Construction of Terpyridine-Ln(III) Coordination Polymers: Structural Diversity, Visible and NIR Luminescence Properties and Response to Nerve-Agent Mimics

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Supporting information

Table S1 Crystallographic data and structure refinement summary for complexes **2-6**, **8**, **10** and **12**

Complex	**2**	**3**	**4**	**5**
Empirical formula	$C_{22}H_{15}N_3O_9S_2Nd$	$C_{22}H_{15}N_3O_9S_2Eu$	$C_{22}H_{15}N_3O_9S_2Tb$	$C_{22}H_{15}N_3O_9S_2Er$
Formula weight	673.73	681.45	688.41	696.75
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	*C*2/c	*C*2/c	*C*2/c	*C*2/c
a / Å	20.199(4)	20.1864(16)	20.084(4)	20.010(3)
b / Å	18.625(3)	18.5532(15)	18.534(4)	18.516(2)
c / Å	13.918(3)	13.8708(11)	13.831(4)	13.7905(18)
α / °	90	90	90	90
β / °	117.069(2)	117.3370(10)	117.639(2)	117.896(2)
γ / °	90	90	90	90
V / $Å^3$	4662.4(15)	4614.8(6)	4560.9(19)	4515.8(10)
Z	8	8	8	8
D / g cm^{-3}	1.920	1.962	2.005	2.047
μ / mm^{-1}	2.467	2.961	3.346	3.964
T / K	298(2)	298(2)	298(2)	298(2)
R^a / wR^b	0.0554 / 0.1211	0.0353 / 0.1093	0.0555 / 0.1529	0.0544 / 0.1336
Total / unique / Rint	11776 / 4092 / 0.1121	13490 / 5043 / 0.0297	13456 / 4980 / 0.0832	10984 / 4866 / 0.0716

Complex	**6**	**8**	**10**	**12**
Empirical formula	$C_{22}H_{15}N_3O_9S_2Yb$	$C_{22}H_{23}N_3O_{13}S_2Yb$	$C_{25}H_{29}N_3O_{15}S_2Yb$	$C_{25}H_{19}N_3O_{10}S_2Dy$
Formula weight	702.53	774.59	849.60	748.05
Crystal system	Monoclinic	Monoclinic	Monoclinic	Triclinic
Space group	*C*2/c	*P*2(1)/c	*C*2/c	*P*-1
a / Å	19.952(7)	8.9698(6)	19.408(6)	10.744(3)
b / Å	18.500(6)	21.7582(15)	13.692(4)	11.964(3)
c / Å	13.756(5)	13.4973(10)	23.830(7)	12.004(6)
α / °	90	90	90	109.647(4)
β / °	117.935(4)	92.1640(10)	90.937(4)	103.175(4)
γ / °	90	90	90	109.375(3)
V / $Å^3$	4486(3)	2632.3(3)	6332(3)	1266.9(8)
Z	8	4	8	2
D / g cm^{-3}	2.080	1.955	1.781	1.961
μ / mm^{-1}	4.419	3.786	3.161	3.181
T / K	298(2)	298(2)	298(2)	298(2)
R^a / wR^b	0.0473 / 0.1197	0.0302 / 0.0792	0.0473 / 0.1245	0.0459 / 0.1222
Total / unique / Rint	12818 / 4880 / 0.0640	15346 / 5708 / 0.0310	17817/ 6895 / 0.0551	6367 / 4381 / 0.0293

Table S**2** Selected bond lengths [Å] and angles[°] for the complexes.[a]

Complex **1**

Gd(1)-O(1W)	2.277(4)	Gd(1)-O(1W)#1	2.297(4)
Gd(1)-O(3W)	2.393(5)	Gd(1)-O(2W)	2.430(5)
Gd(1)-O(4)	2.461(4)	Gd(1)-N(1)#2	2.527(6)
Gd(1)-N(3)#2	2.594(5)	Gd(1)-N(2)#2	2.596(5)
Gd(1)-Gd(1)#1	3.8023(6)		
O(1W)-Gd(1)-O(1W)#1	67.54(16)	O(1W)-Gd(1)-O(3W)	102.79(16)
O(1W)#1-Gd(1)-O(3W)	81.48(17)	O(1W)-Gd(1)-O(2W)	141.10(15)
O(1W)#1-Gd(1)-O(2W)	74.74(16)	O(3W)-Gd(1)-O(2W)	80.1(2)
O(1W)-Gd(1)-O(4)	148.25(14)	O(1W)#1-Gd(1)-O(4)	144.10(14)
O(3W)-Gd(1)-O(4)	84.90(15)	O(2W)-Gd(1)-O(4)	70.27(15)
O(1W)-Gd(1)-N(1)#2	90.79(17)	O(1W)#1-Gd(1)-N(1)#2	85.97(17)
O(3W)-Gd(1)-N(1)#2	156.23(17)	O(2W)-Gd(1)-N(1)#2	77.1(2)
O(4)-Gd(1)-N(1)#2	93.78(17)	O(1W)-Gd(1)-N(3)#2	78.01(15)
O(1W)#1-Gd(1)-N(3)#2	133.56(15)	O(3W)-Gd(1)-N(3)#2	76.70(16)
O(2W)-Gd(1)-N(3)#2	138.57(15)	O(4)-Gd(1)-N(3)#2	73.86(15)
N(1)#2-Gd(1)-N(3)#2	125.76(16)	O(1W)-Gd(1)-N(2)#2	84.56(15)
O(1W)#1-Gd(1)-N(2)#2	138.51(14)	O(3W)-Gd(1)-N(2)#2	136.35(16)
O(2W)-Gd(1)-N(2)#2	120.3(2)	O(4)-Gd(1)-N(2)#2	69.66(14)
N(1)#2-Gd(1)-N(2)#2	63.51(16)	N(3)#2-Gd(1)-N(2)#2	62.68(15)
O(1W)-Gd(1)-Gd(1)#1	33.94(10)	O(1W)#1-Gd(1)-Gd(1)#1	33.60(10)
O(3W)-Gd(1)-Gd(1)#1	92.47(11)	O(2W)-Gd(1)-Gd(1)#1	107.88(12)
O(4)-Gd(1)-Gd(1)#1	176.99(10)	N(1)#2-Gd(1)-Gd(1)#1	88.04(13)
N(3)#2-Gd(1)-Gd(1)#1	106.98(10)	N(2)#2-Gd(1)-Gd(1)#1	113.32(10)

