Supporting information

An unusual bifunctional Tb-MOF for highly sensing of Ba^{2+} ions and remarkable selectivities of CO_2/N_2 and CO_2/CH_4

Yan Yang,[a,b] Feilong Jiang,[a] Lian Chen,*[a] Jiandong Pang,[a,b] Mingyan Wu,[a,b] Xiuyan Wan,[a,b] Jie Pan,[a,b] Jinjie Qian,[a,b] and Maochun Hong*[a]

[a]*State Key Laboratory of Structure Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian, 350002, China*
[b]*University of the Chinese Academy of Sciences, Beijing, 10049, China*

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Table S1. Crystal data and refinement results for **TbL, GdL, EuL and DyL**.

Formula	$C_{57}H_{67}Tb_3N_{11}O_{36}$	$C_{57}H_{67}Gd_3N_{11}O_{36}$
Formula weight	1959.001 (7)	1953.961 (7)
Crystal system	triclinic	triclinic
space group	P-1	P-1
a (Å)	15.1173 (4)	15.0975 (5)
b (Å)	16.7483 (8)	16.7752 (7)
c (Å)	16.9101 (6)	16.9014 (7)
α (°)	110.566 (4)	110.493 (4)
β (°)	90.030 (3)	91.562(3)
γ (°)	100.933 (3)	99.176 (3)
Volume (Å^3)	3925.3 (3)	3942.3 (3)
T (K)	173	173
Z	2	2
F (000)	1548	1542
R_1 (I>2σ(I))	0.0812	0.0806
wR_2 (reflections)	0.2389	0.2305
Goodness of fit on F^2	1.043	0.993
Formula	$C_{57}H_{67}Eu_3N_{11}O_{36}$	$C_{57}H_{67}Dy_3N_{11}O_{36}$
Formula weight	1938.091 (7)	1969.811 (7)
Crystal system	triclinic	triclinic
space group	P-1	P-1
a (Å)	15.1321 (6)	15.1589 (5)
b (Å)	16.9762 (4)	16.8609 (4)
c (Å)	17.0413 (6)	16.9700 (6)
α (°)	110.922 (3)	110.902 (2)
β (°)	93.255 (3)	92.490 (2)
γ (°)	97.511 (3)	98.552 (2)
Volume (Å^3)	4028.6 (3)	3985.0 (0)
T (K)	173	173
Z	2	2
F (000)	1530	1554
R_1 (I>2σ(I))	0.0652	0.0450
wR_2 (reflections)	0.1837	0.1270
Goodness of fit on F^2	1.065	1.028

Table S2. Selected Bond Lengths (Å) for **TbL, GdL, EuL and DyL**.

Bond	Dist.	Bond	Dist.	Bond	Dist.
Tb1—O12^{i}	2.321 (6)	Tb2—O8	2.262 (5)	Tb3—O10^{vi}	2.312 (6)
Tb1—O7	2.338 (6)	Tb2—O9^{vi}	2.288 (6)	Tb3—O16^{v}	2.335 (6)
Tb1—O4	2.359 (6)	Tb2—O17^{v}	2.337 (5)	Tb3—O20^{vii}	2.343 (6)
Tb1—O11^{ii}	2.363 (5)	Tb2—O5	2.364 (5)	Tb3—O19	2.424 (7)
Tb1—O1^{iii}	2.412 (5)	Tb2—O2^{iii}	2.411 (7)	Tb3—O15^{viii}	2.426 (6)

Tb1—O3^{iv}	2.418 (6)	Tb2—O13	2.426 (7)	Tb3—O14	2.463 (6)
Tb1—O17^{v}	2.536 (5)	Tb2—O14	2.502 (6)	Tb3—O6	2.497 (7)
Tb1—O4^{iv}	2.568 (5)	Tb2—O1^{iii}	2.551 (6)	Tb3—O5	2.504 (6)
Tb1—O18^{v}	2.571 (6)			Tb3—O16^{viii}	2.564 (5)

Symmetry codes: (i) x, y, 1+z; (ii) 1-x, -y, -z; (iii) -x, -y, 1-z; (iv) 1-x, -y, 1-z; (v) 2-x, 1-y, 2-z; (vi) 1-x, 1-y, 1-z; (vii) 1-x, 1-y, 2-z; (viii) x-1, y, z.

Bond	Dist.	Bond	Dist.	Bond	Dist.
Gd1—O3^{i}	2.317 (2)	Gd2—O4^{i}	2.274 (3)	Gd3—O6	2.307 (3)
Gd1—O1^{ii}	2.340 (3)	Gd2—O5	2.279(2)	Gd3—O19	2.335 (2)
Gd1—O2^{iii}	2.361 (2)	Gd2—O13	2.334 (2)	Gd3—O15	2.336 (2)
Gd1—O9	2.362 (2)	Gd2—O8	2.358 (3)	Gd3—O20^{ii}	2.399 (3)
Gd1—O10^{iv}	2.423 (2)	Gd2—O11^{v}	2.413 (2)	Gd3—O16^{ii}	2.430 (2)
Gd1—O12^{v}	2.431 (2)	Gd2—O17^{vi}	2.416 (2)	Gd3—O18^{vi}	2.450 (2)
Gd1—O13	2.535 (2)	Gd2—O18^{vi}	2.501 (2)	Gd3—O7	2.501 (2)
Gd1—O14	2.559 (2)	Gd2—O12^{v}	2.527 (2)	Gd3—O8	2.522 (2)
Gd1—O9^{iv}	2.564 (2)		2.545 (2)	Gd3—O15^{ii}	2.569 (2)

Symmetry codes: (i) 1-x, 1-y, -z; (ii) 1-x, 1-y, 1-z; (iii) x, -1+y, -1+z; (iv) 1-x, -y, -z; (v) -x, -y, -z; (vi) 2-x, 1-y, 1-z; (vii) x, 1+y, 1+z.

Bond	Dist.	Bond	Dist.	Bond	Dist.
Eu1—O16^{i}	2.345 (5)	Eu2—O15^{i}	2.297 (5)	Eu3—O14	2.361 (5)
Eu1—O17^{ii}	2.388 (5)	Eu2—O13	2.301 (5)	Eu3—O19	2.369 (5)
Eu1—O4	2.394 (5)	Eu2—O10^{vi}	2.380 (5)	Eu3—O11^{vi}	2.386 (5)
Eu1—O18^{iii}	2.395 (5)	Eu2—O5	2.386 (5)	Eu3—O20^{iii}	2.433 (6)
Eu1—O3^{iv}	2.454 (5)	Eu2—O2^{v}	2.424 (6)	Eu3—O12^{vii}	2.456 (5)
Eu1—O1^{v}	2.463 (5)	Eu2—O7	2.435 (6)	Eu3—O8	2.467 (5)
Eu1—O10^{vi}	2.546 (4)	Eu2—O8	2.540 (4)	Eu3—O5	2.535 (4)
Eu1—O9^{vi}	2.564 (5)	Eu2—O1^{v}	2.559 (5)	Eu3—O6	2.540 (5)
Eu1—O4^{iv}	2.590 (4)			Eu3—O11^{vii}	2.597 (5)

Symmetry codes: (i) 2-x, 2-y, 1-z; (ii) x, -1+y, -1+z; (iii) 2-x, 2-y, 2-z; (iv) 2-x, 1-y, 1-z; (v) 1-x, 1-y, 1-z; (vi) 3-x, 2-y, 2-z; (vii) -1+x, y, z; (viii) 1+x, y, z; (ix) x, 1+y, 1+z.

Bond	Dist.	Bond	Dist.	Bond	Dist.
Dy1—O10^{i}	2.322 (3)	Dy2—O7^{v}	2.278 (3)	Dy3—O8^{v}	2.319 (3)
Dy1—O12	2.335 (4)	Dy2—O4	2.338 (3)	Dy3—O20^{v}	2.340 (3)
Dy1—O11^{ii}	2.356 (3)	Dy2—O16^{iii}	2.351 (3)	Dy3—O5	2.341 (3)
Dy1—O17^{iii}	2.361 (3)	Dy2—O13	2.413 (4)	Dy3—O19	2.411 (4)
Dy1—O18^{iv}	2.418 (3)	Dy2—O2^{vi}	2.418 (4)	Dy3—O6^{v}	2.420 (3)
Dy1—O14	2.443 (3)	Dy2—O1^{vi}	2.527 (3)	Dy3—O1^{vi}	2.468 (3)
Dy1—O4	2.531 (3)	Dy2—O14	2.535 (3)	Dy3—O15^{iii}	2.503 (4)
Dy1—O3	2.557 (3)	Dy2—O7^{v}	2.278 (3)	Dy3—O16^{iii}	2.511 (3)
Dy1—O17^{iv}	2.565 (3)			Dy3—O5^{v}	2.569 (3)

Symmetry codes: (i) x, y, -1+z; (ii) -x, 1-y, -z; (iii) -1-x, 1-y, -z; (iv) 1+x, y, z; (v) -x, 2-y, 1-z; (vi) 1-x, 2-y, 1-z; (vii) x, y, 1+z; (viii) -1+x, y, z.

