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Construction of Structurally Diverse Luminescent Lead (II) Fluorinated Coordination Polymers Based on Auxiliary Ligands

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Table S1 Crystallographic Data collection and refinement result of complexes **1-4**

Complex	**1**	**2**	**3**	**4**
Formula	$C_{18}H_8F_4N_2O_4Pb$	$C_{20}H_8F_4N_2O_4Pb$	$C_{13}H_6F_4NO_5Pb$	$C_{21}H_{14}F_4N_2O_4Pb$
M_r	599.46	623.48	539.39	641.54
Temperature / K	293	293	293	293
Crystal system	monoclinic	monoclinic	triclinic	Orthorhombic
Space group	$P2_1/c$	$P2/c$	P-1	$Pbca$
a / Å	9.962(3)	8.3379(13)	7.722(2)	9.211(2)
b / Å	12.927(3)	12.8358(12)	8.4029(19)	15.947(4)
c / Å	13.826(4)	8.7757(13)	12.016(3)	27.262(7)
α / °	90	90	93.629(3)	90
β / °	103.856(4)	103.116(10)	103.750(9)	90
γ / °	90	90	106.323(11)	90
Volume (Å^3)	1728.7(8)	914.7(2)	719.7(3)	4004.5(17)
Z	4	2	2	8
D_{calcd} (mg/m^3)	2.303	2.264	2.489	2.128
μ (mm^{-1})	9.831	9.295	11.794	8.496
F(000)	1120	584	498	2432
Total/Unique,	14622/3939	6965/2097	8198/4093	29421/4484
R_{int}	0.042	0.032	0.053	0.045
GOF	1.01	1.06	1.07	1.07
R_1,wR_2 [I>2σ(I)]	0.0304, 0.0612	0.0271, 0.0525	0.0445, 0.0885	0.0369, 0.0807
R_1,wR_2 (all data)	0.0379, 0.0649	0.0307, 0.0541	0.0552, 0.0949	0.0478, 0.0865
$(\Delta\rho)_{max}$, $(\Delta\rho)_{min}$ (e Å^{-3})	0.62, -1.41	0.88, -1.20	1.74, -1.48	1.99, -1.35

Table S2 Selected bond distances (Å) and angles (º) for **1-4**

Complex 1

Pb(1)-O(4)#1	2.304(7)	Pb(1)-O(2)	2.439(6)
Pb(1)-N(2)	2.551(8)	Pb(1)-N(1)	2.616(8)
Pb(1)-O(1)#2	2.754(7)	O(4)#1-Pb(1)-O(2)	84.9(3)
O(4)#1-Pb(1)-N(2)	83.7(3)	O(2)-Pb(1)-N(2)	75.8(2)
O(4)#1-Pb(1)-N(1)	75.1(2)	O(2)-Pb(1)-N(1)	135.6(2)
N(2)-Pb(1)-N(1)	63.0(3)	O(4)#1-Pb(1)-O(1)#2	84.2(3)
O(2)-Pb(1)-O(1)#2	135.1(2)	N(2)-Pb(1)-O(1)#2	145.3(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y+1/2,-z+1/2 #2 -x+1,-y+1,-z #3 -x+1,y-1/2,-z+1/2

Complex 2

Pb(1)-O(3)	2.532(3)	Pb(1)-O(3)#1	2.532(3)
Pb(1)-N(1)#1	2.601(3)	Pb(1)-N(1)	2.601(3)
Pb(1)-O(3)#2	2.810(2)	Pb(1)-O(3)#3	2.810(2)
Pb(1)-O(1)#2	2.911(4)	Pb(1)-O(1)#3	2.911(3)
O(3)-Pb(1)-O(3)#1	156.77(12)	O(3)-Pb(1)-N(1)#1	74.64(9)
O(3)#1-Pb(1)-N(1)#1	85.56(9)	N(1)#1-Pb(1)-N(1)	63.61(13)
O(3)-Pb(1)-O(3)#2	118.57(10)	O(3)#1-Pb(1)-O(3)#2	69.15(9)
N(1)#1-Pb(1)-O(3)#2	137.78(9)	N(1)-Pb(1)-O(3)#2	77.02(8)
N(1)#1-Pb(1)-O(3)#3	77.02(8)	O(1)#2-Pb(1)-O(1)#3	102.47(17)
O(3)#3-Pb(1)-O(1)#3	45.03(8)	N(1)#1-Pb(1)-O(1)#3	100.12(10)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+2,-z #2 x+1,y+1,z #3 -x,-y+2,-z