Complex **2**

Nd(1)-O(3)#1	2.421(7)	Nd(1)-O(8)#2	2.443(9)
Nd(1)-O(7)	2.444(8)	Nd(1)-O(5)#3	2.485(7)
Nd(1)-O(4)#4	2.523(8)	Nd(1)-N(3)	2.539(9)
Nd(1)-N(1)	2.540(10)	Nd(1)-N(2)	2.597(8)
O(3)#1-Nd(1)-O(8)#2	75.4(3)	O(3)#1-Nd(1)-O(7)	73.9(3)

O(8)#2-Nd(1)-O(7)	68.3(3)	O(3)#1-Nd(1)-O(5)#3	142.9(3)
O(8)#2-Nd(1)-O(5)#3	80.2(3)	O(7)-Nd(1)-O(5)#3	71.2(3)
O(3)#1-Nd(1)-O(4)#4	140.8(2)	O(8)#2-Nd(1)-O(4)#4	130.6(3)
O(7)-Nd(1)-O(4)#4	138.1(3)	O(5)#3-Nd(1)-O(4)#4	76.1(2)
O(3)#1-Nd(1)-N(3)	75.7(3)	O(8)#2-Nd(1)-N(3)	83.2(3)
O(7)-Nd(1)-N(3)	142.5(3)	O(5)#3-Nd(1)-N(3)	128.7(3)
O(4)#4-Nd(1)-N(3)	79.1(3)	O(3)#1-Nd(1)-N(1)	89.0(3)
O(8)#2-Nd(1)-N(1)	141.9(3)	O(7)-Nd(1)-N(1)	74.1(3)
O(5)#3-Nd(1)-N(1)	93.5(3)	O(4)#4-Nd(1)-N(1)	82.7(3)
N(3)-Nd(1)-N(1)	126.8(3)	O(3)#1-Nd(1)-N(2)	75.0(3)
O(8)#2-Nd(1)-N(2)	140.2(3)	O(7)-Nd(1)-N(2)	126.3(3)
O(5)#3-Nd(1)-N(2)	137.8(3)	O(4)#4-Nd(1)-N(2)	67.2(2)
N(3)-Nd(1)-N(2)	64.2(3)	N(1)-Nd(1)-N(2)	62.7(3)

Complex **3**

Eu(1)-O(3)#1	2.357(4)	Eu(1)-O(8)#2	2.405(4)
Eu(1)-O(7)	2.414(4)	Eu(1)-O(5)#3	2.427(4)
Eu(1)-O(4)#4	2.452(3)	Eu(1)-N(3)	2.502(4)
Eu(1)-N(1)	2.518(5)	Eu(1)-N(2)	2.551(4)
Eu(1)-C(22)#2	3.202(5)	Eu(1)-C(22)	3.228(5)
Eu(1)-S(2)#3	3.4502(12)		
O(3)#1-Eu(1)-O(8)#2	76.49(14)	O(3)#1-Eu(1)-O(7)	74.29(14)
O(8)#2-Eu(1)-O(7)	67.78(13)	O(3)#1-Eu(1)-O(5)#3	144.25(13)
O(8)#2-Eu(1)-O(5)#3	78.00(14)	O(7)-Eu(1)-O(5)#3	73.08(14)
O(3)#1-Eu(1)-O(4)#4	141.88(12)	O(8)#2-Eu(1)-O(4)#4	129.18(12)
O(7)-Eu(1)-O(4)#4	137.28(13)	O(5)#3-Eu(1)-O(4)#4	73.82(12)
O(3)#1-Eu(1)-N(3)	77.25(16)	O(8)#2-Eu(1)-N(3)	82.48(13)
O(7)-Eu(1)-N(3)	142.64(13)	O(5)#3-Eu(1)-N(3)	123.47(15)
O(4)#4-Eu(1)-N(3)	79.16(13)	O(3)#1-Eu(1)-N(1)	89.26(17)
O(8)#2-Eu(1)-N(1)	142.34(14)	O(7)-Eu(1)-N(1)	74.87(14)
O(5)#3-Eu(1)-N(1)	95.97(16)	O(4)#4-Eu(1)-N(1)	82.55(14)
N(3)-Eu(1)-N(1)	128.59(13)	O(3)#1-Eu(1)-N(2)	75.18(12)
O(8)#2-Eu(1)-N(2)	140.26(14)	O(7)-Eu(1)-N(2)	128.35(13)
O(5)#3-Eu(1)-N(2)	138.28(13)	O(4)#4-Eu(1)-N(2)	67.73(11)
N(3)-Eu(1)-N(2)	64.51(13)	N(1)-Eu(1)-N(2)	64.09(13)
O(3)#1-Eu(1)-C(22)#2	71.66(13)	O(8)#2-Eu(1)-C(22)#2	20.10(14)
O(7)-Eu(1)-C(22)#2	47.77(13)	O(5)#3-Eu(1)-C(22)#2	75.76(13)
O(4)#4-Eu(1)-C(22)#2	142.47(12)	N(3)-Eu(1)-C(22)#2	100.25(13)
N(1)-Eu(1)-C(22)#2	122.26(14)	N(2)-Eu(1)-C(22)#2	145.95(12)
O(3)#1-Eu(1)-C(22)	70.60(13)	O(8)#2-Eu(1)-C(22)	48.10(14)
O(7)-Eu(1)-C(22)	19.78(14)	O(5)#3-Eu(1)-C(22)	73.75(13)
O(4)#4-Eu(1)-C(22)	146.89(12)	N(3)-Eu(1)-C(22)	125.37(13)
N(1)-Eu(1)-C(22)	94.35(14)	N(2)-Eu(1)-C(22)	139.62(12)
C(22)#2-Eu(1)-C(22)	28.03(19)	O(3)#1-Eu(1)-S(2)#3	151.29(10)
O(8)#2-Eu(1)-S(2)#3	75.10(10)	O(7)-Eu(1)-S(2)#3	91.13(9)
O(5)#3-Eu(1)-S(2)#3	20.70(11)	O(4)#4-Eu(1)-S(2)#3	63.76(8)
N(3)-Eu(1)-S(2)#3	102.90(9)	N(1)-Eu(1)-S(2)#3	111.04(11)
N(2)-Eu(1)-S(2)#3	131.41(9)	C(22)#2-Eu(1)-S(2)#3	80.20(9)
C(22)-Eu(1)-S(2)#3	87.25(9)		