Table S3. Selected Bond Angles (°) for **TbL, GdL, EuL and DyL**.

Angle	(º)	Angle	(º)
O12^{i}—Tb1—O7	144.7 (2)	O11^{ii}—Tb1—O17^{v}	147.55 (18)
O12^{i}—Tb1—O4	68.5 (2)	O1^{iii}—Tb1—O17^{v}	67.38 (19)
O7—Tb1—O4	143.3 (2)	O3^{iv}—Tb1—O17^{v}	120.2 (2)
O12^{i}—Tb1—O11^{ii}	136.5 (2)	O12^{i}—Tb1—O4^{iv}	73.6 (2)
O7—Tb1—O11^{ii}	77.2 (2)	O7—Tb1—O4^{iv}	122.62 (19)
O4—Tb1—O11^{ii}	77.9 (2)	O4—Tb1—O4^{iv}	72.3 (2)
O12^{i}—Tb1—O1^{iii}	113.4 (2)	O11^{ii}—Tb1—O4^{iv}	70.3 (2)
O7—Tb1—O1^{iii}	74.1 (2)	O1^{iii}—Tb1—O4^{iv}	142.7 (2)
O4—Tb1—O1^{iii}	76.6 (2)	O3^{iv}—Tb1—O4^{iv}	52.32 (19)
O11^{ii}—Tb1—O1^{iii}	83.54 (19)	O17^{v}—Tb1—O4^{iv}	142.16 (19)
O12^{i}—Tb1—O3^{iv}	99.2 (2)	O12^{i}—Tb1—O18^{v}	68.5 (2)
O7—Tb1—O3^{iv}	75.4 (2)	O7—Tb1—O18^{v}	77.1 (2)
O4—Tb1—O3^{iv}	124.11 (19)	O4—Tb1—O18^{v}	136.4 (2)
O11^{ii}—Tb1—O3^{iv}	77.1 (2)	O11^{ii}—Tb1—O18^{v}	142.3 (2)
O1^{iii}—Tb1—O3^{iv}	146.7 (2)	O1^{iii}—Tb1—O18^{v}	115.01 (19)
O12^{i}—Tb1—O17^{v}	71.6 (2)	O3^{iv}—Tb1—O18^{v}	70.0 (2)
O7—Tb1—O17^{v}	81.06 (19)	O17^{v}—Tb1—O18^{v}	51.29 (18)
O4—Tb1—O17^{v}	107.4 (2)	O4^{iv}—Tb1—O18^{v}	101.78 (19)
O8—Tb2—O9^{vi}	93.0 (2)	O2^{iii}—Tb2—O13	158.7 (2)
O8—Tb2—O17^{v}	91.4 (2)	O8—Tb2—O14	125.5 (2)
O9^{vi}—Tb2—O17^{v}	168.0 (2)	O9^{vi}—Tb2—O14	74.2 (2)
O8—Tb2—O5	164.0 (2)	O17^{v}—Tb2—O14	94.16 (19)
O9^{vi}—Tb2—O5	97.6 (2)	O5—Tb2—O14	69.3 (2)
O17^{v}—Tb2—O5	80.7 (2)	O2^{iii}—Tb2—O14	131.9 (2)
O8—Tb2—O2^{iii}	91.7 (2)	O13—Tb2—O14	53.09 (18)
O9^{vi}—Tb2—O2^{iii}	74.5 (2)	O8—Tb2—O1^{iii}	71.2 (2)
O17^{v}—Tb2—O2^{iii}	116.6 (2)	O9^{vi}—Tb2—O1^{iii}	123.8 (2)
O5—Tb2—O2^{iii}	79.7 (2)	O17^{v}—Tb2—O1^{iii}	68.21 (18)
O8—Tb2—O13	74.6 (2)	O5—Tb2—O1^{iii}	92.90 (19)
O9^{vi}—Tb2—O13	89.8 (2)	O2^{iii}—Tb2—O1^{iii}	53.45 (18)
O17^{v}—Tb2—O13	80.6 (2)	O13—Tb2—O1^{iii}	132.39 (17)
O5—Tb2—O13	117.2 (2)	O14—Tb2—O1^{iii}	157.26 (19)
O10^{vi}—Tb3—O16^{v}	144.1 (2)	O19—Tb3—O6	67.7 (2)
O10^{vi}—Tb3—O20^{vii}	78.7 (2)	O15^{viii}—Tb3—O6	71.5 (2)
O16^{v}—Tb3—O20^{vii}	80.9 (2)	O14—Tb3—O6	116.1 (2)
O10^{vi}—Tb3—O19	141.5 (2)	O10^{vi}—Tb3—O5	77.5 (2)
O16^{v}—Tb3—O19	68.1 (2)	O16^{v}—Tb3—O5	104.59 (19)
O20^{vii}—Tb3—O19	138.6 (2)	O20^{vii}—Tb3—O5	145.1 (2)
O10^{vi}—Tb3—O15^{viii}	77.8 (2)	O19—Tb3—O5	72.0 (2)
O16^{v}—Tb3—O15^{viii}	125.18 (19)	O15^{viii}—Tb3—O5	122.3 (2)
O20^{vii}—Tb3—O15^{viii}	76.3 (2)	O14—Tb3—O5	67.75 (19)
O19—Tb3—O15^{viii}	99.3 (2)	O6—Tb3—O5	52.1 (2)

O10^{vi}—Tb3—O14	72.7 (2)	O10^{vi}—Tb3—O16^{viii}	125.21 (19)
O16^{v}—Tb3—O14	75.12 (19)	O16^{v}—Tb3—O16^{viii}	73.0 (2)
O20^{vii}—Tb3—O14	81.0 (2)	O20^{vii}—Tb3—O16^{viii}	69.5 (2)
O19—Tb3—O14	114.8 (2)	O19—Tb3—O16^{viii}	75.4 (2)
O15^{viii}—Tb3—O14	145.6 (2)	O15^{viii}—Tb3—O16^{viii}	52.42 (18)
O10^{vi}—Tb3—O6	75.1 (2)	O14—Tb3—O16^{viii}	139.2 (2)
O16^{v}—Tb3—O6	134.8 (2)	O6—Tb3—O16^{viii}	104.4 (2)
O20^{vii}—Tb3—O6	141.9 (2)	O5—Tb3—O16^{viii}	145.36 (19)

Symmetry codes: (i) x, y, 1+z; (ii) 1-x, -y, -z; (iii) -x, -y, 1-z; (iv) 1-x, -y, 1-z; (v) 2-x, 1-y, 2-z; (vi) 1-x, 1-y, 1-z; (vii) 1-x, 1-y, 2-z; (viii) x-1, y, z.

