Supplementary Material

New Topologically Unique Metal-Organic Architectures Driven by a Pyridine-Tricarboxylate Building Block

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Supplementary material contains:

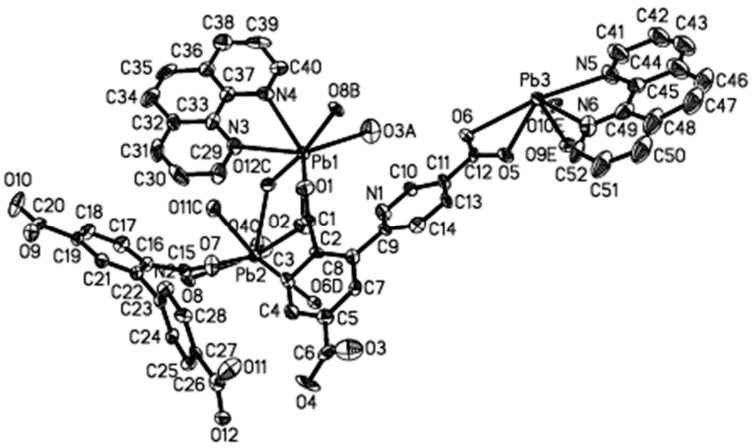

Figure S1. Ortep drawing of the asymmetric unit of compound **1** with 30% probability thermal ellipsoids; H atoms are omitted for clarity. Symmetry code: A = *x* + 1/2, –*y*, *z* + 1/2; B = *x*, *y* + 1, *z*; C = *x* + 1/2, –*y* – 1, *z* + 1/2; D = *x*, *y* – 1, *z*; E = *x* – 1/2, –*y*, *z* + 1/2.

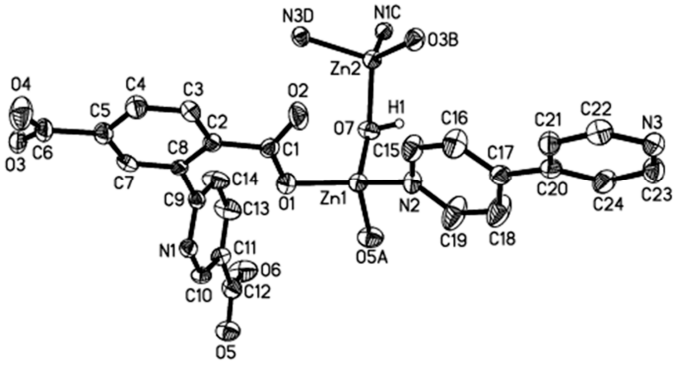

Figure S2. Ortep drawing of the asymmetric unit of compound **2** with 30% probability thermal ellipsoids; H atoms are omitted for clarity except the H of the OH groups. Symmetry code: A = –*x*, –*y*, –*z*; B = –*x* + 1/2, *y* + 1/2, –*z* + 1/2; C = *x*, –*y*, *z* + 1/2; D = –*x* + 1/2, *y* – 1/2, –*z* + 1/2.

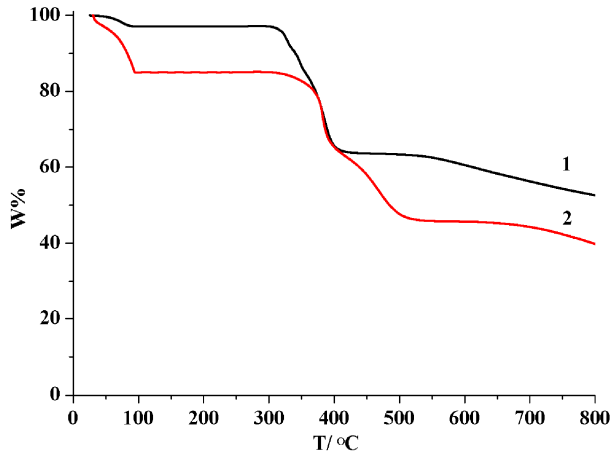

Figure S3. TGA curves for compounds **1** and **2**.

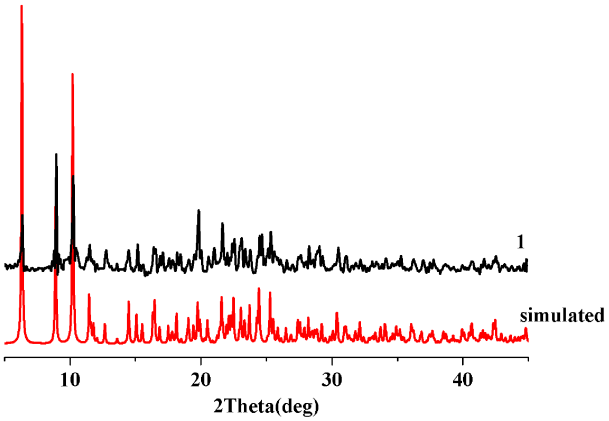

Figure S4. The PXRD patterns of compound **1** at room temperature.

