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Supporting Information

Central-metal Exchange, Improved Catalytic Activity, Photoluminescence Properties of A New Family of d^{10} Coordination Polymers Based on 5,5'-(1H-2,3,5-triazole-1,4-diyl)diisophthalic Acid Ligand

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Contents

1. PXRD analysis of 1-5.

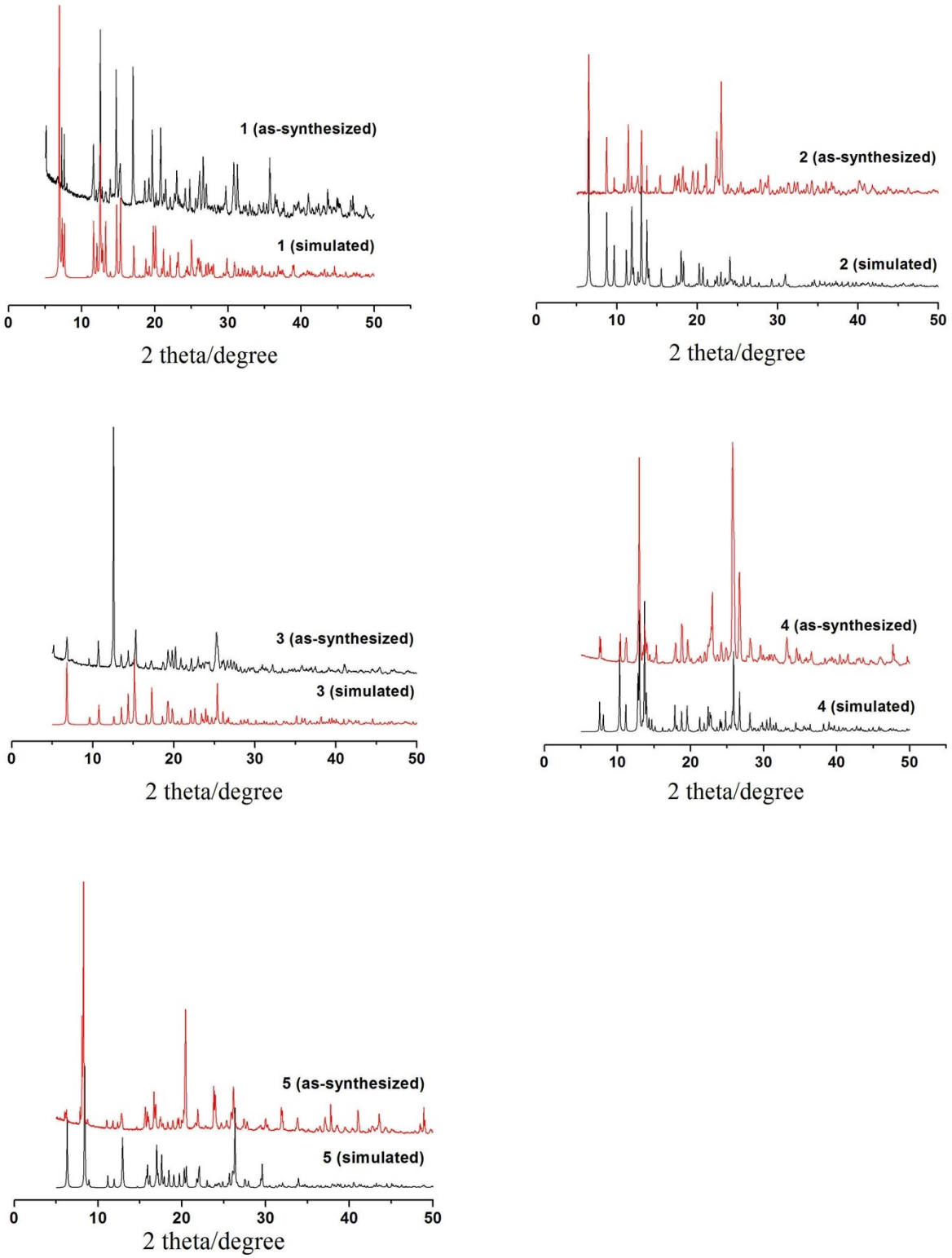


Fig. S1 Experimental and simulated PXRD patterns of **1**-**5 (**as-synthesized**).**

2. TGA analysis of 1-5.

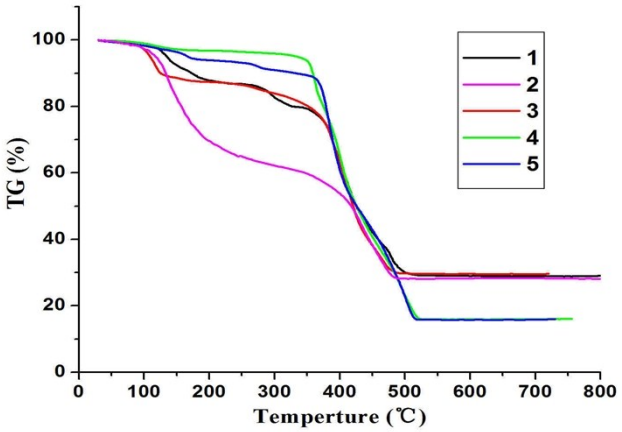


Fig. S2 TGA curves of **1-5**.

