Supporting Information File

Influence of coordination environment in slow magnetic relaxation and photoluminescence behavior in two mononuclear dysprosium (III) based single molecule magnets

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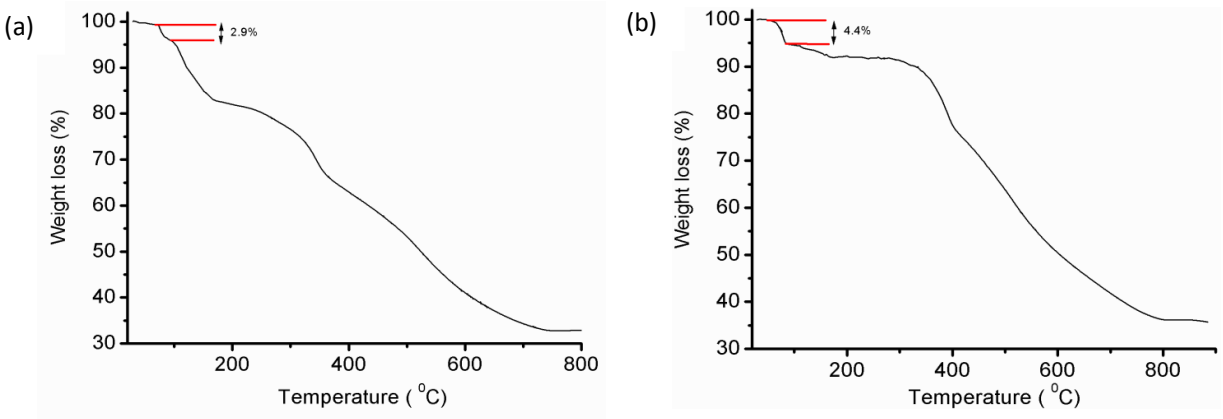

Fig. S1. Thermogravimetric profiles for complexes **1** (a) and **2** (b).

Table S1. Bond distances (Å) around Dy(III) found in **1** and **2**.

1		**2**	
Dy – N1	2.548(3)	Dy – N1	2.521(5)
Dy – N2	2.528(4)	Dy – N2	2.504(5)
Dy – N4	2.540(4)	Dy – N4	2.532(5)
Dy – O1	2.394(4)	Dy – O1	2.450(5)
Dy – O2	2.351(3)	Dy – O2	2.351(5)
Dy – O3	2.373(3)	Dy – O3	2.530(5)
Dy – O6	2.372(3)	Dy – O6	2.439(5)
Dy – O7	2.399(3)	Dy – O7	2.305(5)
Dy – O11	2.455(3)	Dy – O11	2.472(5)

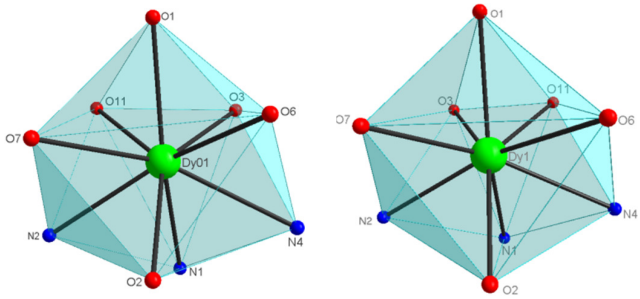

Fig. S2. Distorted muffin coordination geometry around the Dy(III) metal ions in **1** (left) and **2** (right).

Shape analysis

Table S2: Summary of SHAPE analysis for complex **1** and **2**.

```
EP-9            1  D9h     Enneagon
OPY-9           2  C8v     Octagonal pyramid
HBPY-9          3  D7h     Heptagonal bipyramid
JTC-9           4  C3v     Johnson triangular cupola  J3
JCCU-9          5  C4v     Capped cube  J8
CCU-9           6  C4v     Spherical-relaxed capped cube
JCSAPR-9        7  C4v     Capped square antiprism  J10
CSAPR-9         8  C4v     Spherical capped square antiprism
JTCTPR-9        9  D3h     Tricapped trigonal prism  J51
TCTPR-9         10  D3h    Spherical tricapped trigonal prism
JTDIC-9         11  C3v    Tridiminished icosahedron  J63
HH-9            12  C2v    Hula-hoop
MFF-9           13  Cs     Muffin
```

