Supproting Information

Temperature-dependent assemblies from 2-D triple-stranded *meso*-helical layer to 3-D chain-layer metal-organic framework

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Contents

Table **S1**

	1	**2**
Chemical formula	$C_{27}H_{25}N_3O_{14}Dy_2$	$C_{27}H_{29}N_3O_{16}Dy_2$
M	940.50	976.53
Crystal system	Orthorhombic	Monoclinic
Space group	*Pbca*	*C*2/*c*
a /Å	21.746(5)	10.5222(14)
b /Å	14.338(3)	14.6134(19)
c /Å	23.216(5)	39.044(5)
α /°	90	90
β /°	90	92.677(2)
γ /°	90	90
V/Å^3	7239(3)	5997.0(14)
Z	8	8
T /K	298(2)	298(2)
F(000)	3696	3776
D_{calcd} / g cm^{-3}	1.726	2.163
μ /mm^{-1}	4.160	5.030
λ /Å	0.71073	0.71073
R_{int}	0.1023	0.0776
data/restraint/parm	6495 / 6 / 422	5392 / 30 / 464
GOF	1.023	0.978
R_1 $[I = 2\sigma(I)]^a$	0.0649	0.0444
wR_2 $[I = 2\sigma(I)]^b$	0.1153	0.0705

^{a} $R_1 = \Sigma||F_o| - |F_c||/|F_o|$, ^{b} $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$, where w = $1/[\sigma^2(F_o^2) + (aP)_2 + bP]$. $P = (F_o^2 + 2F_c^2)/3$.

Table **S2**.

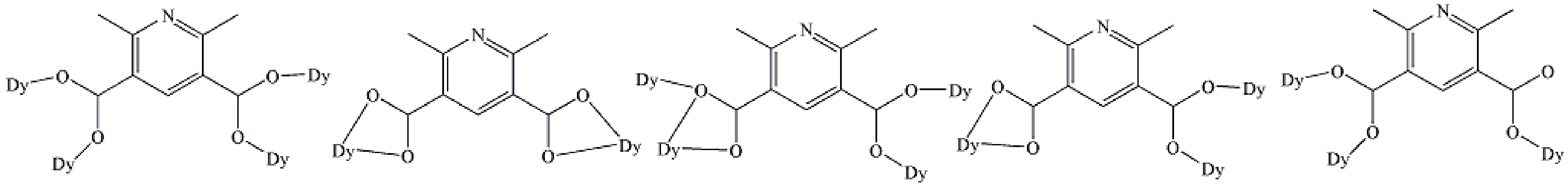
	Complex **1**		
Dy(1)-O(13)#1	2.186(6)	Dy(1)-O(9)	2.260(7)
Dy(1)-O(7)#1	2.223(5)	Dy(1)-O(10)	2.262(5)
Dy(1)-O(11)	2.231(6)	Dy(1)-O(4)#2	2.265(8)
Dy(1)-O(3)#2	2.432(7)	Dy(2)-O(12)	2.196(6)
Dy(2)-O(6)	2.237(6)	Dy(2)-O(14)#1	2.258(5)
Dy(2)-O(5)	2.263(4)	Dy(2)-O(8)#3	2.285(6)
Dy(2)-O(1)	2.290(7)	Dy(2)-O(2)	2.414(6)
O(13)#1-Dy(1)-O(7)#1	87.0(2)	O(13)#1-Dy(1)-O(9)	79.9(2)
O(13)#1-Dy(1)-O(11)	96.2(2)	O(7)#1-Dy(1)-O(9)	87.0(2)
O(7)#1-Dy(1)-O(11)	174.3(3)	O(11)-Dy(1)-O(9)	98.2(2)
