Four New Lead(II)-Iridium(III) Heterobimetallic Coordination Frameworks: Synthesis, Structures, Luminescence and Oxygen-sensing Properties

Yi-Ting Chen,[a] Chun-Yen Lin,[a] Gene-Hsiang Lee,[b] and Mei-Lin Ho[a*]

[a] Department of Chemistry, Soochow University, Taipei, Taiwan.

[b] Instrumentation Center, National Taiwan University, Taipei, Taiwan.

E-mail: meilin_ho@scu.edu.tw

RECEIVED DATE (to be automatically inserted after your manuscript is accepted if required according to the journal that you are submitting your paper to)

Department of Chemistry, Soochow University, Taipei, Taiwan. Fax: +886-2-28811053; Tel: +886-2-28819471 ext 6827; E-mail: meilin_ho@scu.edu.tw

Supplementary materials:

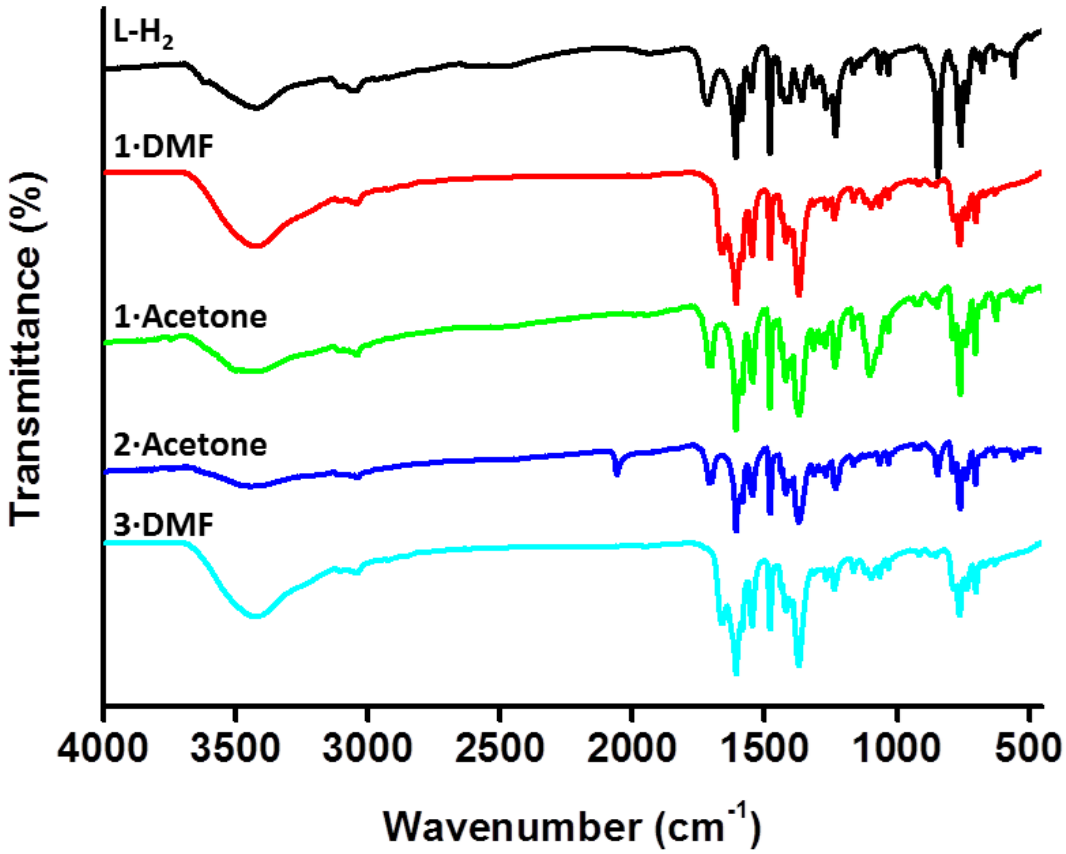

Fig. S1 FT-IR spectra of **L-H$_2$**, **1·DMF**, **1·Acetone**, **2·Acetone** and **3·DMF**.