Angle	(º)	Angle	(º)
O3^{i}—Gd1—O1^{ii}	144.26 (8)	O9—Gd1—O13	107.36 (7)
O3^{i}—Gd1—O2^{iii}	77.30 (7)	O10^{iv}—Gd1—O13	120.57 (6)
O1^{ii}—Gd1—O2^{iii}	136.64 (8)	O12^{v}—Gd1—O13	67.70 (7)
O3^{i}—Gd1—O9	143.16 (9)	O3^{i}—Gd1—O14	76.98 (8)
O1^{ii}—Gd1—O9	69.12 (9)	O1^{ii}—Gd1—O14	67.98 (8)
O2^{iii}—Gd1—O9	77.91 (8)	O2^{iii}—Gd1—O14	142.81 (8)
O3^{i}—Gd1—O10^{iv}	75.19 (8)	O9—Gd1—O14	136.31 (8)
O1^{ii}—Gd1—O10^{iv}	98.99 (9)	O10^{iv}—Gd1—O14	70.90 (7)
O2^{iii}—Gd1—O10^{iv}	76.86 (8)	O12^{v}—Gd1—O14	115.18 (7)
O9—Gd1—O10^{iv}	124.34 (7)	O13—Gd1—O14	50.94 (7)
O3^{i}—Gd1—O12^{v}	74.32 (8)	O3^{i}—Gd1—O9^{iv}	122.66 (8)
O1^{ii}—Gd1—O12^{v}	114.20 (9)	O1^{ii}—Gd1—O9^{iv}	73.35 (8)
O2^{iii}—Gd1—O12^{v}	82.69 (8)	O2^{iii}—Gd1—O9iv	70.37 (8)
O9—Gd1—O12^{v}	75.86 (8)	O9—Gd1—O9^{iv}	72.56 (9)
O10^{iv}—Gd1—O12^{v}	146.27 (8)	O10^{iv}—Gd1—O9^{iv}	52.38 (7)
O3^{i}—Gd1—O13	80.55 (7)	O12^{v}—Gd1—O9^{iv}	141.89 (7)
O1^{ii}—Gd1—O13	72.24 (8)	O13—Gd1—O9^{iv}	142.75 (8)
O2^{iii}—Gd1—O13	146.87 (8)	O14—Gd1—O9^{iv}	102.40 (8)
O4^{i}—Gd2—O5	93.10 (9)	O11^{v}—Gd2—O17^{vi}	158.89 (9)
O4^{i}—Gd2—O13	91.85 (9)	O4^{i}—Gd2—O18^{vi}	124.65 (8)
O5—Gd2—O13	167.38 (7)	O5—Gd2—O18^{vi}	73.31 (8)
O4^{i}—Gd2—O8	164.85 (7)	O13—Gd2—O18^{vi}	94.35 (7)
O5—Gd2—O8	96.78 (8)	O8—Gd2—O18^{vi}	69.50 (7)
O13—Gd2—O8	80.90 (8)	O11^{v}—Gd2—O18^{vi}	131.50 (8)
O4^{i}—Gd2—O11^{v}	92.13 (9)	O17vi—Gd2—O18^{vi}	52.99 (7)
O5—Gd2—O11^{v}	74.38 (8)	O4i—Gd2—O12^{v}	71.87 (7)
O13—Gd2—O11^{v}	117.03 (8)	O5—Gd2—O12^{v}	123.64 (8)
O8—Gd2—O11^{v}	79.57 (8)	O13—Gd2—O12^{v}	68.96 (7)
O4^{i}—Gd2—O17^{vi}	74.29 (8)	O8—Gd2—O12^{v}	93.07 (7)
O5—Gd2—O17^{vi}	90.01 (9)	O11^{v}—Gd2—O12^{v}	53.22 (7)
O13—Gd2—O17^{vi}	80.17 (8)	O17^{vi}—Gd2—O12^{v}	132.66 (7)
O8—Gd2—O17^{vi}	117.04 (7)	O18^{vi}—Gd2—O12^{v}	158.03 (8)
O6—Gd3—O19	78.19 (8)	O20^{ii}—Gd3—O7	67.83 (9)

O6—Gd3—O15	144.07 (9)	O16^{ii}—Gd3—O7	71.32 (7)
O19—Gd3—O15	80.38 (8)	O18^{vi}—Gd3—O7	116.33 (7)
O6—Gd3—O20^{ii}	142.28 (8)	O6—Gd3—O8	78.58 (7)
O19—Gd3—O20^{ii}	138.07 (8)	O19—Gd3—O8	145.43 (8)
O15—Gd3—O20^{ii}	68.31 (9)	O15—Gd3—O8	104.86 (7)
O6—Gd3—O16^{ii}	77.19 (9)	O20^{ii}—Gd3—O8	72.13 (7)
O19—Gd3—O16^{ii}	76.60 (8)	O16^{ii}—Gd3—O8	122.13 (7)
O15—Gd3—O16^{ii}	124.90 (7)	O18^{vi}—Gd3—O8	68.20 (7)
O20^{ii}—Gd3—O16^{ii}	98.68 (9)	O7—Gd3—O8	51.97 (7)
O6—Gd3—O18^{vi}	73.25 (9)	O6—Gd3—O15^{ii}	124.19 (8)
O19—Gd3—O18^{vi}	80.76 (8)	O19—Gd3—O15^{ii}	69.53 (8)
O15—Gd3—O18^{vi}	75.10 (8)	O15—Gd3—O15^{ii}	72.99 (8)
O20^{ii}—Gd3—O18^{vi}	115.25 (9)	O20^{ii}—Gd3—O15^{ii}	74.95 (8)
O16^{ii}—Gd3—O18^{vi}	145.77 (9)	O16^{ii}—Gd3—O15^{ii}	52.15 (7)
O6—Gd3—O7	75.54 (8)	O18^{vi}—Gd3—O15^{ii}	139.24 (6)
O19—Gd3—O7	142.11 (9)	O7—Gd3—O15^{ii}	104.15 (7)
O15—Gd3—O7	135.10 (8)	O8—Gd3—O15^{ii}	144.99 (7)

Symmetry codes: (i) 1-x, 1-y, -z; (ii) 1-x, 1-y, 1-z; (iii) x, -1+y, -1+z; (iv) 1-x, -y, -z; (v) -x, -y, -z; (vi) 2-x, 1-y, 1-z; (vii) x, 1+y, 1+z.

Angle	(º)	Angle	(º)
O16^{i}—Eu1—O17^{ii}	77.32 (17)	O18^{iii}—Eu1—O10^{vi}	71.84 (16)
O16^{i}—Eu1—O4	143.37 (18)	O3^{iv}—Eu1—O10^{vi}	121.02 (15)
O17^{ii}—Eu1—O4	79.17 (17)	O1^{v}—Eu1—O10^{vi}	68.12 (15)
O16^{i}—Eu1—O18^{iii}	143.95 (18)	O16^{i}—Eu1—O9^{vi}	76.85 (17)
O17^{ii}—Eu1—O18^{iii}	136.88 (17)	O17^{ii}—Eu1—O9^{vi}	143.34 (17)
O4—Eu1—O18^{iii}	68.72 (19)	O4—Eu1—O9^{vi}	135.15 (17)
O16^{i}—Eu1—O3^{iv}	76.55 (17)	O18^{iii}—Eu1—O9^{vi}	67.70 (18)
O17^{ii}—Eu1—O3^{iv}	77.63 (17)	O3i^{v}—Eu1—O9^{vi}	71.38 (16)
O4—Eu1—O3^{iv}	124.76 (16)	O1^{v}—Eu1—O9^{vi}	114.78 (16)
O18^{iii}—Eu1—O3^{iv}	97.42 (19)	O10^{vi}—Eu1—O9^{vi}	50.53 (15)
O16^{i}—Eu1—O1^{v}	73.69 (18)	O16^{i}—Eu1—O4^{iv}	122.64 (16)
O17^{ii}—Eu1—O1^{v}	81.88 (17)	O17^{ii}—Eu1—O4^{iv}	69.60 (16)
O4—Eu1—O1^{v}	75.51 (16)	O4—Eu1—O4^{iv}	73.20 (17)
O18^{iii}—Eu1—O1^{v}	115.25 (18)	O18^{iii}—Eu1—O4^{iv}	73.97 (17)
O3^{iv}—Eu1—O1^{v}	146.85 (17)	O3^{iv}—Eu1—O4^{iv}	51.80 (15)
O16^{i}—Eu1—O10^{vi}	80.96 (16)	O1^{v}—Eu1—O4^{iv}	140.79 (16)
O17^{ii}—Eu1—O10^{vi}	146.88 (16)	O10^{vi}—Eu1—O4^{iv}	143.47 (15)
O4—Eu1—O10^{vi}	105.32 (15)	O9^{vi}—Eu1—O4^{iv}	104.04 (16)
O15^{i}—Eu2—O13	92.56 (19)	O2^{v}—Eu2—O7	159.6 (2)
O15^{i}—Eu2—O10^{vi}	93.55 (18)	O15^{i}—Eu2—O8	124.94 (17)
O13—Eu2—O10^{vi}	166.45 (18)	O13—Eu2—O8	73.45 (18)
O15^{i}—Eu2—O5	165.19 (16)	O10^{vi}—Eu2—O8	93.16 (16)
O13—Eu2—O5	96.69 (18)	O5—Eu2—O8	69.08 (15)
O10^{vi}—Eu2—O5	79.97 (16)	O2^{v}—Eu2—O8	132.44 (17)

