## **SUPPORTING INFORMATION**

## Self assembly of a tren-derivative hydrogenated Schiff base with

## transition metal ions: syntheses, crystal structures and

## photoluminescent properties

Yuehong Wen,<sup>a</sup> Tianlu Sheng,<sup>a</sup> Qilong Zhu,<sup>a</sup> Shengmin Hu,<sup>a</sup> Chunhong Tan,<sup>a</sup> Ruibiao Fu,<sup>a</sup> and

Xintao Wu\*<sup>a</sup>

State Key Laboratory of Structure Chemistry Fujian Institute of Research on the Structure of

Matter, Chinese Academy of Sciences, Fuzhou, 350002, China.

E-mail: wxt@fjirsm.ac.cn; Fax: +86-591-83719238; Tel: +86-591-83719238

$\begin{array}{llllllllllllllllllllllllllllllllllll$				
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Zn(1)-O(1)	2.067(3)	N(3)-Zn(1)-N(1)	83.12(14)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Zn(1)-N(3)	2.100(3)	N(2)-Zn(1)-N(1)	82.32(14)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Zn(1)-N(2)	2.101(3)	N(4)- $Zn(1)$ - $N(1)$	81.60(13)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Zn(1)-N(4)	2.114(3)	$N(5)^{a}$ -Zn(2)-N(5)	180
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Zn(1)-N(1)	2.205(3)	$N(5)^{a}$ -Zn(2)-O(3)	90.60(12)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Zn(2)-N(5)	2.137(3)	N(5)-Zn(2)-O(3)	89.40(12)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	$Zn(2) - N(5)^{a}$	2.137(3)	$N(5)^{a}$ -Zn(2)-O(3) <sup>a</sup>	89.40(12)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Zn(2)-O(3)	2.146(3)	$N(5)-Zn(2)-O(3)^{a}$	90.60(12)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	$Zn(2) - O(3)^{a}$	2.146(3)	O(3)-Zn(2)-O(3) <sup>a</sup>	180
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Zn(2)-O(2)	2.148(3)	$N(5)^{a}$ -Zn(2)-O(2)	90.75(11)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	$Zn(2) - O(2)^{a}$	2.148(3)	N(5)-Zn(2)-O(2)	89.25(11)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	N(8)-O(7)	1.236(7)	O(3)-Zn(2)-O(2)	89.62(13)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	N(8)-O(8)	1.245(6)	$O(3)^{a}$ -Zn(2)-O(2)	90.38(12)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	N(8)-O(9)	1.262(6)	$N(5)^{a}$ -Zn(2)-O(2) <sup>a</sup>	89.25(11)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	N(9)-O(5)	1.210(6)	$N(5)-Zn(2)-O(2)^{a}$	90.75(11)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	N(9)-O(4)	1.214(7)	$O(3)$ -Zn(2)- $O(2)^{a}$	90.38(12)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	N(9)-O(6)	1.224(6)	$O(3)^{a}$ -Zn(2)-O(2) <sup>a</sup>	89.62(13)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	N(10)-O(21)	1.212(8)	$O(2)-Zn(2)-O(2)^{a}$	180
$\begin{array}{llllllllllllllllllllllllllllllllllll$	N(10)-O(23)	1.217(8)	O(7)-N(8)-O(8)	119.6(6)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	N(10)-O(22)	1.312(8)	O(7)-N(8)-O(9)	121.0(5)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	O(1)-Zn(1)-N(3)	97.31(13)	O(8)-N(8)-O(9)	119.4(6)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	O(1)-Zn(1)-N(2)	100.10(13)	O(5)-N(9)-O(4)	116.0(5)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	N(3)-Zn(1)-N(2)	112.45(15)	O(5)-N(9)-O(6)	121.6(5)
N(3)-Zn(1)-N(4)125.70(16)O(21)-N(10)-O(23)122.8(10)N(2)-Zn(1)-N(4)116.55(15)O(21)-N(10)-O(22)117.2(10)O(1)-Zn(1)-N(1)177.12(13)O(23)-N(10)-O(22)115.9(9)	O(1)-Zn(1)-N(4)	95.88(13)	O(4)-N(9)-O(6)	122.1(5)
N(2)-Zn(1)-N(4)116.55(15)O(21)-N(10)-O(22)117.2(10)O(1)-Zn(1)-N(1)177.12(13)O(23)-N(10)-O(22)115.9(9)	N(3)-Zn(1)-N(4)	125.70(16)	O(21)-N(10)-O(23)	122.8(10)
O(1)-Zn(1)-N(1) 177.12(13) O(23)-N(10)-O(22) 115.9(9)	N(2)-Zn(1)-N(4)	116.55(15)	O(21)-N(10)-O(22)	117.2(10)
	O(1)-Zn(1)-N(1)	177.12(13)	O(23)-N(10)-O(22)	115.9(9)

Table S1 Selected bond lengths (Å) and angles (°) of complex 1.