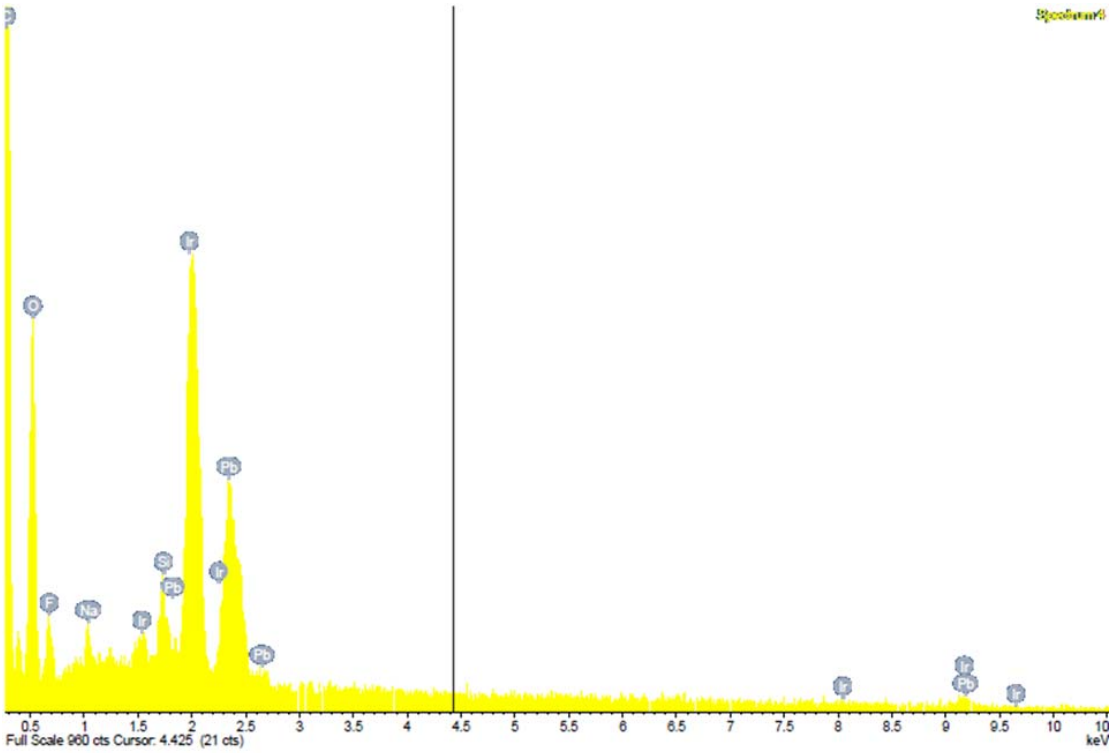

Fig. S2 EDX data for **2·Acetone**.

