Near-White Light Emission from Lead(II) Metal-Organic Frameworks

Supporting Information

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1.1 X-ray Crystallographic Structures

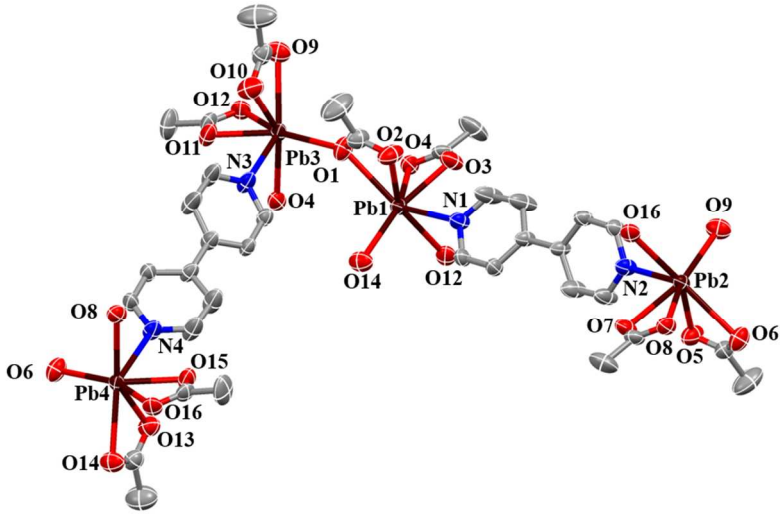

Figure S1. A view of the asymmetric unit in **1** (50% probability ellipsoid) showing the coordination environment of Pb1, Pb2, Pb3 and Pb4 (C-H hydrogen atoms are omitted for clarity).

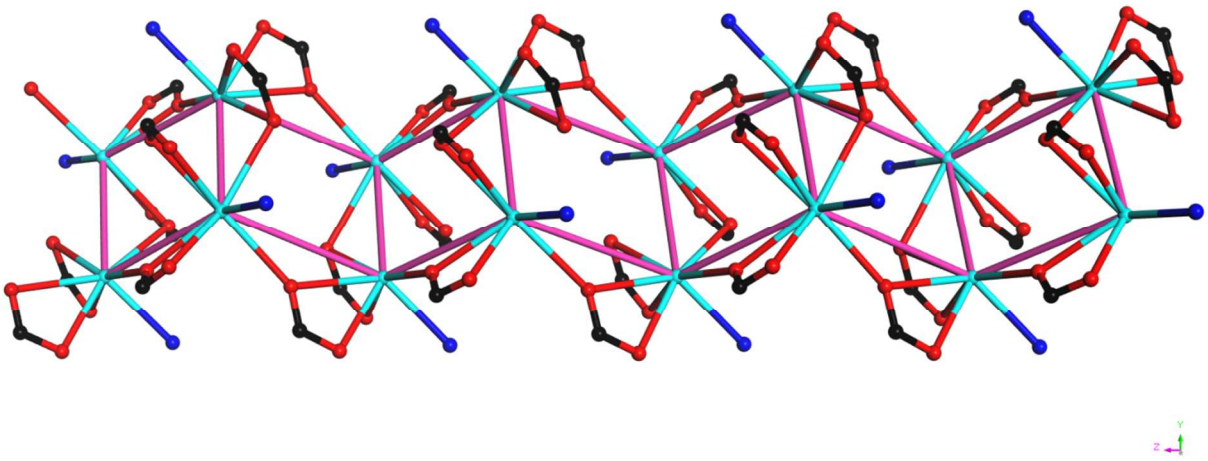

Figure S2. Illustration of zig-zag ladders (connectivity: magenta color) in the **sra** net of **1** view along x-axis.

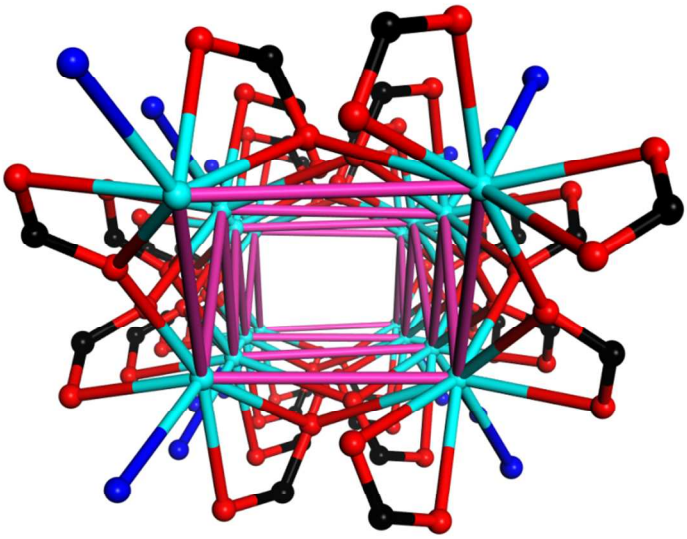

Figure S3. Illustration of zig-zag ladders (connectivity: magenta color) in the **sra** net of **1** view along z-axis.

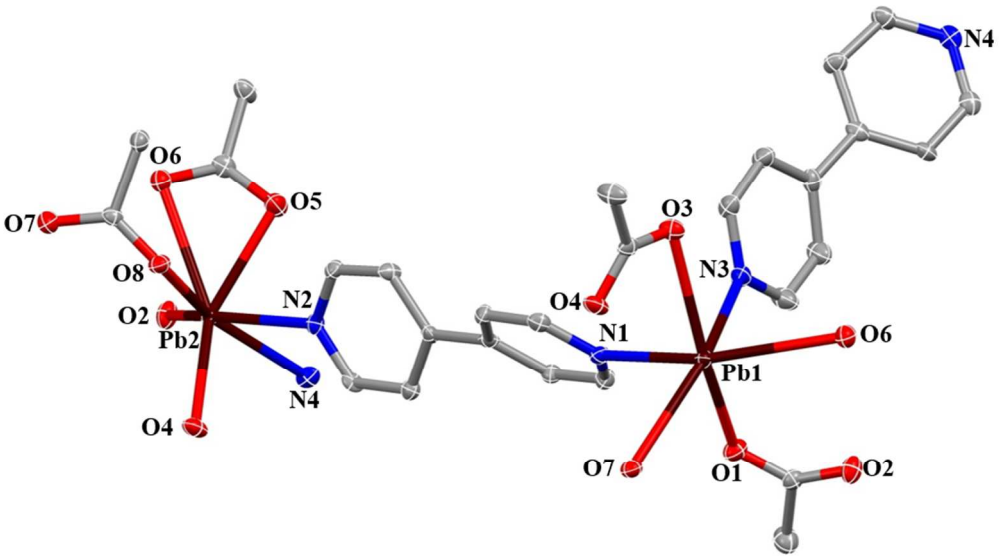

Figure S4. Asymmetric unit in **2** (50% probability ellipsoid) showing the coordination environment of Pb1 and Pb2 (C-H hydrogen atoms, disordered atoms are omitted for clarity).

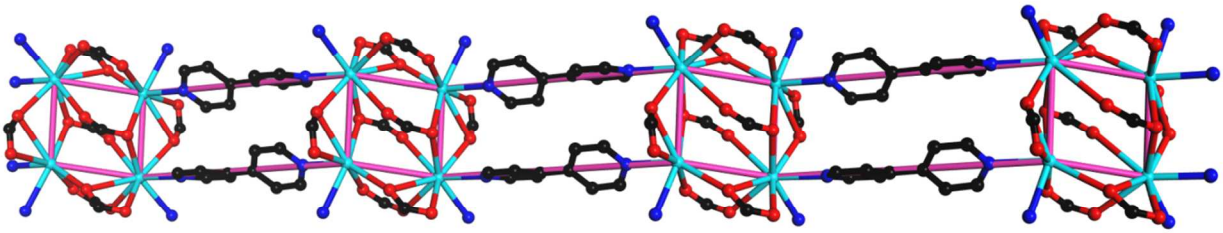

Figure S5. Illustration of zig-zag ladders (connectivity: magenta color) in the **sra** net of **2** view along y-axis.