3. Photoluminescence Properties of H_4L and 1-5.

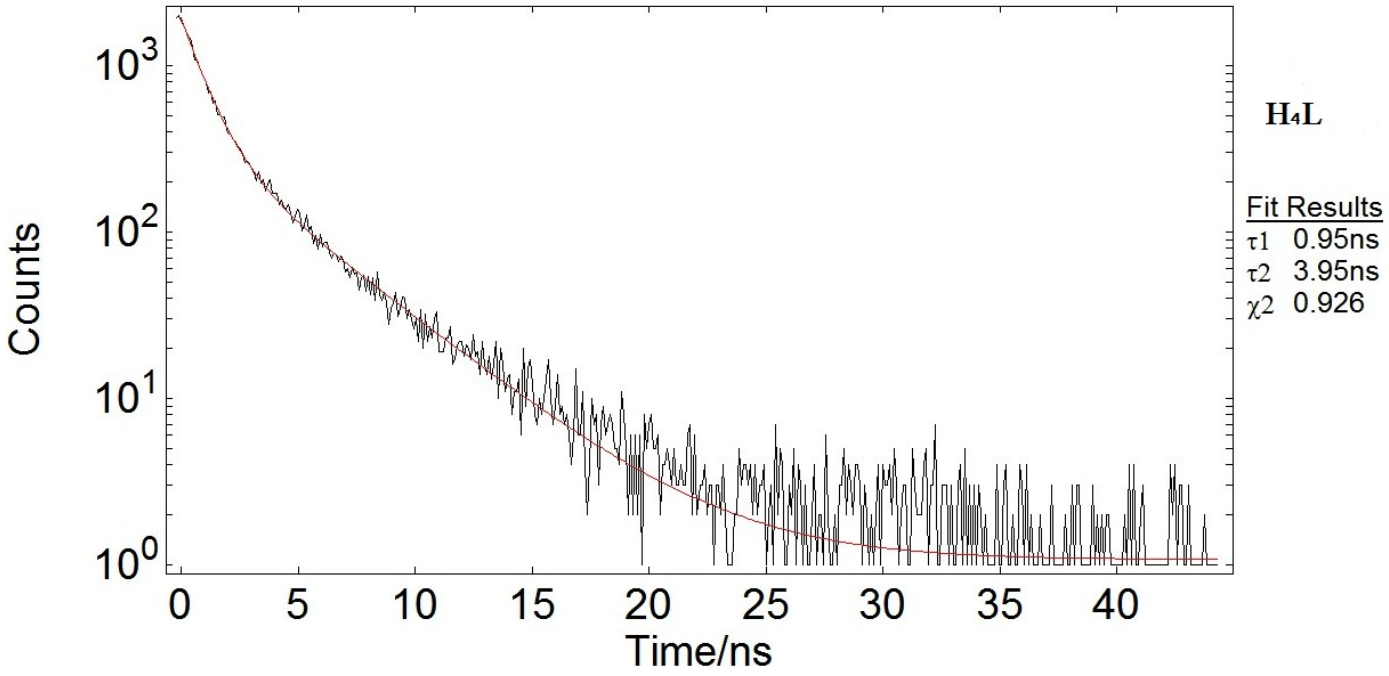


Fig. S3 Emission decay trace and biexponential fit for the free ligand **H_4L** at room temperature.

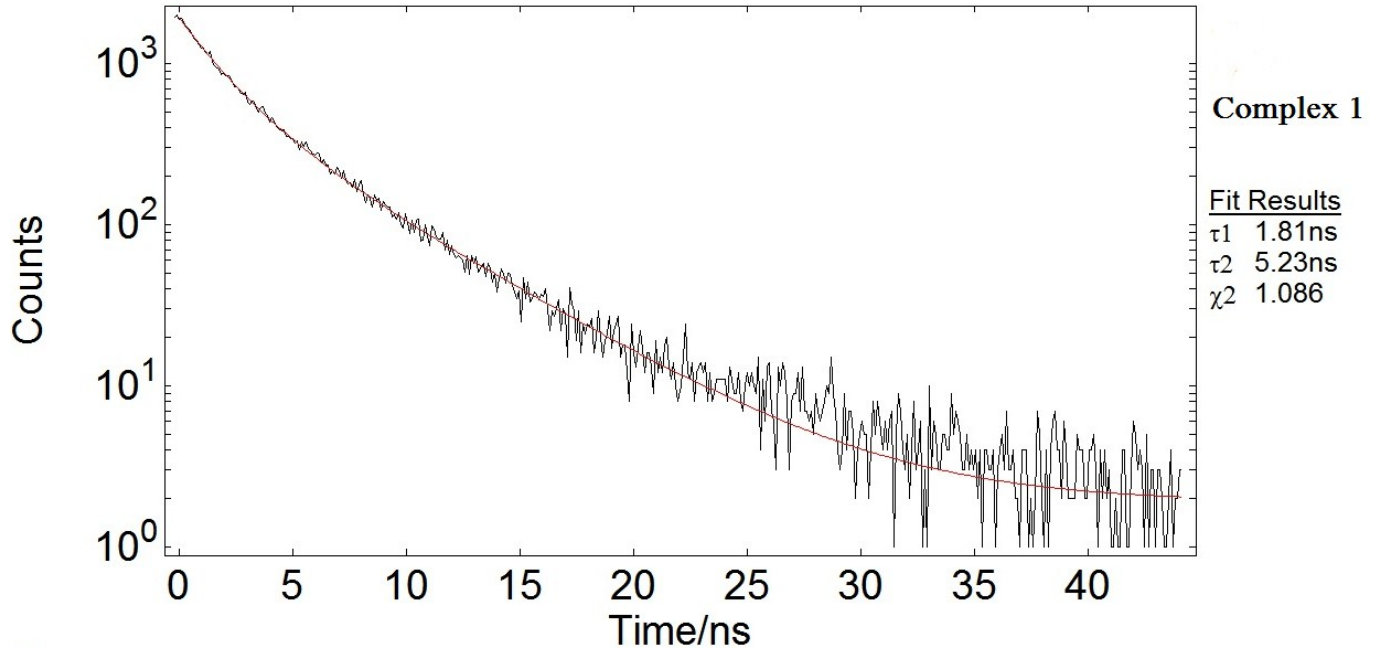


Fig. S4 Emission decay trace and biexponential fit for **1** (λ_{em} = 439 nm) at room temperature.