Complex **1**:

```
Structure [ML9 ]          EP-9        OPY-9       HBPY-9        JTC-9
JCCU-9        CCU-9     JCSAPR-9      CSAPR-9

Dy1             ,         31.797,     24.550,     15.960,       15.741,
6.857,        5.768,     3.367,      2.901,

JTCTPR-9      TCTPR-9      JTDIC-9         HH-9        MFF-9

2.510,        2.522,       12.500,         7.051,      2.347
```

Complex **2**:

```
Structure [ML9 ]          EP-9        OPY-9       HBPY-9        JTC-9
JCCU-9        CCU-9     JCSAPR-9      CSAPR-9

Dy1             ,         34.684,      26.194,     16.889,      16.816,
8.820,        7.467,     5.341,       4.823,

JTCTPR-9      TCTPR-9      JTDIC-9         HH-9        MFF-9

4.464,        4.656,       14.108,         8.806,      4.320
```

Table S3. H-bond parameters found in complex **1.**

D– H···A	D–H(Å)	H···A(Å)	D···A (Å)	<D-H-A(°)	Symmetry[#]
O2—H2A···O7	0.938	2.431	2.836	105.91	0
O2—H2A···N2	0.938	2.965	2.987	82.23	0
O2—H2B···N4	0.938	2.876	2.990	87.72	0
O2—H2B···O6	0.938	2.678	3.022	102.43	0
O2—H2B···O15	0.938	2.365	2.677	98.97	0
N3—H3···O5	1.030	1.788	2.563	128.86	0
O1—H1A···O11	0.938	2.397	2.819	107.06	0
O1—H1A···N10	0.938	2.669	3.346	129.56	0
O1—H1A···O19	0.938	2.269	3.052	140.50	0
O1—H1B···O3	0.938	2.740	2.923	91.74	0
O1—H1B···O6	0.938	2.597	2.704	86.29	0
O3—H3A···N4	0.938	2.389	2.782	104.94	0
O3—H3A···N5	0.938	2.800	3.429	125.38	0
O3—H3B···O1	0.938	2.553	2.923	103.84	0
O3—H3B···O11	0.938	2.641	2.661	81.02	0

N5—H5···O4	1.030	1.841	2.611	128.67	0
C1—H1···O9	1.080	2.930	3.533	115.61	0
C1—H1···O8	1.080	2.573	3.581	155.06	0
C2—H2···O9	1.080	2.923	3.544	116.84	0
C7—H7B···N3	1.080	2.747	2.819	82.59	0
C7—H7B···O20	1.080	2.793	3.602	131.67	0
C23—H23···O7	1.080	2.440	2.783	96.82	0
C12—H12···O6	1.080	2.427	2.768	96.68	0
C9—H9A···N5	1.080	2.632	2.792	86.98	0
O2—H2A···O8	0.938	1.999	2.914	164.37	0
O2—H2A···N6	0.938	2.682	3.456	140.19	1
O2—H2A···O9	0.938	2.689	3.213	115.98	1
O15—H15A···O17	0.938	2.211	2.951	135.14	1
O1—H1A···O10	0.938	2.840	3.322	113.11	2
O3—H3A···O13	0.938	2.034	2.737	130.47	2
O3—H3B···O9	0.938	2.507	3.154	126.19	2
O3—H3B···O10	0.938	1.978	2.835	150.95	2
C9—H9A···O13	1.080	2.816	3.417	115.08	2
C9—H9C···O18	1.080	2.938	3.362	103.68	2
O3—H3B···N6	0.938	2.606	3.427	146.36	2
C13—H13···O8	1.080	2.790	3.800	155.71	3
C13—H13···N6	1.080	2.663	3.634	149.39	3
O1—H1B···N9	0.938	2.896	3.464	120.18	3
O1—H1B···O18	0.938	2.475	3.252	140.17	3
O1—H1B···O17	0.938	2.566	2.861	98.58	3
C13—H13···O9	1.080	2.826	3.793	149.06	3
C2—H2···O15	1.080	2.778	3.828	163.88	4
C2—H2···O2	1.080	2.638	3.360	123.72	4
C7—H7C···O19	1.080	2.511	3.462	146.33	5
C3—H3C···O19	1.080	2.167	3.232	168.02	5
O5—H5A···O13	0.938	1.866	2.623	136.08	6
O5—H5A···O17	0.938	2.721	3.110	105.74	6
O5—H5A···N9	0.938	2.609	3.184	120.08	6
C7—H7B···O17	1.080	2.815	3.399	113.88	6
C24—H24···O11	1.080	2.544	3.499	146.88	6
C24—H24···O20	1.080	2.869	3.674	131.42	6
C21—H21···O9	1.080	2.851	3.631	129.17	6
O4—H4···O10	0.938	1.780	2.708	169.64	7
O4—H4···O8	0.938	2.763	3.455	131.30	7
C15—H15···O10	1.080	2.875	3.549	120.67	7
O4—H4···N6	0.938	2.608	3.485	155.88	7
C22—H22···O18	1.080	2.508	3.330	132.10	8
O15—H15A···O5	0.938	2.724	3.459	135.86	9
C9—H9B···O20	1.080	2.239	3.241	153.45	9
O15—H15B···O20	0.938	1.943	2.867	167.94	9