Complex 3

Pb(1)-O(1)#1	2.440(6)	Pb(1)-O(3)#2	2.496(5)
Pb(1)-N(1)	2.707(7)	Pb(1)-O(1)	2.711(6)
Pb(1)-O(4)#2	2.730(6)	Pb(1)-O(5)	2.795(7)
Pb(1)-O(3)#3	2.835(6)	Pb(1)-O(2)	2.892(7)
O(1)#1-Pb(1)-O(3)#2	97.5(2)	O(1)#1-Pb(1)-N(1)	83.7(2)
O(3)#2-Pb(1)-N(1)	76.4(2)	O(1)#1-Pb(1)-O(1)	67.6(2)
O(3)#2-Pb(1)-O(1)	119.7(2)	N(1)-Pb(1)-O(1)	147.9(2)
O(1)#1-Pb(1)-O(4)#2	76.22(19)	O(3)#2-Pb(1)-O(4)#2	49.00(18)
N(1)-Pb(1)-O(4)#2	117.0(2)	O(1)-Pb(1)-O(4)#2	70.80(18)
O(1)#1-Pb(1)-O(5)	80.9(2)	O(3)#2-Pb(1)-O(5)	158.4(2)
N(1)-Pb(1)-O(5)	81.9(2)	O(1)-Pb(1)-O(5)	79.9(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2 #2 x,-y,z-1/2 #3 -x,-y,-z+1

Complex 4

Pb(1)-O(3)#1	2.455(6)	Pb(1)-O(2)	2.468(6)
Pb(1)-N(1)	2.631(7)	Pb(1)-N(2)#2	2.717(7)
Pb(1)-O(4)#1	2.758(7)	O(3)#1-Pb(1)-N(1)	80.4(2)
O(3)#1-Pb(1)-O(2)	72.7(2)	O(3)#1-Pb(1)-N(2)#2	77.3(2)
O(2)-Pb(1)-N(1)	73.7(2)	O(2)-Pb(1)-N(2)#2	79.0(2)
N(1)-Pb(1)-N(2)#2	148.8(2)	O(3)#1-Pb(1)-O(4)#1	50.4(2)
O(2)-Pb(1)-O(4)#1	121.9(2)	N(1)-Pb(1)-O(4)#1	103.8(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y-1/2,-z+3/2 #2 x,-y+1/2,z-1/2