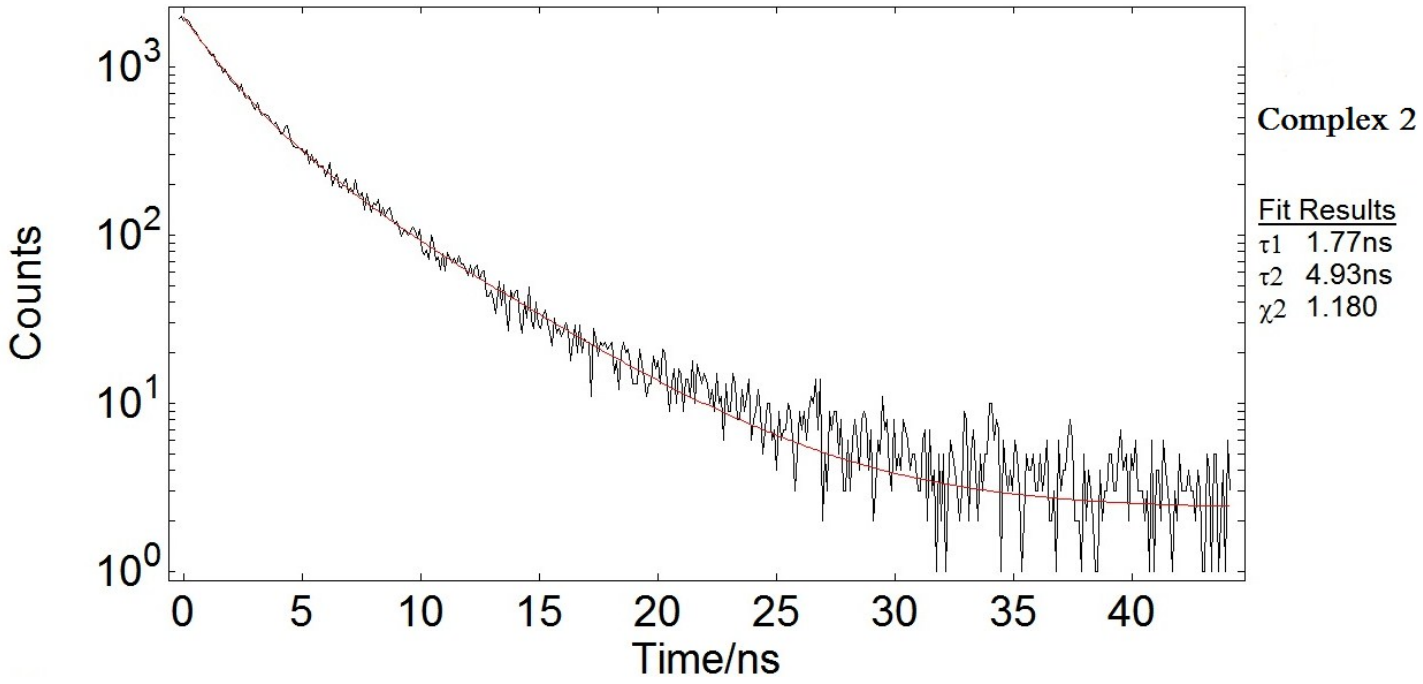


Fig. S5 Emission decay trace and biexponential fit for **2** (λ_{em} = 423 nm) at room temperature.

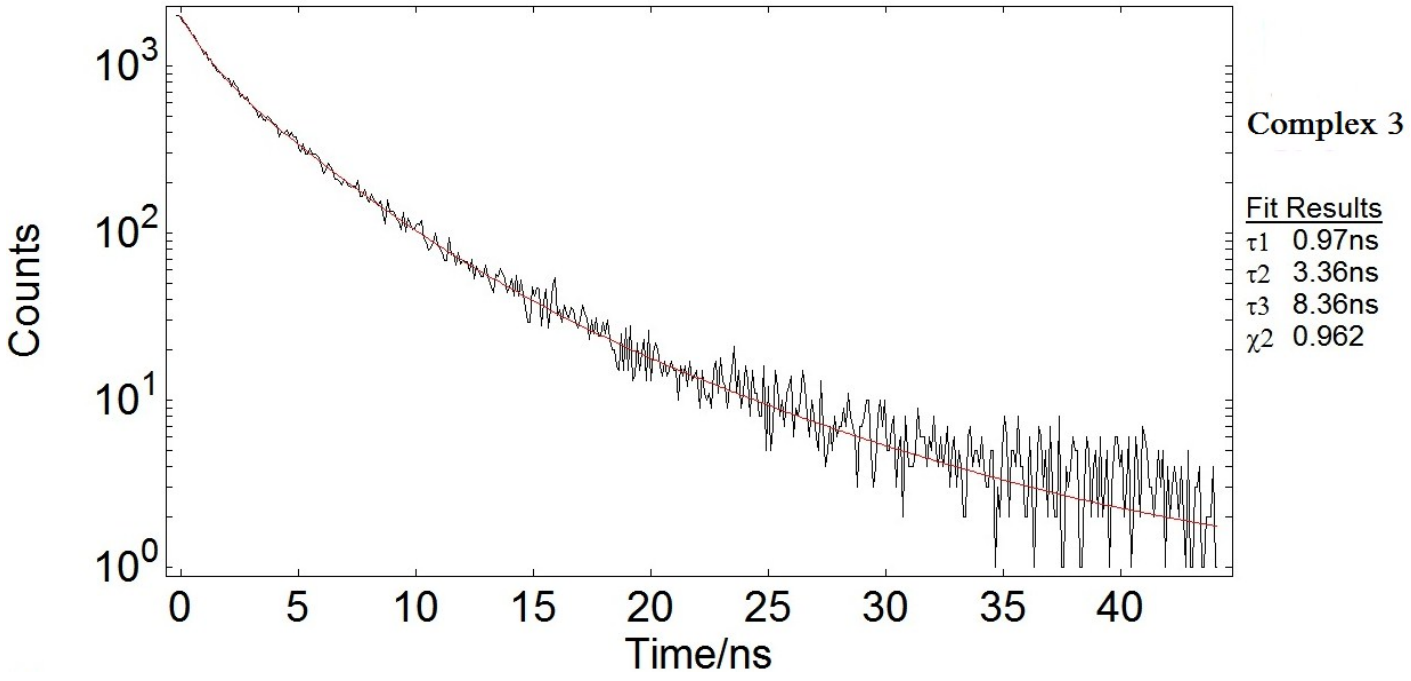


Fig. S6 Emission decay trace and triexponential fit for **3** (λ_{em} = 441 nm) at room temperature.