Symmetry codes: (a) -x, -y+1, -z+2.

Table S2 Selected bond lengths (Å) and angles (°) of complex 2.

$Cd(1)-N(2)^{a}$	2.425(4)	$N(2)^{a}-Cd(1)-Cl(4)$	84.22(10)
Cd(1)-N(1)	2.442(4)	N(1)-Cd(1)-Cl(4)	89.33(10)
Cd(1)-Cl(3)	2.4988(13)	Cl(3)-Cd(1)-Cl(4)	146.20(6)
Cd(1)- $Cl(2)$	2.5037(15)	Cl(2)-Cd(1)-Cl(4)	109.19(5)
Cd(1)-Cl(4)	2.5216(14)	N(5)-Cd(2)-N(4)	133.04(15)
Cd(2)-N(5)	2.354(4)	N(5)-Cd(2)-N(6)	111.24(15)
Cd(2)-N(4)	2.369(4)	N(4)-Cd(2)-N(6)	97.27(14)
Cd(2)-N(6)	2.375(4)	N(5)-Cd(2)-N(7)	76.30(15)
Cd(2)-N(7)	2.413(4)	N(4)-Cd(2)-N(7)	76.26(14)
Cd(2)-Cl(1)	2.4702(16)	N(6)-Cd(2)-N(7)	74.87(14)

12)
,
1)
1)
11)
1

Symmetry codes: (a) -x+2, y+3/2, -z+5/2; (b) -x+2, y-3/2, -z+5/2.

Table S3 Selected bond lengths (Å) and angles (°) of complex 3.

Cd(1)-N(4)	2.27(2)	N(2)-Cd(1)-N(1)	75.6(2)
Cd(1)-N(3)	2.353(5)	N(4')-Cd(1)-N(1)	74.9(5)
Cd(1)-N(2)	2.372(6)	O(2)-Cd(1)-N(1)	148.13(17)
Cd(1)-N(4')	2.38(2)	N(4)-Cd(1)-O(1)	88.5(6)
Cd(1)-O(2)	2.407(5)	N(3)-Cd(1)-O(1)	134.21(19)
Cd(1)-N(1)	2.440(6)	N(2)-Cd(1)-O(1)	88.0(2)
Cd(1)-O(1)	2.456(5)	N(4')-Cd(1)-O(1)	84.0(5)
Cd(2)-O(4)	2.317(5)	O(2)-Cd(1)-O(1)	51.79(18)
$Cd(2)-O(4)^{a}$	2.317(5)	N(1)-Cd(1)-O(1)	150.2(2)
$Cd(2)-N(7)^{b}$	2.372(5)	$O(4)-Cd(2)-O(4)^{a}$	180
$Cd(2)-N(7)^{c}$	2.372(5)	$O(4)-Cd(2)-N(7)^{b}$	90.25(19)
Cd(2)-N(6)	2.383(5)	$O(4)^{a}-Cd(2)-N(7)^{b}$	89.75(19)
$Cd(2)-N(6)^{a}$	2.383(5)	$O(4)-Cd(2)-N(7)^{c}$	89.75(19)
$N(7)-Cd(2)^{d}$	2.372(5)	$O(4)^{a}-Cd(2)-N(7)^{c}$	90.25(19)
N(8)-O(1)	1.226(8)	$N(7)^{b}$ -Cd(2)-N(7) <sup>c</sup>	180
N(8)-O(3)	1.238(7)	O(4)-Cd(2)-N(6)	84.68(18)
N(8)-O(2)	1.250(7)	$O(4)^{a}-Cd(2)-N(6)$	95.32(18)
N(9)-O(5)	1.161(9)	$N(7)^{b}$ -Cd(2)-N(6)	86.40(18)
N(9)-O(7)	1.175(12)	$N(7)^{c}-Cd(2)-N(6)$	93.60(18)
N(9)-O(6)	1.297(13)	$O(4)-Cd(2)-N(6)^{a}$	95.32(18)
N(10)-O(10)	1.158(12)	$O(4)^{a}-Cd(2)-N(6)^{a}$	84.68(18)
N(10)-O(8)	1.255(12)	$N(7)^{b}$ -Cd(2)-N(6) <sup>a</sup>	93.60(18)
N(10)-O(9)	1.288(13)	$N(7)^{c}-Cd(2)-N(6)^{a}$	86.40(18)
N(4)-C(7)	1.48(2)	$N(6)-Cd(2)-N(6)^{a}$	180
N(4)-Cd(1)-N(3)	114.7(4)	O(1)-N(8)-O(3)	121.0(6)
N(4)-Cd(1)-N(2)	115.4(4)	O(1)-N(8)-O(2)	118.2(6)
N(3)-Cd(1)-N(2)	112.9(2)	O(3)-N(8)-O(2)	120.8(6)
N(4)-Cd(1)-N(4')	15.7(6)	O(5)-N(9)-O(7)	132.8(11)
N(3)-Cd(1)-N(4')	127.7(5)	O(5)-N(9)-O(6)	111.8(11)
N(2)-Cd(1)-N(4')	100.1(6)	O(7)-N(9)-O(6)	107.8(10)
N(4)-Cd(1)-O(2)	135.1(6)	O(10)-N(10)-O(8)	122.6(15)
N(3)-Cd(1)-O(2)	87.73(18)	O(10)-N(10)-O(9)	123.8(15)
N(2)-Cd(1)-O(2)	86.74(19)	O(8)-N(10)-O(9)	113.3(10)
N(4')-Cd(1)-O(2)	135.2(5)	N(8)-O(1)-Cd(1)	94.1(4)
N(4)-Cd(1)-N(1)	76.8(6)	N(8)-O(2)-Cd(1)	95.8(4)
N(3)-Cd(1)-N(1)	75.52(19)		