(0) x,y,z; (1) -x+1,+y-1/2,-z+1; (2) -x+1,+y-1/2,-z; (3) x,+y-1,+z (4) –x+1,+y+1/2,-z+1; (5) -x+2,+y+1/2,-z+1 (6) -x+2,+ y-1/2,-z+1; (7) -x, + y-1/2,-z; (8) x+1,+y-1,+z+1; (9) x-1,+y,+z-1/2; (10) y+1/2,-x+1,+z.

Table S4. H-bond parameters found in complex **2.**

D– H···A	**D–H(Å)**	**H···A(Å)**	**D···A (Å)**	**<D-H-A(°)**	**Symmetry[#]**
O4—H1···N5	0.938	1.963	2.646	127.95	0
O5—H2···N3	0.938	1.716	2.546	145.65	0
N5—H4···O4	1.030	1.870	2.646	129.29	0
O2—H2B···O6	0.938	2.678	3.022	102.43	0
C8—H8C···O4	1.080	2.793	3.843	164.12	0
C8—H8C···N5	1.080	2.284	2.745	103.48	0
C9—H9C···N3	1.080	2.684	2.780	83.67	0
O1—H1A···N10	0.938	2.669	3.346	129.56	0
C12—H12···O6	1.080	2.490	2.795	94.75	0
C19—H19···O7	1.080	2.508	2.855	97.37	0
O4—H1···O9	0.938	2.718	2.825	86.81	1
C8—H8A···O12	1.080	2.305	3.351	162.54	1
C8—H8C···O9	1.080	2.427	3.226	129.73	1

C1—H1A···O9	1.080	2.188	3.263	173.20	2
C1—H1A···N16	1.080	2.769	3.804	160.61	2
C5—H5···O12	1.080	2.470	3.257	128.75	2
C1—H1A···O10	1.080	2.615	3.443	132.99	2
C8—H8B···O12	1.080	2.698	3.479	128.86	2
C8—H8B···N6	1.080	2.786	3.770	151.43	2
C13—H13···O12	1.080	2.785	3.419	117.41	3
C14—H14···O12	1.080	2.564	3.306	125.12	3
C13—H13···O3	1.080	2.784	3.662	138.36	3
C15—H15···O11	1.080	2.320	3.184	135.72	4
C21—H21···O3	1.080	2.552	3.274	123.47	5

(0) x,y,z; (1) -x+2,-y+1,-z; (2) x+1,+y,+z; (3) x,+y+1,+z (4) –x+2,-y+2,-z; (5) -x+1,-y+1,-z+1.

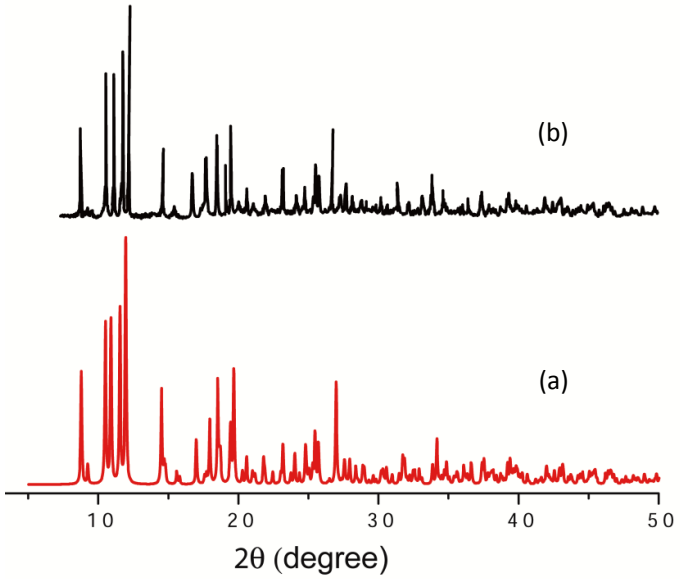

Fig. S3. PXRD patterns of **1**; (a) simulated, (b) as-synthesized.