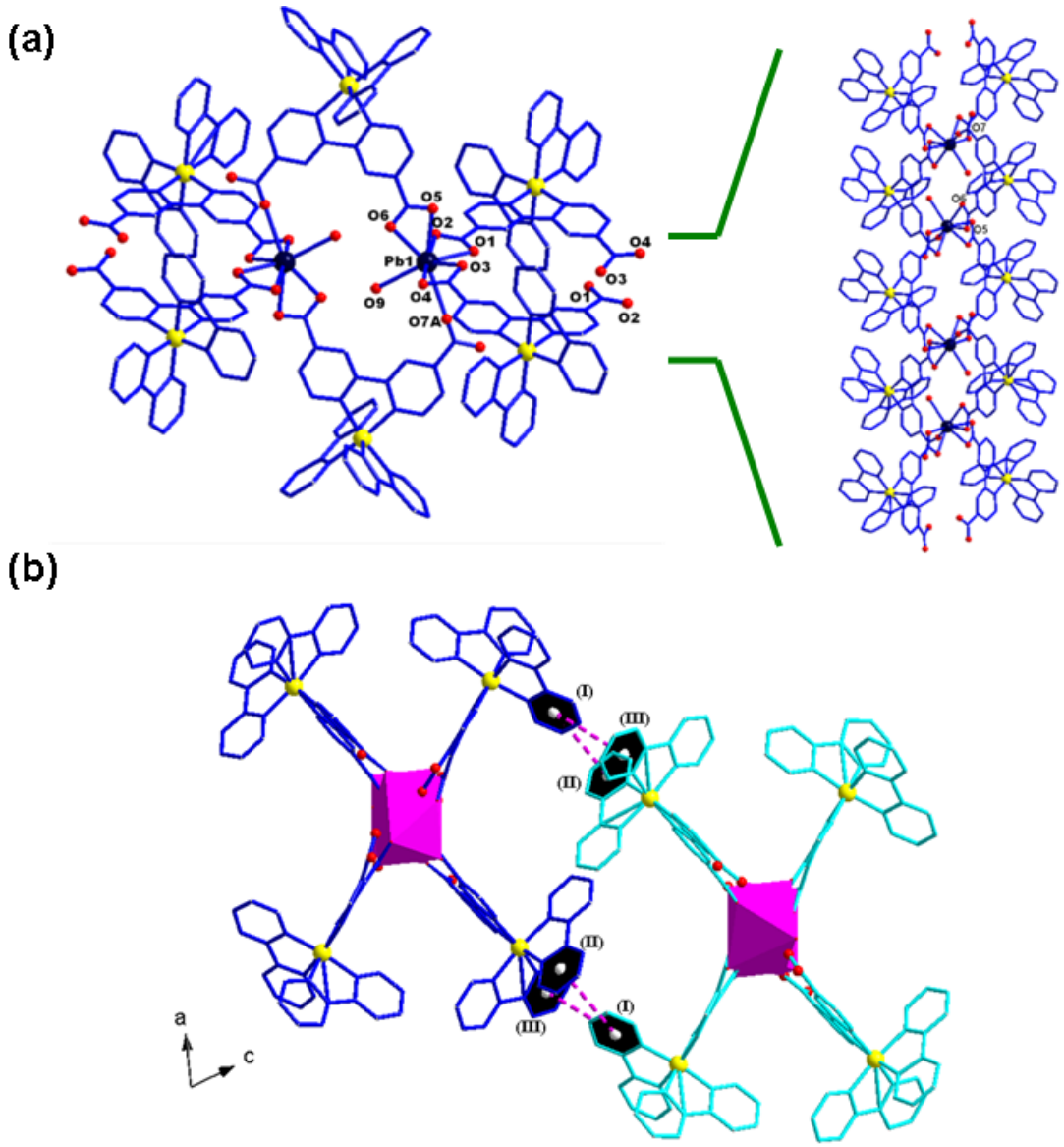

Fig. S3 (a) The coordination environment of Pb(II) in **1·Acetone**. Hydrogen atoms are omitted for clarity. (right) View of a 1D linear chain in **1·Acetone** along the crystallographic *a*-axis. (b) Polyhedral representation of the alternation in an AB/fashion (in blue and cyan) of **1·Acetone** viewed down the *b*-axis. Magenta colored polyhedral represent Pb(II) centers. Dotted lines indicate the π – π interactions found.