O(13)#1-Dy(1)-O(10)	154.3(2)	O(7)#1-Dy(1)-O(10)	95.1(2)
O(11)-Dy(1)-O(10)	84.1(2)	O(9)-Dy(1)-O(10)	74.6(2)
O(13)#1-Dy(1)-O(4)#2	132.8(3)	O(7)#1-Dy(1)-O(4)#2	84.9(3)
O(11)-Dy(1)-O(4)#2	89.4(3)	O(9)-Dy(1)-O(4)#2	145.6(3)
O(10)-Dy(1)-O(4)#2	72.9(2)	O(13)#1-Dy(1)-O(3)#2	79.3(2)
O(7)#1-Dy(1)-O(3)#2	90.3(2)	O(11)-Dy(1)-O(3)#2	85.7(2)
O(9)-Dy(1)-O(3)#2	159.1(2)	O(10)-Dy(1)-O(3)#2	126.3(2)
O(4)#2-Dy(1)-O(3)#2	54.4(2)	O(13)#1-Dy(1)-C(4)#2	105.6(3)
O(7)#1-Dy(1)-C(4)#2	87.8(2)	O(11)-Dy(1)-C(4)#2	86.8(3)
O(9)-Dy(1)-C(4)#2	172.2(3)	O(10)-Dy(1)-C(4)#2	100.1(2)
O(4)#2-Dy(1)-C(4)#2	27.8(3)	O(3)#2-Dy(1)-C(4)#2	26.7(2)
O(12)-Dy(2)-O(6)	77.3(2)	O(12)-Dy(2)-O(14)#1	106.8(2)
O(6)-Dy(2)-O(14)#1	80.2(2)	O(12)-Dy(2)-O(5)	75.28(19)
O(6)-Dy(2)-O(5)	144.3(2)	O(14)#1-Dy(2)-O(5)	86.3(2)
O(12)-Dy(2)-O(8)#3	88.2(3)	O(6)-Dy(2)-O(8)#3	117.4(2)
O(14)#1-Dy(2)-O(8)#3	159.5(2)	O(5)-Dy(2)-O(8)#3	84.2(2)
O(12)-Dy(2)-O(1)	152.0(2)	O(6)-Dy(2)-O(1)	80.8(2)
O(14)#1-Dy(2)-O(1)	86.2(2)	O(5)-Dy(2)-O(1)	131.30(18)
O(8)#3-Dy(2)-O(1)	86.5(3)	O(12)-Dy(2)-O(2)	152.1(2)
O(6)-Dy(2)-O(2)	130.0(2)	O(14)#1-Dy(2)-O(2)	76.8(2)
O(5)-Dy(2)-O(2)	77.37(17)	O(8)#3-Dy(2)-O(2)	83.4(2)
O(1)-Dy(2)-O(2)	54.1(2)		
	Complex **2**		
Dy(1)-O(7)	2.268(6)	Dy(1)-O(1)#4	2.355(6)
Dy(1)-O(6)	2.300(6)	Dy(1)-O(3)#5	2.371(6)
Dy(1)-O(4)	2.328(6)	Dy(1)-O(2)#6	2.443(6)
Dy(1)-O(5)	2.339(7)	Dy(1)-O(1)#6	2.497(6)
Dy(2)-O(14)#7	2.285(7)	Dy(2)-O(11)#9	2.303(6)
Dy(2)-O(14)#8	2.285(7)	Dy(2)-O(10)#9	2.353(6)
Dy(2)-O(11)	2.303(6)	Dy(2)-O(10)	2.353(6)