O15^{i}—Eu2—O2^{v}	91.3 (2)	O7—Eu2—O8	52.76 (16)
O13—Eu2—O2^{v}	75.4 (2)	O15^{i}—Eu2—O1^{v}	72.47 (17)
O10^{vi}—Eu2—O2^{v}	116.46 (17)	O13—Eu2—O1^{v}	124.33 (18)
O5—Eu2—O2^{v}	79.95 (19)	O10^{vi}—Eu2—O1^{v}	69.13 (15)
O15^{i}—Eu2—O7	74.94 (19)	O5—Eu2—O1^{v}	92.75 (15)
O13—Eu2—O7	89.9 (2)	O2^{v}—Eu2—O1^{v}	52.53 (16)
O10^{vi}—Eu2—O7	80.00 (18)	O7—Eu2—O1^{v}	132.84 (17)
O5—Eu2—O7	116.48 (16)	O8—Eu2—O1^{v}	157.02 (16)
O14—Eu3—O19	78.05 (18)	O20^{iii}—Eu3—O5	72.26 (17)
O14—Eu3—O11^{vi}	143.22 (18)	O12^{vii}—Eu3—O5	122.07 (16)
O19—Eu3—O11^{vi}	80.25 (18)	O8—Eu3—O5	67.95 (14)
O14—Eu3—O20^{iii}	142.65 (19)	O14—Eu3—O6	75.59 (18)
O19—Eu3—O20^{iii}	137.77 (18)	O19—Eu3—O6	142.20 (18)
O11^{vi}—Eu3—O20^{iii}	68.73 (19)	O11^{vi}—Eu3—O6	135.44 (17)
O14—Eu3—O12^{vii}	77.95 (18)	O20^{iii}—Eu3—O6	68.04 (19)
O19—Eu3—O12^{vii}	76.67 (18)	O12^{vii}—Eu3—O6	71.71 (16)
O11^{vi}—Eu3—O12^{vi}i	124.92 (16)	O8—Eu3—O6	115.30 (15)
O20^{iii}—Eu3—O12^{vii}	97.90 (19)	O5—Eu3—O6	51.31 (15)
O14—Eu3—O8	72.73 (18)	O14—Eu3—O11^{vii}	124.23 (17)
O19—Eu3—O8	81.32 (16)	O19—Eu3—O11^{vii}	69.36 (16)
O11^{vi}—Eu3—O8	74.92 (16)	O11^{vi}—Eu3—O11^{vii}	73.49 (18)
O20^{iii}—Eu3—O8	115.45 (18)	O20^{iii}—Eu3—O11^{vii}	74.69 (17)
O12^{vii}—Eu3—O8	146.32 (17)	O12^{vii}—Eu3—O11^{vii}	51.66 (16)
O14—Eu3—O5	78.72 (17)	O8—Eu3—O11^{vii}	139.77 (15)
O19—Eu3—O5	145.78 (16)	O5—Eu3—O11^{vii}	144.83 (15)
O11^{vi}—Eu3—O5	104.75 (16)	O6—Eu3—O11^{vii}	104.65 (16)

Symmetry codes: (i) 2-x, 2-y, 1-z; (ii) x, -1+y, -1+z; (iii) 2-x, 2-y, 2-z; (iv) 2-x, 1-y, 1-z; (v) 1-x, 1-y, 1-z; (vi) 3-x, 2-y, 2-z; (vii) -1+x, y, z; (viii) 1+x, y, z; (ix) x, 1+y, 1+z.

Angle	(º)	Angle	(º)
O10^{i}—Dy1—O12	144.56 (13)	O17^{iii}—Dy1—O4	106.07 (11)
O10^{i}—Dy1—O11^{ii}	77.11 (12)	O18^{iv}—Dy1—O4	121.08 (11)
O12—Dy1—O11^{ii}	136.52 (12)	O14—Dy1—O4	67.41 (10)
O10^{i}—Dy1—O17^{iii}	143.34 (12)	O10^{i}—Dy1—O3	77.04 (12)
O12—Dy1—O17^{iii}	68.58 (13)	O12—Dy1—O3	68.18 (13)
O11^{ii}—Dy1—O17^{iii}	78.45 (12)	O11^{ii}—Dy1—O3	142.87 (12)
O10^{i}—Dy1—O18^{iv}	75.81 (12)	O17^{iii}—Dy1—O3	135.85 (11)
O12—Dy1—O18^{iv}	98.21 (13)	O18^{iv}—Dy1—O3	70.74 (11)
O11^{ii}—Dy1—O18^{iv}	77.39 (12)	O14—Dy1—O3	114.85 (11)
O17^{iii}—Dy1—O18^{iv}	124.32 (11)	O4—Dy1—O3	51.32 (10)
O10^{i}—Dy1—O14	73.94 (12)	O10^{i}—Dy1—O17^{iv}	122.74 (11)
O12—Dy1—O14	114.52 (12)	O12—Dy1—O17^{iv}	73.37 (12)
O11^{ii}—Dy1—O14	82.59 (11)	O11^{ii}—Dy1—O17^{iv}	70.08 (11)
O17^{iii}—Dy1—O14	76.17 (11)	O17^{iii}—Dy1—O17^{iv}	72.37 (12)

O18^{iv}—Dy1—O14	146.70 (11)	O18^{iv}—Dy1—O17^{iv}	52.34 (11)
O10^{i}—Dy1—O4	81.38 (11)	O14—Dy1—O17^{iv}	141.58 (11)
O12—Dy1—O4	71.93 (11)	O4—Dy1—O17^{iv}	142.91 (10)
O11^{ii}—Dy1—O4	146.95 (11)	O3—Dy1—O17^{iv}	103.07 (11)
O9^{i}—Dy2—O7^{v}	92.16 (12)	O13—Dy2—O2^{vi}	159.38 (13)
O9^{i}—Dy2—O4	93.19 (12)	O9^{i}—Dy2—O1^{vi}	124.94 (12)
O7^{v}—Dy2—O4	167.07 (12)	O7^{v}—Dy2—O1^{vi}	73.42 (11)
O9^{i}—Dy2—O16^{iii}	165.22 (12)	O4—Dy2—O1^{vi}	93.89 (11)
O7^{v}—Dy2—O16^{iii}	96.75 (12)	O16^{iii}—Dy2—O1^{vi}	69.18 (11)
O4—Dy2—O16^{iii}	80.62 (11)	O13—Dy2—O1^{vi}	132.03 (12)
O9^{i}—Dy2—O13	91.23 (14)	O2^{vi}—Dy2—O1^{vi}	52.92 (11)
O7^{v}—Dy2—O13	75.04 (13)	O9^{i}—Dy2—O14	71.93 (12)
O4—Dy2—O13	116.58 (12)	O7^{v}—Dy2—O14	124.01 (11)
O16^{iii}—Dy2—O13	79.78 (13)	O4—Dy2—O14	68.89 (10)
O9^{i}—Dy2—O2^{vi}	74.93 (12)	O16^{iii}—Dy2—O14	93.30 (11)
O7^{v}—Dy2—O2^{vi}	90.03 (13)	O13—Dy2—O14	52.95 (11)
O4—Dy2—O2^{vi}	80.02 (12)	O2^{vi}—Dy2—O14	132.41 (11)
O16^{iii}—Dy2—O2^{vi}	116.69 (11)	O1^{vi}—Dy2—O14	157.69 (11)
O8^{v}—Dy3—O20^{v}	78.12 (13)	O19—Dy3—O15^{iii}	67.48 (13)
O8^{v}—Dy3—O5	143.78 (13)	O6^{v}—Dy3—O15^{iii}	71.43 (12)
O20^{v}—Dy3—O5	80.27 (12)	O1^{vi}—Dy3—O15^{iii}	115.85 (11)
O8^{v}—Dy3—O19	142.40 (13)	O8^{v}—Dy3—O16^{iii}	78.72 (12)
O20^{v}—Dy3—O19	137.90 (12)	O20^{v}—Dy3—O16^{iii}	145.39 (11)
O5—Dy3—O19	68.61 (13)	O5—Dy3—O16^{iii}	104.69 (11)
O8^{v}—Dy3—O6^{v}	77.70 (12)	O19—Dy3—O16^{iii}	72.37 (12)
O20^{v}—Dy3—O6^{v}	76.85 (13)	O6^{v}—Dy3—O16^{iii}	122.31 (11)
O5—Dy3—O6^{v}	124.71 (11)	O1^{vi}—Dy3—O16^{iii}	67.69 (10)
O19—Dy3—O6^{v}	97.85 (14)	O15^{iii}—Dy3—O16^{iii}	51.97 (11)
O8^{v}—Dy3—O1^{vi}	72.89 (12)	O8^{v}—Dy3—O5^{v}	124.40 (12)
O20^{v}—Dy3—O1^{vi}	81.08 (12)	O20^{v}—Dy3—O5^{v}	69.14 (12)
O5—Dy3—O1^{vi}	75.30 (11)	O5—Dy3—O5^{v}	72.63 (12)
O19—Dy3—O1^{vi}	115.61 (13)	O19—Dy3—O5^{v}	74.81 (12)
O6^{v}—Dy3—O1^{vi}	146.19 (12)	O6^{v}—Dy3—O5^{v}	52.27 (10)
O8^{v}—Dy3—O15^{iii}	75.90 (13)	O1^{vi}—Dy3—O5^{v}	139.11 (11)
O20^{v}—Dy3—O15^{iii}	142.41 (12)	O15^{iii}—Dy3—O5^{v}	104.74 (11)
O5—Dy3—O15^{iii}	134.94 (12)	O16^{iii}—Dy3—O5^{v}	145.38 (11)