Complex **4**

Tb(1)-O(3)#1	2.322(8)	Tb(1)-O(8)#2	2.379(9)
Tb(1)-O(7)	2.388(8)	Tb(1)-O(5)#3	2.396(9)
Tb(1)-O(4)#4	2.409(8)	Tb(1)-N(3)	2.462(10)
Tb(1)-N(1)	2.491(10)	Tb(1)-N(2)	2.514(9)
O(3)#1-Tb(1)-O(8)#2	76.3(3)	O(3)#1-Tb(1)-O(7)	74.7(3)
O(8)#2-Tb(1)-O(7)	68.1(3)	O(3)#1-Tb(1)-O(5)#3	144.4(3)
O(8)#2-Tb(1)-O(5)#3	77.2(3)	O(7)-Tb(1)-O(5)#3	73.5(3)

O(3)#1-Tb(1)-O(4)#4	142.1(3)	O(8)#2-Tb(1)-O(4)#4	128.8(3)
O(7)-Tb(1)-O(4)#4	137.0(3)	O(5)#3-Tb(1)-O(4)#4	73.5(3)
O(3)#1-Tb(1)-N(3)	77.7(3)	O(8)#2-Tb(1)-N(3)	81.3(3)
O(7)-Tb(1)-N(3)	142.6(3)	O(5)#3-Tb(1)-N(3)	121.0(3)
O(4)#4-Tb(1)-N(3)	79.1(3)	O(3)#1-Tb(1)-N(1)	90.0(4)
O(8)#2-Tb(1)-N(1)	142.8(3)	O(7)-Tb(1)-N(1)	75.0(3)
O(5)#3-Tb(1)-N(1)	97.0(3)	O(4)#4-Tb(1)-N(1)	82.3(3)
N(3)-Tb(1)-N(1)	129.9(3)	O(3)#1-Tb(1)-N(2)	75.1(3)
O(8)#2-Tb(1)-N(2)	139.5(3)	O(7)-Tb(1)-N(2)	128.9(3)
O(5)#3-Tb(1)-N(2)	139.0(3)	O(4)#4-Tb(1)-N(2)	68.0(3)
N(3)-Tb(1)-N(2)	65.1(3)	N(1)-Tb(1)-N(2)	64.8(3)

Complex **5**

Er(1)-O(3)#1	2.291(6)	Er(1)-O(7)	2.352(6)
Er(1)-O(5)#2	2.358(6)	Er(1)-O(8)#3	2.360(6)
Er(1)-O(4)#4	2.389(6)	Er(1)-N(1)	2.447(9)
Er(1)-N(3)	2.447(8)	Er(1)-N(2)	2.487(7)
O(3)#1-Er(1)-O(7)	75.0(2)	O(3)#1-Er(1)-O(5)#2	145.1(2)
O(7)-Er(1)-O(5)#2	74.5(2)	O(3)#1-Er(1)-O(8)#3	77.6(2)
O(7)-Er(1)-O(8)#3	68.9(2)	O(5)#2-Er(1)-O(8)#3	76.0(2)
O(3)#1-Er(1)-O(4)#4	142.7(2)	O(7)-Er(1)-O(4)#4	136.0(2)
O(5)#2-Er(1)-O(4)#4	72.1(2)	O(8)#3-Er(1)-O(4)#4	127.4(2)
O(3)#1-Er(1)-N(1)	90.0(3)	O(7)-Er(1)-N(1)	74.7(2)
O(5)#2-Er(1)-N(1)	97.8(3)	O(8)#3-Er(1)-N(1)	143.4(3)
O(4)#4-Er(1)-N(1)	82.2(2)	O(3)#1-Er(1)-N(3)	79.3(3)
O(7)-Er(1)-N(3)	143.1(2)	O(5)#2-Er(1)-N(3)	117.7(2)
O(8)#3-Er(1)-N(3)	80.2(2)	O(4)#4-Er(1)-N(3)	79.1(2)
N(1)-Er(1)-N(3)	131.6(3)	O(3)#1-Er(1)-N(2)	75.1(2)
O(7)-Er(1)-N(2)	129.7(2)	O(5)#2-Er(1)-N(2)	138.8(2)
O(8)#3-Er(1)-N(2)	139.5(2)	O(4)#4-Er(1)-N(2)	68.5(2)
N(1)-Er(1)-N(2)	65.9(3)	N(3)-Er(1)-N(2)	65.7(3)

Complex **6**

Yb(1)-O(3)#1	2.255(6)	Yb(1)-O(5)#2	2.341(5)
Yb(1)-O(8)#3	2.343(6)	Yb(1)-O(7)	2.348(5)
Yb(1)-O(4)#4	2.374(5)	Yb(1)-N(1)	2.432(7)
Yb(1)-N(3)	2.442(7)	Yb(1)-N(2)	2.450(6)
Yb(1)-C(22)#3	3.141(9)	Yb(1)-C(22)	3.149(8)
O(3)#1-Yb(1)-O(5)#2	145.9(2)	O(3)#1-Yb(1)-O(8)#3	77.7(2)
O(5)#2-Yb(1)-O(8)#3	76.1(2)	O(3)#1-Yb(1)-O(7)	76.1(2)
O(5)#2-Yb(1)-O(7)	74.4(2)	O(8)#3-Yb(1)-O(7)	69.34(19)
O(3)#1-Yb(1)-O(4)#4	142.20(18)	O(5)#2-Yb(1)-O(4)#4	71.91(18)
O(8)#3-Yb(1)-O(4)#4	127.27(18)	O(7)-Yb(1)-O(4)#4	135.5(2)
O(3)#1-Yb(1)-N(1)	90.8(2)	O(5)#2-Yb(1)-N(1)	97.6(2)
O(8)#3-Yb(1)-N(1)	143.8(2)	O(7)-Yb(1)-N(1)	74.6(2)
O(4)#4-Yb(1)-N(1)	81.9(2)	O(3)#1-Yb(1)-N(3)	78.9(2)
O(5)#2-Yb(1)-N(3)	116.8(2)	O(8)#3-Yb(1)-N(3)	79.5(2)
O(7)-Yb(1)-N(3)	143.4(2)	O(4)#4-Yb(1)-N(3)	79.1(2)
N(1)-Yb(1)-N(3)	132.3(2)	O(3)#1-Yb(1)-N(2)	74.8(2)
O(5)#2-Yb(1)-N(2)	138.5(2)	O(8)#3-Yb(1)-N(2)	139.5(2)
O(7)-Yb(1)-N(2)	129.73(19)	O(4)#4-Yb(1)-N(2)	68.35(19)
N(1)-Yb(1)-N(2)	65.8(2)	N(3)-Yb(1)-N(2)	66.5(2)
O(3)#1-Yb(1)-C(22)#3	73.5(2)	O(5)#2-Yb(1)-C(22)#3	74.3(2)
O(8)#3-Yb(1)-C(22)#3	20.6(2)	O(7)-Yb(1)-C(22)#3	48.8(2)
O(4)#4-Yb(1)-C(22)#3	140.21(19)	N(1)-Yb(1)-C(22)#3	123.2(2)
N(3)-Yb(1)-C(22)#3	98.4(2)	N(2)-Yb(1)-C(22)#3	147.0(2)
O(3)#1-Yb(1)-C(22)	73.1(2)	O(5)#2-Yb(1)-C(22)	73.3(2)
O(8)#3-Yb(1)-C(22)	49.0(2)	O(7)-Yb(1)-C(22)	20.3(2)