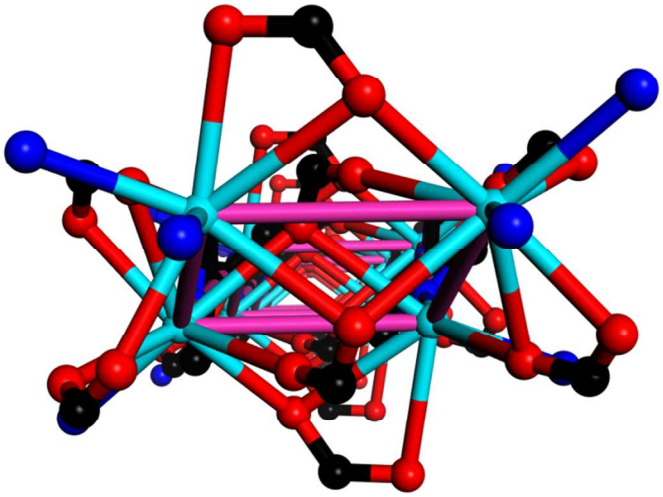

Figure S6. Illustration of zig-zag ladders (connectivity: magenta color) in the **sra** net of **2** view along z-axis.

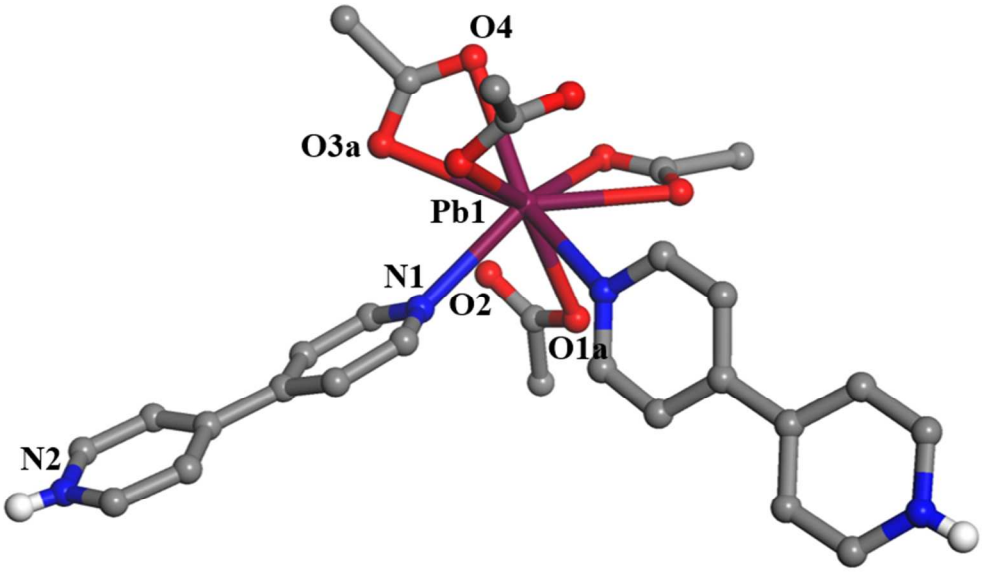

Figure S7. The coordination geometry at Pb(II) metal center in **3**. C-H hydrogen atoms, disordered atoms are omitted for clarity.

Table S1. Selected bond distances (Å) and angles (°) for **1**.

Pb(1)-O(3)	2.410(5)
Pb(1)-O(2)	2.440(6)
Pb(1)-N(1)	2.617(5)
Pb(1)-O(1)	2.648(5)
Pb(2)-O(7)	2.419(5)
Pb(2)-O(5)	2.430(6)
Pb(2)-N(2)	2.583(5)
Pb(2)-O(6)	2.667(5)
Pb(2)-O(9)	2.731(5)
Pb(3)-O(11)	2.406(5)
Pb(3)-O(10)	2.449(6)
Pb(3)-N(3)	2.579(5)
Pb(3)-O(9)	2.647(6)
Pb(4)-O(13)	2.426(5)
Pb(4)-O(15)	2.429(5)
Pb(4)-N(4)	2.627(6)
Pb(4)-O(14)	2.653(5)
Pb(4)-O(6)$^{\#1}$	2.738(5)
O(1)-C(1)	1.217(9)
O(2)-C(1)	1.258(9)
O(3)-C(3)	1.271(9)
O(4)-C(3)	1.244(9)
O(7)-C(17)	1.272(9)

O(8)-C(17)	1.236(8)
O(5)-C(15)	1.245(9)
O(6)-C(15)	1.230(9)
O(6)-Pb(4)$^{\#1}$	2.738(5)
O(9)-C(19)	1.260(9)
O(10)-C(19)	1.249(9)
O(11)-C(21)	1.257(9)
O(12)-C(21)	1.256(9)
O(15)-C(35)	1.258(9)
O(16)-C(35)	1.250(8)
O(13)-C(33)	1.267(9)
O(14)-C(33)	1.238(10)
N(1)-C(9)	1.317(9)
N(1)-C(5)	1.334(8)
N(2)-C(10)	1.318(9)
N(2)-C(14)	1.336(8)
N(3)-C(23)	1.308(9)
N(3)-C(27)	1.342(8)
N(4)-C(32)	1.322(8)
N(4)-C(28)	1.330(9)
C(1)-C(2)	1.523(13)
C(3)-C(4)	1.513(11)
C(5)-C(6)	1.378(9)
C(6)-C(7)	1.384(9)
C(7)-C(8)	1.378(10)
C(7)-C(12)	1.485(9)
C(8)-C(9)	1.390(10)
C(10)-C(11)	1.388(9)
C(11)-C(12)	1.406(9)
C(12)-C(13)	1.375(9)
C(13)-C(14)	1.370(9)
C(15)-C(16)	1.525(12)
C(17)-C(18)	1.516(11)
C(19)-C(20)	1.499(13)
C(21)-C(22)	1.521(10)
C(23)-C(24)	1.382(10)
C(24)-C(25)	1.403(10)
C(25)-C(26)	1.364(8)
C(25)-C(30)	1.495(9)
C(26)-C(27)	1.370(9)
C(28)-C(29)	1.382(10)
C(29)-C(30)	1.396(10)
C(30)-C(31)	1.372(9)
C(31)-C(32)	1.382(9)
C(33)-C(34)	1.497(13)
C(35)-C(36)	1.509(10)

O(3)-Pb(1)-O(2)	81.3(2)
O(3)-Pb(1)-N(1)	76.38(18)
O(2)-Pb(1)-N(1)	76.95(19)

O(3)-Pb(1)-O(1)	93.45(19)
O(2)-Pb(1)-O(1)	50.12(17)
N(1)-Pb(1)-O(1)	127.06(19)
O(7)-Pb(2)-O(5)	80.1(2)
O(7)-Pb(2)-N(2)	75.92(18)
O(5)-Pb(2)-N(2)	77.27(19)
O(7)-Pb(2)-O(6)	96.13(18)
O(5)-Pb(2)-O(6)	50.15(17)
N(2)-Pb(2)-O(6)	127.27(19)
O(7)-Pb(2)-O(9)	151.34(17)
O(5)-Pb(2)-O(9)	87.9(2)
N(2)-Pb(2)-O(9)	76.09(19)
O(6)-Pb(2)-O(9)	95.83(18)
O(11)-Pb(3)-O(10)	81.2(2)
O(11)-Pb(3)-N(3)	76.16(18)
O(10)-Pb(3)-N(3)	76.2(2)
O(11)-Pb(3)-O(9)	92.16(19)
O(10)-Pb(3)-O(9)	50.14(18)
N(3)-Pb(3)-O(9)	126.3(2)
O(13)-Pb(4)-O(15)	80.35(19)
O(13)-Pb(4)-N(4)	77.65(19)
O(15)-Pb(4)-N(4)	76.08(18)
O(13)-Pb(4)-O(14)	50.44(18)
O(15)-Pb(4)-O(14)	97.22(18)
N(4)-Pb(4)-O(14)	127.84(19)
O(13)-Pb(4)-O(6)$^{\#1}$	87.47(18)
O(15)-Pb(4)-O(6)$^{\#1}$	153.90(17)
N(4)-Pb(4)-O(6)$^{\#1}$	78.81(19)
O(14)-Pb(4)-O(6)$^{\#1}$	92.51(18)
C(1)-O(1)-Pb(1)	89.4(5)
C(1)-O(2)-Pb(1)	98.3(5)
C(3)-O(3)-Pb(1)	104.6(4)
C(17)-O(7)-Pb(2)	102.5(4)
C(15)-O(5)-Pb(2)	99.0(5)
C(15)-O(6)-Pb(2)	88.0(4)
C(15)-O(6)-Pb(4)$^{\#1}$	145.9(5)
Pb(2)-O(6)-Pb(4)$^{\#1}$	126.1(2)
C(19)-O(9)-Pb(3)	90.0(5)
C(19)-O(9)-Pb(2)	142.4(5)
Pb(3)-O(9)-Pb(2)	126.4(2)
C(19)-O(10)-Pb(3)	99.7(5)
C(21)-O(11)-Pb(3)	103.3(4)
C(35)-O(15)-Pb(4)	104.0(4)
C(33)-O(13)-Pb(4)	99.5(5)
C(33)-O(14)-Pb(4)	89.4(5)
C(9)-N(1)-C(5)	117.5(6)
C(9)-N(1)-Pb(1)	122.3(5)
C(5)-N(1)-Pb(1)	120.1(4)
C(10)-N(2)-C(14)	117.4(6)
C(10)-N(2)-Pb(2)	122.0(4)
C(14)-N(2)-Pb(2)	120.6(4)

