Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Enhancement of near-infrared luminescence of ytterbium in triple-stranded binuclear helicates

Bing Li, Hongfeng Li,* Peng Chen, Wenbin Sun, Cheng Wang, Ting Gao and Pengfei Yan*

Key Laboratory of Functional Inorganic Material Chemistry (MOE), P. R. China; School of Chemistry and Materials Science, Heilongjiang University; No. 74, Xuefu Road, Nangang District, Harbin 150080, P. R. China.

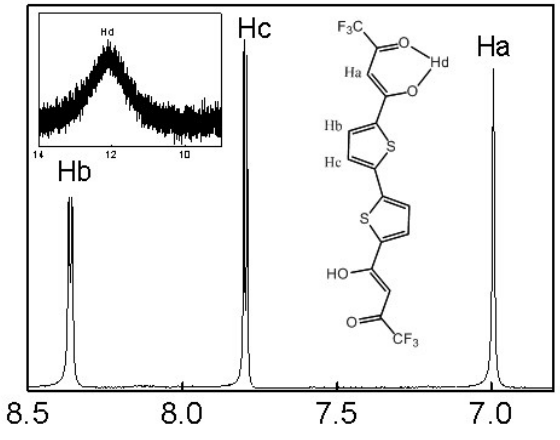


Figure S1 400 MHz ^{1}H NMR spectrum of BTT in $CDCl_3$

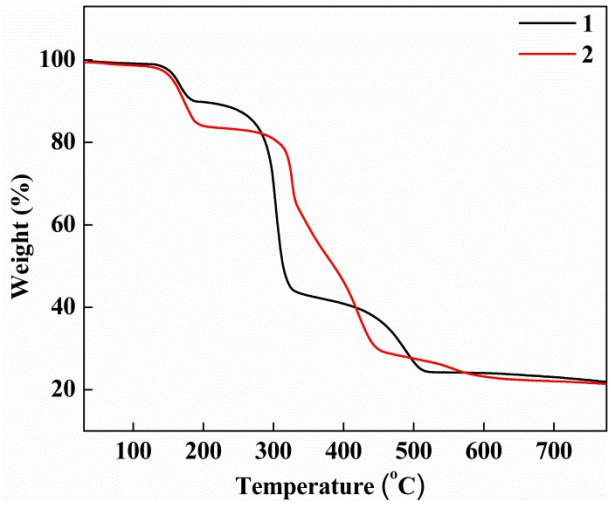


Figure S2 Thermogravimetric curves of **1** and **2**.

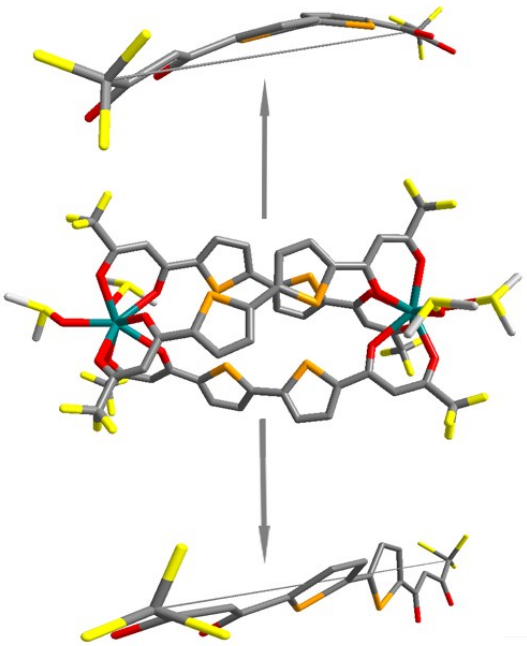


Figure S3 The bending patterns of the ligands in **2**.