O(4)#4-Yb(1)-C(22)	144.2(2)	N(1)-Yb(1)-C(22)	94.8(2)
N(3)-Yb(1)-C(22)	125.0(2)	N(2)-Yb(1)-C(22)	142.0(2)
C(22)#3-Yb(1)-C(22)	28.5(3)	O(5)#2-Yb(1)-C(22)	

Complex **7**

Lu(1)-O(3)#1	2.252(5)	Lu(1)-O(8)#2	2.327(6)
Lu(1)-O(5)#3	2.335(5)	Lu(1)-O(7)	2.337(5)
Lu(1)-O(4)#4	2.361(5)	Lu(1)-N(3)	2.423(6)
Lu(1)-N(1)	2.436(7)	Lu(1)-N(2)	2.442(6)
O(3)#1-Lu(1)-O(8)#2	77.6(2)	O(3)#1-Lu(1)-O(5)#3	145.8(2)
O(8)#2-Lu(1)-O(5)#3	76.1(2)	O(3)#1-Lu(1)-O(7)	76.2(2)
O(8)#2-Lu(1)-O(7)	69.86(19)	O(5)#3-Lu(1)-O(7)	74.46(19)
O(3)#1-Lu(1)-O(4)#4	142.13(19)	O(8)#2-Lu(1)-O(4)#4	127.00(19)
O(5)#3-Lu(1)-O(4)#4	72.02(18)	O(7)-Lu(1)-O(4)#4	135.57(18)
O(3)#1-Lu(1)-N(3)	79.2(2)	O(8)#2-Lu(1)-N(3)	78.9(2)
O(5)#3-Lu(1)-N(3)	116.3(2)	O(7)-Lu(1)-N(3)	143.5(2)
O(4)#4-Lu(1)-N(3)	78.7(2)	O(3)#1-Lu(1)-N(1)	91.0(2)
O(8)#2-Lu(1)-N(1)	143.4(2)	O(5)#3-Lu(1)-N(1)	97.2(2)
O(7)-Lu(1)-N(1)	73.7(2)	O(4)#4-Lu(1)-N(1)	82.4(2)
N(3)-Lu(1)-N(1)	133.4(2)	O(3)#1-Lu(1)-N(2)	74.8(2)
O(8)#2-Lu(1)-N(2)	139.1(2)	O(5)#3-Lu(1)-N(2)	138.7(2)
O(7)-Lu(1)-N(2)	129.8(2)	O(4)#4-Lu(1)-N(2)	68.31(19)
N(3)-Lu(1)-N(2)	66.7(2)	N(1)-Lu(1)-N(2)	66.8(2)

Complex **8**

Yb(1)-O(6)#1	2.269(3)	Yb(1)-O(8)#2	2.295(3)
Yb(1)-O(1W)	2.304(3)	Yb(1)-O(2)#3	2.309(3)
Yb(1)-O(7)	2.329(3)	Yb(1)-N(1)	2.456(3)
Yb(1)-N(2)	2.461(3)	Yb(1)-N(3)	2.483(3)
Yb(1)-C(22)#2	3.091(4)	Yb(1)-C(22)	3.119(4)
O(6)#1-Yb(1)-O(8)#2	84.09(10)	O(6)#1-Yb(1)-O(1W)	79.77(11)
O(8)#2-Yb(1)-O(1W)	141.09(10)	O(6)#1-Yb(1)-O(2)#3	102.15(11)
O(8)#2-Yb(1)-O(2)#3	147.14(10)	O(1W)-Yb(1)-O(2)#3	71.38(11)
O(6)#1-Yb(1)-O(7)	80.05(11)	O(8)#2-Yb(1)-O(7)	70.42(9)
O(1W)-Yb(1)-O(7)	72.04(11)	O(2)#3-Yb(1)-O(7)	142.27(10)
O(6)#1-Yb(1)-N(1)	152.40(12)	O(8)#2-Yb(1)-N(1)	97.11(11)
O(1W)-Yb(1)-N(1)	82.34(12)	O(2)#3-Yb(1)-N(1)	91.75(12)
O(7)-Yb(1)-N(1)	74.51(11)	O(6)#1-Yb(1)-N(2)	138.92(11)
O(8)#2-Yb(1)-N(2)	72.00(11)	O(1W)-Yb(1)-N(2)	138.43(12)
O(2)#3-Yb(1)-N(2)	83.18(11)	O(7)-Yb(1)-N(2)	120.00(11)
N(1)-Yb(1)-N(2)	65.78(11)	O(6)#1-Yb(1)-N(3)	76.56(11)
O(8)#2-Yb(1)-N(3)	76.35(11)	O(1W)-Yb(1)-N(3)	132.25(11)
O(2)#3-Yb(1)-N(3)	73.94(11)	O(7)-Yb(1)-N(3)	140.90(11)
N(1)-Yb(1)-N(3)	130.66(11)	N(2)-Yb(1)-N(3)	65.76(11)
O(6)#1-Yb(1)-C(22)#2	80.50(10)	O(8)#2-Yb(1)-C(22)#2	20.66(9)
O(1W)-Yb(1)-C(22)#2	120.81(11)	O(2)#3-Yb(1)-C(22)#2	167.77(10)
O(7)-Yb(1)-C(22)#2	49.79(10)	N(1)-Yb(1)-C(22)#2	90.95(11)
N(2)-Yb(1)-C(22)#2	87.07(11)	N(3)-Yb(1)-C(22)#2	95.34(11)
O(6)#1-Yb(1)-C(22)	78.51(10)	O(8)#2-Yb(1)-C(22)	49.60(9)
O(1W)-Yb(1)-C(22)	92.34(11)	O(2)#3-Yb(1)-C(22)	163.13(10)
O(7)-Yb(1)-C(22)	20.86(9)	N(1)-Yb(1)-C(22)	81.41(11)
N(2)-Yb(1)-C(22)	107.59(11)	N(3)-Yb(1)-C(22)	122.05(11)
C(22)#2-Yb(1)-C(22)	28.94(13)		

