Supplementary Information for

Lanthanide-titanium $LnTi_{11}$ oxo-cluster, a potential molecular based fluorescent labelling agent and photocatalyst

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Figures

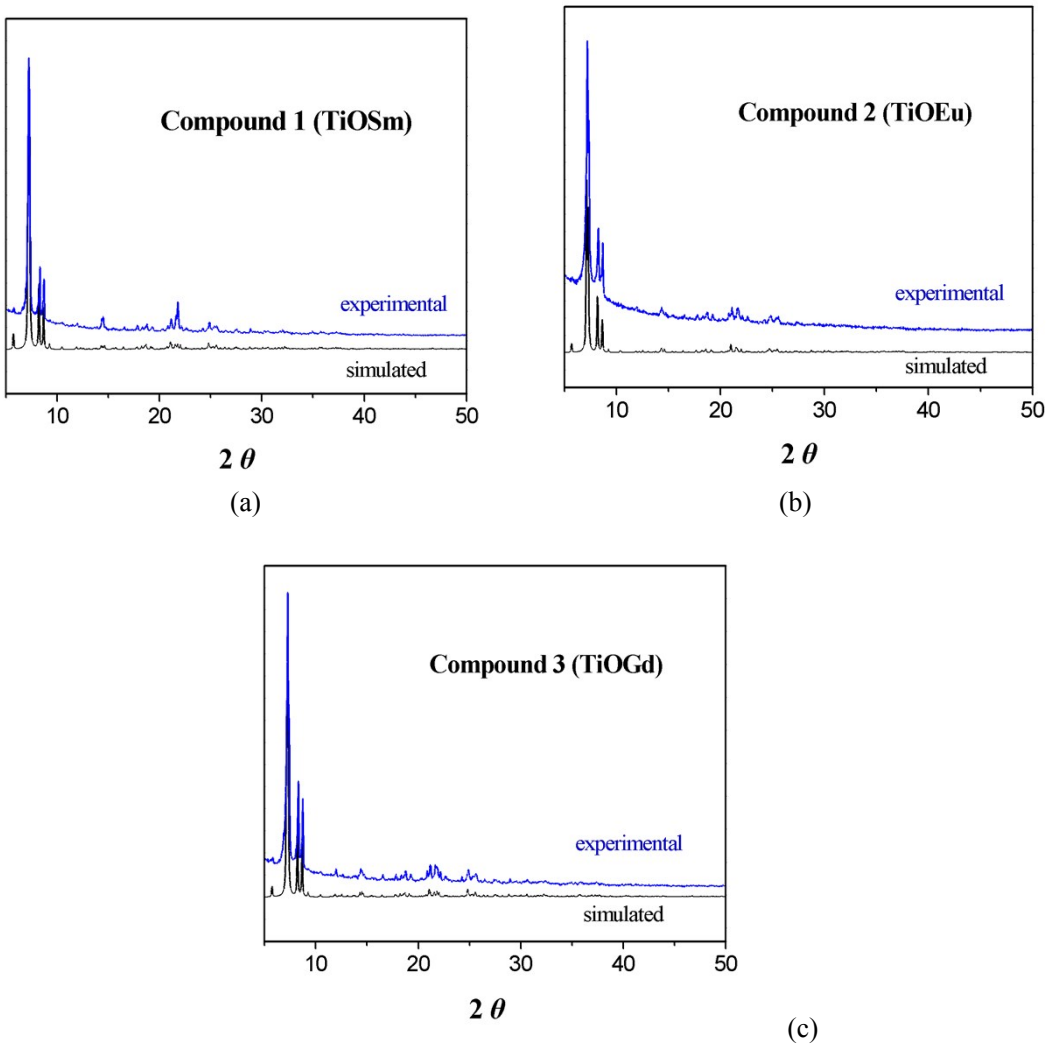


Fig. S1 XRD patterns of the microcrystal samples and that simulated from the data of single-crystal analysis.

