Supplementary Material (ESI) for CrystEngComm.

Journal Supporting Information

Ln-MOFs using a Compartmental Ligand with an Unique Combination of *hard-soft* Terminals and Their Magnetic, Gas Adsorption and Luminescence Properties

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- **S1. SHAPE calculations**
- **Powder XRD patterns**
- **TGA plot**
- **Luminescence Study**
- **Circular dichroism spectra**
- **Crystal data and refinement parameters**
- **Selected bond lengths and bond angles**
- **Plot of Debye Equation**

Table S1- Lanthanide geometry analysis by using Continuous Shape Measurements (CShM)

MOF-1(Gd)	**EP-9(D_{9h})**	**OPY-9(C_{8v})**	**HBPY-9(D_{7h})**	**JTC-9(C_{3v})**	**JCCU-9(C_{4v})**	**CCU-9($C4v$)**	**JCSAPR-9(C_{4v})**	**CSAPR-9(C_{4v})**	**JTCTPR-9(D_{3h})**	**TCTPR-9(D_{3h})**
	32.73053	24.39959	19.44356	12.62698	10.67158	9.56392	2.66004	1.70136	1.77566	1.42769
MOF-2(Dy)	**EP-9(D_{9h})**	**OPY-9(C_{8v})**	**HBPY-9(D_{7h})**	**JTC-9(C_{3v})**	**JCCU-9(C_{4v})**	**CCU-9(C_{4v})**	**JCSAPR-9(C_{4v})**	**CSAPR-9(C_{4v})**	**JTCTPR-9(D_{3h})**	**TCTPR-9(D_{3h})**
	34.45702	24.27753	19.94488	13.24954	10.98856	9.65949	2.59881	1.44980	2.08421	1.01514

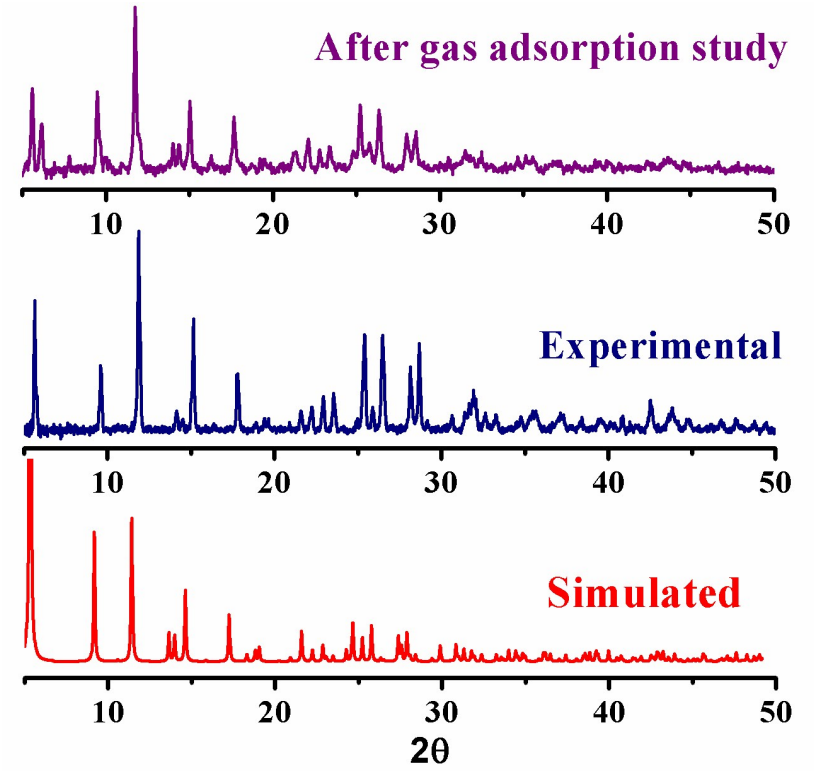
Ideal structures ML9

EP-9 = Enneagon, OPY-9 = Octagonal pyramid, HBPY-9 = Heptagonal bipyramid, JTC-9 = Johnson triangular cupola J3, JCCU-9 = Capped cube J8, CCU-9 = Spherical-relaxed capped cube, JCSAPR-9 = Capped square antiprism J10, CSAPR-9 = Spherical capped square antiprism, JTCTPR-9 = Tricapped trigonal prism J51, TCTPR-9= Spherical tricapped trigonal prism

