Electronic Supporting Information

Sn(II)-Doped One-Dimensional Hybrid Metal Halide $[C_5H_{14}NO]CdCl_3$ Single Crystals With Broadband Greenish-Yellow Light Emission.

Haiming Cheng,[1a] *Chi Cao,*[1a] *Shiyong Teng,*[d] *Zhinan Zhang,*[a] *Ying Zhang,*[a] *Dayang Wang,*[a] *Wensheng Yang,*[abc] *and Renguo Xie**[a]

[a] State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry Jilin University, Changchun 130012, China.

[b] Engineering Center for Nanomaterials, Henan University, Kaifeng, 475004, China

[c] Institute of Molecular Plus, Tianjin University, Tianjin, 300072, China.

[d] First Hospital, Jilin University, Changchun 130021, China.

[*]E-mail: renguoxie@jlu.edu.cn

Table of contents

Table S1. Crystal data and structure refinement for $[C_5H_{14}NO]CdCl_3$.

Formula	$[C_5H_{14}NO]CdCl_3$
Formula mass	322.92
Crystal system	orthorhombic
Space group	$Pna2_1$
a (Å)	16.8879 (4)
b (Å)	8.1763 (2)
c (Å)	7.7975 (2)
α (°)	90
β (°)	90
γ (°)	90
V (Å^3)	1076.68 (5)
Z	4
ρ_{calcd} (g/cm^3)	1.992
Temperature (K)	293
λ (Å)	0.71073
F(000)	632
μ (mm^{-1})	2.72
$R1$, $wR2$ ($I > 2\sigma(I)$)[a]	0.0175/0.0339
GOF on F^2	-0.004(19)

Table S2. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $[C_5H_{14}NO]CdCl_3$. $U_{(eq)}$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

atom	x	y	z	U_{eq} ($Å^2$)
Cd1	4903.5(2)	4835.6(2)	4003.5(6)	26.37(7)
Cl1	4011.5(5)	2369.8(9)	4580.6(9)	35.86(18)
Cl2	4246.0(4)	6502.7(9)	6529.2(11)	31.09(16)
Cl3	5968.8(4)	4119.6(9)	6382.7(10)	30.96(16)
O1	5632.1(13)	7253(2)	3349(3)	31.0(5)
N1	6805.8(15)	9500(3)	5155(3)	26.5(5)
C1	5456.6(17)	8921(3)	3770(4)	29.7(7)
C2	5912.7(17)	9476(4)	5323(4)	27.0(6)
C3	7134(2)	10360(4)	6692(5)	44.2(9)
C4	7058(2)	10392(5)	3581(5)	57.5(12)
C5	7140(2)	7809(4)	5157(5)	47.9(9)

Table S3. Selected bond lengths (Å) and angles (deg) for $[C_5H_{14}NO]CdCl_3$.

Cd1—Cl1	2.5566(7)	O1—C1	1.433(3)
Cd1—Cl2[1]	2.6424(9)	N1—C2	1.514(4)
Cd1—Cl2	2.6400(9)	N1—C3	1.495(4)
Cd1—Cl3	2.6497(9)	N1—C4	1.490(4)
Cd1—Cl3[1]	2.6601(9)	N1—C5	1.494(4)
Cd1—O1	2.3838(19)	C1—C2	1.505(4)
Cl1—Cd1—Cl2	91.61(3)	O1—Cd1—Cl3	89.01(6)
Cl1—Cd1—Cl2[1]	97.02(3)	O1—Cd1—Cl3[1]	81.66(6)
Cl1—Cd1—Cl3[1]	93.57(3)	Cd1—Cl2—Cd1[2]	95.87(2)
Cl1—Cd1—Cl3	95.89(3)	Cd1—Cl3—Cd1[2]	95.22(2)
Cl2—Cd1—Cl2[1]	170.783(9)	C1—O1—Cd1	129.27(17)
Cl2[1]—Cd1—Cl3[1]	82.71(3)	C3—N1—C2	107.8(2)
Cl2—Cd1—Cl3[1]	100.04(2)	C4—N1—C2	111.2(3)
Cl2—Cd1—Cl3	82.96(3)	C4—N1—C3	108.9(3)
Cl2[1]—Cd1—Cl3	92.90(2)	C4—N1—C5	110.2(3)
Cl3—Cd1—Cl3[1]	170.005(18)	C5—N1—C2	111.4(2)
O1—Cd1—Cl1	174.73(6)	C5—N1—C3	107.1(2)
O1—Cd1—Cl2[1]	84.63(5)	O1—C1—C2	111.4(2)
O1—Cd1—Cl2	87.06(5)	C1—C2—N1	116.4(2)