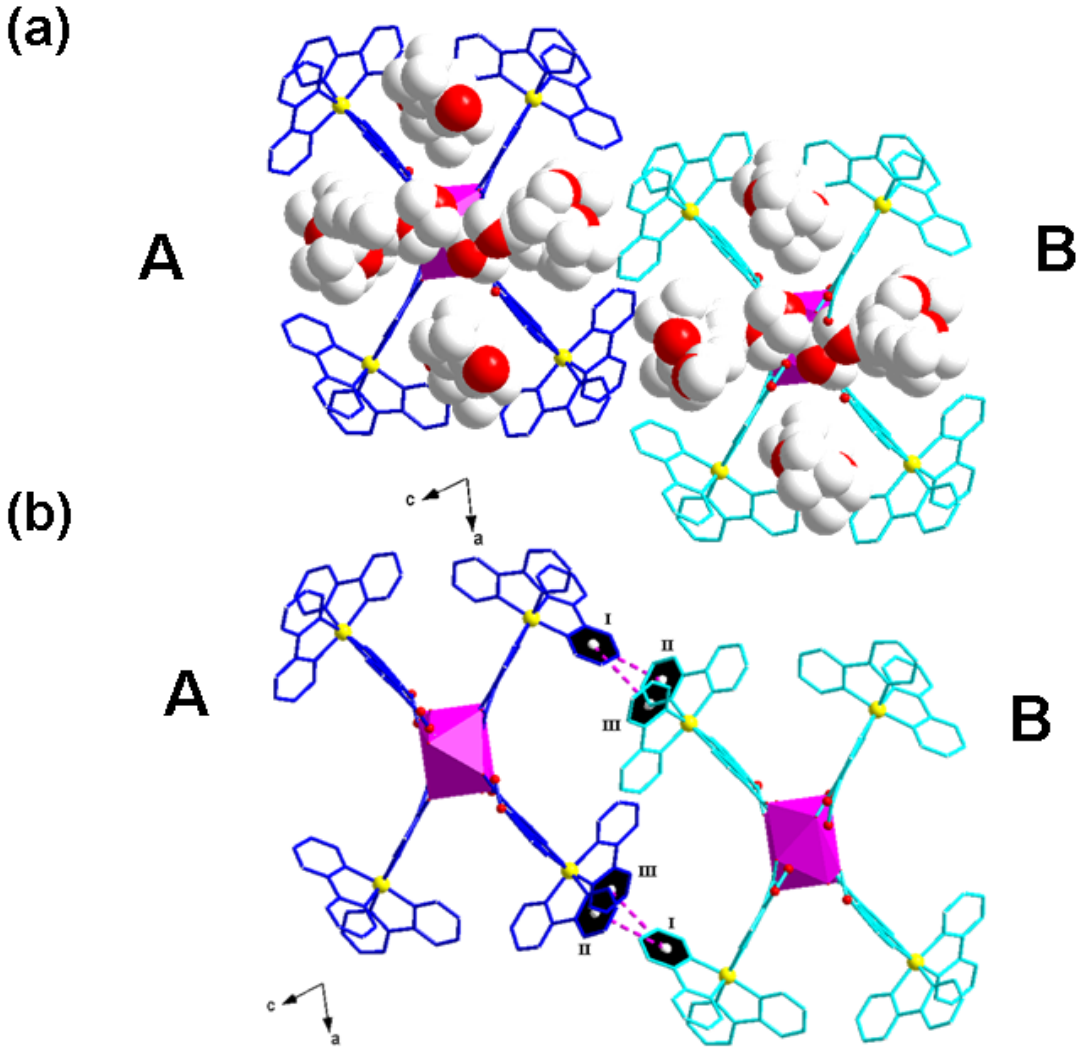

Fig. S4 (a) Polyhedral representation of the alternation in an AB/fashion (in blue and green) of **2·Acetone** viewed down the *b*-axis. Magenta colored polyhedral represent Pb(II) centers. (b) Dotted lines indicate the π – π interactions found.

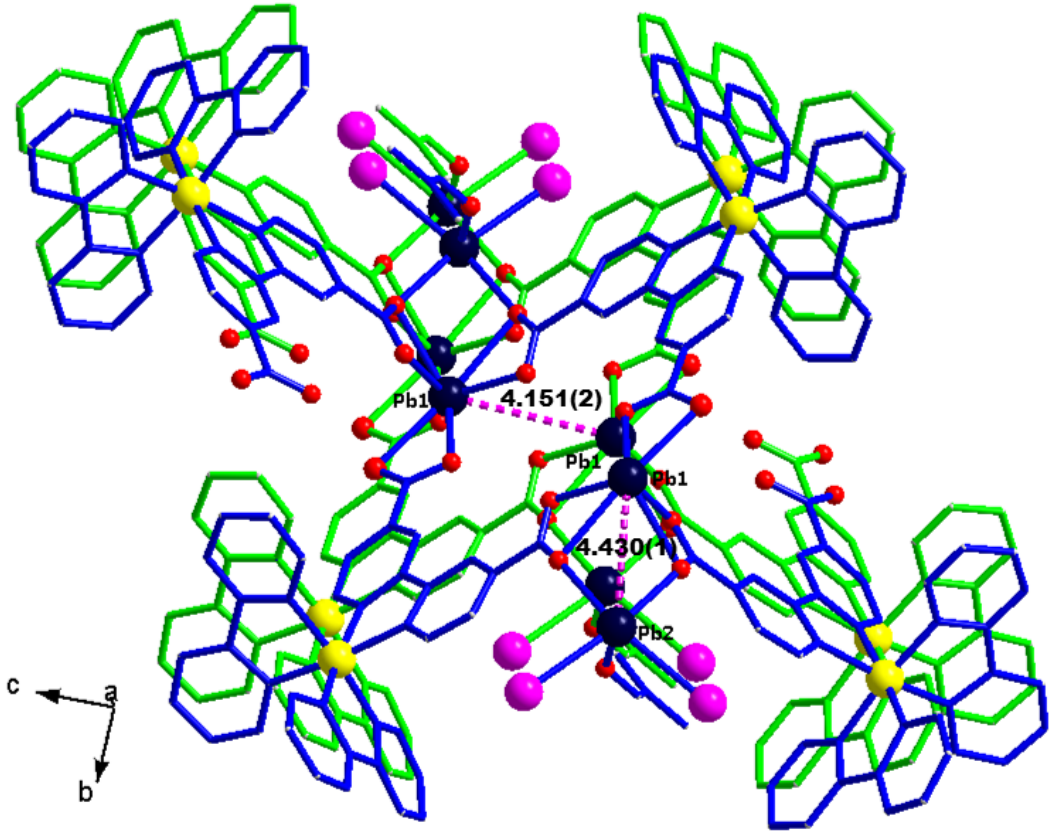

Fig. S5 Selected pairs of molecules from the structure of **3·DMF** along the *a*-axis. Dotted lines indicate the edge-to-face interactions found. Blue color denoted the upper layer, and the green color denoted the next layer.