C(23)-N(3)-C(27)	117.4(6)
C(23)-N(3)-Pb(3)	122.0(5)
C(27)-N(3)-Pb(3)	120.6(4)
C(32)-N(4)-C(28)	117.2(6)
C(32)-N(4)-Pb(4)	120.6(4)
C(28)-N(4)-Pb(4)	121.7(4)
O(1)-C(1)-O(2)	121.8(8)
O(1)-C(1)-C(2)	120.3(8)
O(2)-C(1)-C(2)	117.9(8)
O(4)-C(3)-O(3)	120.9(7)
O(4)-C(3)-C(4)	121.6(8)
O(3)-C(3)-C(4)	117.5(7)
N(1)-C(5)-C(6)	122.1(6)
C(5)-C(6)-C(7)	120.4(6)
C(8)-C(7)-C(6)	117.3(6)
C(8)-C(7)-C(12)	120.9(6)
C(6)-C(7)-C(12)	121.7(6)
C(7)-C(8)-C(9)	118.4(7)
N(1)-C(9)-C(8)	124.2(7)
N(2)-C(10)-C(11)	122.9(7)
C(10)-C(11)-C(12)	119.8(6)
C(13)-C(12)-C(11)	115.8(6)
C(13)-C(12)-C(7)	122.2(6)
C(11)-C(12)-C(7)	121.9(6)
C(14)-C(13)-C(12)	120.5(6)
N(2)-C(14)-C(13)	123.4(6)
O(6)-C(15)-O(5)	122.5(8)
O(6)-C(15)-C(16)	119.1(7)
O(5)-C(15)-C(16)	118.3(8)
O(8)-C(17)-O(7)	121.8(7)
O(8)-C(17)-C(18)	120.2(8)
O(7)-C(17)-C(18)	118.0(7)
O(10)-C(19)-O(9)	119.4(8)
O(10)-C(19)-C(20)	120.0(8)
O(9)-C(19)-C(20)	120.6(8)
O(12)-C(21)-O(11)	122.4(7)
O(12)-C(21)-C(22)	119.7(8)
O(11)-C(21)-C(22)	117.8(7)
N(3)-C(23)-C(24)	122.6(7)
C(23)-C(24)-C(25)	119.9(7)
C(26)-C(25)-C(24)	116.5(6)
C(26)-C(25)-C(30)	121.7(6)
C(24)-C(25)-C(30)	121.7(6)
C(25)-C(26)-C(27)	119.8(6)
N(3)-C(27)-C(26)	123.5(6)
N(4)-C(28)-C(29)	123.8(7)
C(28)-C(29)-C(30)	118.3(7)
C(31)-C(30)-C(29)	117.6(6)
C(31)-C(30)-C(25)	121.8(6)
C(29)-C(30)-C(25)	120.4(7)
C(30)-C(31)-C(32)	119.7(6)

N(4)-C(32)-C(31)	123.1(6)
O(14)-C(33)-O(13)	120.4(8)
O(14)-C(33)-C(34)	120.5(8)
O(13)-C(33)-C(34)	119.1(8)
O(16)-C(35)-O(15)	121.5(7)
O(16)-C(35)-C(36)	120.4(7)
O(15)-C(35)-C(36)	118.1(7)

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

Table S2. Selected bond distances (Å) and angles (°) for **2**

Pb(1)-O(1)	2.508(4)
Pb(1)-N(1)	2.531(4)
Pb(1)-N(3)	2.604(5)
Pb(1)-O(3)	2.678(4)
Pb(1)-O(7)$^{\#1}$	2.728(4)
Pb(2)-O(5)	2.503(4)
Pb(2)-N(2)	2.536(4)
Pb(2)-O(4)$^{\#1}$	2.609(4)
Pb(2)-O(7)	2.623(4)
Pb(2)-N(4)$^{\#2}$	2.651(5)
N(1)-C(5)	1.334(7)
N(1)-C(1)	1.348(7)
N(2)-C(10)	1.325(7)
N(2)-C(6)	1.337(7)
N(3)-C(11)	1.333(7)
N(3)-C(15)	1.343(7)
N(4)-C(20)	1.338(8)
N(4)-C(16)	1.344(7)
N(4)-Pb(2)$^{\#3}$	2.651(5)
O(1)-C(21)	1.247(7)
O(2)-C(21)	1.224(7)
O(3)-C(23)	1.227(7)
O(4)-C(23)	1.252(7)
O(4)-Pb(2)$^{\#1}$	2.609(4)
O(5)-C(25)	1.257(7)
O(6)-C(25)	1.228(7)
O(7)-C(27)	1.263(6)
O(7)-Pb(1)$^{\#1}$	2.728(4)
O(8)-C(27)	1.231(7)
F(10)-C(28)	1.337(6)
F(11)-C(28)	1.333(7)
F(12)-C(28)	1.337(6)
C(1)-C(2)	1.393(7)
C(2)-C(3)	1.376(8)
C(3)-C(4)	1.389(7)

C(3)-C(8)	1.487(7)
C(4)-C(5)	1.386(8)
C(6)-C(7)	1.377(7)
C(7)-C(8)	1.396(7)
C(8)-C(9)	1.390(7)
C(9)-C(10)	1.394(7)
C(11)-C(12)	1.389(8)
C(12)-C(13)	1.390(8)
C(13)-C(14)	1.387(8)
C(13)-C(18)	1.478(8)
C(14)-C(15)	1.385(8)
C(16)-C(17)	1.396(8)
C(17)-C(18)	1.400(8)
C(18)-C(19)	1.391(8)
C(19)-C(20)	1.380(8)
C(21)-C(22)	1.538(8)
C(22)-F(2B)	1.336(5)
C(22)-F(2A)	1.343(5)
C(22)-F(1A)	1.345(5)
C(22)-F(3B)	1.351(5)
C(22)-F(1B)	1.363(5)
C(22)-F(3A)	1.369(5)
C(23)-C(24)	1.538(8)
C(24)-F(4B)	1.316(4)
C(24)-F(6A)	1.330(5)
C(24)-F(5A)	1.335(5)
C(24)-F(6B)	1.341(5)
C(24)-F(5B)	1.347(4)
C(24)-F(4A)	1.360(5)
C(25)-C(26B)	1.555(10)
C(25)-C(26A)	1.557(9)
C(27)-C(28)	1.545(7)
C(26A)-F(9A)	1.337(5)
C(26A)-F(7A)	1.339(5)
C(26A)-F(8A)	1.340(5)
C(26B)-F(9B)	1.337(5)
C(26B)-F(7B)	1.339(5)
C(26B)-F(8B)	1.339(5)
C(1S)-Cl(1)	1.747(7)
C(1S)-Cl(3)	1.756(7)
C(1S)-Cl(2)	1.760(7)
O(1)-Pb(1)-N(1)	77.25(14)
O(1)-Pb(1)-N(3)	80.86(14)
N(1)-Pb(1)-N(3)	73.84(14)
O(1)-Pb(1)-O(3)	156.62(12)
N(1)-Pb(1)-O(3)	90.39(13)
N(3)-Pb(1)-O(3)	76.63(13)
O(1)-Pb(1)-O(7)$^{\#1}$	81.63(13)
N(1)-Pb(1)-O(7)$^{\#1}$	82.70(13)
N(3)-Pb(1)-O(7)$^{\#1}$	153.28(13)

