Electronic Supplementary Material (ESI) for Photochemical & Photobiological Science

Supporting information

A series of mononuclear lanthanide complexes featuring 3-D supramolecular networks: Synthesis, characterization and luminescent properties for sensing guest molecules

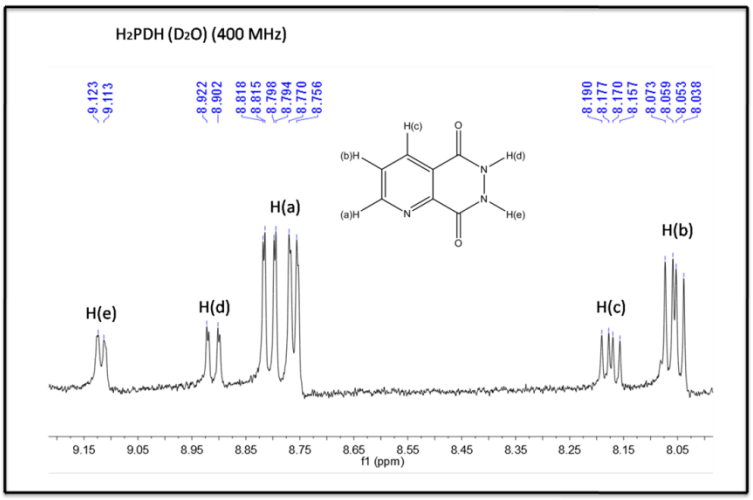

Figure S1. ^{1}HNMR spectrum of 6,7-dihydropyrido(2,3-d)pyridazine-5,8-dione at 400 MHz by using D_2O as solvent.

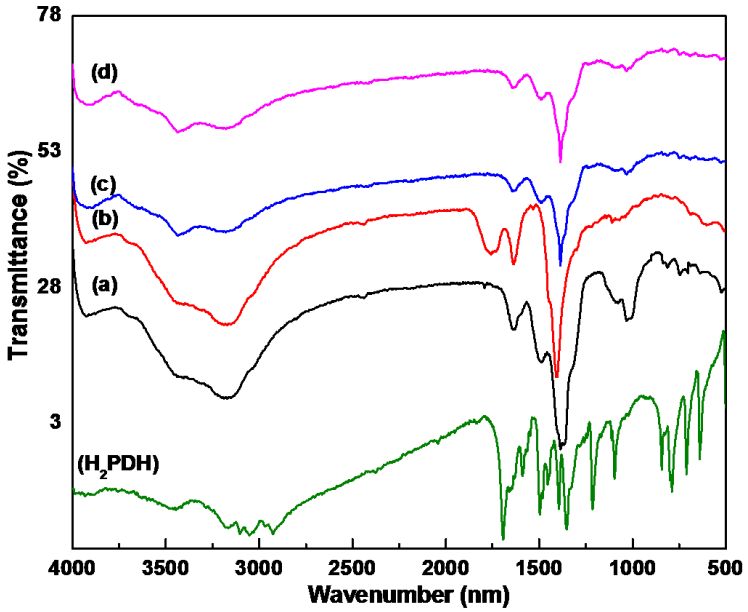

Figure S2. Infrared (IR) spectra of ligand H_2PDH and complexes **1** (a), **2** (b), **3** (c) and **4** (d).

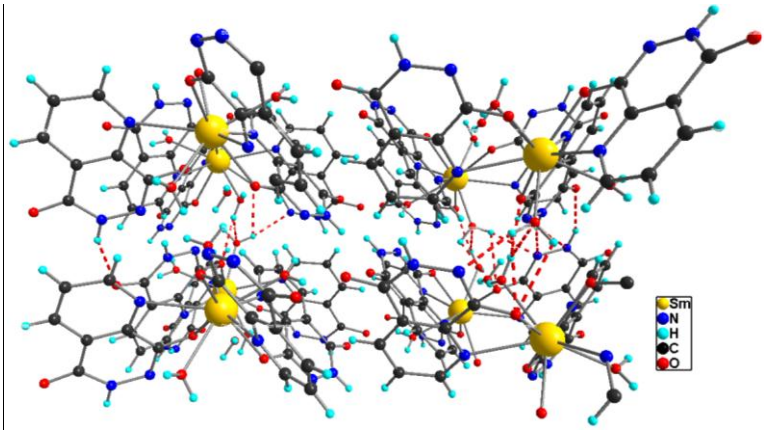

Figure S3. Hydrogen bonding interactions shown with dotted lines in red between two adjacent 2D layers.