Symmetry codes: (i) x, y, -1+z; (ii) -x, 1-y, -z; (iii) -1-x, 1-y, -z; (iv) 1+x, y, z; (v) -x, 2-y, 1-z; (vi) 1-x, 2-y, 1-z; (vii) x, y, 1+z; (viii) -1+x, y, z.

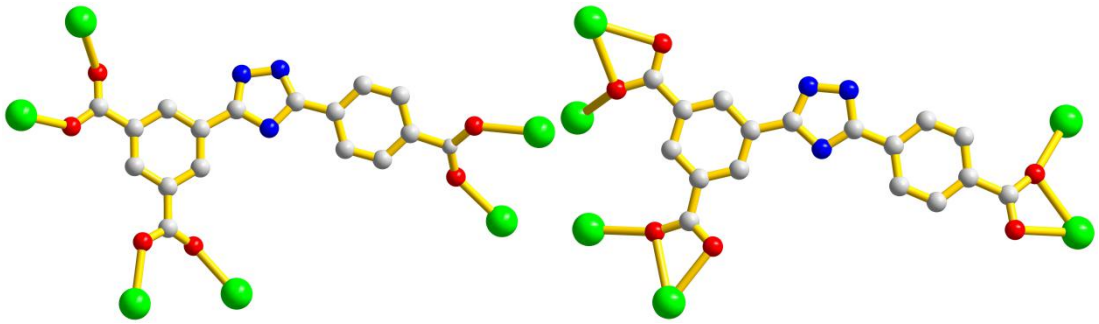

Fig. S1 The coordination modes of three L^{3-} in **TbL**: (a) μ_2-bridging mode. (b) μ_3-bridging mode.

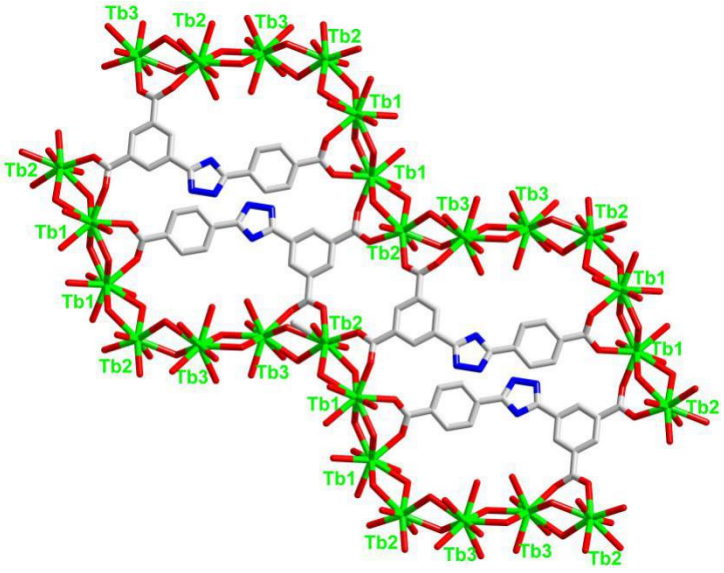

Fig. S2 The peanut-shaped structure of **TbL**.

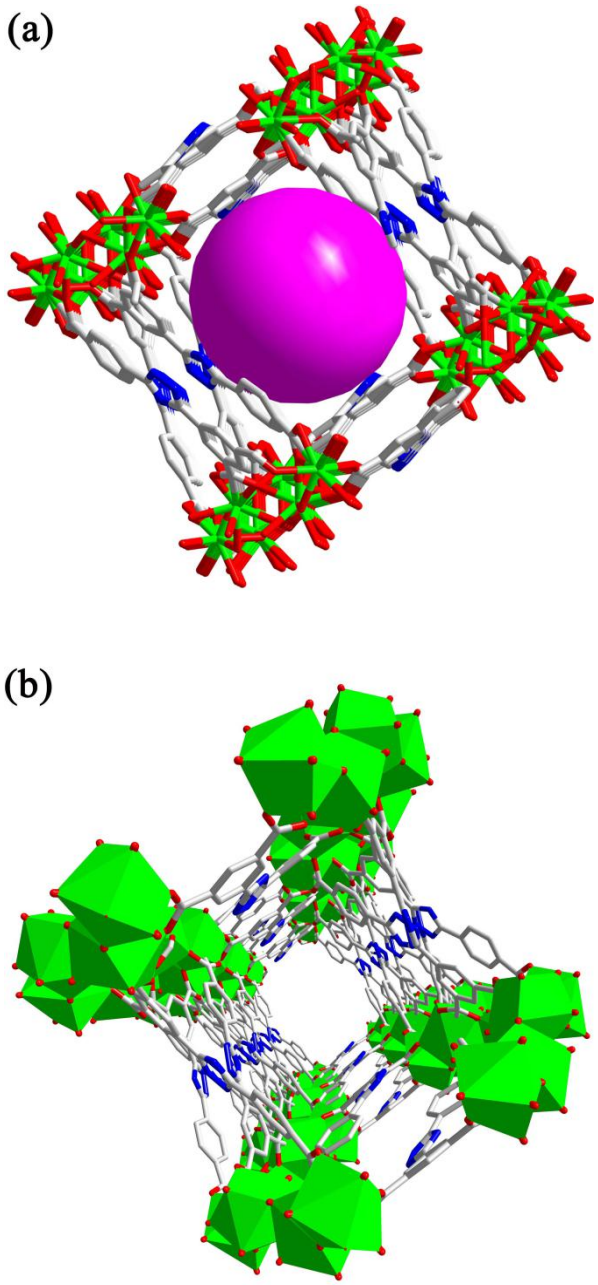

Fig. S3 Open channel of **TbL**.

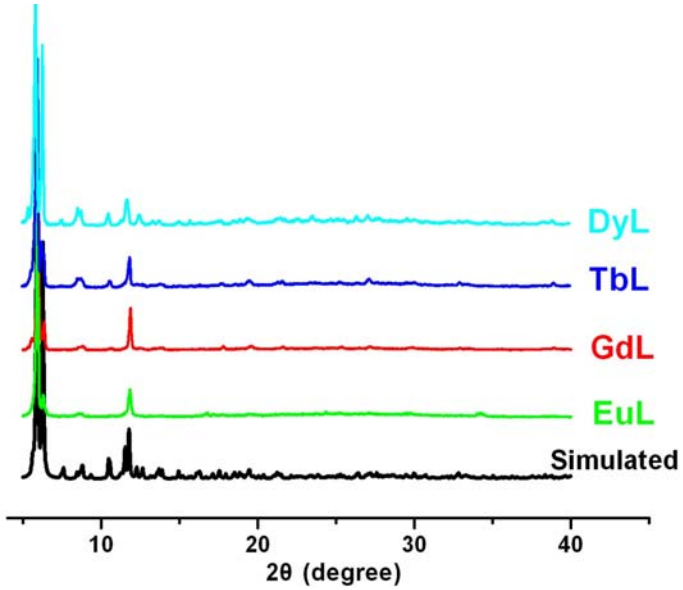

Fig. S4 PXRD patterns of **TbL, GdL, EuL and DyL**.