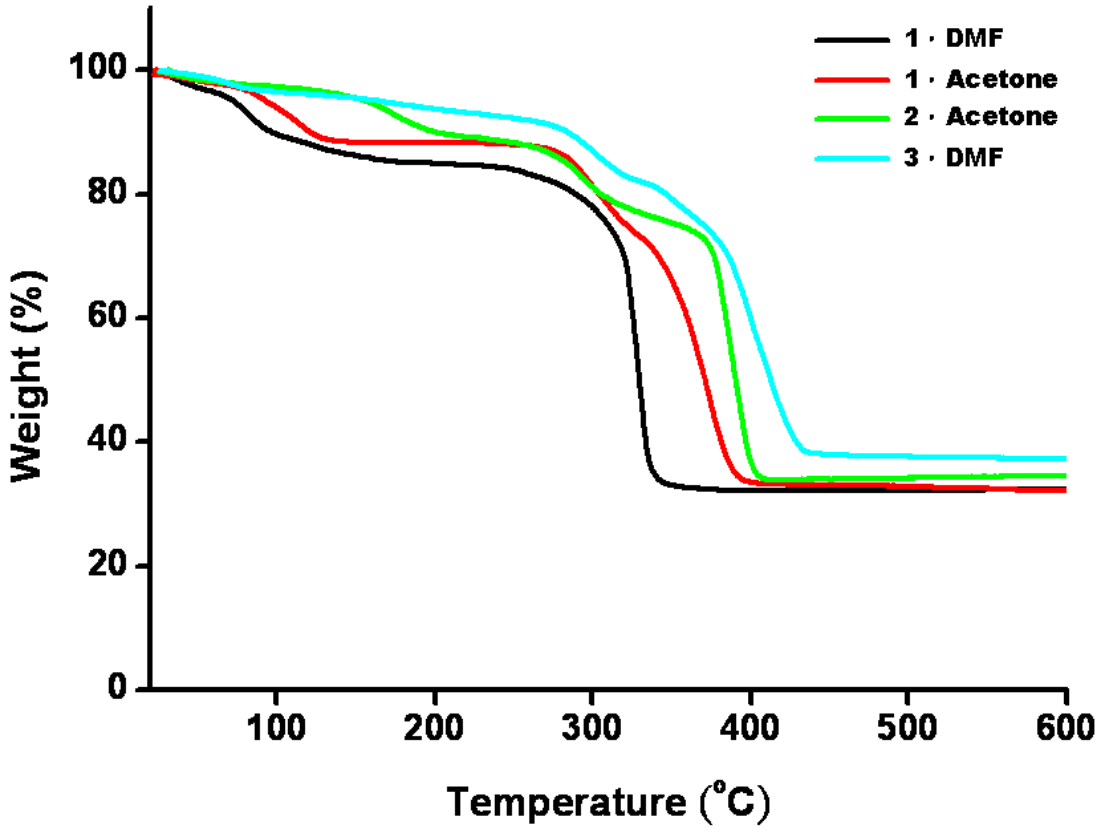

Fig. S6 TG curves of **1·DMF—3·DMF**.