Complex **9**

Lu(1)-O(6)#1	2.265(5)	Lu(1)-O(8)#2	2.284(6)
Lu(1)-O(1W)	2.297(6)	Lu(1)-O(7)	2.327(6)
Lu(1)-O(2)#3	2.324(6)	Lu(1)-N(1)	2.456(7)

Lu(1)-N(2)	2.467(6)	Lu(1)-N(3)	2.498(7)
O(6)#1-Lu(1)-O(8)#2	84.4(2)	O(6)#1-Lu(1)-O(1W)	79.8(2)
O(8)#2-Lu(1)-O(1W)	141.3(2)	O(6)#1-Lu(1)-O(7)	79.74(19)
O(8)#2-Lu(1)-O(7)	70.62(19)	O(1W)-Lu(1)-O(7)	71.9(2)
O(6)#1-Lu(1)-O(2)#3	102.42(19)	O(8)#2-Lu(1)-O(2)#3	146.9(2)
O(1W)-Lu(1)-O(2)#3	71.4(2)	O(7)-Lu(1)-O(2)#3	142.2(2)
O(6)#1-Lu(1)-N(1)	152.2(2)	O(8)#2-Lu(1)-N(1)	96.9(2)
O(1W)-Lu(1)-N(1)	82.2(2)	O(7)-Lu(1)-N(1)	74.6(2)
O(2)#3-Lu(1)-N(1)	91.6(2)	O(6)#1-Lu(1)-N(2)	139.2(2)
O(8)#2-Lu(1)-N(2)	71.6(2)	O(1W)-Lu(1)-N(2)	138.3(2)
O(7)-Lu(1)-N(2)	119.9(2)	O(2)#3-Lu(1)-N(2)	83.2(2)
N(1)-Lu(1)-N(2)	65.6(2)	O(6)#1-Lu(1)-N(3)	76.5(2)
O(8)#2-Lu(1)-N(3)	76.7(2)	O(1W)-Lu(1)-N(3)	131.9(2)
O(7)-Lu(1)-N(3)	141.0(2)	O(2)#3-Lu(1)-N(3)	73.7(2)
N(1)-Lu(1)-N(3)	131.0(2)	N(2)-Lu(1)-N(3)	66.3(2)

Complex**10**

Yb(1)-O(1W)	2.257(6)	Yb(1)-O(1)	2.278(4)
Yb(1)-O(2W)	2.280(5)	Yb(1)-O(8)	2.327(5)
Yb(1)-O(7)	2.375(4)	Yb(1)-N(3)#1	2.440(6)
Yb(1)-N(2)#1	2.465(5)	Yb(1)-N(1)#1	2.487(5)
Yb(1)-C(22)	2.695(7)		
O(1W)-Yb(1)-O(1)	108.5(2)	O(1W)-Yb(1)-O(2W)	74.8(2)
O(1)-Yb(1)-O(2W)	81.21(16)	O(1W)-Yb(1)-O(8)	155.0(2)
O(1)-Yb(1)-O(8)	83.03(16)	O(2W)-Yb(1)-O(8)	129.81(16)
O(1W)-Yb(1)-O(7)	147.6(2)	O(1)-Yb(1)-O(7)	76.82(15)
O(2W)-Yb(1)-O(7)	74.58(17)	O(8)-Yb(1)-O(7)	55.46(16)
O(1W)-Yb(1)-N(3)#1	89.0(2)	O(1)-Yb(1)-N(3)#1	151.39(16)
O(2W)-Yb(1)-N(3)#1	81.83(17)	O(8)-Yb(1)-N(3)#1	90.40(17)
O(7)-Yb(1)-N(3)#1	76.55(17)	O(1W)-Yb(1)-N(2)#1	80.2(2)
O(1)-Yb(1)-N(2)#1	138.19(16)	O(2W)-Yb(1)-N(2)#1	138.99(16)
O(8)-Yb(1)-N(2)#1	76.84(16)	O(7)-Yb(1)-N(2)#1	117.92(16)
N(3)#1-Yb(1)-N(2)#1	65.62(16)	O(1W)-Yb(1)-N(1)#1	79.9(2)
O(1)-Yb(1)-N(1)#1	75.61(16)	O(2W)-Yb(1)-N(1)#1	137.92(17)
O(8)-Yb(1)-N(1)#1	81.75(17)	O(7)-Yb(1)-N(1)#1	131.18(17)
N(3)#1-Yb(1)-N(1)#1	131.07(17)	N(2)#1-Yb(1)-N(1)#1	65.56(17)
O(1W)-Yb(1)-C(22)	172.3(2)	O(1)-Yb(1)-C(22)	77.34(17)
O(2W)-Yb(1)-C(22)	101.68(19)	O(8)-Yb(1)-C(22)	28.18(17)
O(7)-Yb(1)-C(22)	27.33(17)	N(3)#1-Yb(1)-C(22)	83.77(19)
N(2)#1-Yb(1)-C(22)	98.94(18)	N(1)#1-Yb(1)-C(22)	106.75(19)

Complex **11**

Lu(1)-O(1W)	2.243(4)	Lu(1)-O(1)	2.267(3)
Lu(1)-O(2W)	2.274(3)	Lu(1)-O(8)	2.321(3)
Lu(1)-O(7)	2.362(3)	Lu(1)-N(3)#1	2.435(5)
Lu(1)-N(2)#1	2.466(4)	Lu(1)-N(1)#1	2.493(4)
Lu(1)-C(22)	2.696(5)		
O(1W)-Lu(1)-O(1)	107.21(14)	O(1W)-Lu(1)-O(2W)	74.74(14)
O(1)-Lu(1)-O(2W)	81.07(12)	O(1W)-Lu(1)-O(8)	154.78(15)
O(1)-Lu(1)-O(8)	83.53(12)	O(2W)-Lu(1)-O(8)	130.19(13)
O(1W)-Lu(1)-O(7)	147.93(15)	O(1)-Lu(1)-O(7)	77.31(13)
O(2W)-Lu(1)-O(7)	74.71(13)	O(8)-Lu(1)-O(7)	55.72(12)
O(1W)-Lu(1)-N(3)#1	89.47(16)	O(1)-Lu(1)-N(3)#1	151.75(13)
O(2W)-Lu(1)-N(3)#1	81.63(13)	O(8)-Lu(1)-N(3)#1	90.82(13)
O(7)-Lu(1)-N(3)#1	76.67(14)	O(1W)-Lu(1)-N(2)#1	80.31(14)
O(1)-Lu(1)-N(2)#1	138.16(12)	O(2W)-Lu(1)-N(2)#1	138.92(13)
O(8)-Lu(1)-N(2)#1	76.84(12)	O(7)-Lu(1)-N(2)#1	118.12(13)
N(3)#1-Lu(1)-N(2)#1	65.86(13)	O(1W)-Lu(1)-N(1)#1	79.06(15)