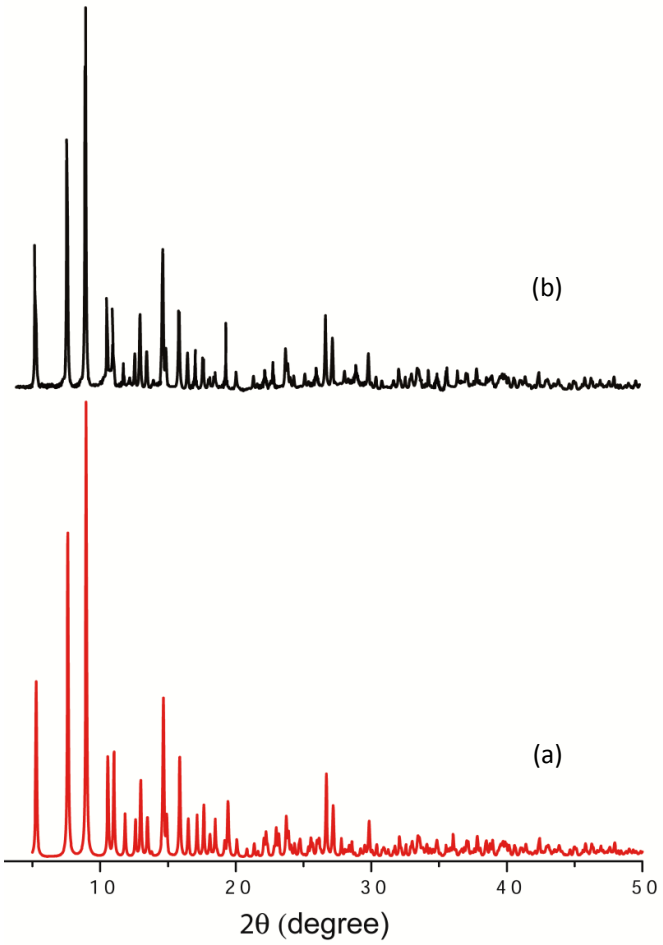

Fig. S4. PXRD patterns of **2**; (a) simulated, (b) as-synthesized.

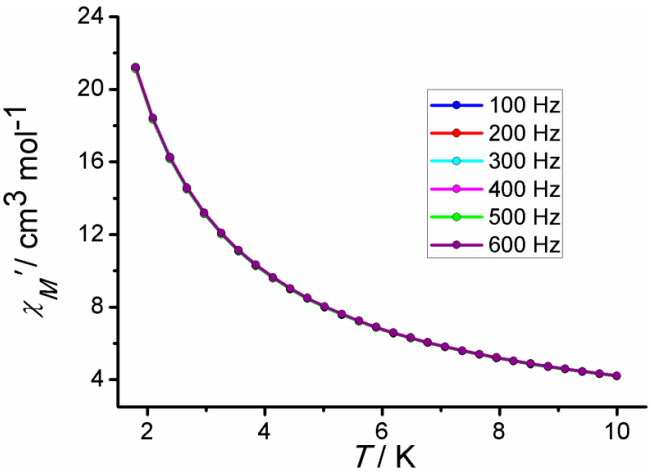

Fig. S5. χ_M' vs T for complex **1** at 0 Oe.