Dy(2)-O(9)	2.382(6)	Dy(2)-O(9)#9	2.382(6)
Dy(3)-O(13)	2.217(6)	Dy(3)-O(12)#9	2.276(6)
Dy(3)-O(13)#6	2.217(6)	Dy(3)-O(16)#10	2.362(6)
Dy(3)-O(12)	2.276(6)	Dy(3)-O(16)#4	2.362(7)
Dy(3)-O(15)#10	2.738(9)	Dy(3)-O(15)#4	2.738(9)
O(7)-Dy(1)-O(6)	88.0(2)	O(7)-Dy(1)-O(4)	105.9(2)
O(6)-Dy(1)-O(4)	145.9(2)	O(7)-Dy(1)-O(5)	75.3(2)
O(6)-Dy(1)-O(5)	76.9(2)	O(4)-Dy(1)-O(5)	76.9(2)
O(7)-Dy(1)-O(1)#4	84.5(2)	O(6)-Dy(1)-O(1)#4	142.3(2)
O(4)-Dy(1)-O(1)#4	71.1(2)	O(5)-Dy(1)-O(1)#4	135.5(2)
O(7)-Dy(1)-O(3)#5	88.1(2)	O(6)-Dy(1)-O(3)#5	70.9(2)
O(4)-Dy(1)-O(3)#5	138.8(2)	O(5)-Dy(1)-O(3)#5	144.1(2)
O(1)#4-Dy(1)-O(3)#5	72.0(2)	O(7)-Dy(1)-O(2)#6	149.3(2)
O(6)-Dy(1)-O(2)#6	77.5(2)	O(4)-Dy(1)-O(2)#6	75.0(2)
O(5)-Dy(1)-O(2)#6	75.2(2)	O(1)#4-Dy(1)-O(2)#6	123.1(2)
O(3)#5-Dy(1)-O(2)#6	111.7(2)	O(7)-Dy(1)-O(1)#6	158.1(2)
O(6)-Dy(1)-O(1)#6	100.8(2)	O(4)-Dy(1)-O(1)#6	77.9(2)
O(5)-Dy(1)-O(1)#6	126.1(2)	O(1)#4-Dy(1)-O(1)#6	76.3(2)
O(3)#5-Dy(1)-O(1)#6	76.2(2)	O(2)#6-Dy(1)-O(1)#6	52.5(2)
O(14)#7-Dy(2)-O(14)#8	87.5(4)	O(14)#7-Dy(2)-O(11)	110.5(2)
O(14)#8-Dy(2)-O(11)	141.0(2)	O(14)#7-Dy(2)-O(11)#9	141.0(2)
O(14)#8-Dy(2)-O(11)#9	110.5(2)	O(11)-Dy(2)-O(11)#9	77.4(3)
O(14)#7-Dy(2)-O(10)#9	79.9(3)	O(14)#8-Dy(2)-O(10)#9	68.6(2)
O(11)-Dy(2)-O(10)#9	146.4(2)	O(11)#9-Dy(2)-O(10)#9	75.6(2)
O(14)#8-Dy(2)-O(10)	68.6(2)	O(14)#8-Dy(2)-O(10)	79.9(3)
O(11)-Dy(2)-O(10)	75.6(2)	O(11)#9-Dy(2)-O(10)	146.4(2)
O(10)#9-Dy(2)-O(10)	136.1(4)	O(14)#7-Dy(2)-O(9)	76.1(2)
O(14)#8-Dy(2)-O(9)	143.0(2)	O(11)-Dy(2)-O(9)	76.0(2)
O(11)#9-Dy(2)-O(9)	68.9(2)	O(10)#9-Dy(2)-O(9)	76.0(2)
O(10)-Dy(2)-O(9)	122.1(3)	O(14)#7-Dy(2)-O(9)#9	143.0(2)
O(14)#8-Dy(2)-O(9)#9	76.1(2)	O(11)-Dy(2)-O(9)#9	68.9(2)
O(11)#9-Dy(2)-O(9)#9	76.0(2)	O(10)#9-Dy(2)-O(9)#9	122.1(3)
O(10)-Dy(2)-O(9)#9	76.0(2)	O(9)-Dy(2)-O(9)#9	134.6(3)
O(13)-Dy(3)-O(13)#9	171.8(4)	O(13)-Dy(3)-O(12)	86.4(2)
O(13)#9-Dy(3)-O(12)	87.9(3)	O(13)-Dy(3)-O(12)#9	87.9(3)
O(13)#9-Dy(3)-O(12)#9	86.4(2)	O(12)-Dy(3)-O(12)#9	92.7(3)
O(13)-Dy(3)-O(16)#10	80.4(2)	O(13)#9-Dy(3)-O(16)#10	103.7(3)
O(12)-Dy(3)-O(16)#10	161.5(2)	O(12)#9-Dy(3)-O(16)#10	73.9(2)
O(13)-Dy(3)-O(16)#4	103.7(3)	O(13)#9-Dy(3)-O(16)#4	80.4(2)
O(12)-Dy(3)-O(16)#4	73.9(2)	O(12)#9-Dy(3)-O(16)#4	161.5(2)
O(16)#10-Dy(3)-O(16)#4	121.8(3)	O(13)-Dy(3)-O(15)#10	115.9(2)
O(13)#9-Dy(3)-O(15)#10	71.6(3)	O(12)-Dy(3)-O(15)#10	148.8(2)
O(12)#9-Dy(3)-O(15)#10	108.7(3)	O(16)#10-Dy(3)-O(15)#10	49.7(2)