O(3)-Pb(1)-O(7)$^{\#1}$	116.81(11)
O(5)-Pb(2)-N(2)	77.05(13)
O(5)-Pb(2)-O(4)$^{\#1}$	148.83(12)
N(2)-Pb(2)-O(4)$^{\#1}$	71.98(13)
O(5)-Pb(2)-O(7)	92.92(13)
N(2)-Pb(2)-O(7)	77.95(13)
O(4)#1-Pb(2)-O(7)	77.44(12)
O(5)-Pb(2)-N(4)$^{\#2}$	83.74(14)
N(2)-Pb(2)-N(4)$^{\#2}$	75.51(14)
O(4)#1-Pb(2)-N(4)$^{\#2}$	91.81(14)
O(7)-Pb(2)-N(4)$^{\#2}$	153.33(13)
C(5)-N(1)-C(1)	117.7(5)
C(5)-N(1)-Pb(1)	120.9(4)
C(1)-N(1)-Pb(1)	121.1(3)
C(10)-N(2)-C(6)	118.0(4)
C(10)-N(2)-Pb(2)	120.7(3)
C(6)-N(2)-Pb(2)	121.2(3)
C(11)-N(3)-C(15)	117.3(5)
C(11)-N(3)-Pb(1)	120.4(4)
C(15)-N(3)-Pb(1)	120.7(4)
C(20)-N(4)-C(16)	117.0(5)
C(20)-N(4)-Pb(2)$^{\#3}$	109.8(4)
C(16)-N(4)-Pb(2)$^{\#3}$	133.0(4)
C(21)-O(1)-Pb(1)	130.2(4)
C(23)-O(3)-Pb(1)	97.9(3)
C(23)-O(4)-Pb(2)$^{\#1}$	142.9(3)
C(25)-O(5)-Pb(2)	97.5(3)
C(27)-O(7)-Pb(2)	120.3(3)
C(27)-O(7)-Pb(1)$^{\#1}$	101.7(3)
Pb(2)-O(7)-Pb(1)$^{\#1}$	103.34(12)
N(1)-C(1)-C(2)	122.0(5)
C(3)-C(2)-C(1)	119.8(5)
C(2)-C(3)-C(4)	118.2(5)
C(2)-C(3)-C(8)	121.0(5)
C(4)-C(3)-C(8)	120.8(5)
C(5)-C(4)-C(3)	118.8(5)
N(1)-C(5)-C(4)	123.4(5)
N(2)-C(6)-C(7)	123.4(5)
C(6)-C(7)-C(8)	119.0(5)
C(9)-C(8)-C(7)	117.6(5)
C(9)-C(8)-C(3)	121.1(5)
C(7)-C(8)-C(3)	121.2(5)
C(8)-C(9)-C(10)	119.1(5)
N(2)-C(10)-C(9)	122.8(5)
N(3)-C(11)-C(12)	123.8(5)
C(11)-C(12)-C(13)	118.8(5)
C(14)-C(13)-C(12)	117.1(5)
C(14)-C(13)-C(18)	120.7(5)
C(12)-C(13)-C(18)	122.0(5)
C(15)-C(14)-C(13)	120.3(6)
N(3)-C(15)-C(14)	122.3(6)

N(4)-C(16)-C(17)	123.6(5)
C(16)-C(17)-C(18)	118.3(5)
C(19)-C(18)-C(17)	118.1(5)
C(19)-C(18)-C(13)	119.4(5)
C(17)-C(18)-C(13)	122.5(5)
C(20)-C(19)-C(18)	119.3(5)
N(4)-C(20)-C(19)	123.7(5)
O(2)-C(21)-O(1)	131.1(5)
O(2)-C(21)-C(22)	116.2(5)
O(1)-C(21)-C(22)	112.7(4)
F(2A)-C(22)-F(1A)	107.7(4)
F(2B)-C(22)-F(3B)	107.8(5)
F(2B)-C(22)-F(1B)	106.7(4)
F(3B)-C(22)-F(1B)	105.3(4)
F(2A)-C(22)-F(3A)	105.3(4)
F(1A)-C(22)-F(3A)	102.6(7)
F(2B)-C(22)-C(21)	120.6(6)
F(2A)-C(22)-C(21)	116.2(5)
F(1A)-C(22)-C(21)	116.2(6)
F(3B)-C(22)-C(21)	112.1(7)
F(1B)-C(22)-C(21)	103.0(6)
F(3A)-C(22)-C(21)	107.4(5)
O(3)-C(23)-O(4)	127.7(5)
O(3)-C(23)-C(24)	116.6(4)
O(4)-C(23)-C(24)	115.7(5)
F(6A)-C(24)-F(5A)	107.7(4)
F(4B)-C(24)-F(6B)	108.0(4)
F(4B)-C(24)-F(5B)	108.0(4)
F(6B)-C(24)-F(5B)	105.2(4)
F(6A)-C(24)-F(4A)	105.2(4)
F(5A)-C(24)-F(4A)	105.1(4)
F(4B)-C(24)-C(23)	116.7(5)
F(6A)-C(24)-C(23)	118.9(6)
F(5A)-C(24)-C(23)	114.8(5)
F(6B)-C(24)-C(23)	109.1(5)
F(5B)-C(24)-C(23)	109.3(5)
F(4A)-C(24)-C(23)	103.7(5)
O(6)-C(25)-O(5)	128.0(5)
O(6)-C(25)-C(26B)	112.9(5)
O(5)-C(25)-C(26B)	118.8(5)
O(6)-C(25)-C(26A)	119.2(5)
O(5)-C(25)-C(26A)	112.7(5)
O(8)-C(27)-O(7)	129.0(5)
O(8)-C(27)-C(28)	115.4(5)
O(7)-C(27)-C(28)	115.5(5)
F(11)-C(28)-F(12)	107.3(5)
F(11)-C(28)-F(10)	106.4(5)
F(12)-C(28)-F(10)	106.5(4)
F(11)-C(28)-C(27)	110.9(5)
F(12)-C(28)-C(27)	112.3(4)
F(10)-C(28)-C(27)	113.1(4)

F(9A)-C(26A)-F(7A)	107.2(4)
F(9A)-C(26A)-F(8A)	107.1(4)
F(7A)-C(26A)-F(8A)	106.8(4)
F(9A)-C(26A)-C(25)	110.2(5)
F(7A)-C(26A)-C(25)	110.6(6)
F(8A)-C(26A)-C(25)	114.5(6)
F(9B)-C(26B)-F(7B)	107.2(5)
F(9B)-C(26B)-F(8B)	107.2(5)
F(7B)-C(26B)-F(8B)	107.0(5)
F(9B)-C(26B)-C(25)	113.4(7)
F(7B)-C(26B)-C(25)	112.0(8)
F(8B)-C(26B)-C(25)	109.8(8)
Cl(1)-C(1S)-Cl(3)	109.7(4)
Cl(1)-C(1S)-Cl(2)	110.7(4)
Cl(3)-C(1S)-Cl(2)	110.4(4)

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

Table S3. Selected bond distances (Å) and angles (°) for **3**.

Pb(1)-O(1)	2.661(2)
Pb(1)-O(1)$^{\#1}$	2.661(2)
Pb(1)-N(1)$^{\#1}$	2.677(3)
Pb(1)-N(1)	2.677(3)
F(1)-C(12)	1.296(5)
F(2)-C(12)	1.346(6)
F(3)-C(12)	1.323(4)
O(1)-C(11)	1.259(4)
O(2)-C(11)	1.231(4)
O(3)-C(13)	1.251(4)
N(1)-C(1)	1.336(4)
N(1)-C(5)	1.342(4)
N(2)-C(10)	1.338(5)
N(2)-C(6)	1.347(4)
C(1)-C(2)	1.397(4)
C(2)-C(3)	1.395(4)
C(3)-C(4)	1.396(4)
C(3)-C(8)	1.488(4)
C(4)-C(5)	1.380(4)
C(6)-C(7)	1.377(5)
C(7)-C(8)	1.399(4)
C(8)-C(9)	1.398(4)
C(9)-C(10)	1.375(4)
C(11)-C(12)	1.543(5)
C(13)-O(4A)	1.235(9)
C(13)-O(4B)	1.241(13)
C(13)-C(14A)	1.526(11)
C(13)-C(14B)	1.562(17)