O(1)-Lu(1)-N(1)#1	75.29(12)	O(2W)-Lu(1)-N(1)#1	137.37(13)
O(8)-Lu(1)-N(1)#1	81.91(13)	O(7)-Lu(1)-N(1)#1	131.48(13)
N(3)#1-Lu(1)-N(1)#1	131.40(13)	N(2)#1-Lu(1)-N(1)#1	65.69(13)
O(1W)-Lu(1)-C(22)	173.18(16)	O(1)-Lu(1)-C(22)	77.94(13)
O(2W)-Lu(1)-C(22)	102.08(15)	O(8)-Lu(1)-C(22)	28.17(14)
O(7)-Lu(1)-C(22)	27.61(14)	N(3)#1-Lu(1)-C(22)	84.06(14)
N(2)#1-Lu(1)-C(22)	98.92(14)	N(1)#1-Lu(1)-C(22)	106.88(14)

Complex **12**

Dy(1)-O(7)#1	2.259(5)	Dy(1)-O(8)	2.285(5)
Dy(1)-O(2)	2.318(5)	Dy(1)-O(6)#2	2.362(5)
Dy(1)-O(5)#3	2.413(5)	Dy(1)-N(2)#4	2.498(6)
Dy(1)-N(1)#4	2.549(6)	Dy(1)-N(3)#4	2.553(6)
O(7)#1-Dy(1)-O(8)	114.3(2)	O(7)#1-Dy(1)-O(2)	89.11(18)
O(8)-Dy(1)-O(2)	139.26(19)	O(7)#1-Dy(1)-O(6)#2	76.53(19)
O(8)-Dy(1)-O(6)#2	75.4(2)	O(2)-Dy(1)-O(6)#2	78.68(19)
O(7)#1-Dy(1)-O(5)#3	77.68(19)	O(8)-Dy(1)-O(5)#3	70.3(2)
O(2)-Dy(1)-O(5)#3	150.2(2)	O(6)#2-Dy(1)-O(5)#3	122.70(19)
O(7)#1-Dy(1)-N(2)#4	139.8(2)	O(8)-Dy(1)-N(2)#4	87.9(2)
O(2)-Dy(1)-N(2)#4	94.77(19)	O(6)#2-Dy(1)-N(2)#4	143.40(19)
O(5)#3-Dy(1)-N(2)#4	79.46(18)	O(7)#1-Dy(1)-N(1)#4	154.2(2)
O(8)-Dy(1)-N(1)#4	69.9(2)	O(2)-Dy(1)-N(1)#4	75.22(19)
O(6)#2-Dy(1)-N(1)#4	80.37(19)	O(5)#3-Dy(1)-N(1)#4	125.29(19)
N(2)#4-Dy(1)-N(1)#4	63.24(19)	O(7)#1-Dy(1)-N(3)#4	78.0(2)
O(8)-Dy(1)-N(3)#4	134.6(2)	O(2)-Dy(1)-N(3)#4	80.8(2)
O(6)#2-Dy(1)-N(3)#4	147.3(2)	O(5)#3-Dy(1)-N(3)#4	70.4(2)
N(2)#4-Dy(1)-N(3)#4	63.34(19)	N(1)#4-Dy(1)-N(3)#4	118.3(2)

Complex **13**

Er(1)-O(7)#1	2.242(3)	Er(1)-O(8)	2.267(3)
Er(1)-O(2)	2.306(3)	Er(1)-O(6)#2	2.336(4)
Er(1)-O(5)#3	2.396(3)	Er(1)-N(2)#4	2.461(4)
Er(1)-N(1)#4	2.543(4)	Er(1)-N(3)#4	2.544(4)
O(7)#1-Er(1)-O(8)	114.28(13)	O(7)#1-Er(1)-O(2)	89.21(13)
O(8)-Er(1)-O(2)	139.22(13)	O(7)#1-Er(1)-O(6)#2	76.33(13)
O(8)-Er(1)-O(6)#2	75.60(14)	O(2)-Er(1)-O(6)#2	78.68(13)
O(7)#1-Er(1)-O(5)#3	77.96(13)	O(8)-Er(1)-O(5)#3	70.33(13)
O(2)-Er(1)-O(5)#3	150.04(13)	O(6)#2-Er(1)-O(5)#3	123.04(12)
O(7)#1-Er(1)-N(2)#4	139.97(14)	O(8)-Er(1)-N(2)#4	87.73(14)
O(2)-Er(1)-N(2)#4	94.74(13)	O(6)#2-Er(1)-N(2)#4	143.47(13)
O(5)#3-Er(1)-N(2)#4	79.09(13)	O(7)#1-Er(1)-N(1)#4	153.26(14)
O(8)-Er(1)-N(1)#4	69.99(13)	O(2)-Er(1)-N(1)#4	74.67(13)
O(6)#2-Er(1)-N(1)#4	79.62(13)	O(5)#3-Er(1)-N(1)#4	125.86(13)
N(2)#4-Er(1)-N(1)#4	64.08(13)	O(7)#1-Er(1)-N(3)#4	77.91(13)
O(8)-Er(1)-N(3)#4	134.36(14)	O(2)-Er(1)-N(3)#4	81.02(13)
O(6)#2-Er(1)-N(3)#4	147.20(14)	O(5)#3-Er(1)-N(3)#4	69.92(13)
N(2)#4-Er(1)-N(3)#4	63.53(14)	N(1)#4-Er(1)-N(3)#4	119.17(13)

[a]Symmetry transformations used to generate equivalentatoms: #1 –x + 1, -y, -z + 1, #2 –x + 2, y, -z + 3/2 for complex **1**; #1 –x + 1/2, -y + 1/2 , -z, #2 –x + 1/2, -y + 1/2, -z + 1, #3 x, y, z + 1, #4 -x, y, -z - 1/2, #5 x, y, z - 1 for complexes **2-7**; #1 x, y, z + 1, #2 -x, -y + 2, -z #3 x, -y + 3/2, z + 1/2, #4 x, y, z – 1, #5 x, -y + 3/2, z-1/2 for complex **8-9**; #1 –x + 5/2, y - 1/2, -z + 3/2, #2 –x + 5/2, y + 1/2, -z + 3/2 #3 –x + 2, y, -z + 3/2 for complex **10-11**; #1 -x, -y + 1, -z, #2 -x, -y, -z, #3 x, y + 1, z, #4 -x, -y + 1, -z + 1, #5 x, y - 1, z, #6 –x - 1, -y + 1, -z for complex **12-13**.