O(16)#4-Dy(3)-O(15)#10	79.5(3)	O(13)-Dy(3)-O(15)#4	71.6(3)
O(13)#9-Dy(3)-O(15)#4	115.9(2)	O(12)-Dy(3)-O(15)#4	108.7(3)
O(12)#9-Dy(3)-O(15)#4	148.8(2)	O(16)#10-Dy(3)-O(15)#4	79.5(3)
O(16)#4-Dy(3)-O(15)#4	49.7(2)	O(15)#10-Dy(3)-O(15)#4	63.1(4)

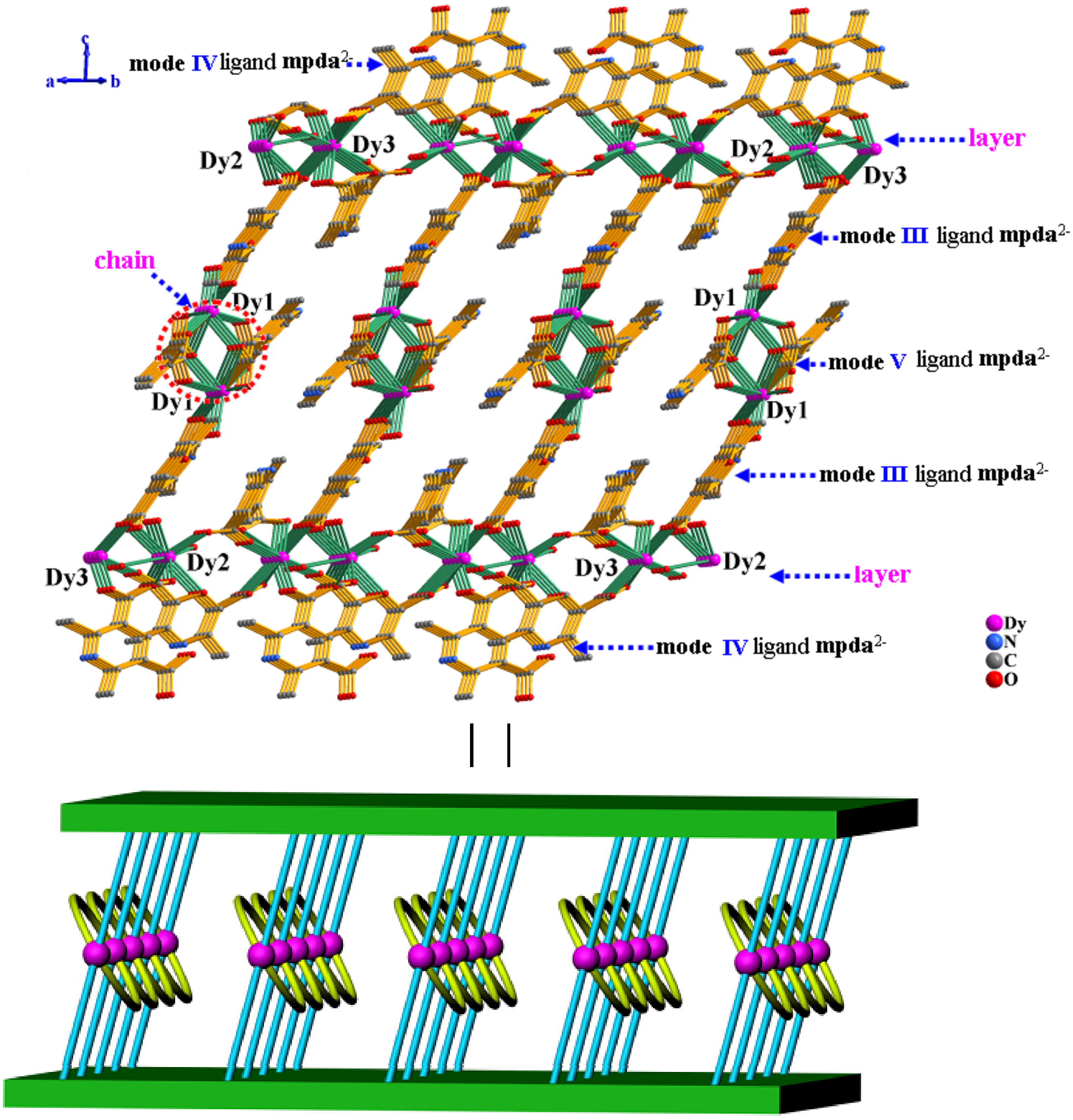
*Symmetry transformations used to generate equivalent atoms: #1 -x,y-1/2,-z+1/2; #2x,-y+1/2,z-1/2; #3-x,y+1/2,-z+1/2; #4x+1/2,y+1/2,z; #5-x+1,-y,-z; #6-x+1/2,-y-1/2,-z； #7 x+1/2,y-1/2,z; #8 -x+1/2,y-1/2,-z+1/2; #9 -x+1,y,-z+1/2; #10 -x+1/2,y+1/2,-z+1/2.