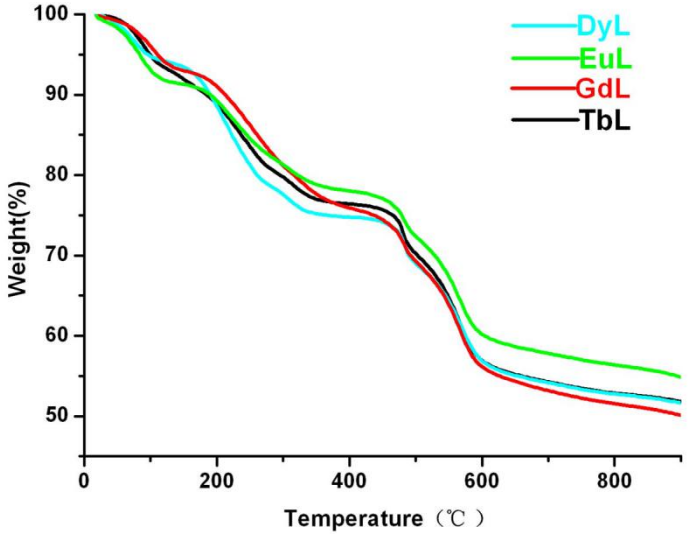

Fig. S5 The TGA curves of **TbL, GdL, EuL and DyL**.

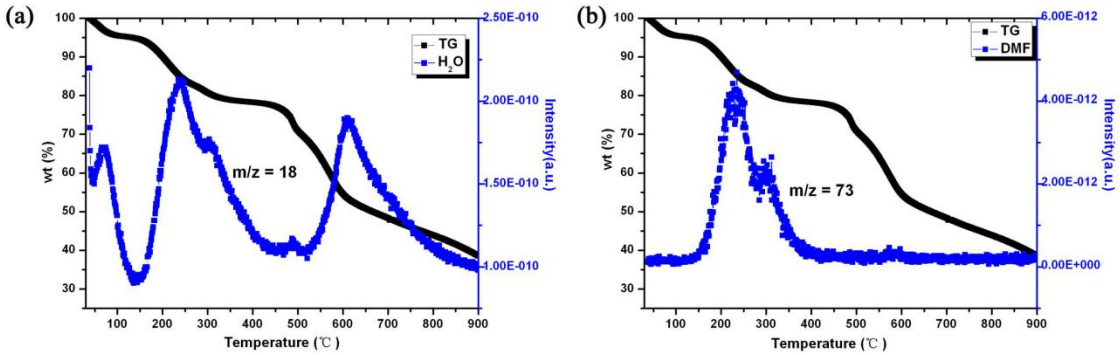

Fig. S6 The TGA curves associated with solvent peaks (left for water molecule m/z = 18 and right for DMF molecule m/z = 73) of **TbL**.

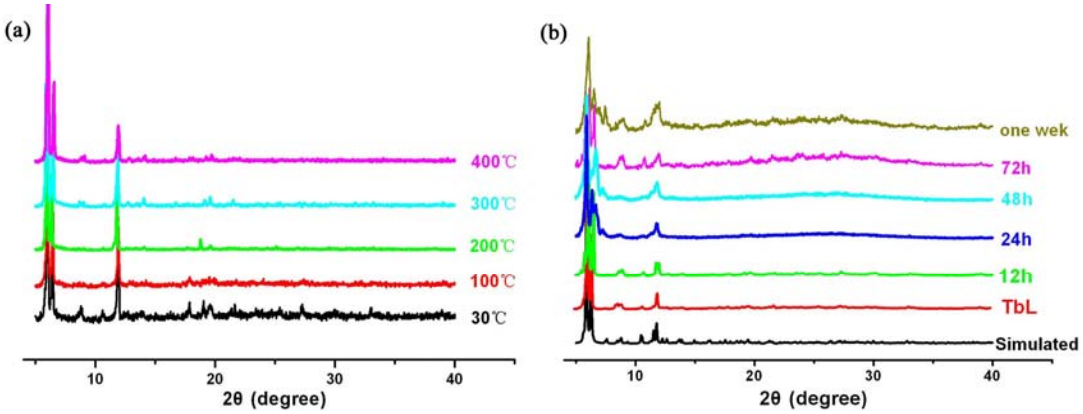

Fig. S7 (a) The X-ray thermodiffractogram of **TbL**. (b) PXRD patterns of **TbL** after exposed to open air containing H_2O vapor for 12 h, 24 h, 48 h, 72 h and one week.

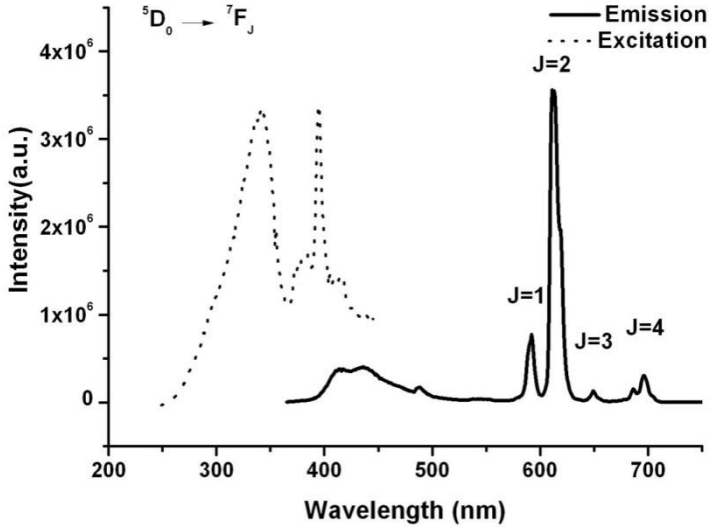

Fig. S8 The excitation (dot, λ_{em}= 613 nm) and emission spectra (solid, λ_{ex}= 341 nm) of **EuL** at room temperature.

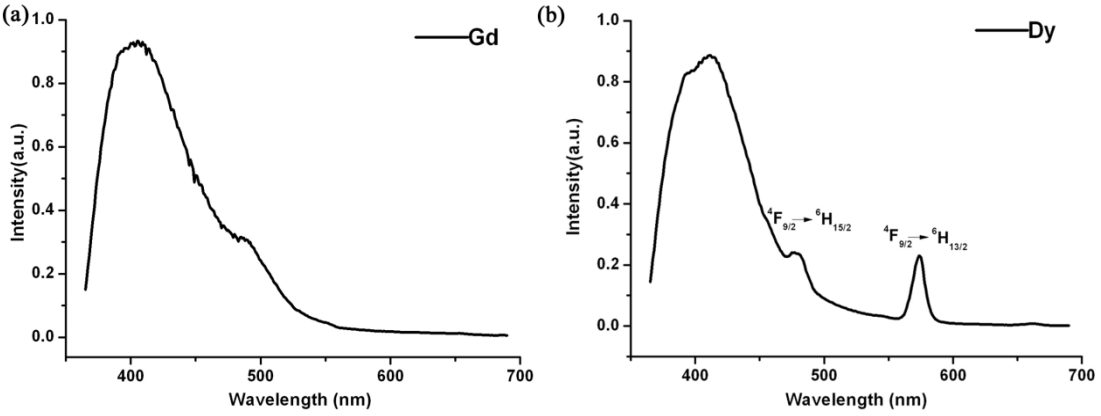

Fig. S9 Emission spectra of (a) **GdL** (excited at 345 nm) and (b) **DyL** (excited at 348 nm) at room temperature.

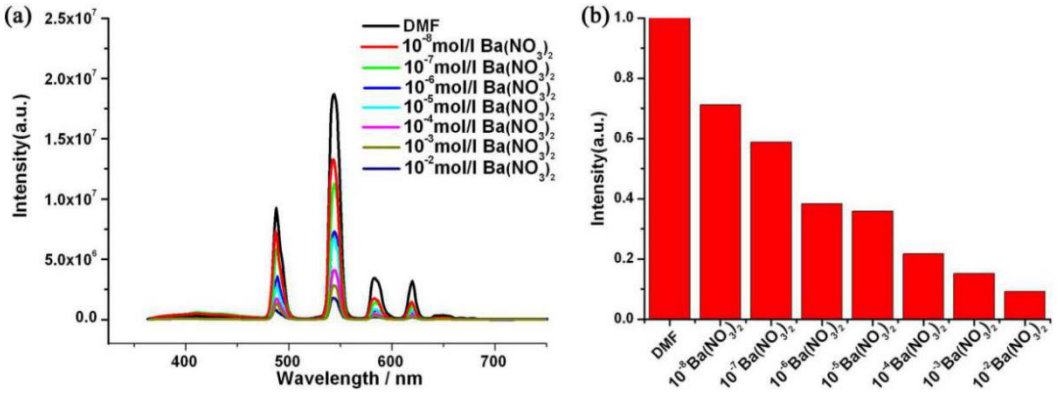

Fig. S10 The luminescence intensity of **TbL** (the $^5D_4$-$^7F_5$ transition) in different concentrations of $Ba(NO_3)_2$.