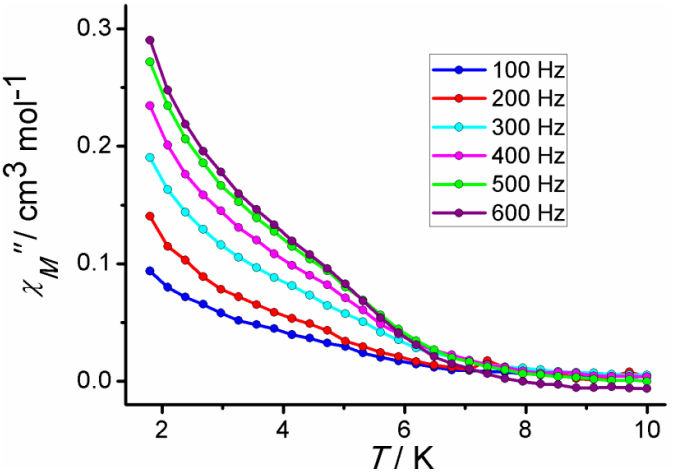

Fig. S6. χ_M'' vs T for complex **1** at 0 Oe.

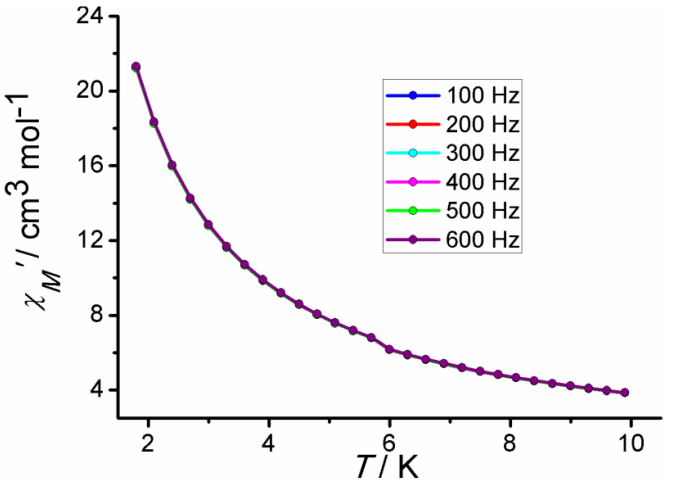

Fig. S7. χ_M' vs T for complex **2** at 0 Oe.

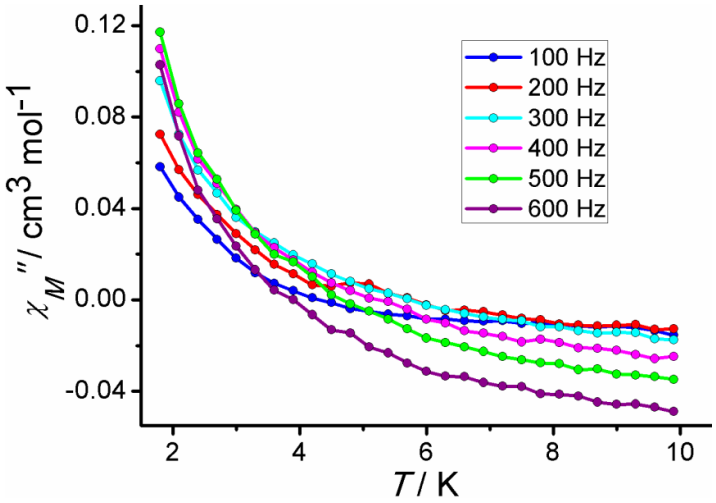

Fig. S8. χ_M'' vs T for complex **2** at 0 Oe.

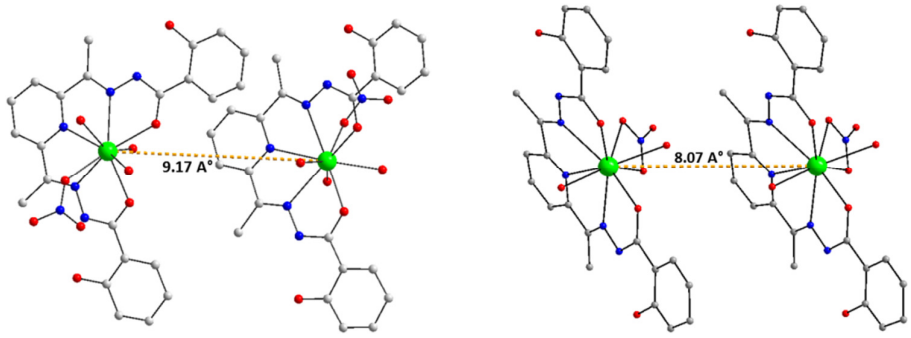

Fig. S9. Intermolecular Dy···Dy distances in complexes **1** (left) and **2** (right).