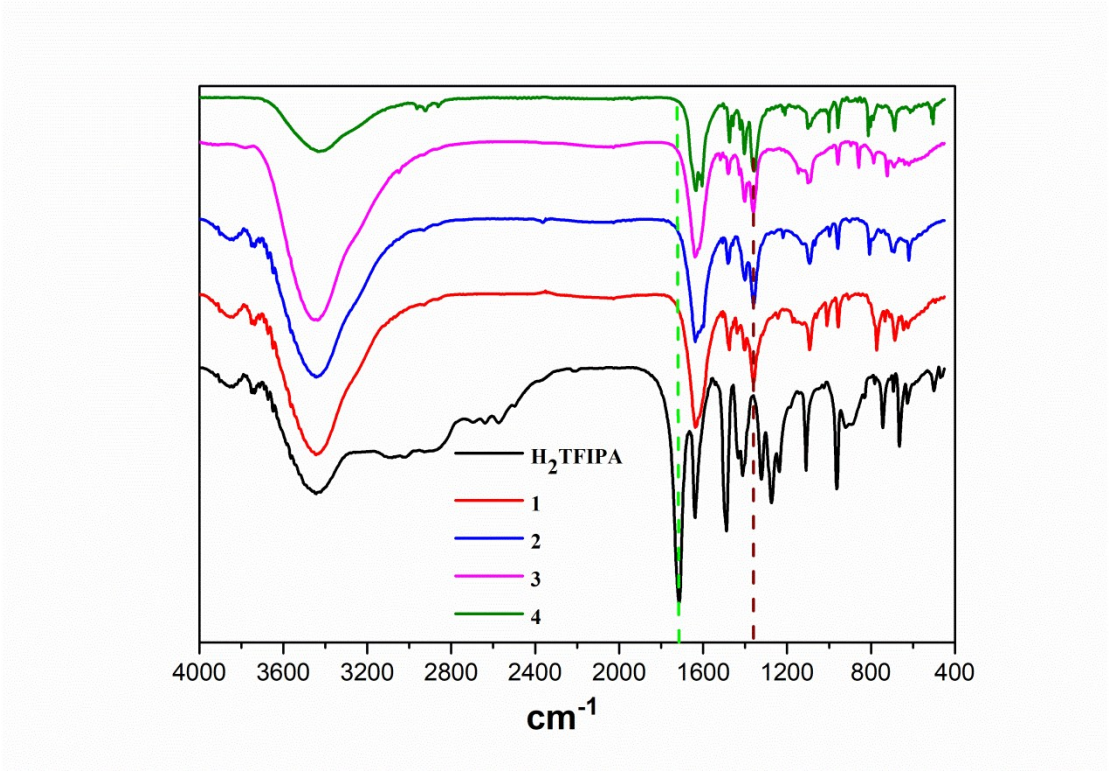

Figure S1. IR spectrum of complexes **1-4** and free H_2TFIPA.

Comparison IR spectrum of complexes **1-4** with free H_2TFIPA, the carboxylate groups of the H_2TFIPA were completely deprotonated in all compounds due to the absence of the absorption band in the range of 1770-1680 cm^{-1} for the protonated carboxylate groups in free H_2TFIPA ligand. And, there has a distinct absorption peak at about 1360 cm^{-1} for complexes **1-4** which should be ascribed the ν(C=N) vibration of N-donor auxiliary ligands.