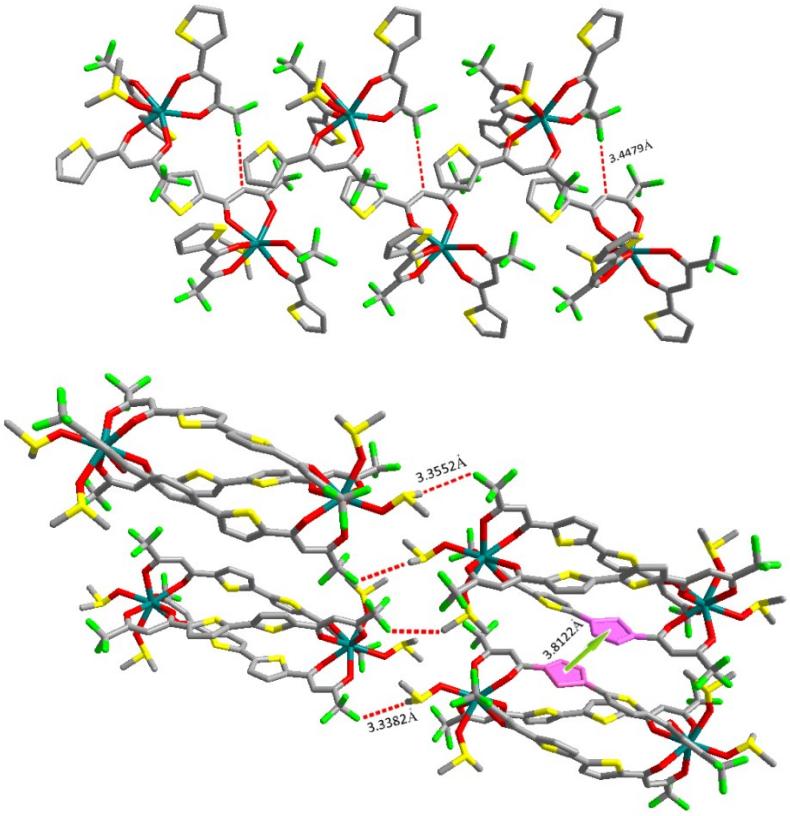


Figure S4 Intermolecular C–H···F and π···π interactions in **1** and **2.**

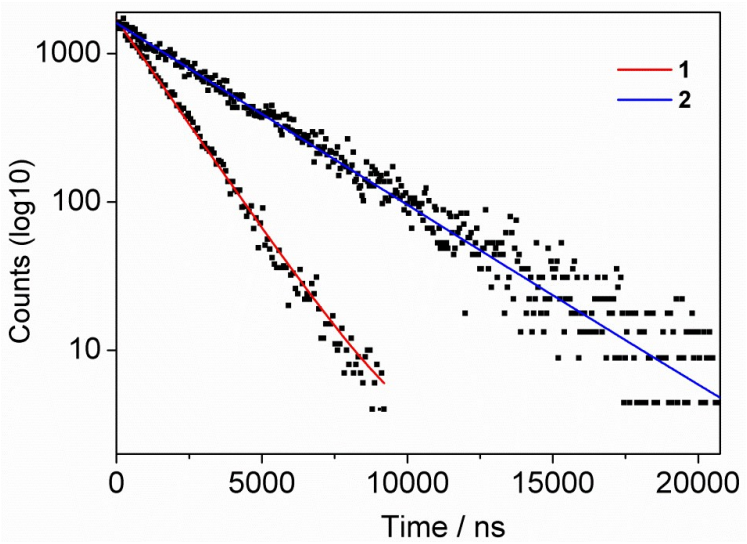


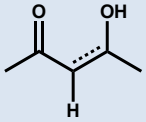
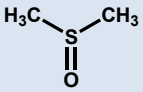
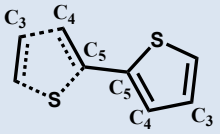
Figure S5 Luminescence decay curves of **1** and **2** monitored at 975 nm.

Table S1 Crystal data and structure refinement for **1** and **2.**

	1	**2**
formula	$C_{26}H_{18}F_9O_7S_4Yb$	$C_{60}H_{54}F_{18}Yb_2O_{18}S_{12}$
Mr	914.68	2135.83
color	colorless	yellow
cryst syst.	orthorhombic	monoclinic
space group	$P2_12_12_1$	$C2/c$
a (Å)	10.9140(3)	41.711(6)
b (Å)	11.4933(5)	11.812(17)
c (Å)	26.0098(10)	16.553(2)
α (deg)	90	90
β (deg)	90	98.582(3)
γ (deg)	90	90
V (Å^3)	3262.6(2)	8064(2)
Z	4	4
ρ (g cm^3)	1.862	1.759
μ (mm^{-1})	3.216	2.719
F (000)	1780	4208
R_1,[$I > 2\sigma(I)$]	0.0519	0.0577

wR_2,[I>2σ (I)]	0.1025	0.1365
R_1, (all data)	0.0635	0.1031
wR_2, (all date)	0.1091	0.1633
GOF on F^2	1.102	0.992

Table S2 Distance of metal centres to C–H bonds

Complexes	 **Methyne**	 **Solvents**	 **Thiophene rings**		
	Yb···$C_{methyne}$	Yb···C_{DMSO}	Yb···C_3	Yb···C_4	Yb···C_5
	3.652	4.196	5.856	6.793	6.526
1	3.680	4.855	5.839	6.846	6.551
	3.627		5.704	6.839	6.528
Average	3.653	4.526	5.866	6.826	6.535
	3.686	4.218	5.598	6.564	
2	3.726	4.224	5.778	6.715	
	3.733	4.869	5.925	6.966	
		4.772			
Average	3.715	4.520	5.767	6.748	