Symmetry codes: (a)-x+1, -y+1, -z+2; (b) x+1/2, -y+1/2, z+1/2; (c)-x+1/2, y+1/2, -z+3/2; (d) -x+1/2, y-1/2, -z+3/2.

Table S4 Selected bond lengths (Å) and angles (°) of complex 4.

	$Mn(1)-N(7)^{a}$	2.300(4)	N(5)-Mn(1)-Cl(2)	88.57(9)
	$Mn(1)-N(7)^{b}$	2.300(4)	$N(7)^{a}-Mn(1)-Cl(2)^{c}$	90.08(11)
	$Mn(1)-N(5)^{c}$	2.348(4)	$N(7)^{b}-Mn(1)-Cl(2)^{c}$	89.92(11)
	Mn(1)-N(5)	2.348(4)	$N(5)^{c}-Mn(1)-Cl(2)^{c}$	88.57(9)
	Mn(1)-Cl(2)	2.5027(11)	$N(5)-Mn(1)-Cl(2)^{c}$	91.43(9)
	$Mn(1)$ - $Cl(2)^{c}$	2.5027(11)	$Cl(2)-Mn(1)-Cl(2)^{c}$	180
	Mn(2)-O(1)	2.239(4)	O(1)-Mn(2)-N(2)	84.03(14)
	Mn(2)-N(2)	2.301(4)	O(1)-Mn(2)-N(4)	85.97(18)
	Mn(2)-N(4)	2.324(4)	N(2)-Mn(2)-N(4)	146.71(15)
	Mn(2)-N(3)	2.327(4)	O(1)-Mn(2)-N(3)	176.01(15)
	Mn(2)-N(1)	2.331(4)	N(2)-Mn(2)-N(3)	93.55(14)
	Mn(2)- $Cl(1)$	2.4471(15)	N(4)-Mn(2)-N(3)	94.40(18)
	$N(7)-Mn(1)^d$	2.300(4)	O(1)-Mn(2)-N(1)	100.03(14)
	$N(7)^{a}-Mn(1)-N(7)^{b}$	180	N(2)-Mn(2)-N(1)	76.28(13)
	$N(7)^{a}-Mn(1)-N(5)^{c}$	87.04(14)	N(4)-Mn(2)-N(1)	74.34(14)
	$N(7)^{b}-Mn(1)-N(5)^{c}$	92.96(14)	N(3)-Mn(2)-N(1)	76.27(14)
	$N(7)^{a}-Mn(1)-N(5)$	92.96(14)	O(1)-Mn(2)-Cl(1)	90.97(12)
	$N(7)^{b}-Mn(1)-N(5)$	87.04(14)	N(2)-Mn(2)-Cl(1)	112.53(10)
	$N(5)^{c}-Mn(1)-N(5)$	180	N(4)-Mn(2)-Cl(1)	99.29(12)
	$N(7)^{a}-Mn(1)-Cl(2)$	89.92(11)	N(3)-Mn(2)-Cl(1)	92.89(11)
	$N(7)^{b}-Mn(1)-Cl(2)$	90.08(11)	N(1)-Mn(2)-Cl(1)	166.74(11)
_	$N(5)^{c}-Mn(1)-Cl(2)$	91.43(9)		

Symmetry codes: (a) x+1/2, -y-1/2, z-1/2;(b) -x+1/2, y+1/2, -z+1/2;(c) -x+1, -y, -z; (d) -x+1/2, y-1/2, -z+1/2.

Figure S1 Comparison of experimental and calculated powder X-ray diffraction patterns of complex 1.



Figure S2 Comparison of experimental and calculated powder X-ray diffraction patterns of complex 2.



Figure S3 Comparison of experimental and calculated powder X-ray diffraction

patterns of complex 3.



Figure S4 Comparison of experimental and calculated powder X-ray diffraction patterns of complex 4.