Scheme S1



mode I: μ_4-η^1:η^1:η^1:η^1 mode II: μ_2-η^1:η^1:η^1:η^1 mode III: μ_4-η^2:η^1:η^1:η^1 mode IV: μ_3-η^1:η^1:η^1:η^1 mode V: μ_3-η^1:η^1:η^1

Figure S1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b
mode IV ligand mpda2-
Dy2
Dy3
Dy2
Dy3
layer
mode III ligand mpda2-
chain
Dy1
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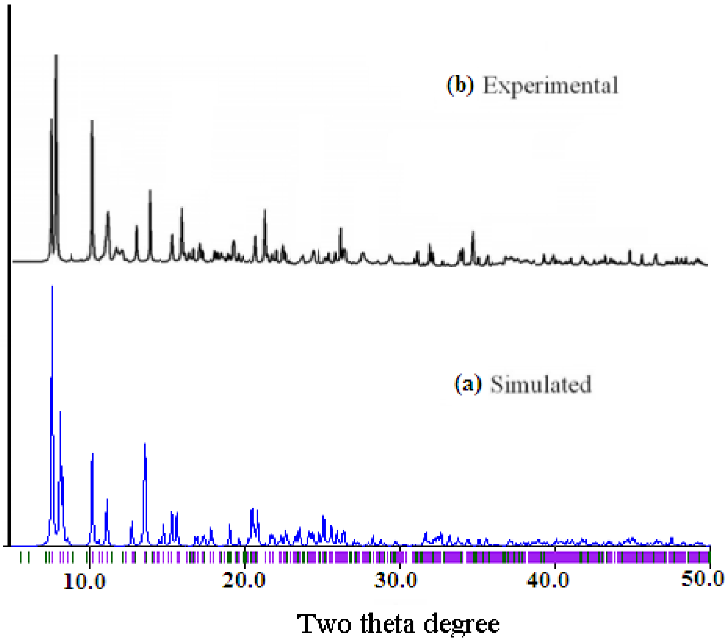
mode V ligand mpda2-
Dy1
Dy1
mode III ligand mpda2-
Dy3
Dy2
Dy3
Dy2
layer
mode IV ligand mpda2-
Dy
N
C
O