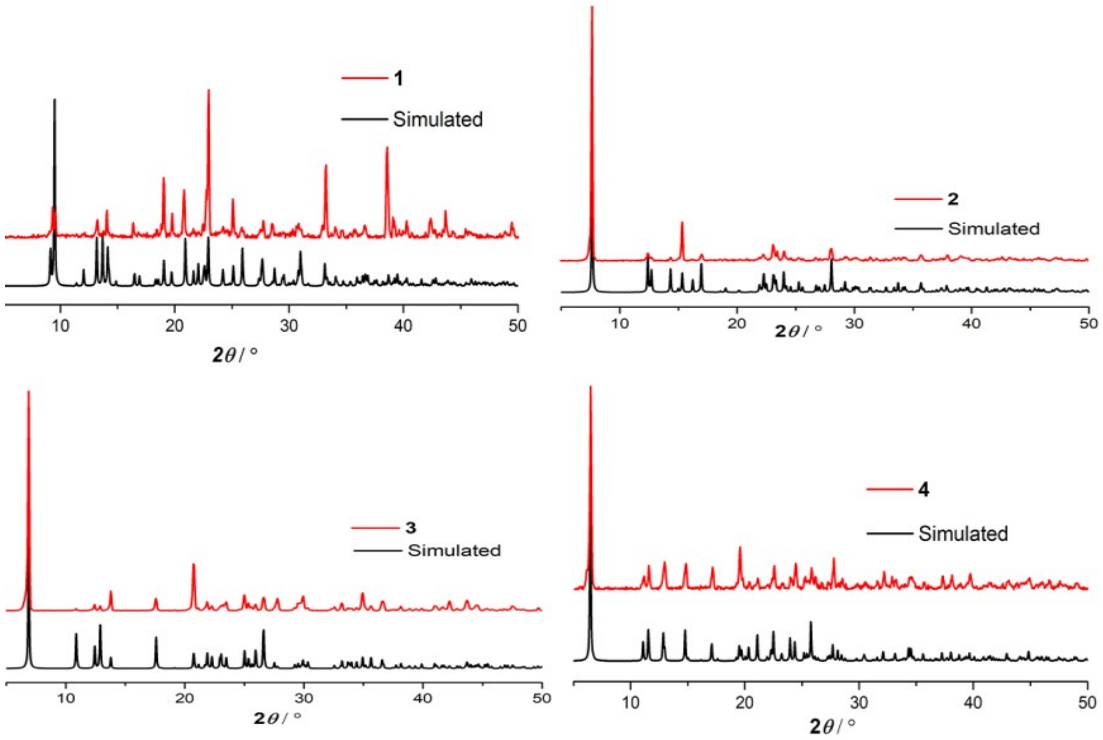

Figure S2. PXRD patterns of complexes **1-4** for simulated (black) and the as-synthesized (red).

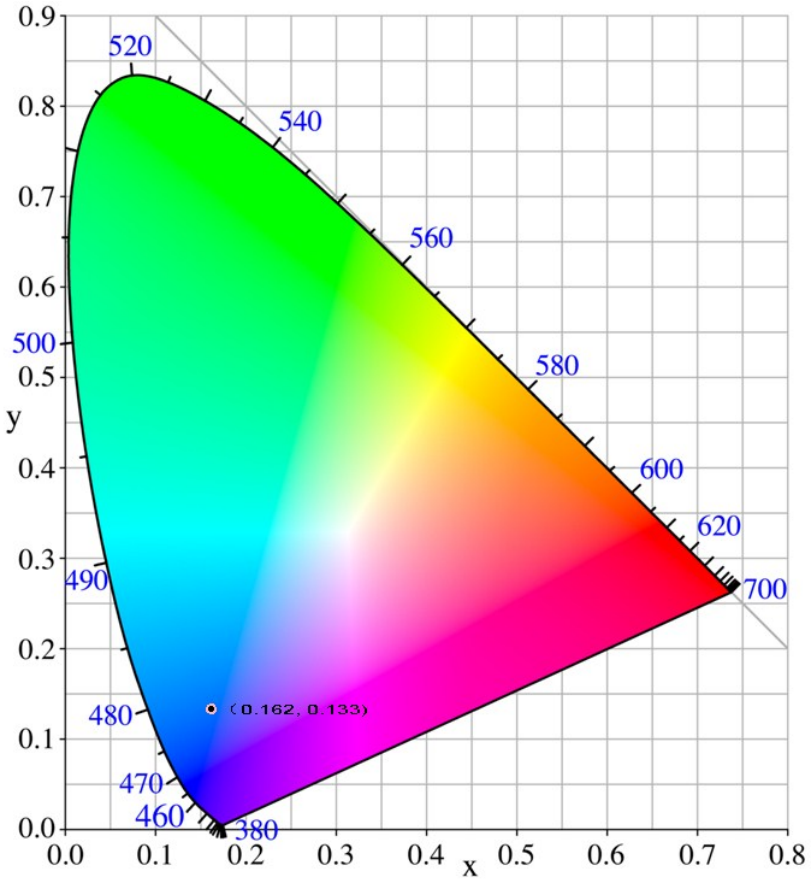

Figure S3. Plot of colour coordinates on the CIE 1931 chromaticity diagram for **3**