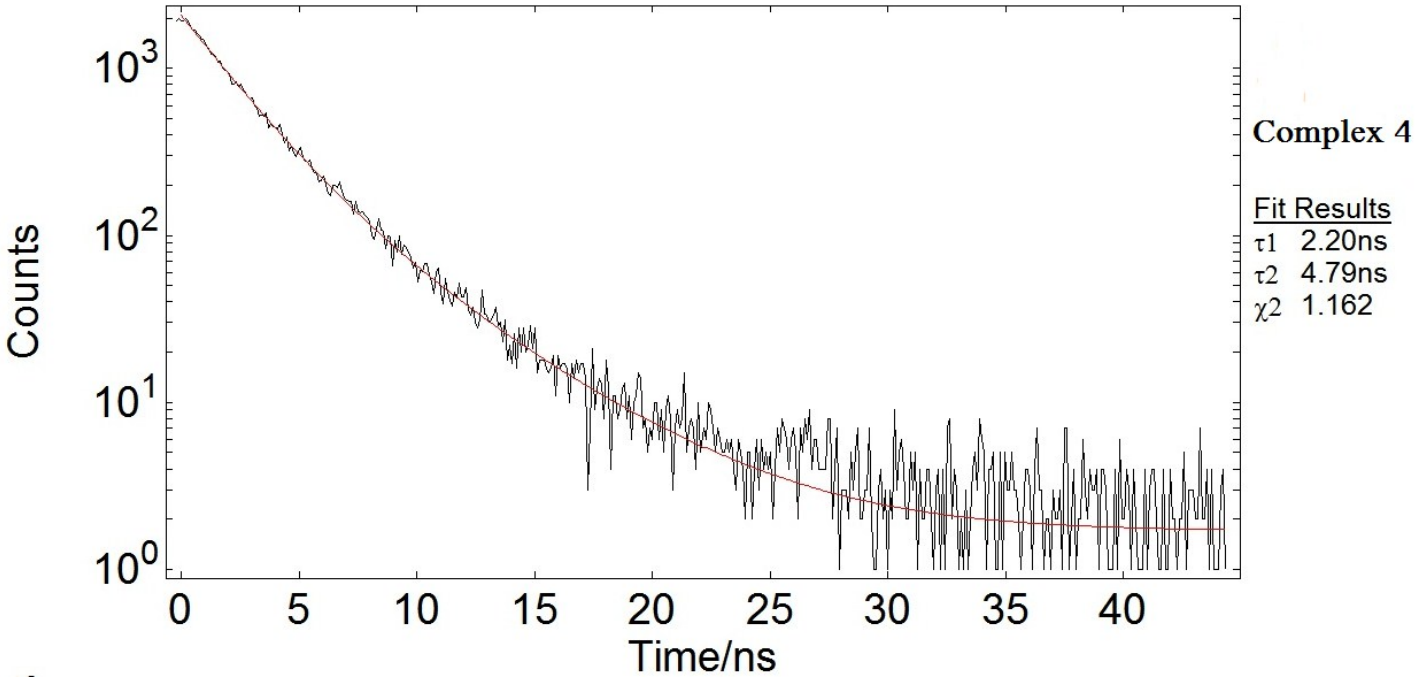


Fig. S7 Emission decay trace and biexponential fit for **4** (λ_{em} = 442 nm) at room temperature.