C(14A)-F(4A)	1.316(13)
C(14A)-F(5A)	1.336(10)
C(14A)-F(6A)	1.336(11)
C(14B)-F(6B)	1.289(13)
C(14B)-F(5B)	1.327(15)
C(14B)-F(4B)	1.330(16)
O(1)-Pb(1)-O(1)$^{\#1}$	143.11(10)
O(1)-Pb(1)-N(1)$^{\#1}$	78.75(8)
O(1)#1-Pb(1)-N(1)$^{\#1}$	73.34(8)
O(1)-Pb(1)-N(1)	73.34(8)
O(1)#1-Pb(1)-N(1)	78.75(8)
N(1)#1-Pb(1)-N(1)	80.80(12)
C(11)-O(1)-Pb(1)	102.1(2)
C(1)-N(1)-C(5)	117.1(3)
C(1)-N(1)-Pb(1)	125.4(2)
C(5)-N(1)-Pb(1)	115.9(2)
C(10)-N(2)-C(6)	122.2(3)
N(1)-C(1)-C(2)	123.2(3)
C(3)-C(2)-C(1)	119.4(3)
C(2)-C(3)-C(4)	117.0(3)
C(2)-C(3)-C(8)	121.9(3)
C(4)-C(3)-C(8)	121.1(3)
C(5)-C(4)-C(3)	119.7(3)
N(1)-C(5)-C(4)	123.6(3)
N(2)-C(6)-C(7)	119.4(3)
C(6)-C(7)-C(8)	120.4(3)
C(9)-C(8)-C(7)	117.8(3)
C(9)-C(8)-C(3)	120.5(3)
C(7)-C(8)-C(3)	121.6(3)
C(10)-C(9)-C(8)	120.0(3)
N(2)-C(10)-C(9)	120.2(3)
O(2)-C(11)-O(1)	128.0(3)
O(2)-C(11)-C(12)	115.8(3)
O(1)-C(11)-C(12)	116.2(3)
F(1)-C(12)-F(3)	109.4(4)
F(1)-C(12)-F(2)	105.2(4)
F(3)-C(12)-F(2)	106.4(4)
F(1)-C(12)-C(11)	112.0(3)
F(3)-C(12)-C(11)	113.0(3)
F(2)-C(12)-C(11)	110.5(4)
O(4A)-C(13)-O(3)	125.5(9)
O(4B)-C(13)-O(3)	131.3(16)
O(4A)-C(13)-C(14A)	115.2(9)
O(3)-C(13)-C(14A)	119.3(4)
O(4B)-C(13)-C(14B)	117.2(16)
O(3)-C(13)-C(14B)	111.3(6)
F(4A)-C(14A)-F(5A)	105.4(11)
F(4A)-C(14A)-F(6A)	105.6(10)
F(5A)-C(14A)-F(6A)	106.9(8)
F(4A)-C(14A)-C(13)	113.8(10)

F(5A)-C(14A)-C(13)	113.6(8)
F(6A)-C(14A)-C(13)	111.0(7)
F(6B)-C(14B)-F(5B)	111.2(14)
F(6B)-C(14B)-F(4B)	107.0(14)
F(5B)-C(14B)-F(4B)	107.3(16)
F(6B)-C(14B)-C(13)	113.3(11)
F(5B)-C(14B)-C(13)	107.9(11)
F(4B)-C(14B)-C(13)	110.0(15)

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

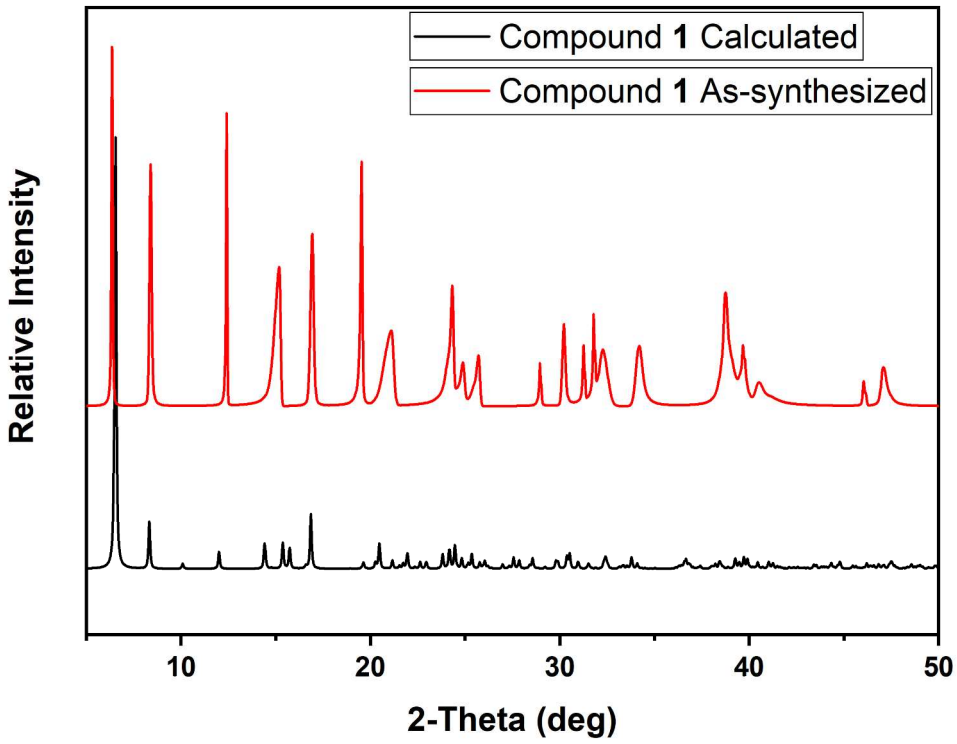

Figure S8. Experimental and calculated PXRD patterns for compound **1**, indicating the purity of the as-synthesized sample.

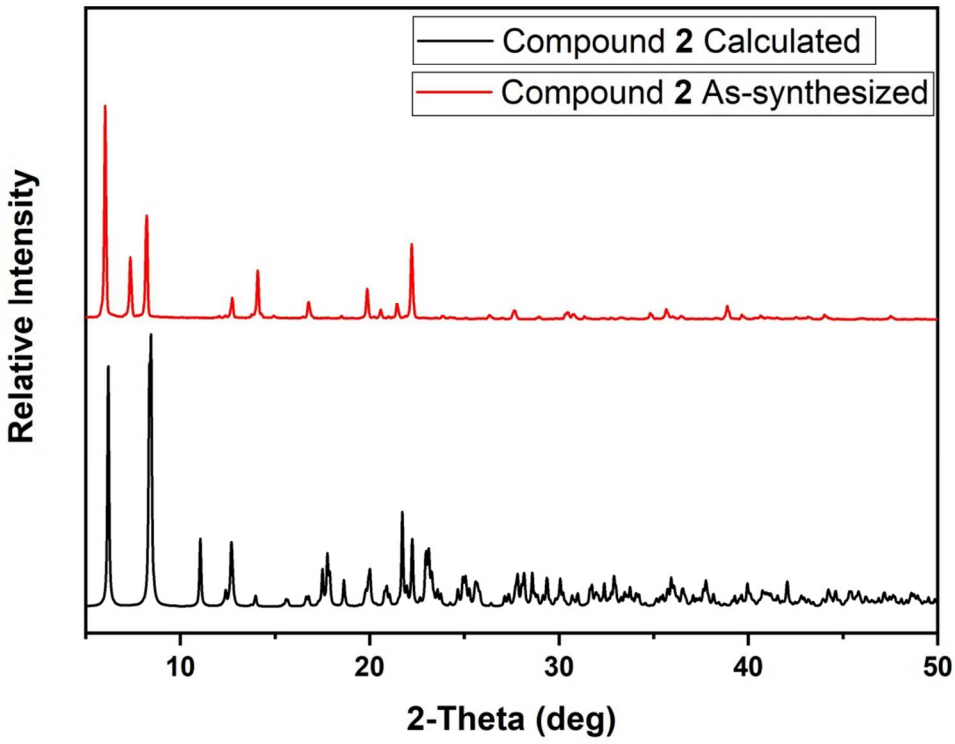

Figure S9. Experimental and calculated PXRD patterns for compound **2**, indicating the purity of the as-synthesized sample.