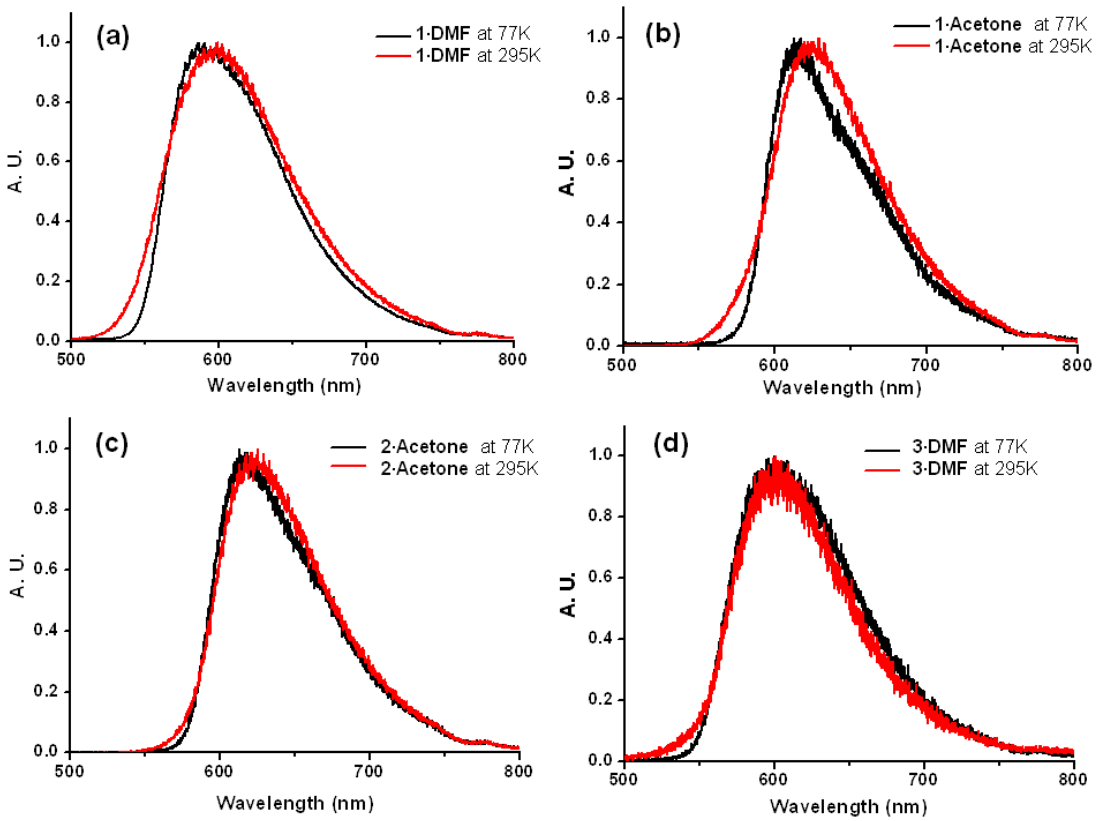

Fig. S7 The normalized emission spectrum of **1·DMF—3·DMF** in single crystal at 295 K and at 77K. λ_{ex} = 405 nm.

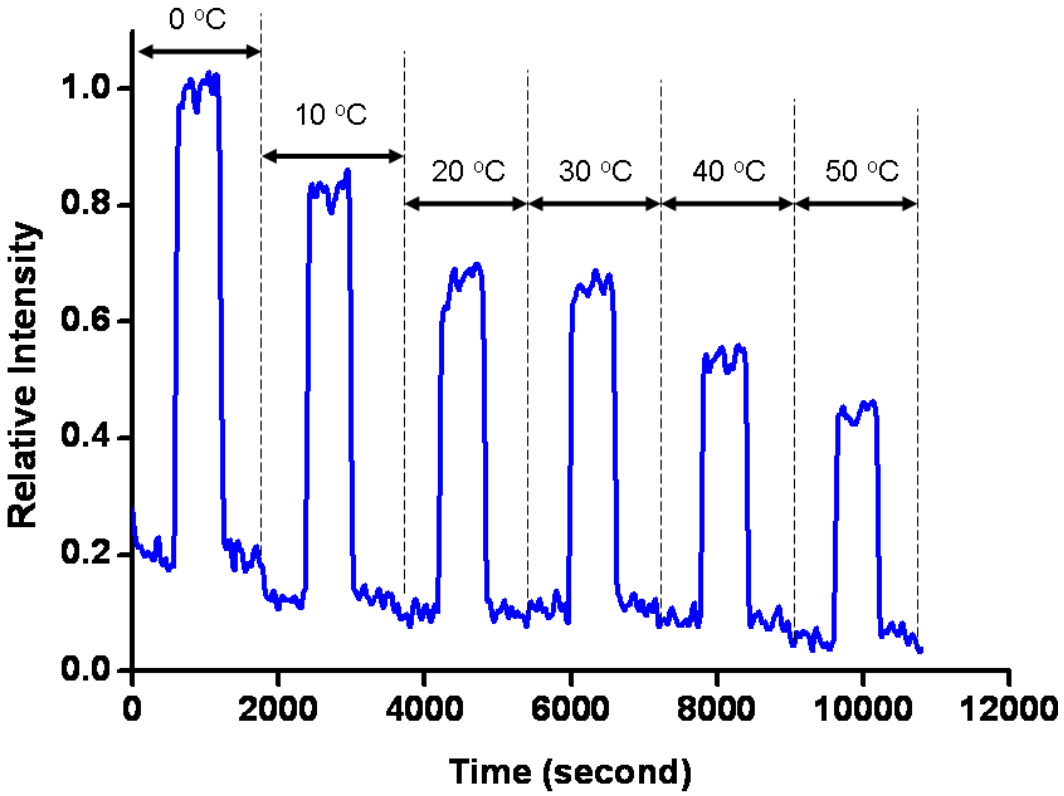

Fig. S8 Relative luminescence changes of **3·DMF** in single crystal at 0, 10, 20, 30, 40, and 50 °C, respectively upon alternating exposure to 100% nitrogen and 100% oxygen atmosphere.