Figure S2

(**a**) for compound **1**



(**b**) for compound **2**

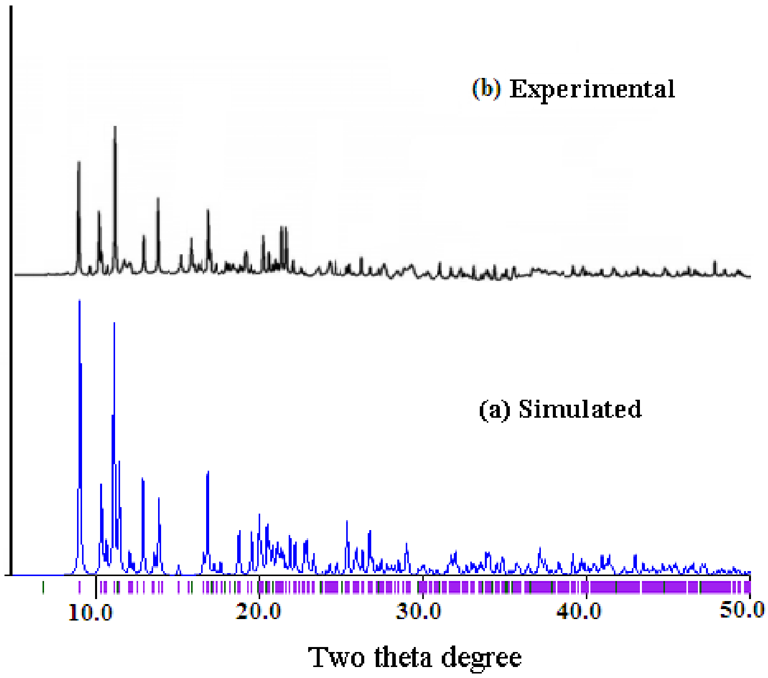


Figure S3

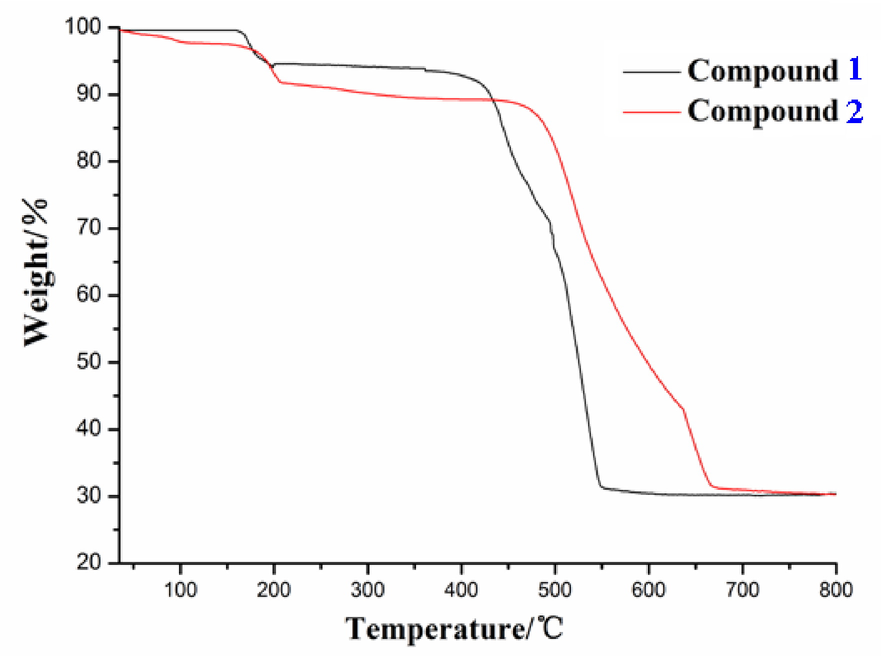

100
90
80
70
60
50
40
30
20
Weight/%
100
200
300
400
500
600
700
800
Temperature/℃
Compound 1
Compound 2

Figure S4

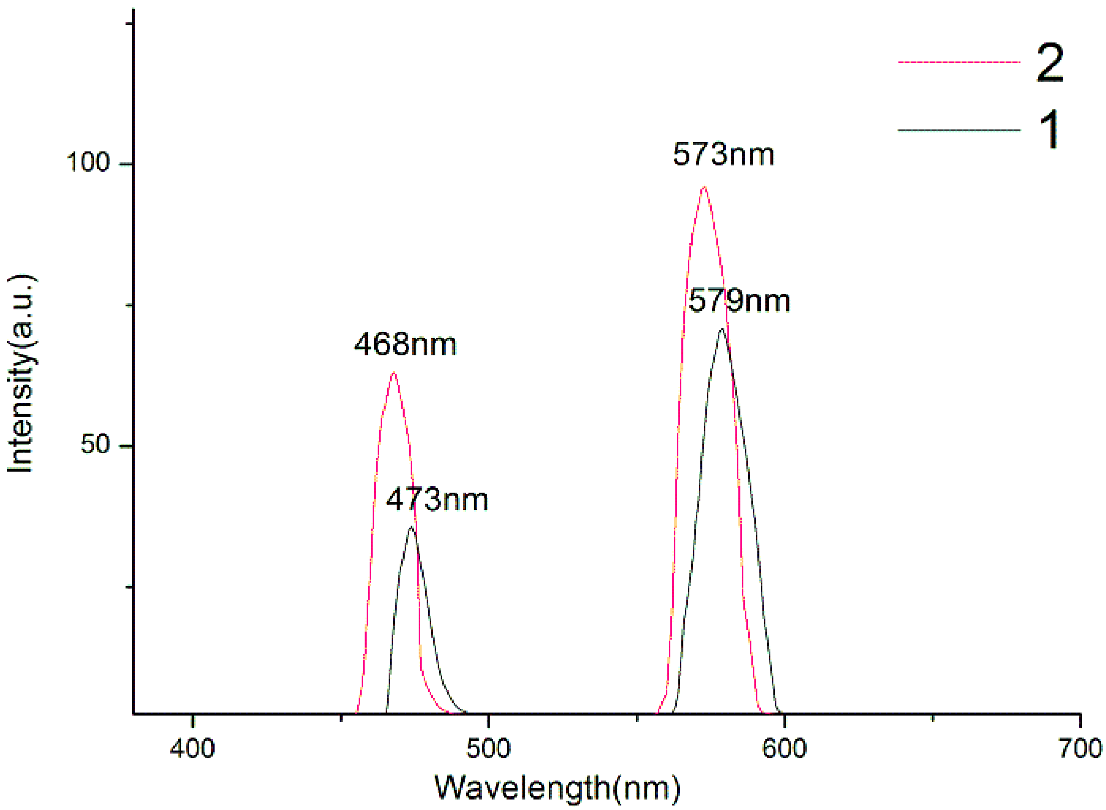

2
1
573nm
579nm
468nm
473nm
100
50
Intensity(a.u.)
400
500
600
700
Wavelength(nm)

Figure S5