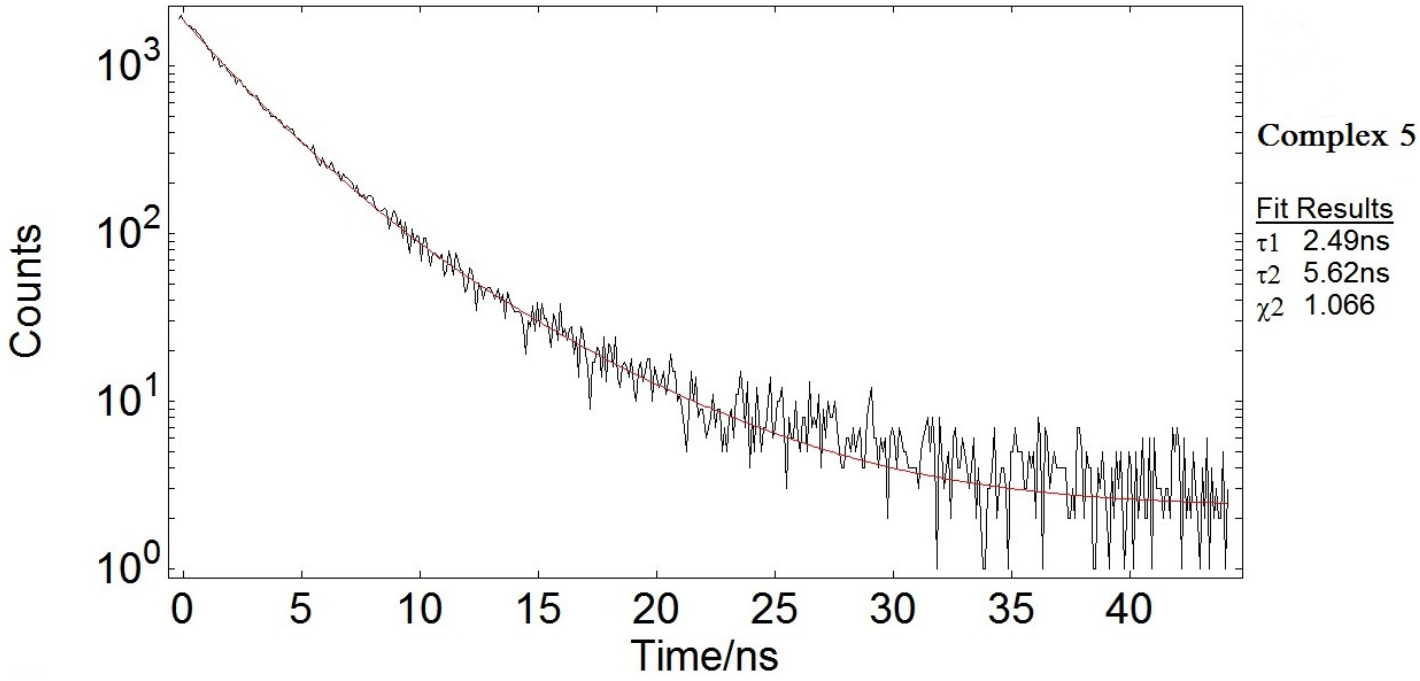


Fig. S8 Emission decay trace and biexponential fit for **5** (λ_{em} = 448 nm) at room temperature.

4. Selected Bond Distances (Å) and Angles (deg) for 1-5.

Table S1 Selected Bond Distances (Å) and Angles (deg) for **1-5**.

1			
Cd(1)-O(1)	2.252(4)	Cd(2)-O(5)#4	2.163(2)
Cd(1)-O(6)#1	2.263(3)	Cd(2)-O(5)#1	2.163(2)
Cd(1)-O(9)	2.290(4)	Cd(2)-O(2)	2.352(3)
Cd(1)-O(8)#2	2.298(3)	Cd(2)-O(2)#5	2.352(3)
Cd(1)-O(3)#3	2.407(3)	Cd(2)-O(3)#6	2.358(3)
Cd(1)-O(7)#2	2.590(3)	Cd(2)-O(3)#3	2.358(3)
Cd(1)-O(4)#3	2.592(4)	O(1)-Cd(1)-O(6)#1	131.28(12)
O(1)-Cd(1)-O(9)	89.44(16)	O(1)-Cd(1)-O(4)#3	75.07(15)
O(6)#1-Cd(1)-O(9)	82.59(14)	O(6)#1-Cd(1)-O(4)#3	129.92(15)
O(1)-Cd(1)-O(8)#2	133.88(11)	O(9)-Cd(1)-O(4)#3	146.41(14)
O(6)#1-Cd(1)-O(8)#2	93.43(11)	O(8)#2-Cd(1)-O(4)#3	84.48(12)
O(9)-Cd(1)-O(8)#2	85.42(14)	O(3)#3-Cd(1)-O(4)#3	51.44(11)
O(1)-Cd(1)-O(3)#3	89.55(13)	O(7)#2-Cd(1)-O(4)#3	69.03(12)
O(6)#1-Cd(1)-O(3)#3	83.20(10)	O(5)#4-Cd(2)-O(5)#1	180.00(13)
O(9)-Cd(1)-O(3)#3	160.13(11)	O(5)#4-Cd(2)-O(2)	88.25(11)
O(8)#2-Cd(1)-O(3)#3	109.25(13)	O(5)#1-Cd(2)-O(2)	91.75(11)
O(1)-Cd(1)-O(7)#2	81.18(12)	O(5)#4-Cd(2)-O(2)#5	91.75(11)
O(6)#1-Cd(1)-O(7)#2	142.59(11)	O(5)#1-Cd(2)-O(2)#5	88.25(11)
O(9)-Cd(1)-O(7)#2	79.38(12)	O(2)-Cd(2)-O(2)#5	180.000(1)
O(8)#2-Cd(1)-O(7)#2	52.81(12)	O(5)#4-Cd(2)-O(3)#6	89.13(10)
O(3)#3-Cd(1)-O(7)#2	120.02(10)	O(5)#1-Cd(2)-O(3)#6	90.87(10)
O(2)-Cd(2)-O(3)#6	98.10(11)	O(2)-Cd(2)-O(3)#3	81.90(11)

O(2)#5-Cd(2)-O(3)#6	81.90(11)	O(2)#5-Cd(2)-O(3)#3	98.10(11)
O(5)#4-Cd(2)-O(3)#3	90.87(10)	O(3)#6-Cd(2)-O(3)#3	180.000(1)
O(5)#1-Cd(2)-O(3)#3	89.13(10)		
		2	
Cd(1)-O(2)#1	2.354(5)	N(2)-Cd(1)-O(4)	91.8(2)
Cd(1)-N(1)	2.369(4)	O(2)#1-Cd(1)-O(5)	141.48(17)
Cd(1)-N(3)	2.364(9)	N(1)-Cd(1)-O(5)	85.37(17)
Cd(1)-N(2)	2.376(4)	N(3)-Cd(1)-O(5)	82.0(3)
Cd(1)-O(4)	2.391(5)	N(2)-Cd(1)-O(5)	92.07(17)
O(2)#1-Cd(1)-N(3)	136.5(3)	O(4)-Cd(1)-O(5)	54.79(17)
N(1)-Cd(1)-N(3)	93.6(3)	O(2)#1-Cd(1)-O(3)#1	54.51(18)
O(2)#1-Cd(1)-N(2)	90.52(19)	N(1)-Cd(1)-O(3)#1	87.85(19)
N(1)-Cd(1)-N(2)	177.44(17)	N(3)-Cd(1)-O(3)#1	82.6(3)
N(3)-Cd(1)-N(2)	86.0(3)	N(2)-Cd(1)-O(3)#1	94.6(2)
O(2)#1-Cd(1)-O(4)	86.72(18)	O(4)-Cd(1)-O(3)#1	140.67(19)
N(1)-Cd(1)-O(4)	86.8(2)	O(5)-Cd(1)-O(3)#1	162.69(19)
N(3)-Cd(1)-O(4)	136.6(3)		
		3	
Cd(1)-O(11)	2.265(7)	Cd(2)-O(1)	2.230(7)
Cd(1)-O(8)	2.295(7)	Cd(2)-O(13)	2.262(7)
Cd(1)-O(9)	2.323(9)	Cd(2)-O(14)	2.339(10)
Cd(1)-O(6)#1	2.369(7)	Cd(2)-O(3)#2	2.350(7)
Cd(1)-O(10)	2.374(9)	Cd(2)-O(4)#2	2.436(7)
Cd(1)-O(5)#1	2.434(7)	Cd(2)-O(12)	2.444(10)
Cd(1)-O(7)	2.502(7)	O(11)-Cd(1)-O(8)	139.2(3)
O(11)-Cd(1)-O(9)	109.1(3)	O(1)-Cd(2)-O(13)	124.6(3)
O(8)-Cd(1)-O(9)	84.8(3)	O(1)-Cd(2)-O(14)	102.6(3)