Table S1. Selected Bond Lengths (Å) and Angles (°) for complexes

1·DMF—3·DMF.[a]

1·DMF							
Pb(1)-O(1)	2.476(9)	O(1)-Pb(1)-O(7A)	96.8(3)	O(1)-Pb(1)-O(20B)	84.4(4)	O(5)-Pb(1)-O(2)	118.4(3)
Pb(1)-O(7A)	2.521(9)	O(1)-Pb(1)-O(5)	79.2(3)	O(7A)-Pb(1)-O(20B)	156.4(4)	O(6)-Pb(1)-O(2)	128.8(3)
Pb(1)-O(5)	2.606(5)	O(7A)-Pb(1)-O(5)	128.0(3)	O(5)-Pb(1)-O(20B)	75.5(3)	O(20B)-Pb(1)-O(2)	73.8(4)
Pb(1)-O(6)	2.637(6)	O(1)-Pb(1)-O(6)	85.9(3)	O(6)-Pb(1)-O(20B)	125.4(4)		
Pb(1)-O(2)	2.703(11)	O(7A)-Pb(1)-O(6)	78.2(3)	O(1)-Pb(1)-O(2)	45.9(3)		
Pb(1)-O(20B)	2.684(15)	O(5)-Pb(1)-O(6)	49.90(17)	O(7A)-Pb(1)-O(2)	90.0(3)		
1·Acetone							
Pb(1)-O(3)	2.409(7)	O(3)-Pb(1)-O(1)	78.5(2)	O(3)-Pb(1)-O(9)	140.4(3)	O(2)-Pb(1)-O(4)	169.8(3)
Pb(1)-O(6)	2.475(7)	O(6)-Pb(1)-O(1)	125.9(3)	O(6)-Pb(1)-O(9)	79.7(3)	O(9)-Pb(1)-O(4)	95.3(2)
Pb(1)-O(1)	2.507(6)	O(3)-Pb(1)-O(5)	78.8(3)	O(1)-Pb(1)-O(9)	130.6(3)	O(3)-Pb(1)-O(7A)	69.3(3)
Pb(1)-O(5)	2.591(8)	O(6)-Pb(1)-O(5)	49.3(2)	O(5)-Pb(1)-O(9)	126.0(2)	O(6)-Pb(1)-O(7A)	144.5(3)
Pb(1)-O(2)	2.596(7)	O(1)-Pb(1)-O(5)	80.7(2)	O(2)-Pb(1)-O(9)	93.7(3)	O(1)-Pb(1)-O(7A)	88.4(3)
Pb(1)-O(9)	2.796(8)	O(3)-Pb(1)-O(2)	124.7(2)	O(3)-Pb(1)-O(4)	47.6(2)	O(5)-Pb(1)-O(7A)	147.7(2)
Pb(1)-O(4)	2.804(8)	O(6)-Pb(1)-O(2)	91.6(3)	O(6)-Pb(1)-O(4)	85.3(3)	O(2)-Pb(1)-O(7A)	120.8(3)
Pb(1)-O(7A)	2.815(9)	O(1)-Pb(1)-O(2)	50.4(2)	O(1)-Pb(1)-O(4)	124.9(2)	O(9)-Pb(1)-O(7A)	83.8(2)
O(3)-Pb(1)-O(6)	105.7(3)	O(5)-Pb(1)-O(2)	74.2(3)	O(5)-Pb(1)-O(4)	96.6(3)	O(4)-Pb(1)-O(7A)	65.2(3)
2·Acetone							
Pb(1)-O(3A)	2.426(5)	O(3A)-Pb(1)-O(2)	123.49(19)	O(3A)-Pb(1)-O(7B)	81.5(4)	O(5)-Pb(1)-O(4A)	102.2(3)
Pb(1)-O(6)	2.536(5)	O(6)-Pb(1)-O(2)	97.2(2)	O(6)-Pb(1)-O(7B)	155.6(4)	O(7B)-Pb(1)-O(4A)	81.2(5)
Pb(1)-O(2)	2.620(6)	O(3A)-Pb(1)-O(1)	75.64(17)	O(2)-Pb(1)-O(7B)	97.1(5)	O(3A)-Pb(1)-O(9)	135.9(2)
Pb(1)-O(1)	2.624(5)	O(6)-Pb(1)-O(1)	127.7(2)	O(1)-Pb(1)-O(7B)	76.4(4)	O(6)-Pb(1)-O(9)	75.2(2)
Pb(1)-O(5)	2.645(6)	O(2)-Pb(1)-O(1)	49.94(17)	O(5)-Pb(1)-O(7B)	153.3(4)	O(2)-Pb(1)-O(9)	99.3(2)
Pb(1)-O(7B)	2.71(2)	O(3A)-Pb(1)-O(5)	80.7(2)	O(3A)-Pb(1)-O(4A)	50.3(2)	O(1)-Pb(1)-O(9)	138.96(19)
Pb(1)-O(4A)	2.758(7)	O(6)-Pb(1)-O(5)	50.35(19)	O(6)-Pb(1)-O(4A)	86.5(2)	O(5)-Pb(1)-O(9)	123.47(17)
Pb(1)-O(9)	2.814(6)	O(2)-Pb(1)-O(5)	76.6(2)	O(2)-Pb(1)-O(4A)	173.70(19)	O(7A)-Pb(1)-O(9)	83.0(4)
O(3A)-Pb(1)-O(6)	106.5(2)	O(1)-Pb(1)-O(5)	79.99(17)	O(1)-Pb(1)-O(4A)	123.83(18)	O(4A)-Pb(1)-O(9)	86.6(2)
3·DMF							
Pb(1)-O(5)	2.427(8)	Pb(2)-I(1)	3.0732(10)	O(2)-Pb(1)-O(1)	50.1(2)	O(9)-Pb(2)-O(6)	77.0(3)
Pb(1)-O(2)	2.454(8)	Pb(2)-I(2)	3.0479(10)	O(3)-Pb(1)-O(1)	124.3(3)	O(4)-Pb(2)-O(6)	71.9(5)
Pb(1)-O(3)	2.465(8)	O(5)-Pb(1)-O(2)	76.7(3)	O(6)-Pb(1)-O(1)	103.5(3)	O(9)-Pb(2)-I(2)	86.9(2)
Pb(1)-O(6)	2.696(8)	O(5)-Pb(1)-O(3)	81.6(3)	O(5)-Pb(1)-O(4)	92.5(4)	O(4)-Pb(2)-I(2)	93.9(5)