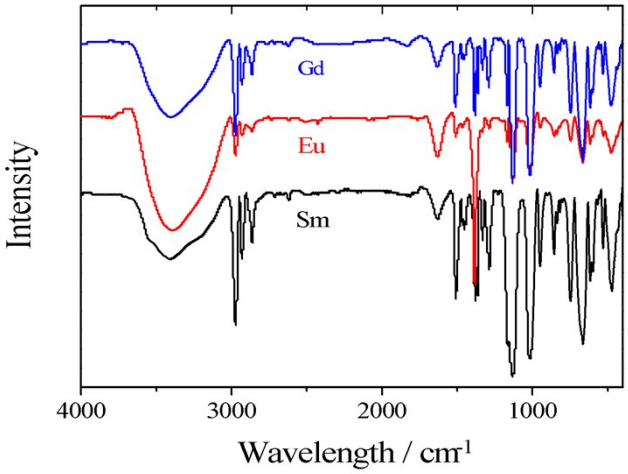


Fig. S2 IR spectra of compounds 1-3.

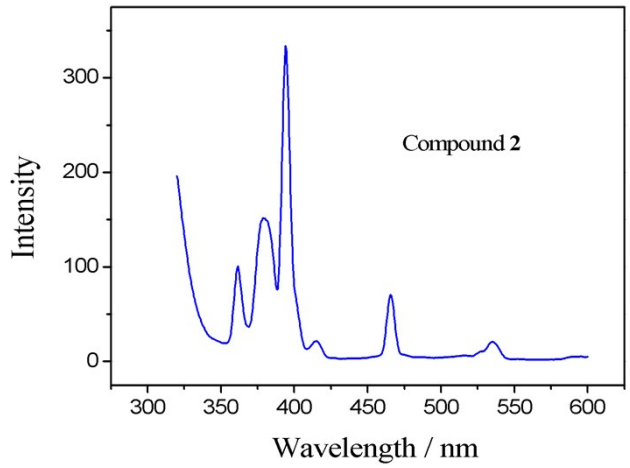
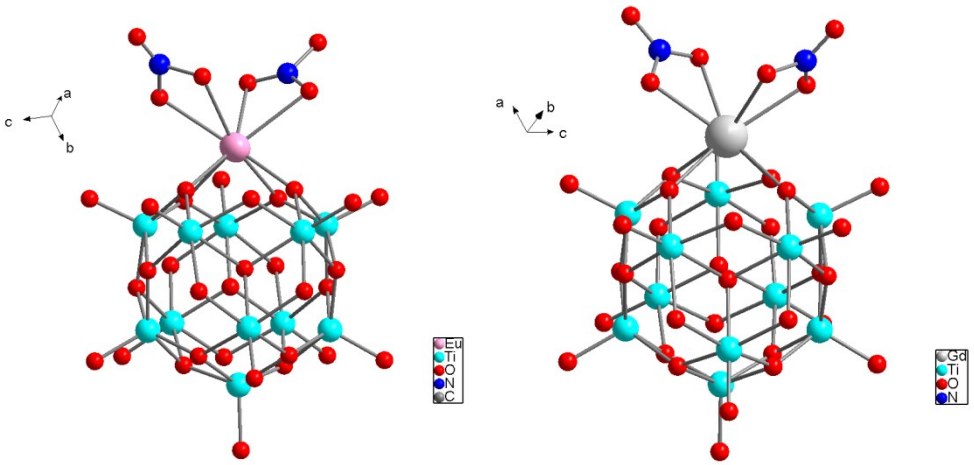


Fig. S3 Excitation spectrum of compound 2 in dichloromethane.



(a) (b)

Fig. S4 Ball-stick views of clusters **2** and **3**. Co-crystallized water molecules, carbon and hydrogen atoms are omitted for clarity.