O(11)-Cd(1)-O(6)#1	125.6(3)	O(13)-Cd(2)-O(14)	89.8(3)
O(8)-Cd(1)-O(6)#1	91.1(2)	O(1)-Cd(2)-O(3)#2	91.2(3)
O(9)-Cd(1)-O(6)#1	90.6(3)	O(13)-Cd(2)-O(3)#2	142.4(3)
O(11)-Cd(1)-O(10)	84.7(3)	O(14)-Cd(2)-O(3)#2	93.0(3)
O(8)-Cd(1)-O(10)	78.9(3)	O(1)-Cd(2)-O(4)#2	145.2(3)
O(9)-Cd(1)-O(10)	163.6(3)	O(13)-Cd(2)-O(4)#2	90.1(3)
O(6)#1-Cd(1)-O(10)	88.1(3)	O(14)-Cd(2)-O(4)#2	76.6(3)
O(11)-Cd(1)-O(5)#1	78.7(3)	O(3)#2-Cd(2)-O(4)#2	54.4(2)
O(8)-Cd(1)-O(5)#1	142.1(2)	O(1)-Cd(2)-O(12)	91.5(3)
O(9)-Cd(1)-O(5)#1	81.5(3)	O(13)-Cd(2)-O(12)	89.9(3)
O(6)#1-Cd(1)-O(5)#1	54.0(2)	O(14)-Cd(2)-O(12)	163.1(3)
O(10)-Cd(1)-O(5)#1	110.6(3)	O(3)#2-Cd(2)-O(12)	77.1(3)
O(11)-Cd(1)-O(7)	86.8(3)	O(4)#2-Cd(2)-O(12)	86.4(3)
O(8)-Cd(1)-O(7)	54.8(2)	O(10)-Cd(1)-O(7)	84.4(3)
O(9)-Cd(1)-O(7)	87.5(3)	O(5)#1-Cd(1)-O(7)	157.8(2)
O(6)#1-Cd(1)-O(7)	145.9(3)		
4			
Zn(1)-O(1)	1.953(4)	Zn(1)-O(5)#2	1.972(4)
Zn(1)-O(7)#1	1.957(4)	Zn(1)-O(3)#3	2.022(4)
O(1)-Zn(1)-O(5)#2	129.27(18)	O(1)-Zn(1)-O(3)#3	108.04(19)
O(7)#1-Zn(1)-O(5)#2	99.95(19)	O(7)#1-Zn(1)-O(3)#3	101.44(19)
O(1)-Zn(1)-O(7)#1	116.21(18)	O(5)#2-Zn(1)-O(3)#3	97.43(18)
5			
Zn(1)-O(7)	1.940(3)	Zn(1)-O(6)#2	2.001(3)
Zn(1)-O(3)#1	1.961(3)	Zn(1)-N(4)	2.018(3)
O(7)-Zn(1)-O(3)#1	101.82(11)	O(7)-Zn(1)-N(4)	120.75(13)
O(7)-Zn(1)-O(6)#2	111.98(12)	O(3)#1-Zn(1)-N(4)	111.16(12)

O(3)#1-Zn(1)-O(6)#2	111.08(11)	O(6)#2-Zn(1)-N(4)	100.28(13)

Symmetry transformations used to generate equivalent atoms:

1: #1 x+1,-y+2,z+1/2; #2 x+1/2,y+1/2,z; #3 x,-y+2,z-1/2; #4 -x,y,-z+3/2; #5 -x+1,-y+2,-z+2; #6 -x+1,y,-z+5/2.

2: #1 -x+1/2,y+1/2,-z+1/2.

3: #1 x,-y+1/2,z+1/2; #2 -x,y-1/2,-z+1/2.

4: #1 x+1,y+1,z; #2 -x+2,y+1/2,-z+1/2; #3 -x+2,-y+2,-z.

5: #1 x+1,y,z+1; #2 -x+2,-y+2,-z+2; #3 x-1,y,z-1; #4 -x+4,-y+1,-z+2.

5. PXRD analysis of 2 and exchange products 2a-2c.

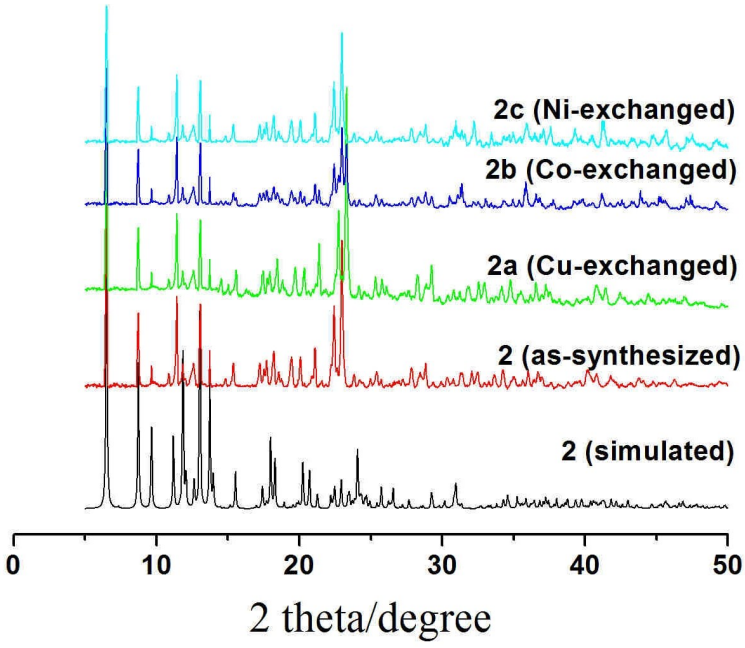


Fig. S9 Experimental and simulated PXRD patterns of **2** and **2a-2c (**as-synthesized).