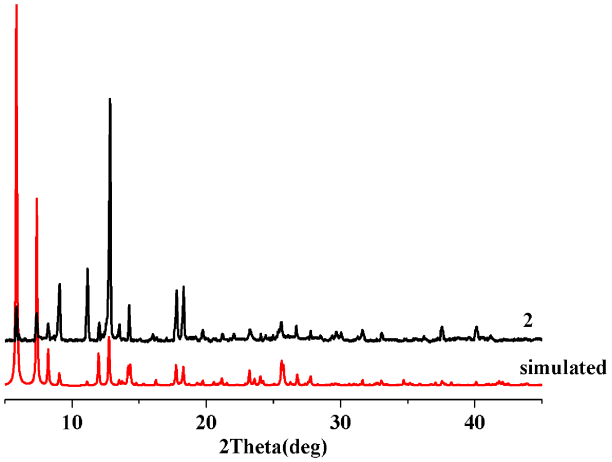

Figure S5. The PXRD patterns of compound **2** at room temperature.

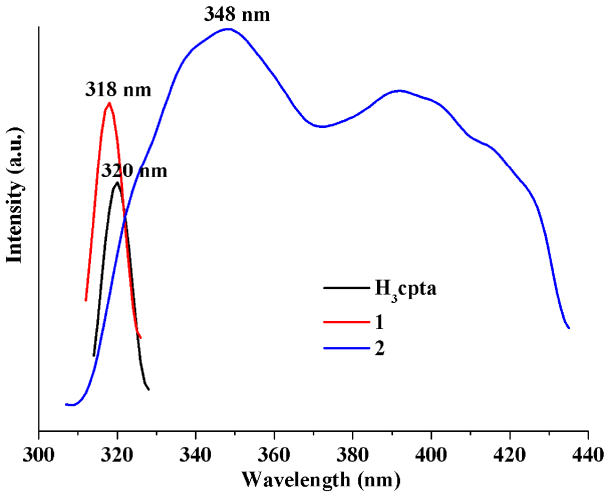

Figure S6. Solid-state excitation spectra of H_3cpta and compounds **1** and **2** at room temperature (λ_{ex} = 470 nm).

Table S1. Selected bond lengths (Å) and bond angles (°) for compounds **1** and **2**.