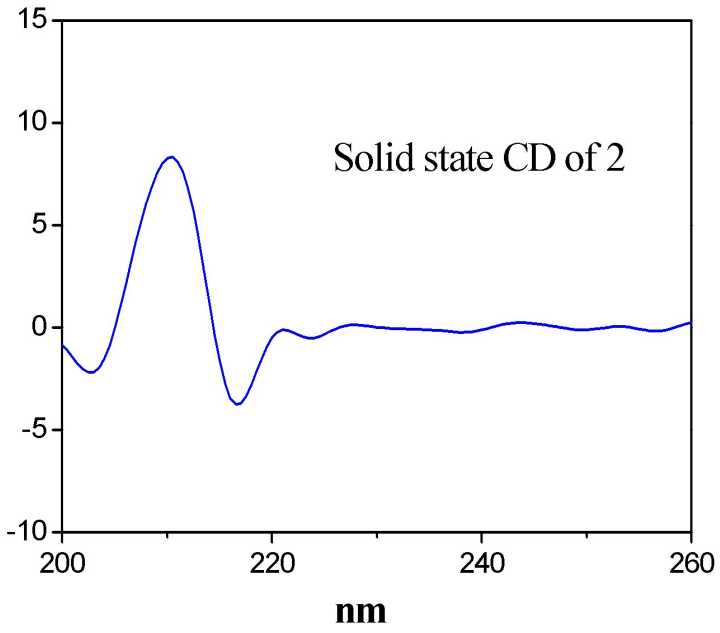


Fig. S5 The CD spectrum of **2** using a large single crystal**.**

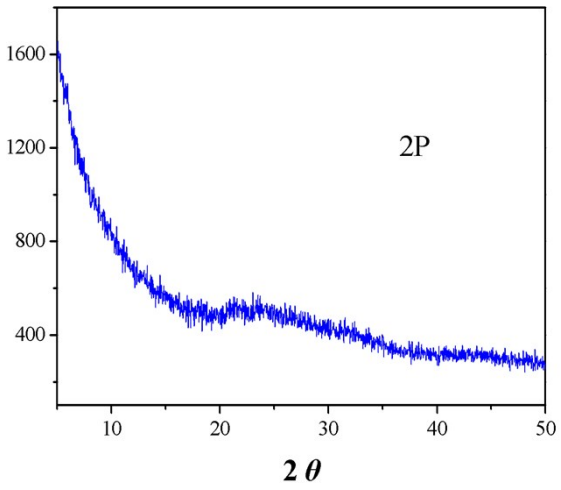


Fig. S6 PXRD result of precipitate **2P**.

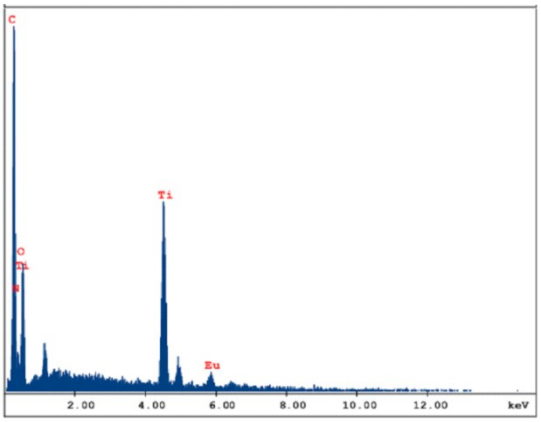


Fig. S7 EDS result of precipitate **2P**.

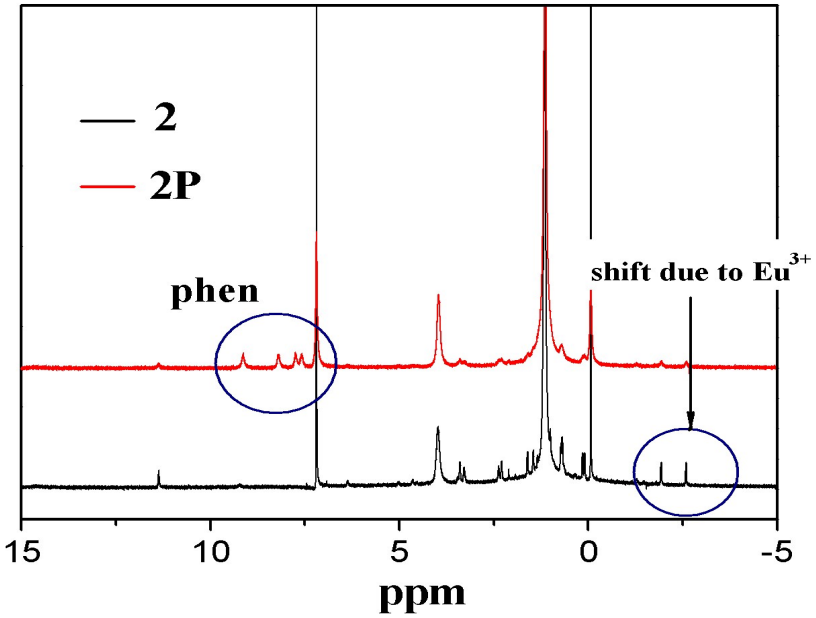
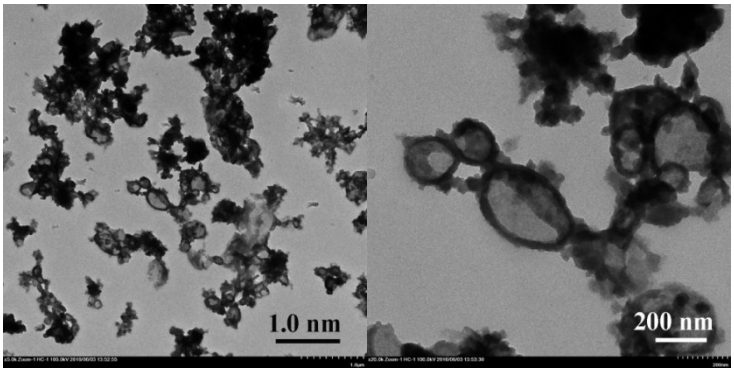