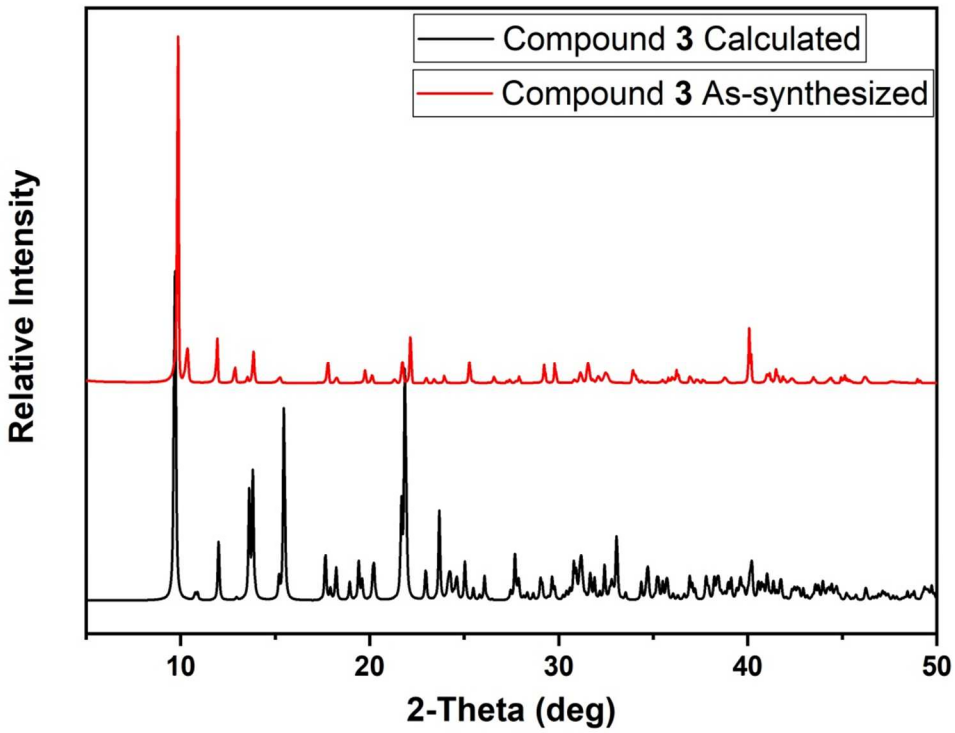

Figure S10. Experimental and calculated PXRD patterns for compound **3**, indicating the purity of the as-synthesized sample.

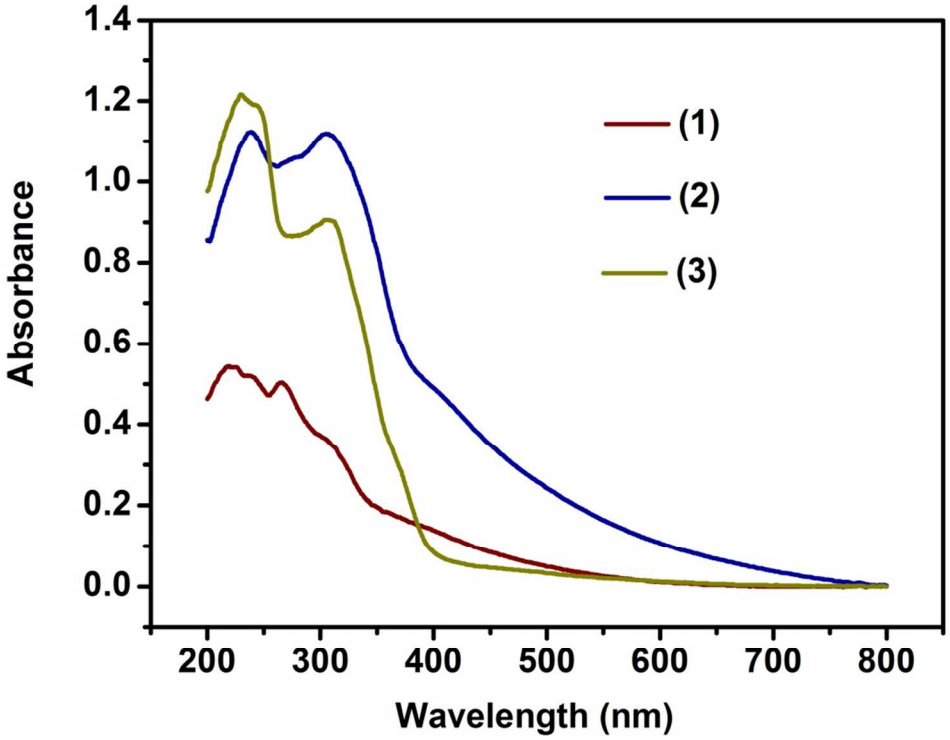

Figure S11. UV/Vis spectra of compounds **1**-**3**.

Table S4: Orbital energies for the $[Pb(bpy)_2(CF_3COO)_4]^{2-}$.

Orbital	Energy (eV)
HOMO	-1.376
LUMO	1.837
HOMO-1	-1.625
LUMO+1	1.868
HOMO-2	-1.817
LUMO+2	2.656
HOME-3	-1.922
LUMO+3	2.677
HOME-4	-2.073
LUMO+4	3.511

HOME-5	-2.154
LUMO+5	3.662

Table S5. XYZ Coordinates for $[Pb(bpy)_2(CF_3COO)_4]^{2-}$ (LANL2DZ and the B3LYP/6-31G(d))

Energy -1944228.8755075

N	5.38030	-6.80549	1.28538
H	4.60965	-2.09321	-0.33658
C	4.55140	-6.35443	2.25570
H	4.50111	-6.95847	3.15669
C	3.79786	-5.18563	2.14315
C	3.88119	-4.41167	0.96888
C	4.74360	-4.88143	-0.04127
H	4.83267	-4.34171	-0.97721
C	5.46102	-6.06165	0.15702
H	6.12559	-6.43884	-0.61429
Pb	0.23832	1.41661	0.04777
F	1.90900	1.91319	-4.52331
F	2.89172	-0.05531	-4.88514
F	0.75871	0.25258	-5.47357
O	1.22591	-1.24479	-2.99732
O	0.84643	0.91282	-2.27084
O	-2.03641	2.64652	-0.16379
N	-1.56838	-0.42571	-0.50167
N	-6.76891	-5.20697	-1.49503
C	-1.34610	-1.53125	-1.25286
H	-0.35851	-1.62966	-1.69646
C	-2.34531	-2.48121	-1.47133
H	-2.11679	-3.36129	-2.06232
C	-3.61945	-2.30313	-0.90177
C	-3.83217	-1.14361	-0.13628
H	-4.80159	-0.92745	0.29729
C	-2.79213	-0.23161	0.04175
H	-2.92908	0.69597	0.57888
C	-5.85920	-4.94118	-2.46138
H	-5.97412	-5.49557	-3.38795
C	-4.82831	-4.01264	-2.31400
H	-4.14391	-3.82679	-3.13412

C	-4.69998	-3.29857	-1.10649
C	-5.64648	-3.57539	-0.10053
H	-5.58527	-3.07488	0.85918
C	-6.64626	-4.52018	-0.33478
H	-7.37996	-4.74821	0.43233
C	1.22355	0.01448	-3.10418
C	1.70103	0.54642	-4.47551
C	-2.70464	3.74268	-0.25493
O	-2.33884	4.91999	-0.48489
F	-4.83568	3.25535	-1.35649
C	-4.24095	3.53278	-0.11637
F	-4.59757	2.46624	0.71970
F	-4.90814	4.64662	0.38830
F	-1.34983	1.94377	4.68534
F	-2.93395	0.37480	4.74118
F	-0.90185	-0.05742	5.56394
O	-1.41621	-1.18731	2.95382
O	-0.50195	0.85420	2.38545
O	4.50133	1.66265	-0.63388
N	1.60616	-0.80241	0.47106
C	1.09799	-1.84269	1.17727
H	0.11067	-1.70895	1.61148
C	1.81314	-3.02687	1.35932
H	1.35430	-3.83953	1.91165
C	3.09781	-3.16311	0.80170
C	3.61144	-2.06917	0.08506
C	2.84678	-0.91012	-0.06281
H	3.25211	-0.03981	-0.57039
H	3.16830	-4.86482	2.96549
C	-1.12456	0.02981	3.14138
C	-1.57113	0.58792	4.51409
C	3.78737	2.51552	-0.03391
O	2.56987	2.44671	0.35932
F	3.67172	4.93056	0.45014
C	4.51087	3.82796	0.35979
F	5.13128	3.70208	1.61364
F	5.52424	4.18049	-0.53170

Table S6: The highest wavelength absorption data from calculations (TD-DFT) for the studied compound 1.