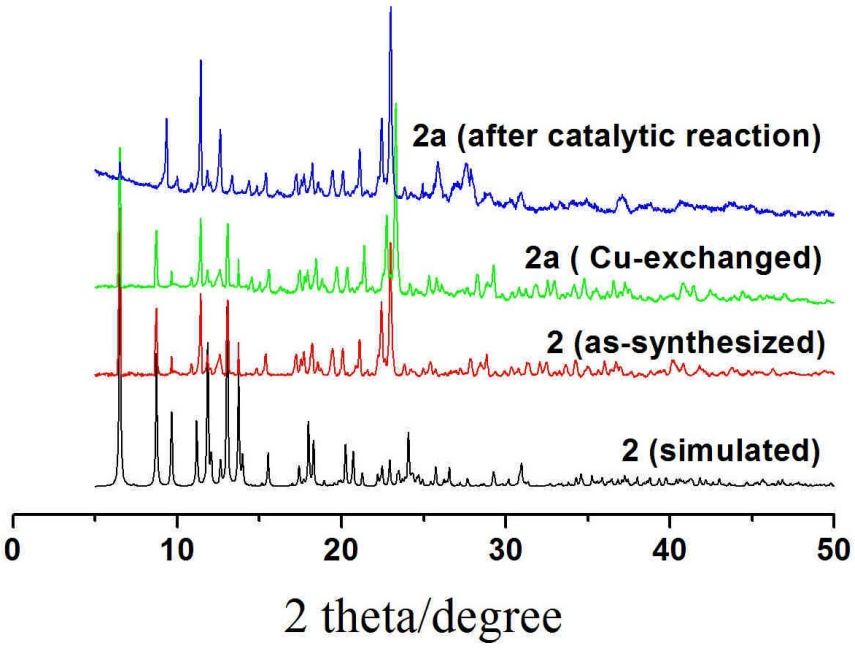


Fig. S10 Comparison of the PXRD patterns of **2a** before and after catalysis.

6. Reusability experiment of 2a.

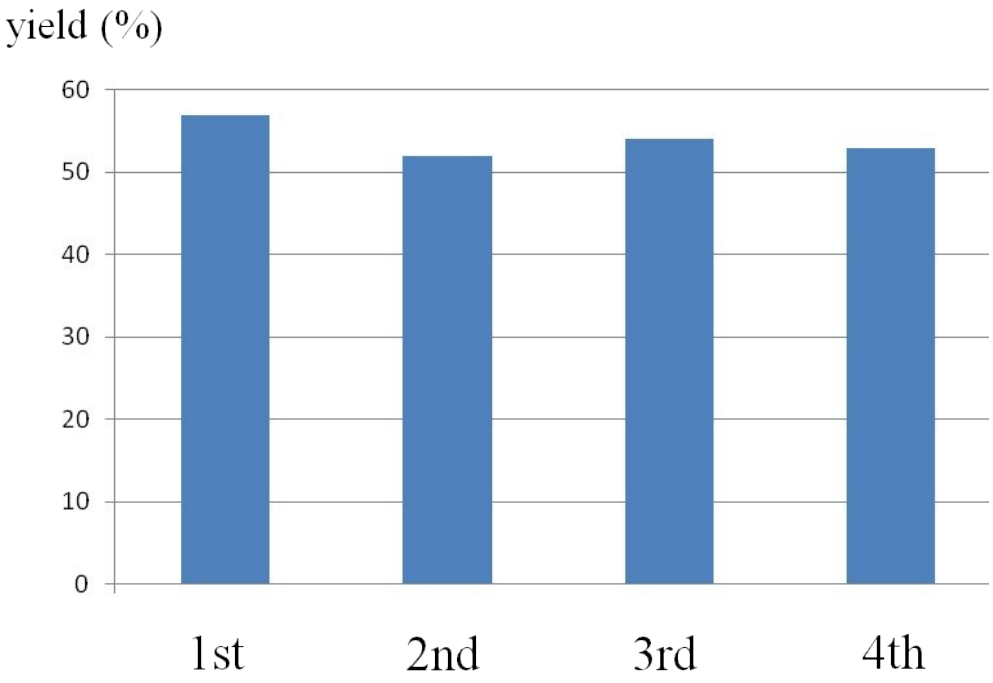


Fig. S11 Recyclability test of complex **2a** for the synthesis of **7b**.

7. 1H NMR spectra for 7a and 7b.