Fig. S8 The NMR results of **2** and freshly prepared **2P** in CD_3Cl.



(a) (b)

Fig. S9 TEM result of precipitate **2P**.

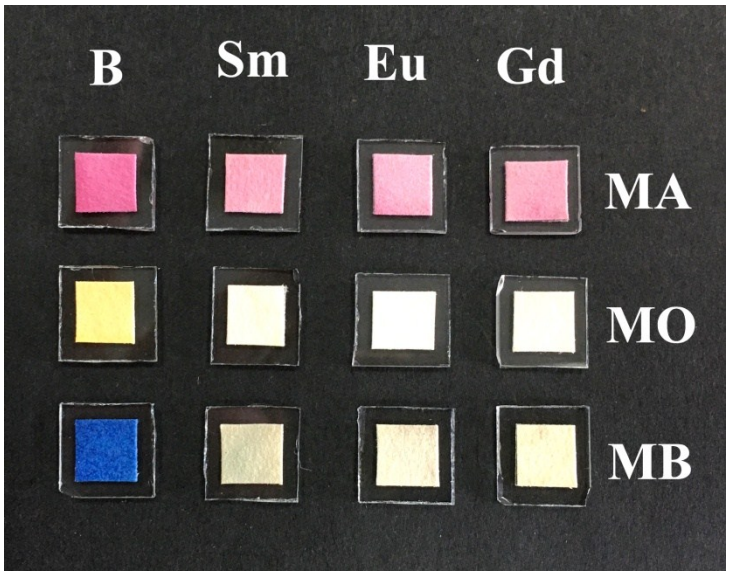


Fig. S10 Photos of the dye colored papers after UV irradiation(5 W, 60 min), (B) blank control group and Sm, Eu, Gd compounds treated groups.

Table S1 Crystal data and structural refinement parameters for **1**–**3**

	1	**2**	**3**
formula	$C_{51}H_{123}N_2O_{39}SmTi_{11}$	$C_{51}H_{123}N_2O_{39}EuTi_{11}$	$C_{51}H_{123}N_2O_{39}GdTi_{11}$
fw	2065.41	2067.01	2072.30
cryst size (mm^3)	0.20×0.60×1.00	0.20×0.50×1.00	0.20×0.45×0.70
cryst syst	monoclinic	monoclinic	monoclinic
space group	$P2_1$	$P2_1$	$P2_1$
a (Å)	15.428(3)	15.526(3)	15.393(5)
b (Å)	15.000(3)	15.035(3)	15.023(4)
c (Å)	20.388(5)	20.443(4)	20.366(6)
α (deg)	90.00	90.00	90.00
β (deg)	90.678(6)	90.31(3)	90.753(7)
γ (deg)	90.00	90.00	90.00
V ($Å^3$)	4717.7(17)	4771.9(17)	4709(2)
Z	2	2	2
ρ_{calcd} ($g\ cm^{-3}$)	1.430	1.436	1.438
F(000)	2082	2112	2086
μ (mm^{-1})	1.559	1.585	1.642
T (K)	293(2)	293(2)	293(2)
reflns collected	33794	35322	19011
unique reflns	14769	16112	13771
observed reflns	12221	8513	10887
no. params	876	853	903
flack	0.22(2)	0.38(3)	0.47(2)
GOF on F^2	1.196	1.189	1.114
R_1 [I>2σ(I)]	0.0806	0.0888	0.0683
$_wR_2$ [I>2σ(I)]	0.1568	0.1648	0.1390