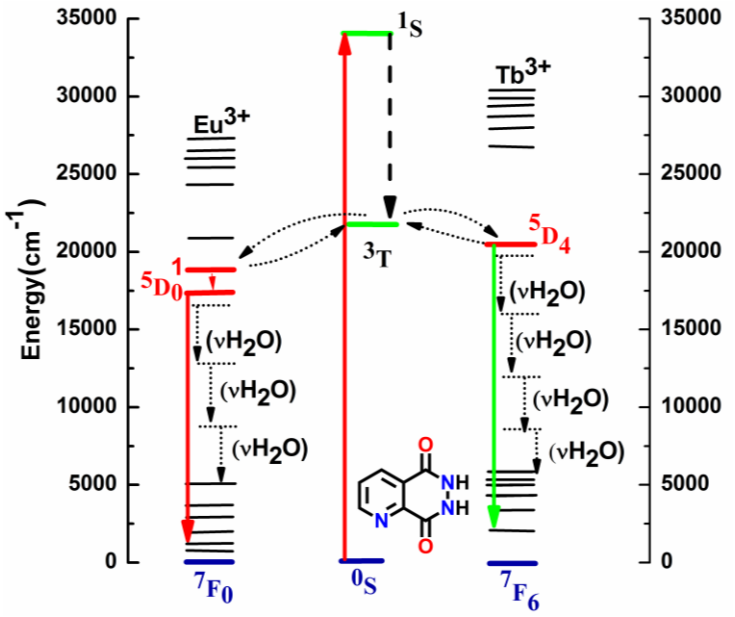

Figure S4. Energy levels of Eu(III) and Tb(III) showing nonradiative deactivation mechanism.

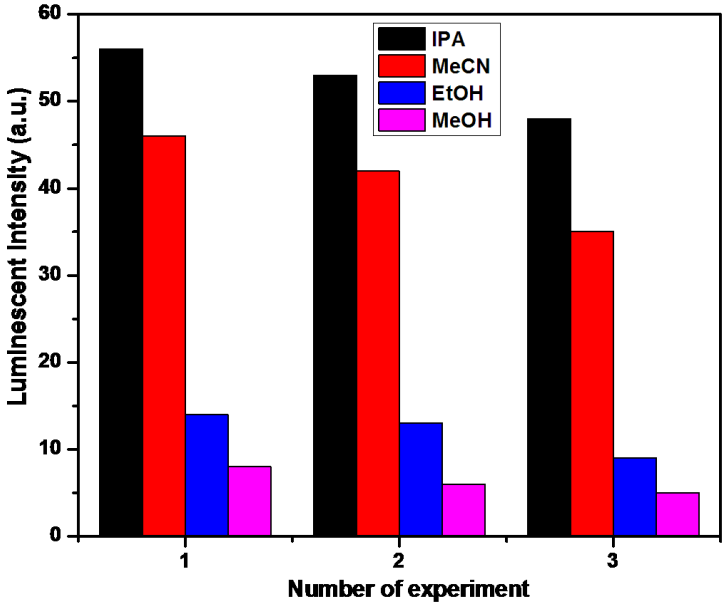

Figure S5. Reusability of the complex **3a** in IPA, MeCN, EtOH and MeOH by filtering off the dispersed solution after use, washing several times with H_2O/EtOH and drying under vacuum at 423 K for 5 h, when excited at 270 nm.

Tables

Table S1 Crystal data and structure refinement of complex **1** and complex **3**.

	Complex **1**	Complex **3**
Formula	$C_{21}H_{20}N_9O_{10}Sm$	$C_{21}H_{20}N_9O_{10}Tb$
*F*w	708.81	717.38
Crystal system	Monoclinic	Monoclinic
space group	$P2_1/c$	$P2_1/c$
a (Å)	6.0157(7)	5.9758(2)
b (Å)	21.542(4)	21.4942(13)
c (Å)	18.412(3)	18.3468(12)
α (°)	90.00	90.00
β (°)	92.247(13)	91.887(4)
γ (°)	90.00	90.00
V , Å^3	2384.2(6)	2355.3(2)
Z	4	4
ρ_{calcd}, mg/m^3	1.975	2.023
Temp, K	101.8	98.6
F(000)	1404	1416
μ, mm^{-1}	2.543	3.083
Reflections collected / unique	10193	9489
R(int)	0.0595	0.0548
*R*1, *wR*2 [I > 2ó(I)]	0.0487, 0.0834	0.0454, 0.0862
*R*1, *wR*2 (all data)	0.0744, 0.0932	0.0646, 0.0953
GOF	1.033	1.044
Largest diff. peak and hole (e·Å^{-3})	1.820 and -0.706	1.971 and -0.745
CCDC numbers	960629	960631

Table S2 Selected bond lengths [Å] and angles [°] for complex **1**.