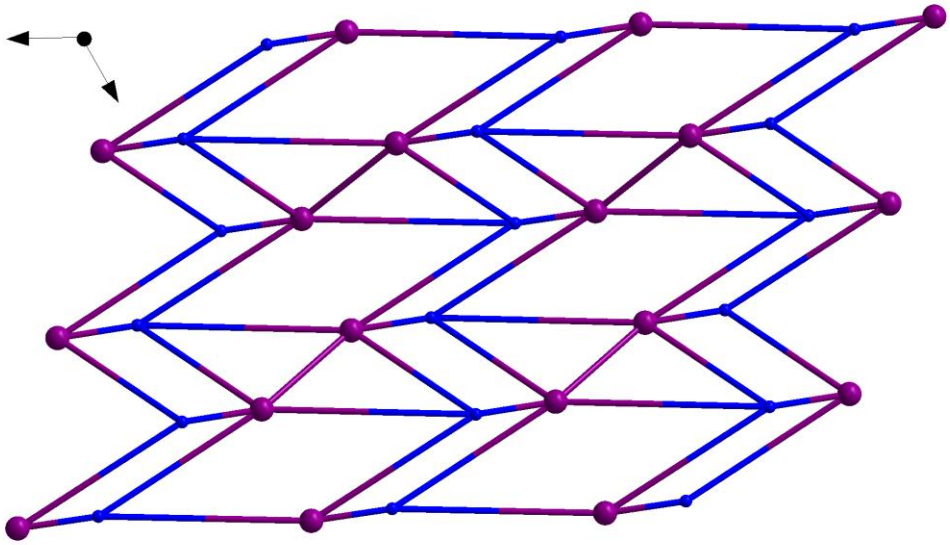

Figure S1. The topology of complex **7** (the purple balls represent for Lu(III) ions and blue balls represent for $BSPT^{2-}$ ligands).

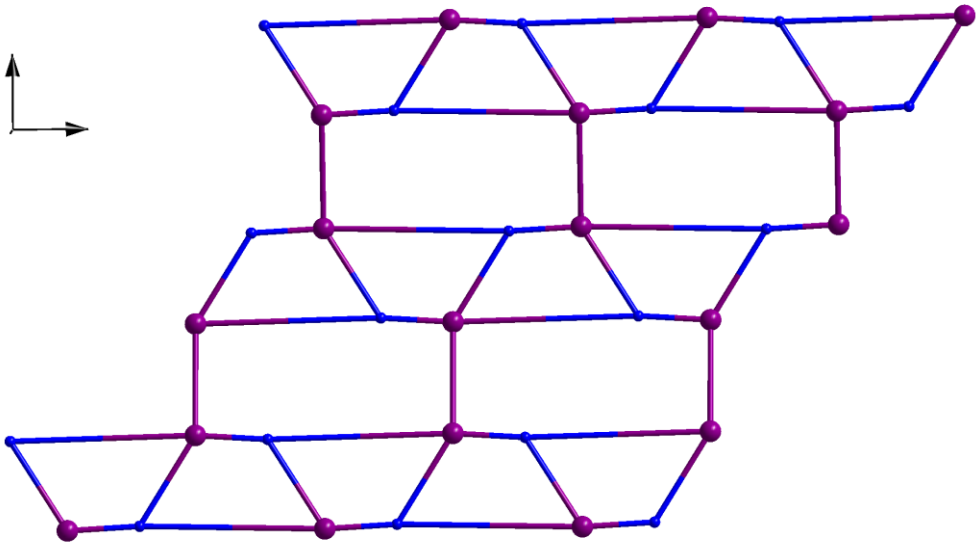

Figure S2. The topology of complex **9** (the purple balls represent for Lu(III) ions and blue balls represent for $BSPT^{2-}$ ligands).

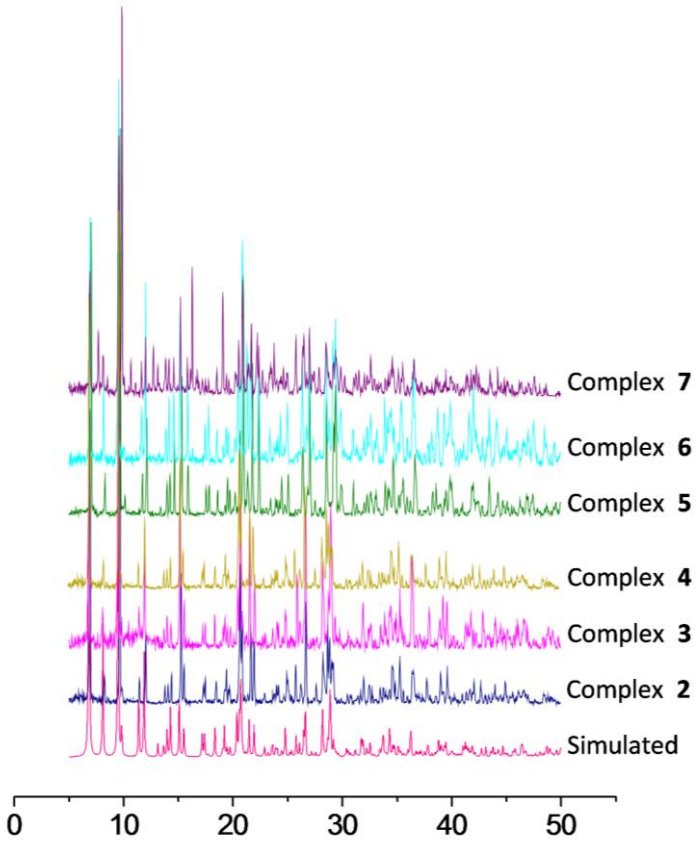

Figure S3. PXRD patterns of simulated based on the X-ray single-crystal diffraction data of **2** and for as-synthesized **2-7**.