Symmetry codes: (i) 1-X,1-Y,-1/2+Z; (ii) 1-X,1-Y,1/2

Table S4. The data of ICP-OES and the molar ratios of $[C_5H_{14}NO]CdCl_3:xSn^{2+}$ ($0 \leq x \leq 0.25$)

Sn / Cd precursors ratio (at%)	ICP-OES-determined	PLQY
2%	0.96%	41.07%
5%	1.12%	80.28%
10%	1.33%	91.27%
15%	1.76%	86.25%
20%	2.14%	83.30%
25%	2.3%	71.72%

Table S5. Chromaticity coordinates of $[C_5H_{14}NO]CdCl_3:Sn^{2+}$ crystals at different temperatures when excited by 288nm UV light.

No.	Temperature (K)	Chromaticity coordinates (x, y)
A	80	0.4632, 0.5011
B	110	0.4656, 0.5025
C	140	0.4415, 0.5144
D	170	0.4187, 0.5184
E	200	0.3790,0.5181
F	230	0.3408, 0.5052
G	260	0.3282, 0.4886
H	290	0.3234, 0.4750
I	320	0.3212, 0.4615

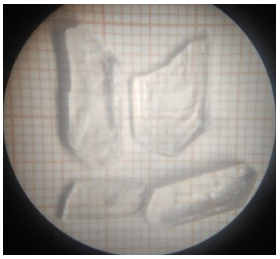

Figure S1. The photographs of $[C_5H_{14}NO]CdCl_3$ crystals were obtained by slow volatilization.

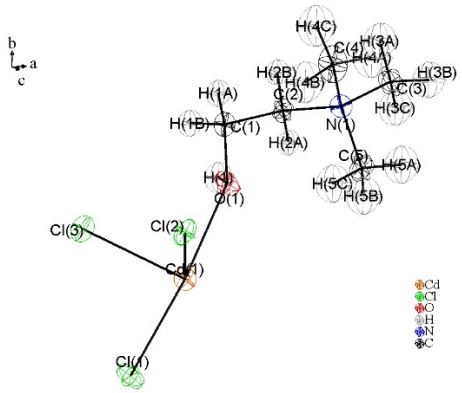

Figure S2. The asymmetric unit of compound $[C_5H_{14}NO]CdCl_3$.

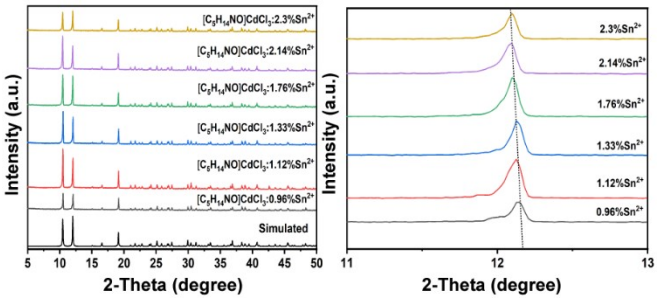

Figure S3. Powder X-ray diffraction (PXRD) patterns (left) and magnified PXRD patterns (right) of $[C_5H_{14}NO]CdCl_3:Sn^{2+}$