Complex **1**			
Bond lengths			
Sm(1)-O(1)	2.351(2)	Sm(1)-O(5)	2.404(3)
Sm(1)-O(3)	2.385(3)	Sm(1)-OW(8)	2.454(4)
Sm(1)-OW(7)	2.401(3)	Sm(1)-OW(9)	2.568(3)
Sm(1)-N(1)	2.695(3)	Sm(1)-N(4)	2.741(5)
Sm(1)-N(7)	2.634(3)		
Bond angles			
O(1)-Sm(1)-N(1)	64.59(4)	O(1)-Sm(1)-O(3)	76.18(4)
O(1)-Sm(1)-OW(7)	136.32(3)	O(3)-Sm(1)-N(1)	67.85(4)
O(1)-Sm(1)-N(4)	132.43(5)	OW(7)-Sm(1)-N(4)	70.68(4)
O(1)-Sm(1)-OW(9)	79.24(4)	OW(7)-Sm(1)-OW(9)	139.26(3)
O(1)-Sm(1)-O(5)	136.76(4)	OW(7)-Sm(1)-O(5)	77.21(4)
O(1)-Sm(1)-N(7)	71.76(4)	OW(7)-Sm(1)-N(7)	132.38(4)
O(1)-Sm(1)-OW(8)	81.61(4)	OW(7)-Sm(1)-OW(8)	78.59(4)
N(1)-Sm(1)-O(3)	67.85(4)	OW(7)-Sm(1)-N(1)	71.93(3)
N(1)-Sm(1)-OW(7)	71.93(3)	N(4)-Sm(1)-OW(9)	69.32(4)
N(1)-Sm(1)-N(4)	115.33(6)	N(4)-Sm(1)-O(5)	76.97(4)
N(1)-Sm(1)-OW(9)	133.90(5)	N(4)-Sm(1)-N(7)	123.42(6)
N(1)-Sm(1)-O(5)	139.42(5)	N(4)-Sm(1)-OW(8)	145.16(4)
N(1)-Sm(1)-N(7)	120.90(5)	OW(9)-Sm(1)-O(5)	86.58(3)
N(1)-Sm(1)-OW(8)	68.07(4)	OW(9)-Sm(1)-N(7)	68.11(4)
O(3)-Sm(1)-OW(7)	91.74(3)	OW(9)-Sm(1)-OW(8)	135.57(4)
O(3)-Sm(1)-N(4)	62.73(4)	O(5)-Sm(1)-N(7)	65.04(4)
O(3)-Sm(1)-OW(9)	76.79(4)	O(5)-Sm(1)-OW(8)	80.62(5)
O(3)-Sm(1)-O(5)	139.57(5)	N(7)-Sm-OW(8)	67.89(4)
O(3)-Sm(1)-OW(8)	135.72(5)		

Table S3 Hydrogen bonds [Å] and angles [°] found in complex **1**

D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	D···H···A (°)
Inter-molecular hydrogen Bonding interaction within 1D chain				
OW8-H8b···O4	0.8464(1)	1.8965(2)	2.7078(3)	160.131(15)
Hydrogen bonding interaction between 1D chains and uncoordinated water molecules				
OW9-H9a···OW10	0.8507(1)	2.2370(3)	3.0124(4)	151.575(13)
Hydrogen bonding interaction between adjacent 2D layers				
N6-H6···O6	0.8600(1)	2.0693(3)	2.8536(4)	151.285(5)
O7-H7b···O3	0.8522(1)	2.6016(3)	2.9587(3)	106.499(6)
N9-H9···N5	0.8601(1)	2.1029(3)	2.9369(4)	163.237(9)
O7-H7a···N5	0.8473(1)	2.2190(3)	3.0550(4)	168.995(12)
O7-H7a···O3	0.8473(1)	2.5136(3)	2.9587(3)	113.777(7)
O9-H9b···O5	0.8436(1)	2.1637(3)	2.9779(3)	162.140(7)
O9-H9b···O7	0.8436(1)	2.6372(3)	3.1301(4)	118.617(8)