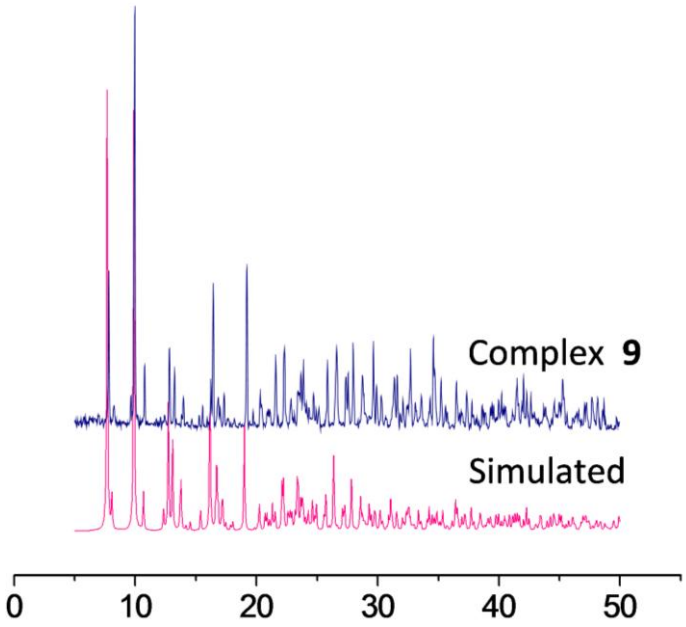

Figure S4. PXRD patterns of simulated based on the X-ray single-crystal diffraction data of **9** and for as-synthesized **9**.

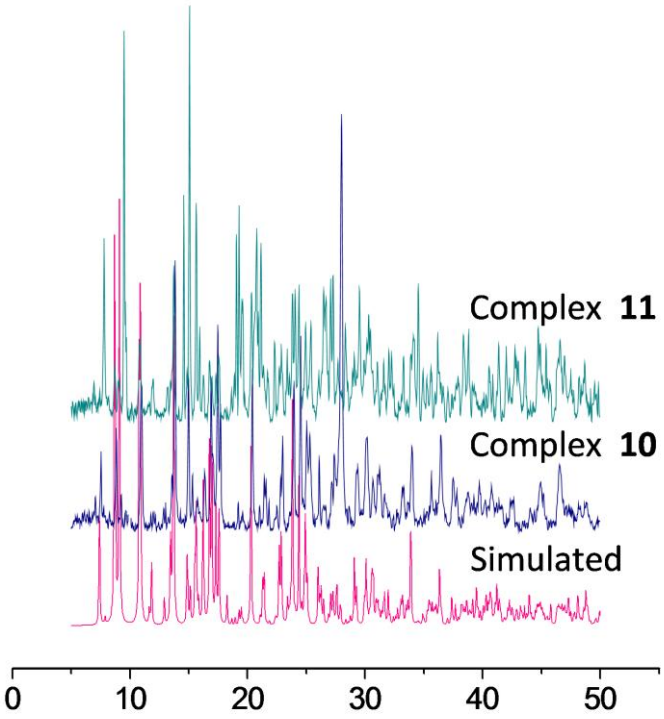

Figure S5. PXRD patterns of simulated based on the X-ray single-crystal diffraction data of **10** and for as-synthesized **10**-**11**.

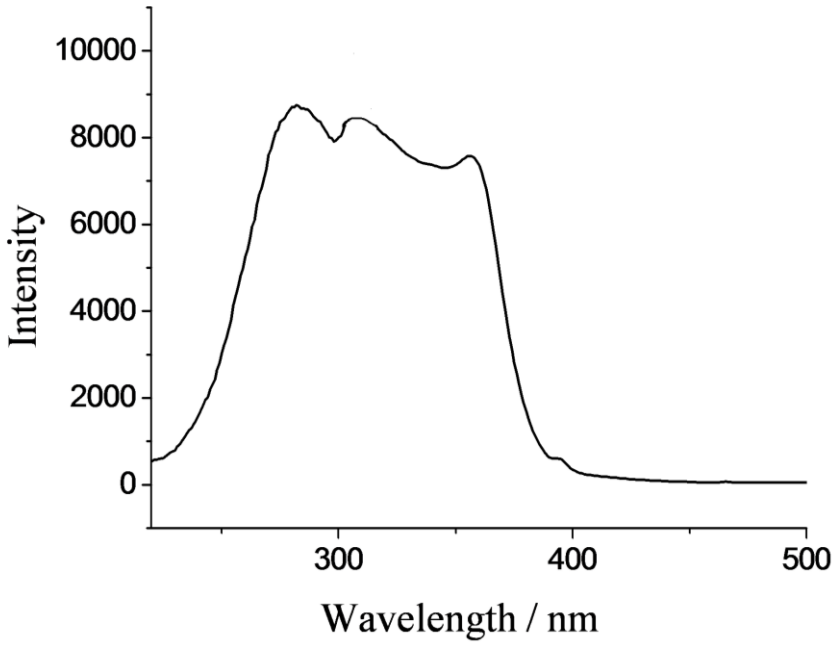

Figure S6. Solid-state excitation spectrum for **3** in the solid state at room temperature.

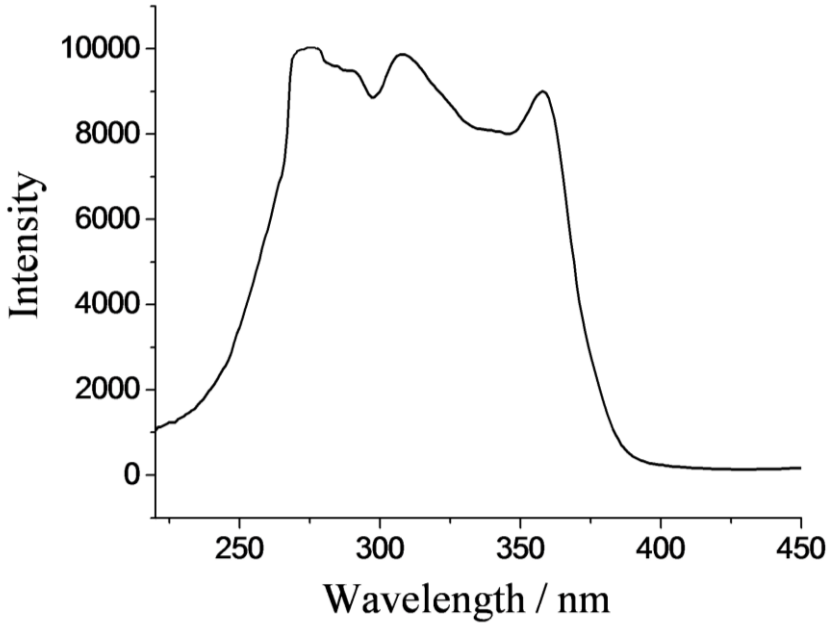

Figure S7. Solid-state excitation spectrum for **4** in the solid state at room temperature.