Experimental information for dilution studies:

Synthesis of [Y(H_4daps)(NO_3)$_2$(MeOH)]·(NO_3)·(MeOH) (3)

H_4daps (43 mg, 0.1 mmol) was dissolved in MeOH (5 ml) and the solution was warmed to 40°C. $Y(NO_3)_3·6H_2O$ (39 mg, 0.1 mmol) dissolved in MeOH (5 ml) was added dropwise to the above ligand solution while stirring. The resulting solution forms an intense yellow mixture that was stirred further for 1 hour. The solution was then filtered off and the filtrate was left at open atmosphere for slow evaporation which gave large X-ray quality yellow needle like crystals of [Y(H_4daps)(NO_3)$_2$(MeOH)]·(NO_3)·(MeOH) (**3**) after 2 days. The crystals were separated, washed with cold water and Et_2O and air-dried. Yield (70 %). Anal. Calcd for $C_{25}H_{28}YN_8O_{15}$: C, 39.02; H, 3.66; N, 14.56 %. Found: C, 39.13; H, 3.83; N, 14.61 %.

Table S5. X-ray Crystallographic Data and Refinement Parameters for **3**.

	3
Formula	$C_{25}H_{28}YN_8O_{15}$
M_w (g mol^{-1})	769.46
Crystal size (mm)	0.32×0.26×0.23
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
T (K)	107(2)
a (Å)	8.6524(6)
b (Å)	18.8655(11)
c (Å)	19.2015(14)
α (°)	90
β (°)	90
γ (°)	90
V (Å^3)	3134.3(4)
Z	4
ρ_{calcd} (g cm^{-3})	1.631
μ(MoKα) (mm^{-1})	1.946
F(000)	1572.0
T_{max}, T_{min}	0.639, 0.550
h, k, l range	$-11 \le h \le 11$, $-25 \le k \le 25$, $-26 \le l \le 26$
Collected reflections	8462
Independent reflections	4723
Goodness-of-fit (GOF) on F^2	0.965
R1, wR2 ($I > 2\sigma I$)	0.0604, 0.1443
R1, wR2 (all data)	0.0926, 0.1617
CCDC Number	1044379

$R1 = \Sigma||Fo| - |Fc||/\Sigma|Fo|$ and $wR2 = |\Sigma w(|Fo|^2 - |Fc|^2)|/\Sigma|w(Fo)^2|^{1/2}$

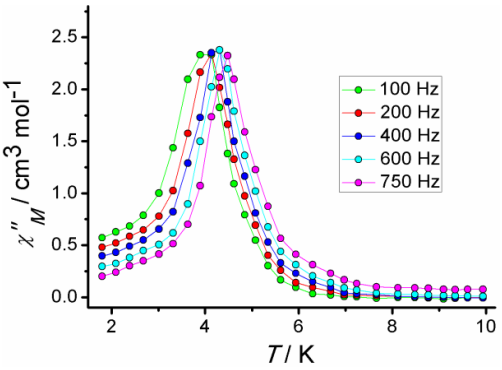

Fig. S10. Out-of-phase (χ_M'') AC magnetic susceptibility plot for a diluted (1:10) sample at 2000 Oe dc field.

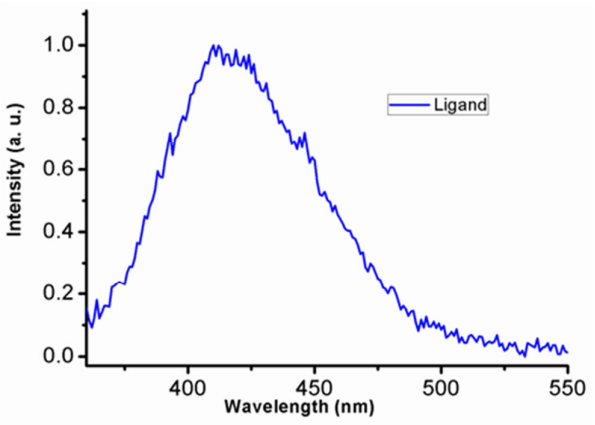

Fig. S11. The emission spectrum of the ligand (H_4daps) in solid state at room temperature with λ_{ex} = 350 nm.