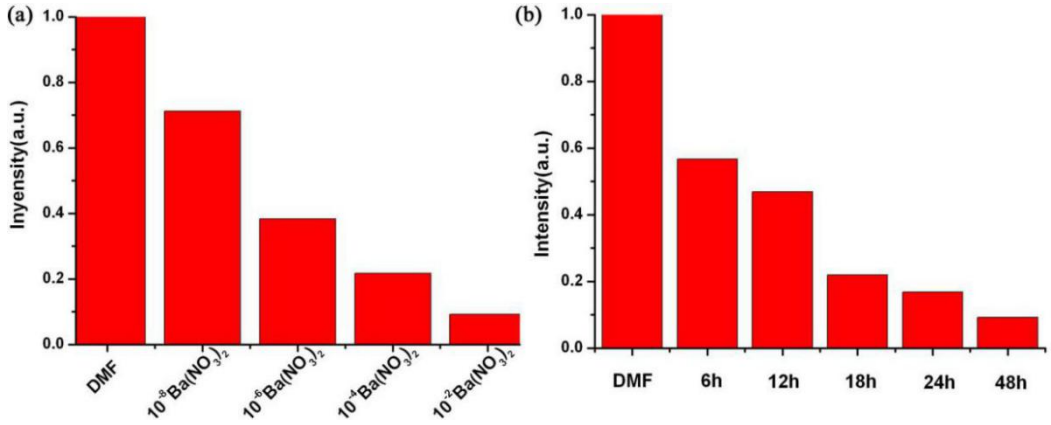

Fig. S11 Column charts of the luminescence intensity of **TbL** (the $^5D_4$-$^7F_5$ transition) (a) in different concentrations of $Ba(NO_3)_2$. (b) at different reaction times of $Ba(NO_3)_2$ DMF solutions.

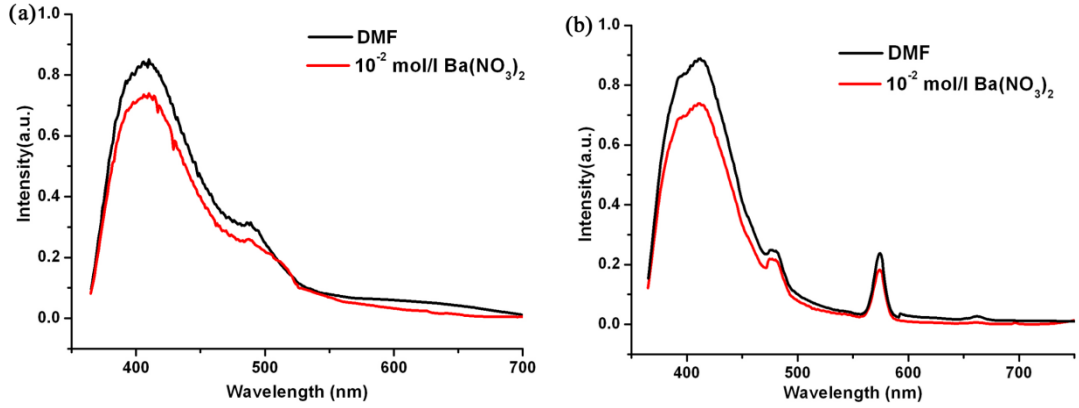

Fig. S12 The luminescence spectra of (a) **GdL** and (b) **DyL** in 10^{-2} M DMF solutions containing $Ba(NO_3)_2$.

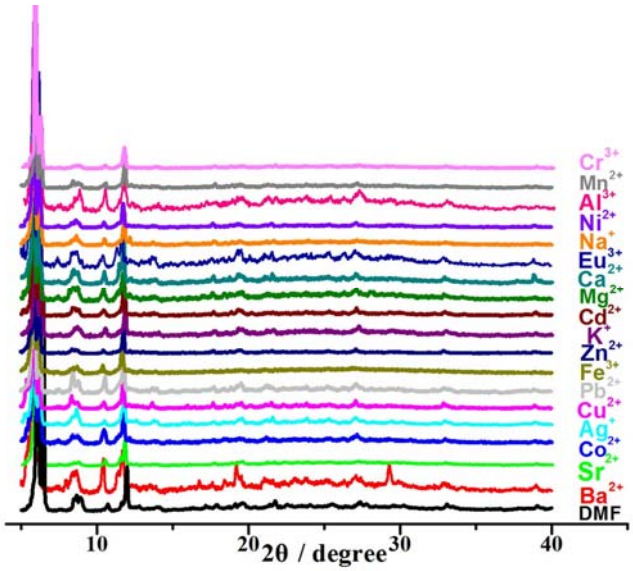

Fig. S13 PXRD patterns of **TbL** after dispersed in different $M(NO_3)_x$ ($M = Na^+$, K^+, Cu^{2+}, Zn^{2+}, Cd^{2+}, Ni^{2+}, Mn^{2+}, Pb^{2+}, Mg^{2+}, Co^{2+}, Ba^{2+}, Cr^{3+}, Ca^{2+}, Sr^{2+}, Eu^{3+}, Al^{3+}, Ag^+, Fe^{3+}) DMF solutions.

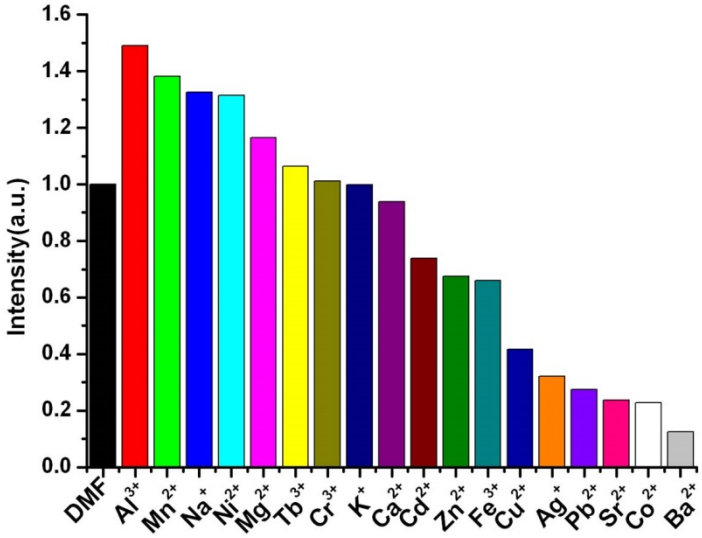

Fig. S14 The emission intensity of the $^5D_0$-$^7F_2$ transition of **EuL** excited at 341 nm in different $M(NO_3)_x$ DMF solutions.

Table S4. Quenching effect coefficients (K_{sv}) of different metal ions on the

luminescence intensity of metal-ion-incorporated **EuL**.

Metal ion	K_{sv}	Metal ion	K_{sv}
Al^{3+}	-33	Cd^{2+}	35
Mn^{2+}	-28	Zn^{2+}	48
Na^{+}	-25	Fe^{3+}	51
Ni^{2+}	-24	Cu^{2+}	140
Mg^{2+}	-14	Ag^{+}	211
Tb^{3+}	-6	Pb^{2+}	263
Cr^{3+}	-1	Sr^{2+}	320
K^{+}	0	Co^{2+}	341
Ca^{2+}	6	Ba^{2+}	700

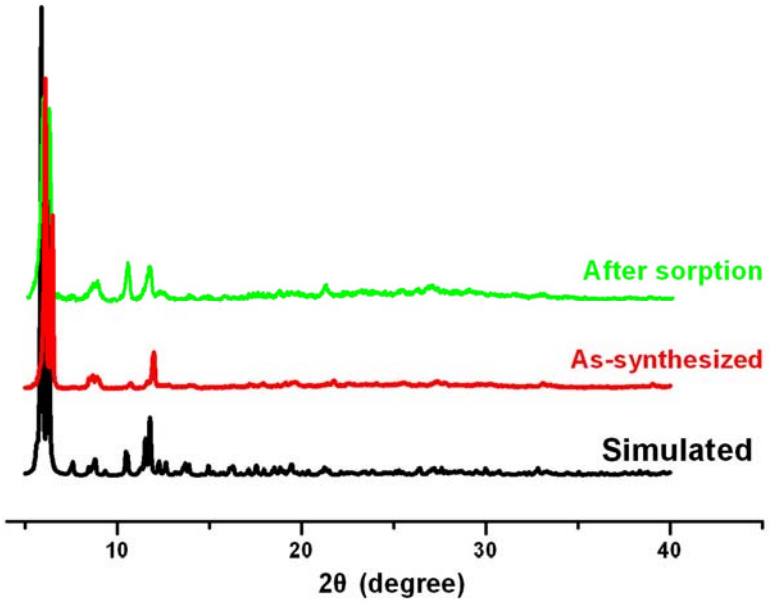

Fig. S15 PXRD patterns of **TbL**: pattern simulated from single-crystal structure in black, experimental pattern for the as-synthesized sample in red and that for the sample after adsorption in green.