Calculated λ (nm)	Oscillator Strength	Major contributions (%)
467.3006	0.0003	HOMO(A)->LUMO(A) (47%), HOMO(B)->LUMO(B) (47%)
459.5922	0.0016	HOMO(A)->L+1(A) (47%), HOMO(B)->L+1(B) (47%)
436.1341	0.0002	H-1(A)->LUMO(A) (47%), H-1(B)->LUMO(B) (47%)
414.6906	0.0004	H-1(A)->L+1(A) (39%), H-1(B)->L+1(B) (39%)
410.7613	0.0013	H-2(A)->L+1(A) (40%), H-2(B)->L+1(B) (40%)
388.9212	0.0008	H-3(A)->LUMO(A) (48%), H-3(B)->LUMO(B) (48%)
380.378	0.0002	H-5(A)->LUMO(A) (18%), H-4(A)->LUMO(A) (25%), H-5(B)->LUMO(B) (18%), H-4(B)->LUMO(B) (25%)
373.9307	0.0004	H-6(A)->LUMO(A) (18%), H-5(A)->LUMO(A) (11%), H-6(B)->LUMO(B) (18%), H-5(B)->LUMO(B) (11%)
373.4576	0.0003	H-4(A)->L+1(A) (40%), H-4(B)->L+1(B) (40%)
371.5662	0.0003	H-5(A)->L+1(A) (21%), H-3(A)->L+1(A) (23%), H-5(B)->L+1(B) (21%), H-3(B)->L+1(B) (23%)
365.2933	0.0009	H-6(A)->L+1(A) (30%), H-3(A)->L+1(A) (14%), H-6(B)->L+1(B) (30%), H-3(B)->L+1(B) (14%)
359.6872	0.0006	H-7(A)->LUMO(A) (35%), H-7(B)->LUMO(B) (35%)
358.5742	0.0001	H-7(A)->L+1(A) (10%), H-5(A)->LUMO(A) (10%), H-4(A)->LUMO(A) (16%), H-7(B)->L+1(B) (10%), H-5(B)->LUMO(B) (10%), H-4(B)->LUMO(B) (16%)
357.984	0.0003	H-7(A)->LUMO(A) (12%), H-7(A)->L+1(A) (30%), H-7(B)->LUMO(B) (12%), H-7(B)->L+1(B) (30%)
343.6941	0.0004	HOMO(A)->L+2(A) (49%), HOMO(B)->L+2(B) (49%)
340.9156	0.0001	H-9(A)->LUMO(A) (37%), H-8(A)->LUMO(A) (12%), H-9(B)->LUMO(B) (37%), H-8(B)->LUMO(B) (12%)
340.3354	0.0012	HOMO(A)->L+3(A) (48%), HOMO(B)->L+3(B) (48%)
338.7269	0.0023	H-9(A)->LUMO(A) (11%), H-8(A)->LUMO(A) (37%), H-9(B)->LUMO(B) (11%), H-8(B)->LUMO(B) (37%)
334.8029	0.0016	H-9(A)->L+1(A) (13%), H-8(A)->L+1(A) (30%), H-9(B)->L+1(B) (13%), H-8(B)->L+1(B) (30%)
333.9192	0.0037	H-10(A)->LUMO(A) (41%), H-10(B)->LUMO(B) (41%)
333.1923	0.0017	H-9(A)->L+1(A) (30%), H-8(A)->L+1(A) (15%), H-9(B)->L+1(B) (30%), H-8(B)->L+1(B) (15%)
331.2871	0.0004	H-10(A)->L+1(A) (46%), H-10(B)->L+1(B) (46%)
323.0522	0.0119	H-11(A)->LUMO(A) (48%), H-11(B)->LUMO(B) (48%)
319.1849	0.0112	H-11(A)->L+1(A) (49%), H-11(B)->L+1(B) (49%)
295.5171	0.0016	HOMO(A)->L+4(A) (44%), HOMO(B)->L+4(B) (44%)
290.2931	0.0001	H-5(A)->L+3(A) (38%), H-5(B)->L+3(B) (38%)
288.1276	0.0018	H-13(A)->LUMO(A) (18%), H-12(A)->LUMO(A) (17%), H-13(B)->LUMO(B) (18%), H-12(B)->LUMO(B) (17%)
286.9539	0.0001	H-6(A)->L+3(A) (40%), H-6(B)->L+3(B) (40%)
286.7416	0.0102	H-12(A)->L+1(A) (33%), H-12(B)->L+1(B) (33%)
284.0807	0.0088	H-13(A)->L+1(A) (14%), H-12(A)->LUMO(A) (12%), H-13(B)->L+1(B) (14%), H-12(B)->LUMO(B) (12%)
283.2629	0.0096	H-13(A)->L+1(A) (15%), H-13(B)->L+1(B) (15%)
283.0108	0.0017	H-7(A)->L+2(A) (44%), H-7(B)->L+2(B) (44%)

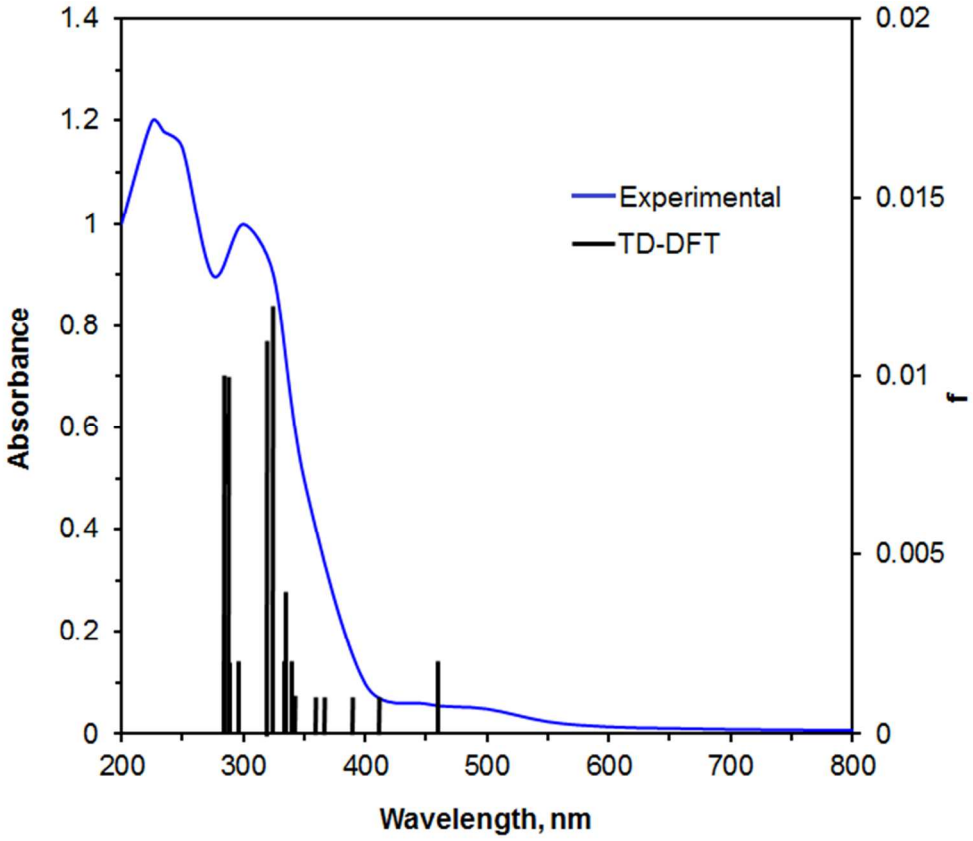

Figure S12. UV-Vis spectrum of $[Pb(bpy)_2(CF_3COO)_4]^{2-}$ experimental (blue) and calculated using TD-DFT (black).

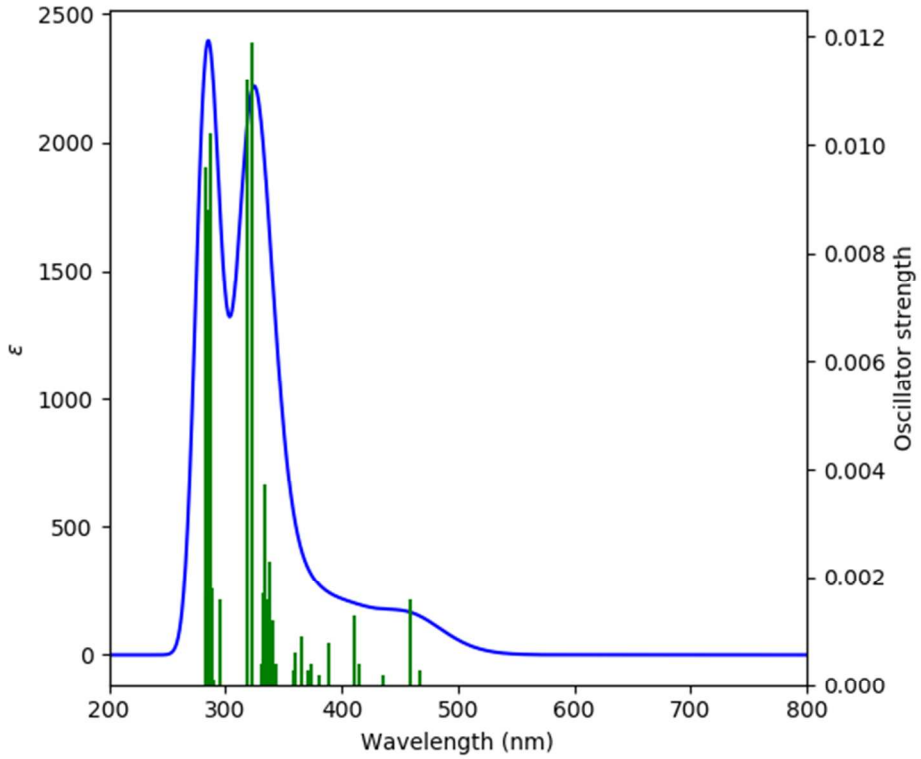

Figure S13. UV-vis spectra of compound $[Pb(bpy)_2(CF_3COO)4]2^{-}$. obtained by TD-DFT calculations.