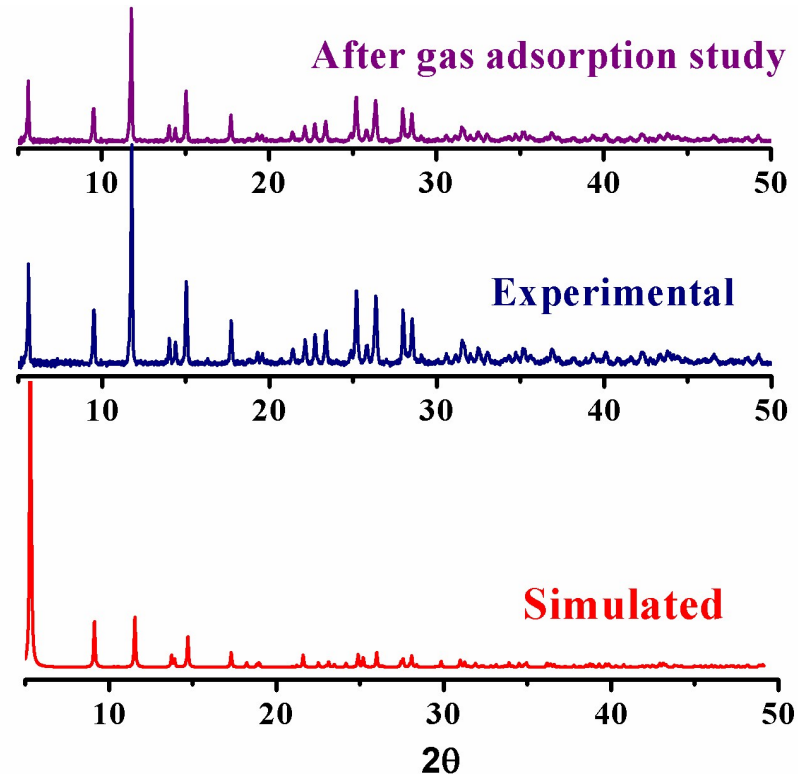
(a) Alvarez, S., Alemany, P., Casanova, D., Cirera, Llunell, J., M., Avnir, D. *Coord. Chem. Rev*., 2005, **249**, 1693-1708;
(b) Casanova, D., Llunell, M., Alemany, P., Alvarez, S. *Chem. Eur. J*., 2005, **11**, 1479-1494.

S1 - Powder XRD patterns:

Compound 1

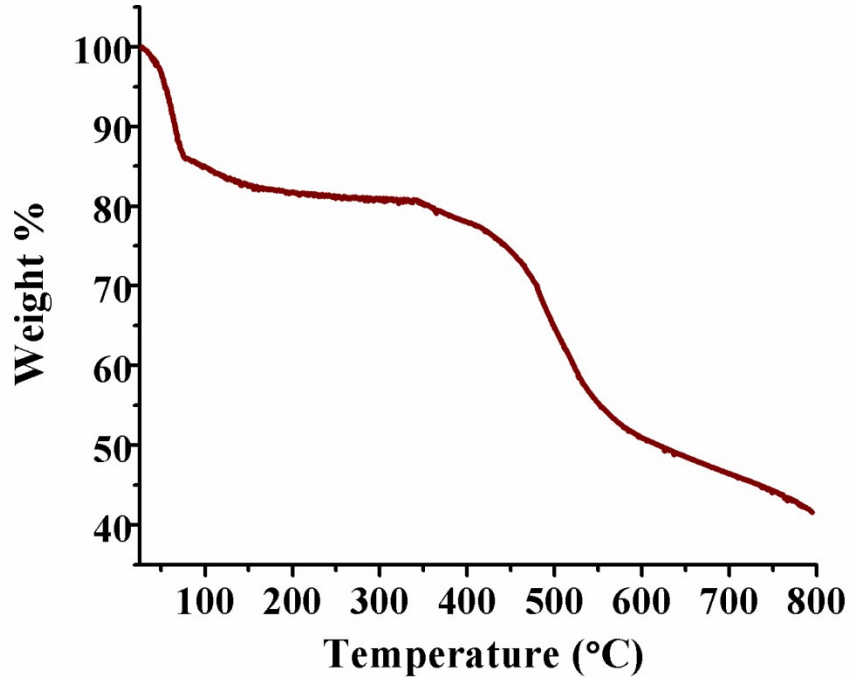


Compound 2

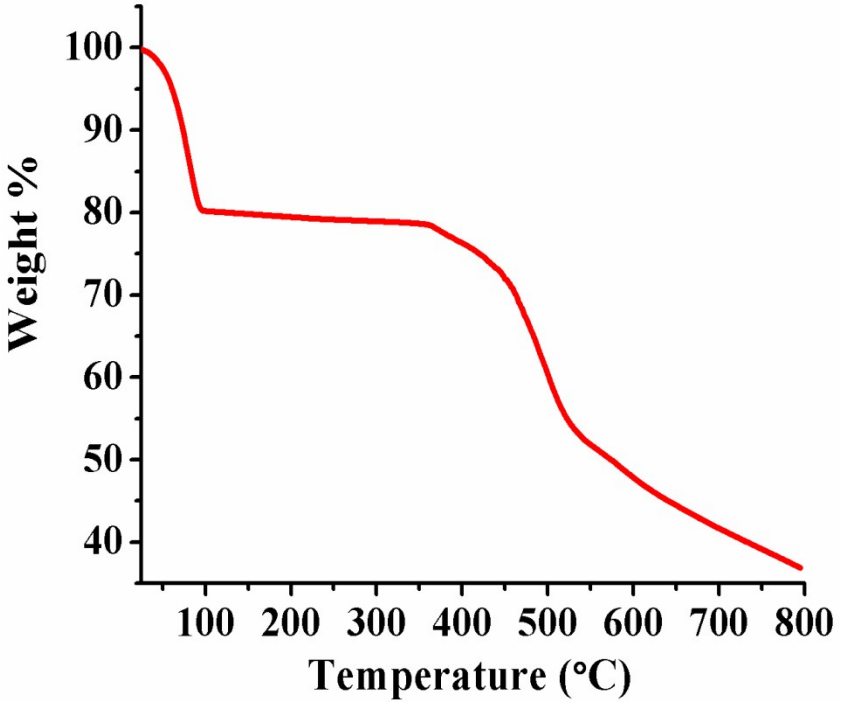


S2 – TGA Plot:

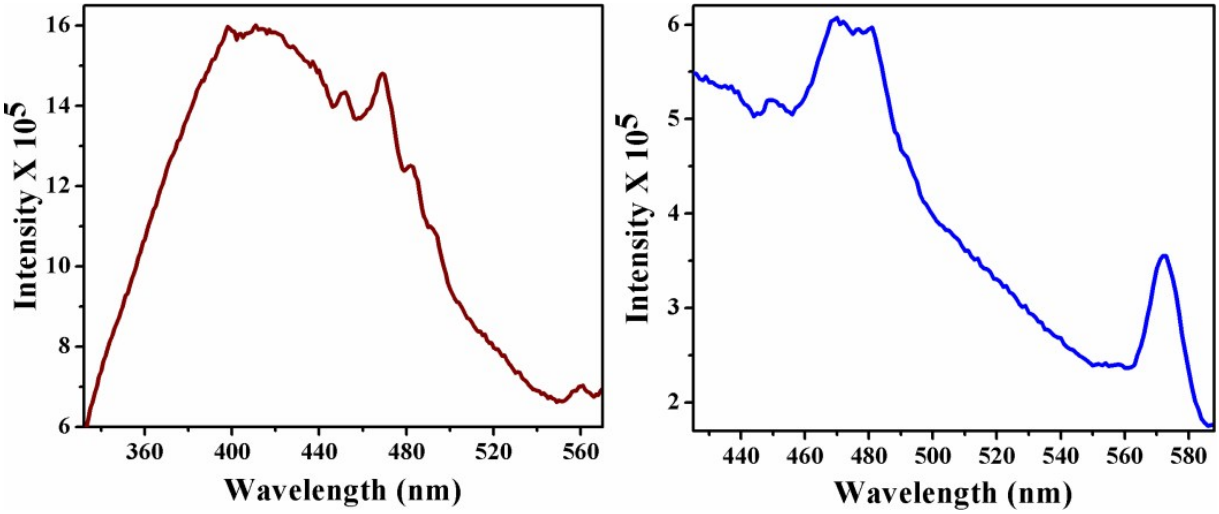
Compound 1



Compound 2



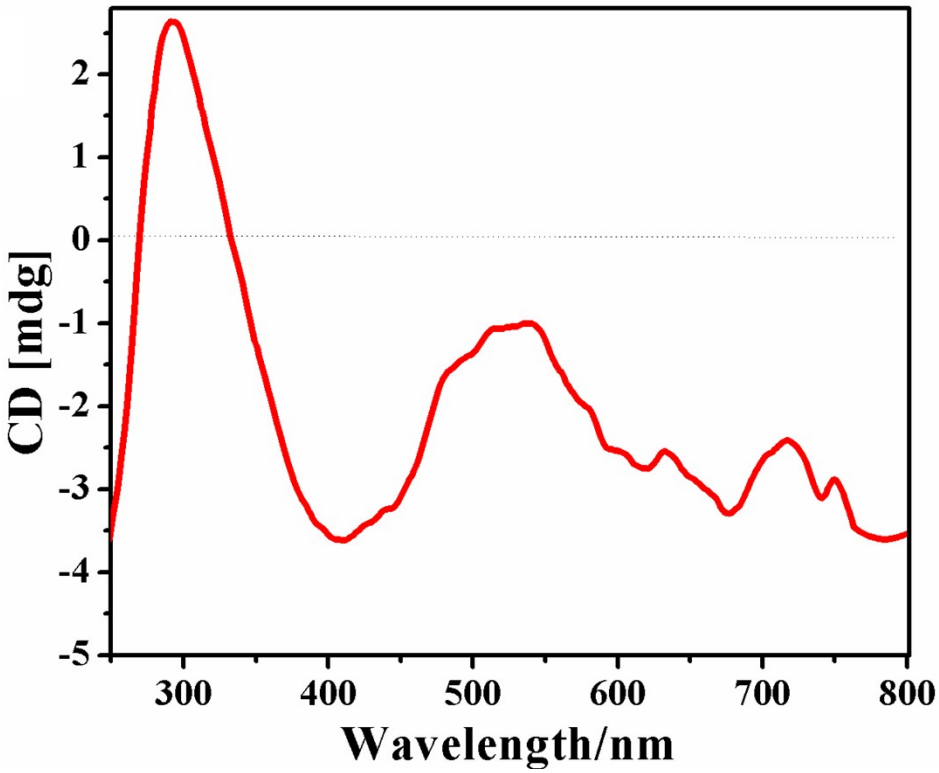
S3-Luminescence Study:



Solid state emission spectra of MOF-**1** and MOF-**2** at 298 K, excited at 320 nm.

S4-Circular dichroism spectra

Compound 1



Compound 2

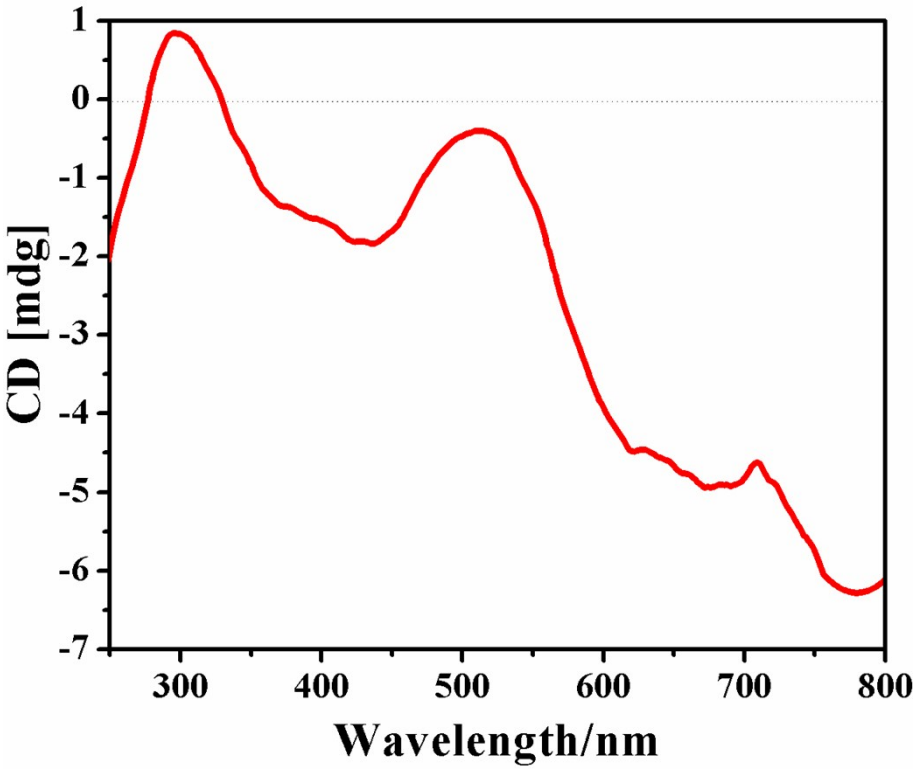

1
0
-1
-2
-3
-4
-5
-6
-7
CD [mdg]
300
400
500
600
700
800
Wavelength/nm

Table S2: Crystallographic data and refinement parameters of MOF 1-2.