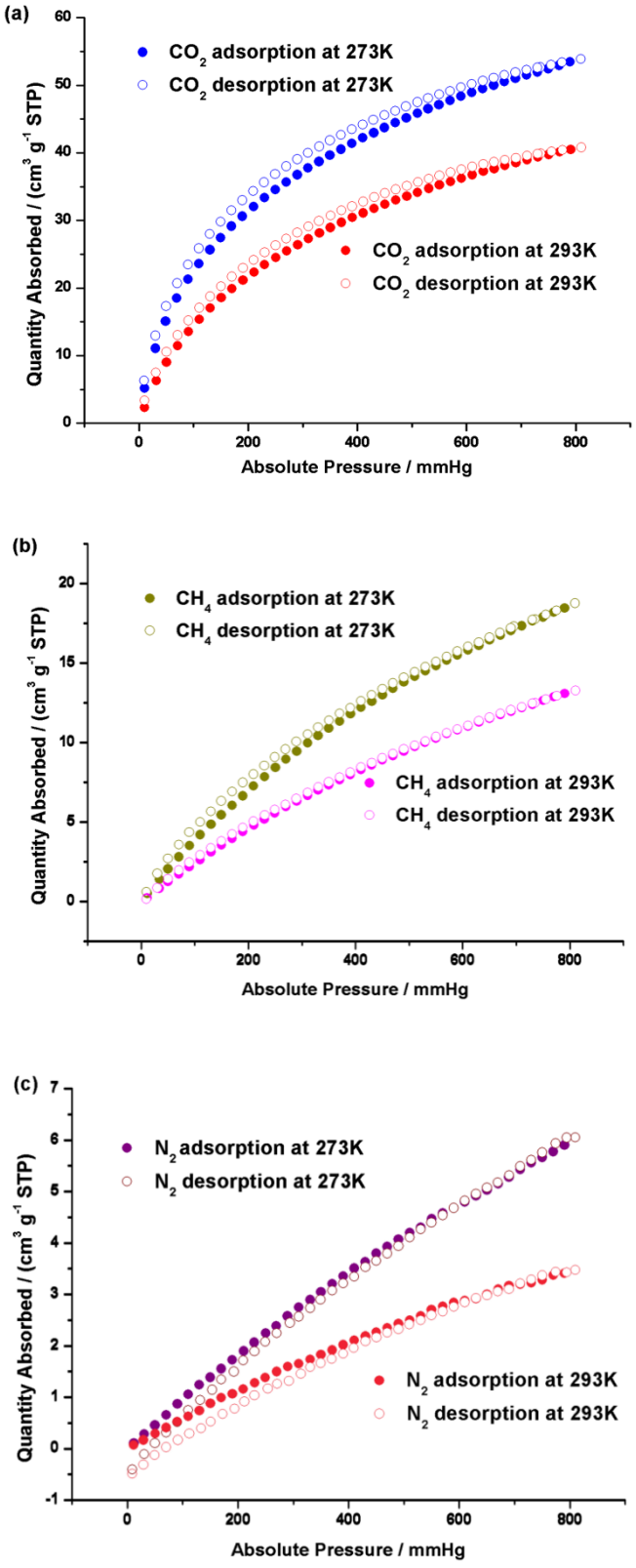

Fig. S16 (a) CO_2 sorption isotherms of **TbL** at 273 K and 293 K. (b) CH_4 sorption isotherms of **TbL** at 273 K and 293 K. (c) N_2 sorption isotherms of **TbL** at 273 K and 293 K.

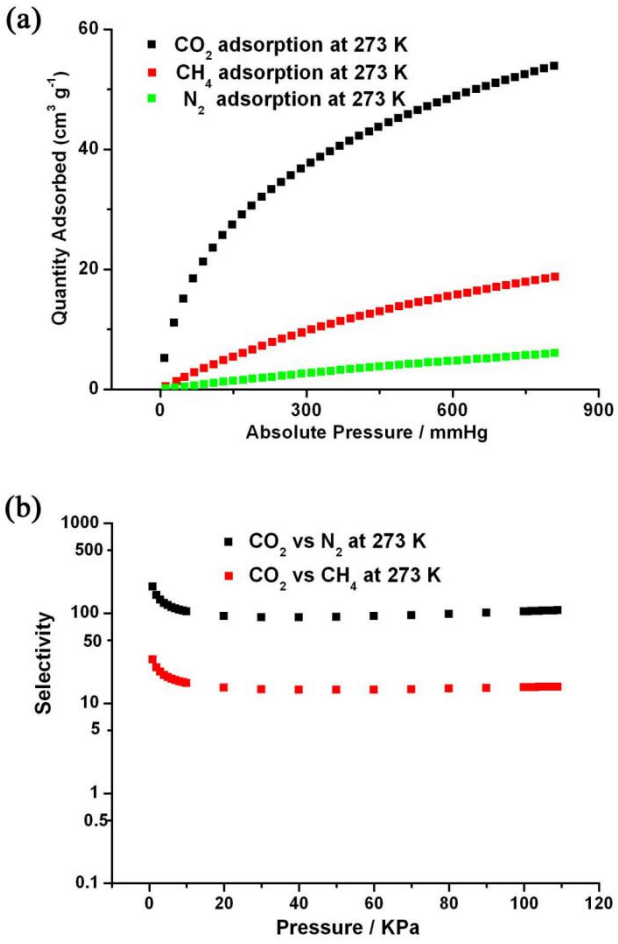

Fig. S17 (a) Adsorption isotherms of **TbL** for CO_2, CH_4 and N_2 at 273 K. (b) Adsorption selectivities of CO_2/N_2 and CO_2/CH_4 (CO_2:N_2=15:85; CO_2:CH_4=50:50) at 273 K.

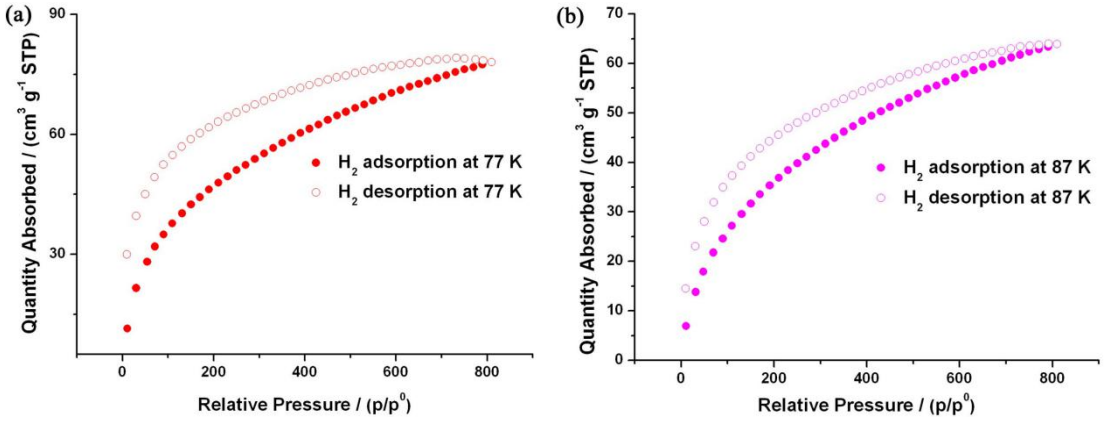

Fig. S18 Adsorption isotherms of **TbL** for H_2 at 77 K (a) and 87 K.