Pb(1)-O(1)	2.742(8)	O(2)-Pb(1)-O(3)	75.1(3)	O(2)-Pb(1)-O(4)	125.9(5)	O(6)-Pb(2)-I(2)	160.4(2)
Pb(1)-O(4)	2.77(2)	O(5)-Pb(1)-O(6)	50.7(3)	O(3)-Pb(1)-O(4)	50.7(5)	O(9)-Pb(2)-I(1)	86.4(2)
Pb(2)-O(9)	2.391(9)	O(2)-Pb(1)-O(6)	126.8(3)	O(6)-Pb(1)-O(4)	70.6(5)	O(4)-Pb(2)-I(1)	156.6(4)
Pb(2)-O(4)	2.61(3)	O(3)-Pb(1)-O(6)	101.2(3)	O(1)-Pb(1)-O(4)	169.3(4)	O(6)-Pb(2)-I(1)	88.41(18)
Pb(2)-O(6)	2.765(9)	O(5)-Pb(1)-O(1)	77.1(3)	O(9)-Pb(2)-O(4)	77.1(5)	I(2)-Pb(2)-I(1)	101.74(3)

[a]Symmetry codes for **1·DMF**: (A) -x+1, -y+1, -z+1; (B) x, y+1, z. Symmetry code for **1·Acetone**: (A) –x+1, -y+1, -z+1. Symmetry code for **2·Acetone**: (A) –x+1, -y+2, -z; (B) -x+1,-y+1,-z.

Table S2. Selected Hydrogen Bond Data for complexes **1·DMF** and **3·DMF**.[a]

D–H···A (Å)	D–H (Å)	H···A (Å)	D···A (Å)	∠ D–H···A(°)
1·DMF				
C(8)-H(8)…O(9)^{iv}	0.95	2.42	3.361(12)	172
C(37)-H(37)…O(10)^{vii}	0.95	2.53	3.443(13)	162
3·DMF				
O(11)-H(11B)…O(7)^{ii}	0.85	2.00	2.844(13)	172
O(11)-H(11A)…O(1)^{i}	0.85	2.21	3.043(13)	166
C(11)-H(11)…O(1)^{ii}	0.93	2.58	3.351(16)	140

[a]Symmetry codes for **1·DMF**: (iv) 1-x, -y, -z; (vii) -1+x, y, z. Symmetry code for **3·DMF**: (i) 1-x, 1-y, 1-z; (ii) -x, 1-y, 1-z.

Table S3. π–π interactions for complexes **1·Acetone**, **2·Acetone**, and **3·DMF**.

Interaction	Ring position	Symmetry code	Distance centroids	Dihedral angle
1·Acetone	I…II	-2-x, 6-y, 2-z	4.828(4)	79.12(61)
	I…III	-2-x, 6-y, 2-z	4.502(3)	76.70(53)
2·Acetone	I…II	x, -1+y, z	4.550(3)	78.24(43)
	I…III	x, -1+y, z	4.930(4)	82.62(42)
3·DMF	I…II	1-x, 1-y, 1-z	3.815(2)	66.22(75)