Table S7: Coordinates for the B3LYP/LANL2DZ/6-31G(d,p) -optimized structure of the compound $[Pb(bpy)_2(CF_3COO)_4]^{2-}$. Energy: -1944872.2348742

	X	Y	Z
N	-5.38030	6.80549	1.28538
H	-4.60965	2.09321	-0.33658
C	-4.55140	6.35443	2.25570
H	-4.50111	6.95847	3.15668
C	-3.79786	5.18563	2.14315
C	-3.88119	4.41167	0.96888
C	-4.74360	4.88143	-0.04127
H	-4.83267	4.34171	-0.97721
C	-5.46102	6.06165	0.15702
H	-6.12559	6.43884	-0.61429
Pb	-0.23832	-1.41661	0.04777
F	-1.90900	-1.91319	-4.52331

F	-2.89172	0.05531	-4.88514
F	-0.75871	-0.25258	-5.47357
O	-1.22591	1.24479	-2.99732
O	-0.84643	-0.91282	-2.27084
O	2.03641	-2.64652	-0.16379
N	1.56838	0.42571	-0.50167
N	6.76891	5.20697	-1.49503
C	1.34610	1.53125	-1.25286
H	0.35851	1.62966	-1.69646
C	2.34531	2.48121	-1.47133
H	2.11679	3.36129	-2.06232
C	3.61945	2.30313	-0.90177
C	3.83217	1.14361	-0.13628
H	4.80159	0.92745	0.29729
C	2.79213	0.23161	0.04175
H	2.92908	-0.69597	0.57888
C	5.85920	4.94118	-2.46138
H	5.97412	5.49557	-3.38795
C	4.82831	4.01264	-2.31400
H	4.14391	3.82679	-3.13412
C	4.69998	3.29857	-1.10649
C	5.64648	3.57539	-0.10053
H	5.58527	3.07488	0.85918
C	6.64626	4.52018	-0.33478
H	7.37996	4.74821	0.43233
C	-1.22355	-0.01448	-3.10418
C	-1.70103	-0.54642	-4.47551
C	2.70464	-3.74268	-0.25493
O	2.33883	-4.91999	-0.48489
F	4.83568	-3.25535	-1.35649
C	4.24095	-3.53278	-0.11636
F	4.59757	-2.46624	0.71970
F	4.90814	-4.64662	0.38830
F	1.34983	-1.94377	4.68534
F	2.93395	-0.37480	4.74118
F	0.90185	0.05742	5.56394
O	1.41621	1.18731	2.95382
O	0.50195	-0.85420	2.38545
O	-4.50133	-1.66265	-0.63388
N	-1.60616	0.80241	0.47106
C	-1.09799	1.84269	1.17727
H	-0.11067	1.70895	1.61148
C	-1.81314	3.02687	1.35932
H	-1.35430	3.83953	1.91165
C	-3.09781	3.16311	0.80170
C	-3.61144	2.06917	0.08506

C	-2.84678	0.91012	-0.06281
H	-3.25211	0.03981	-0.57039
H	-3.16830	4.86482	2.96549
C	1.12456	-0.02981	3.14138
C	1.57113	-0.58792	4.51409
C	-3.78737	-2.51552	-0.03391
O	-2.56987	-2.44671	0.35932
F	-3.67172	-4.93056	0.45014
C	-4.51087	-3.82796	0.35979
F	-5.13128	-3.70208	1.61364
F	-5.52424	-4.18049	-0.53170

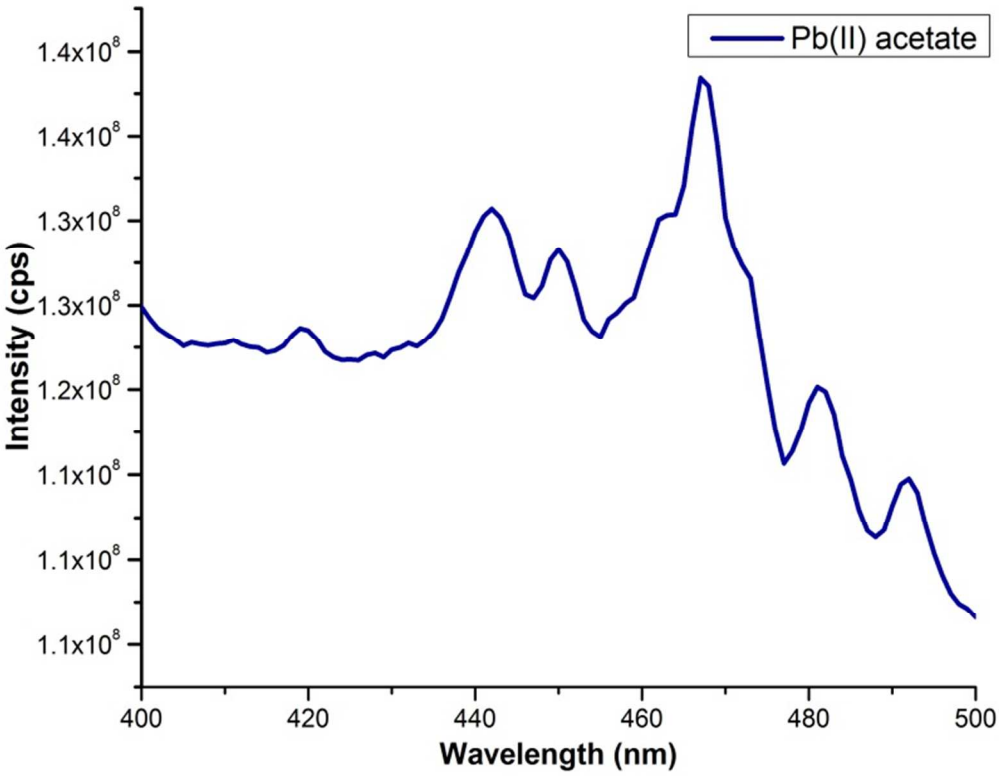

Figure S14. Solid-state luminescent emission spectra of compound $Pb(OAc)_2$ (λ_{ex} = 325 nm) at room temperature.

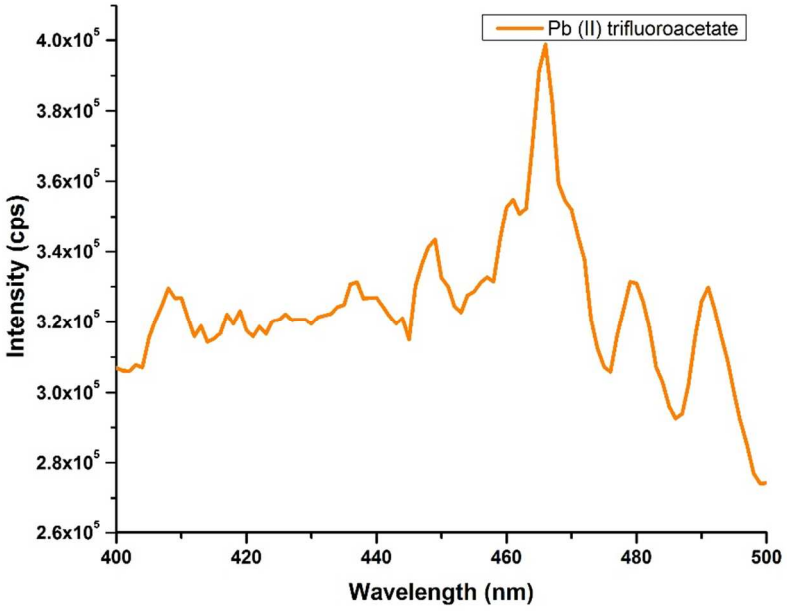

Figure S15. Solid-state luminescent emission spectra of compound $Pb(TFA)_2$ (λ_{ex} = 325 nm) at room temperature.