	1	**2**
Empirical formula	$C_{90}H_{70}Gd_2N_{18}O_{25}$	$C_{90}H_{90}Dy_2N_{18}O_{28}$
Crystal system	trigonal	trigonal
Formula weight	2118.14	2196.79
Space group	*P3*	*P3*
a/Å	19.109(2)	19.1877(19)
b/Å	19.109(2)	19.1877(19)
c/Å	8.6482(11)	8.5095(9)
α/°	90.00	90.00
β/°	90.00	90.00
γ/°	120.00	120.00
V/Å^3	2734.9(6)	2713.2(6)
Reflections collected	40923	42867
Unique reflections	11426	11728
Obsrefls [I> 2σ(I)]	10241	6685
R1 [I> 2σ(I)]	0.0281	0.0728
wR2 [I> 2σ(I)]	0.0752	0.1506
CCDC No.	1459327	1459328

Table S3-Selected bond lengths and bond angles

Compound 1

Bond Length			
Gd1	O1B	2.297(4)	
Gd1	N2A	2.589(4)	
Gd1	N1A	2.727(5)	
Gd2	O1A	2.323(4)	
Gd2	N2B	2.565(4)	
Gd2	N1B	2.706(5)	

Bond Angle			
O1B	Gd1	O1B	82.71(16)
O1B	Gd1	N2A	71.80(14)
O1B	Gd1	N2A	144.25(15)
O1B	Gd1	N2A	69.80(14)
N2A	Gd1	N2A	119.38(3)
N2A	Gd1	N2A	119.38(3)
O1B	Gd1	N1A	82.54(14)
O1B	Gd1	N1A	141.12(12)
O1B	Gd1	N1A	130.43(12)
N2A	Gd1	N1A	60.63(13)
N2A	Gd1	N1A	69.36(13)
N2A	Gd1	N1A	133.14(14)

Bond Angle			
N1A	Gd1	N1A	80.16(16)
O1B	Gd1	N1A	130.42(12)
O1B	Gd1	N1A	82.54(14)
O1B	Gd1	N1A	141.12(12)
O1A	Gd2	O1A	80.81(17)
O1A	Gd2	N2B	144.29(17)
O1A	Gd2	N2B	71.17(14)
O1A	Gd2	N2B	73.37(15)
N2B	Gd2	N2B	118.97(4)
O1A	Gd2	N1B	141.23(13)
O1A	Gd2	N1B	131.85(12)
O1A	Gd2	N1B	84.61(15)
N2B	Gd2	N1B	60.69(14)
N2B	Gd2	N1B	131.07(15)
N2B	Gd2	N1B	67.93(15)
N1B	Gd2	N1B	78.83(16)
N2B	Gd2	N1B	67.93(15)
N2B	Gd2	N1B	60.70(14)
N2B	Gd2	N1B	131.07(15)
N1B	Gd2	N1B	78.83(16)

Compound 2

Bond Length			
Dy1	O1	2.305(16)	
Dy1	N2A	2.494(19)	
Dy1	N1A	2.67(2)	
Dy2	O1A	2.295(16)	
Dy2	N2	2.630(19)	
Dy2	N1	2.70(2)	

Bond Angle			
O1	Dy1	O1	79.9(7)
O1	Dy1	N2A	142.8(6)
O1	Dy1	N2A	71.1(6)
O1	Dy1	N2A	72.6(6)
N2A	Dy1	N2A	119.28(13)
O1	Dy1	N1A	141.2(5)
O1	Dy1	N1A	132.3(5)
O1	Dy1	N1A	85.2(6)

Bond Angle			
N2A	Dy1	N1A	61.2(6)
N2A	Dy1	N1A	68.8(6)
N2A	Dy1	N1A	132.0(6)
N1A	Dy1	N1A	78.8(6)
O1A	Dy2	O1A	82.5(7)
O1A	Dy2	N2	70.4(6)
O1A	Dy2	N2	70.8(6)
O1A	Dy2	N2	143.9(6)
N2	Dy2	N2	119.46(13)
O1A	Dy2	N1	131.4(6)
O1A	Dy2	N1	82.1(6)
O1A	Dy2	N1	139.9(6)
N2	Dy2	N1	61.0(7)
N2	Dy2	N1	134.0(7)
N2	Dy2	N1	69.1(6)
N1	Dy2	N1	80.9(7)

S5-Plot of Debye Equation