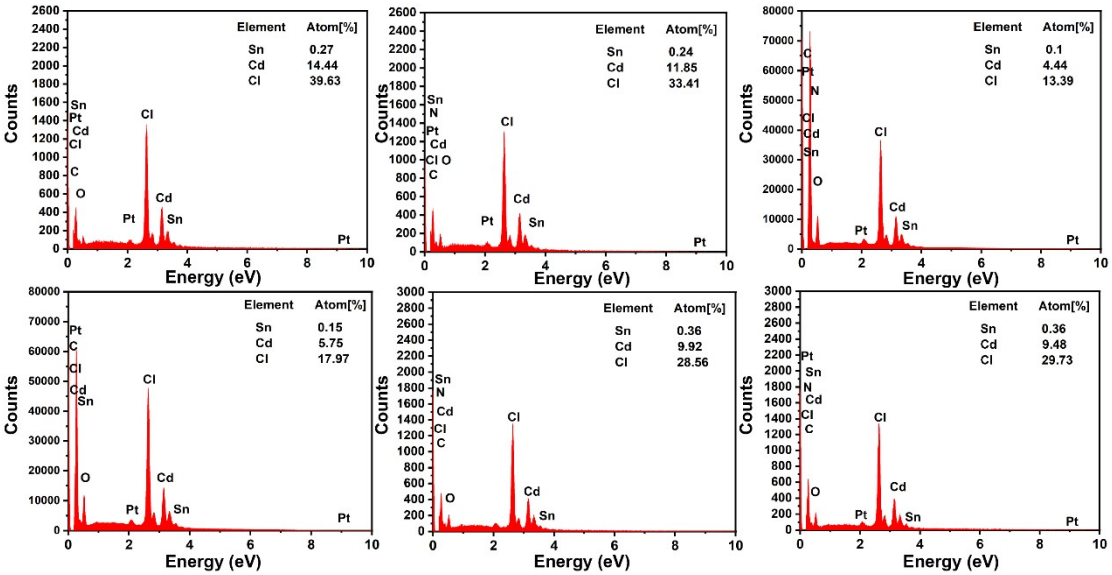

Figure S4. The EDS spectrum of as-synthesized $[C_5H_{14}NO]CdCl_3$:xSn^{2+} samples.

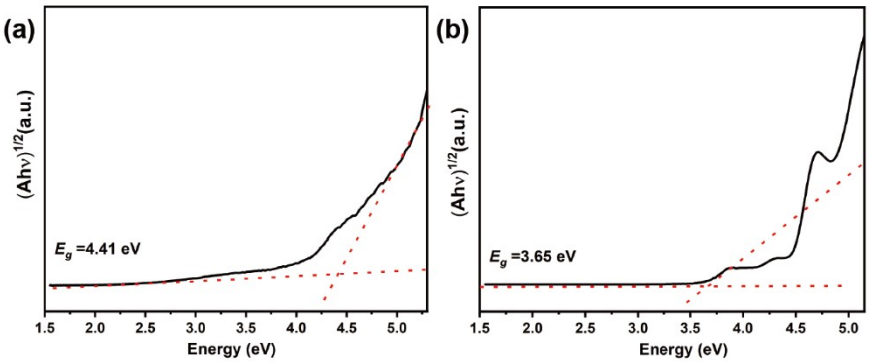

Figure S5. A Tauc plot of the absorption measurements of the $[C_5H_{14}NO]CdCl_3$ and $[C_5H_{14}NO]CdCl_3$:1.33%Sn^{2+}.