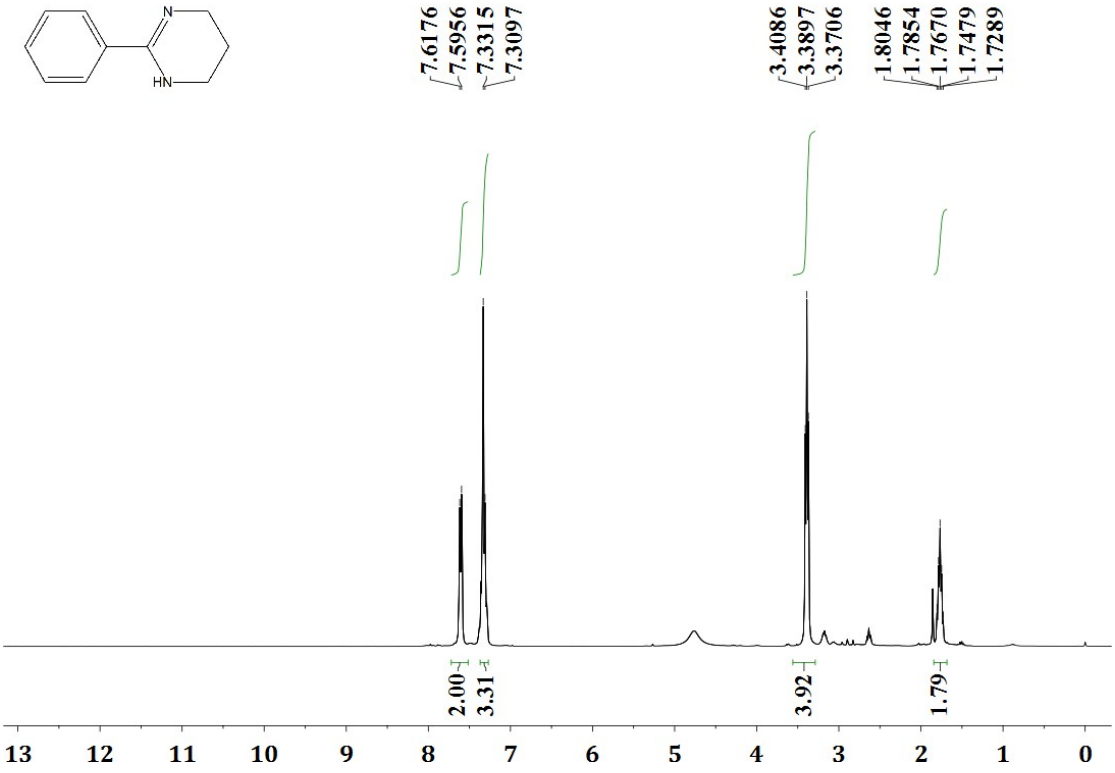
2-Phenyl-1,4,5,6-tetrahydropyrimidine (7a).

^{1}H NMR (300 MHz, CDCl3): δ = 7.62-7.60 (d, *J* = 6.6 Hz, 2 H), 7.36–7.29 (m, 3 H), 3.41-3.37 (t, *J* = 5.7 Hz, 4 H), 1.80–1.73 (m, 2 H).

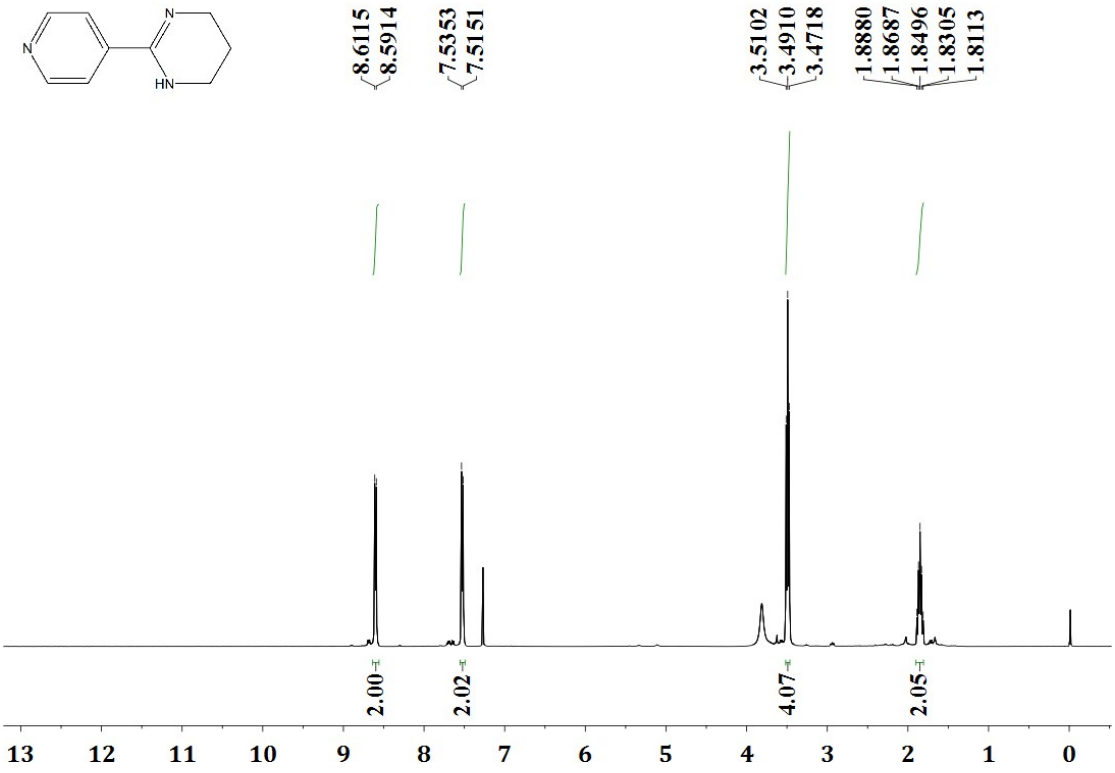
2-(Pyridin-4-yl)-1,4,5,6-tetrahydropyrimidine (7b).

^{1}H NMR (300 MHz, CDCl3): δ = 8.61-8.59 (d, *J* = 8.1 Hz, 2 H), 7.54-7.52 (d, *J* = 8.4 Hz, 2 H), 3.51-3.47 (t, *J* = 5.7 Hz, 4 H), 1.87–1.81 (m, 2 H).

^{1}H NMR data of **7a**-**b** are matched with those in previous papers.[1]



^{1}H NMR spectrum of compound **7a**



^{1}H NMR spectrum of compound **7b**

References:

(1) (*a*) S. J. An, B. Yin, P. Liu, L X. G. i, C. Li, J. L. Li, Z. Shi, *Synthesis*, 2013, **45**, 2525–2532. (*b*) M. Ishihara, H. Togo, *Tetrahedron*, 2007, **63**, 1474–1480.