		1			
Pb(1)–O(1)	2.445(13)	Pb(1)–O(2)	2.715(12)	Pb(1)–O(3)i	2.913(10)
Pb(1)–O(8)ii	2.474(11)	Pb(1)–O(12)iii	2.646(11)	Pb(1)–N(3)	2.577(15)
Pb(1)–N(4)	2.704(17)	Pb(2)–O(2)	2.717(11)	Pb(2)–O(7)	2.650(11)
Pb(2)–O(8)	2.632(10)	Pb(2)–O(4)iii	2.506(14)	Pb(2)–O(6)iv	2.822(12)
Pb(2)–O(11)iii	2.425(14)	Pb(2)–O(12)iii	2.812(13)	Pb(3)–O(5)	2.445(11)
Pb(3)–O(6)	2.897(12)	Pb(3)–O(9)v	2.328(11)	Pb(3)–O(10)v	2.892(11)
Pb(3)–N(5)	2.676(17)	Pb(3)–N(6)	2.620(17)		
O(1)–Pb(1)–O(2)	49.7(4)	O(1)–Pb(1)–O(8)ii	76.4(4)	O(1)–Pb(1)–O(12)iii	115.4(4)
O(1)–Pb(1)–N(3)	79.6(5)	O(1)–Pb(1)–N(4)	132.7(4)	O(1)–Pb(1)–O(3)i	118.8(4)
O(8)ii–Pb(1)–O(2)	120.7(4)	O(12)iii–Pb(1)–O(2)	71.7(3)	N(3)–Pb(1)–O(2)	91.8(5)
N(4)–Pb(1)–O(2)	147.2(4)	O(2)–Pb(1)–O(3)i	110.9(3)	O(8)ii–Pb(1)–O(12)iii	167.6(4)
O(8)ii–Pb(1)–N(3)	102.1(4)	O(8)ii–Pb(1)–N(4)	85.7(4)	O(3)i–Pb(1)–O(8)ii	71.3(4)
O(12)iii–Pb(1)–N(3)	77.6(3)	O(12)iii–Pb(1)–N(4)	83.3(4)	O(3)i–Pb(1)–O(12)iii	104.0(4)
N(3)–Pb(1)–N(4)	61.7(5)	O(3)i–Pb(1)–N(3)	156.7(3)	O(3)i–Pb(1)–N(4)	95.2(4)
O(2)–Pb(2)–O(11)iii	103.1(5)	O(2)–Pb(2)–O(12)iii	69.2(4)	O(2)–Pb(2)–O(6)iv	78.1(4)
O(2)–Pb(2)–O(7)	83.1(5)	O(2)–Pb(2)–O(8)	132.0(5)	O(2)–Pb(2)–O(4)iii	122.4(5)
O(11)iii–Pb(2)–O(12)iii	49.7(6)	O(6)iv–Pb(2)–O(11)iii	161.7(5)	O(7)–Pb(2)–O(11)iii	82.5(4)
O(8)–Pb(2)–O(11)iii	70.1(6)	O(4)iii–Pb(2)–O(11)iii	77.4(5)	O(6)iv–Pb(2)–O(12)iii	116.3(6)
O(7)–Pb(2)–O(12)iii	112.7(6)	O(8)–Pb(2)–O(12)iii	119.7(4)	O(4)iii–Pb(2)–O(12)iii	69.3(5)
O(6)iv–Pb(2)–O(7)	115.7(5)	O(6)iv–Pb(2)–O(8)	122.9(6)	O(4)iii–Pb(2)–O(6)iv	86.4(5)
O(8)–Pb(2)–O(7)	49.1(4)	O(4)iii–Pb(2)–O(7)	150.5(6)	O(4)iii–Pb(2)–O(7)	103.0(6)
O(5)–Pb(3)–O(6)	48.1(5)	O(5)-Pb(3)-N(5)	135.0(6)	O(5)-Pb(3)-N(6)	75.0(5)
O(5)–Pb(3)–O(9)v	81.32(5)	O(5)–Pb(3)–O(10)v	113.3(6)	O(6)–Pb(3)–N(5)	161.9(5)
O(6)–Pb(3)–N(6)	123.0(5)	O(6)–Pb(3)–O(9)v	89.2(6)	O(6)–Pb(3)–O(10)v	85.3(5)
N(6)–Pb(3)–N(5)	63.0(6)	O(9)v–Pb(3)–N(5)	75.0(5)	O(10)v–Pb(3)–N(5)	77.6(5)
O(9)v–Pb(3)–N(6)	77.9(6)	O(10)v–Pb(3)–N(6)	120.2(5)	Pb(1)–O(2)–Pb(2)	108.9(4)
		2			
Zn(1)–O(1)	1.936(5)	Zn(1)–O(5)i	1.952(5)	Zn(1)–O(7)	1.936(5)
Zn(1)–N(2)	2.030(6)	Zn(2)–O(7)	1.937(5)	Zn(2)–O(3)ii	1.977(5)
Zn(2)–N(1)iii	2.050(6)	Zn(2)–N(3)iv	2.049(6)		
O(1)–Zn(1)–O(7)	108.2(2)	O(1)–Zn(1)–O(5)i	107.4(2)	O(7)–Zn(1)–O(5)i	98.4(2)
O(1)–Zn(1)–N(2)	120.1(2)	O(7)–Zn(1)–N(2)	111.2(2)	O(5)i–Zn(1)–N(2)	109.3(3)
O(7)–Zn(2)–O(3)ii	111.2(2)	O(7)–Zn(2)–N(3)iv	106.0(2)	O(3)ii–Zn(2)–N(3)iv	108.1(2)
O(7)–Zn(2)–N(1)iii	107.3(2)	O(3)ii–Zn(2)–N(1)iii	121.5(2)	N(3)iv–Zn(2)–N(1)iii	101.4(2)
O(7)–Zn(2)–O(3)ii	85.37(10)	O(7)–Zn(2)–O(3)ii	96.99(10)	O(7)–Zn(2)–O(3)ii	176.51(10)
Zn(1)–O(7)–Zn(2)	128.4(2)				

Symmetry codes: (**1**) i: $x + 1/2, -y, z + 1/2$; ii: $x, y + 1, z$; iii: $x + 1/2, -y - 1, z + 1/2$; iv: $x, y - 1, z$; v: $x - 1/2, -y, z + 1/2$; (**2**) i: $-x, -y, -z$; ii: $-x + 1/2, y + 1/2, -z + 1/2$; iii: $x, -y, z + 1/2$; iv: $-x + 1/2, y - 1/2, -z + 1/2$.

Table S2. Hydrogen bonds in crystal packing [Å, °] of compounds **1** and **2**.

Compound	D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠DHA	Symmetry code
1	O(13)–H(1W)···O(4)	0.85	2.42	2.905	116.6	$x + 1, y + 1, z$
	O(13)–H(2W)···O(14)	0.85	1.96	2.792	167.2	
2	O(11)–H(7W)···O(2)	0.85	1.93	2.778	178.6	