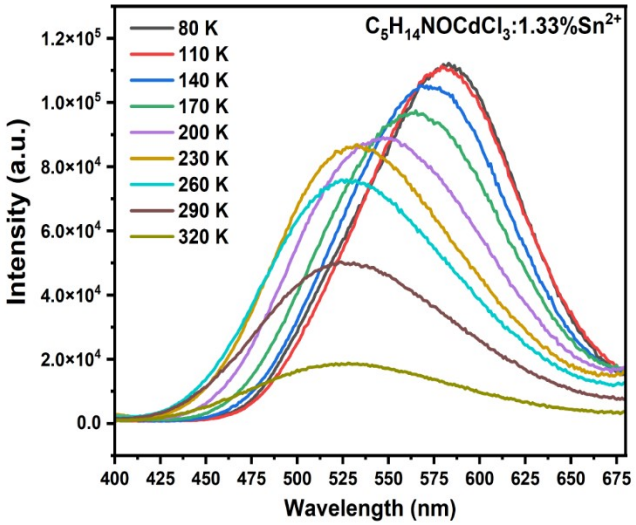

Figure S6. Emission spectra of Sn^{2+}-doped $[C_5H_{14}NO]CdCl_3$ samples at different temperatures.

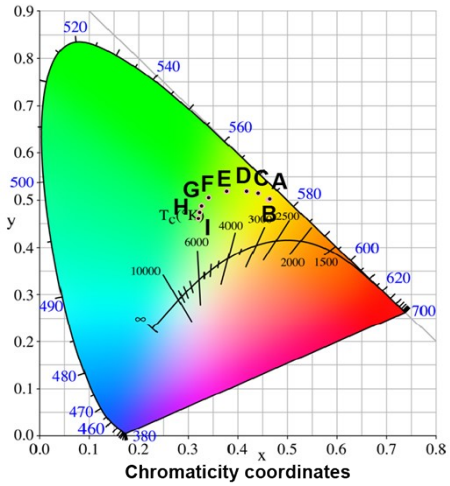

Figure S7. Chromaticity coordinate diagram of $[C_5H_{14}NO]CdCl_3$:1.33%Sn^{2+} sample under different temperature conditions.

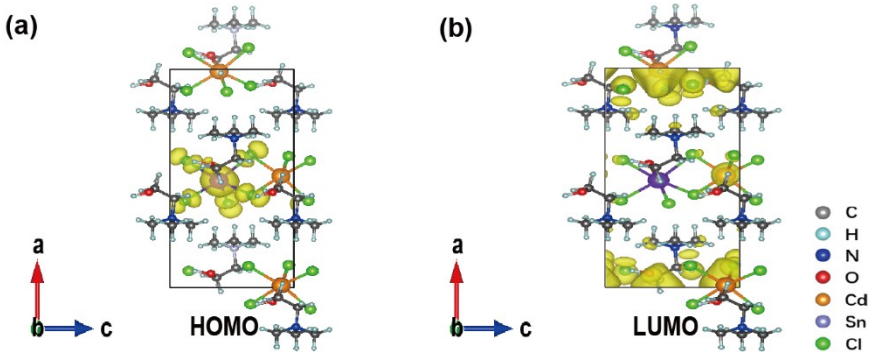

Figure S8. Charge densities of the VBM (a) and CBM (b) for Sn^{2+}-doped $[C_5H_{14}NO]CdCl_3$.

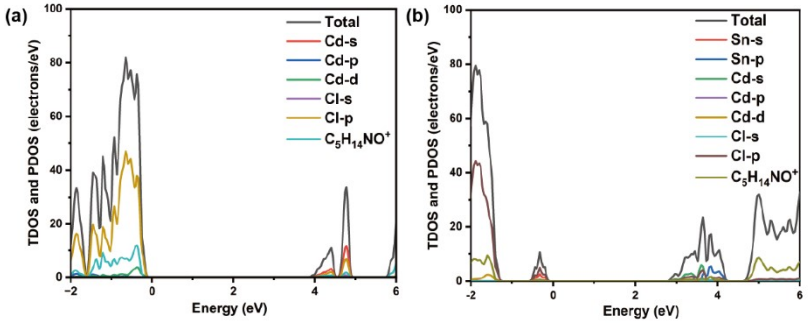

Figure S9. The calculated partial DOS of (a) $[C_5H_{14}NO]CdCl_3$ and (b) Sn^{2+}-doped $[C_5H_{14}NO]CdCl_3$.