Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information for

Metal Organic Frameworks with Uni-, Di-, Tri-nuclear Cd(II) SBU Prepared from 1,3-bis(4-pyridyl)propane and Different Dicarboxylate ligands: Syntheses, Structures and Luminescent Properties

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Content

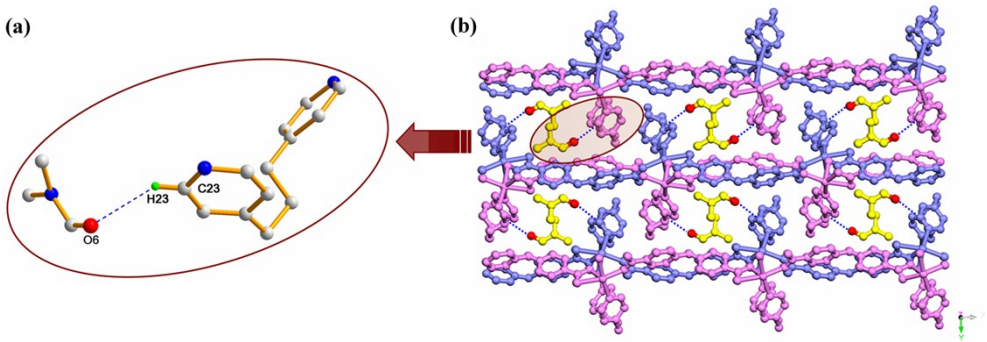

Figure S1. Schematic illustration of (a) details of H-bond ($d_{(H23\cdots O6)}$ = 2.54 Å, $d_{(C23\cdots O6)}$ = 3.327(10) Å, ∠C23-H23⋯O6 = 143°), symmetry code: 1-x, -1/2+y, 3/2-z; (b) H-bonds between the free DMF guest molecules and the double layers.

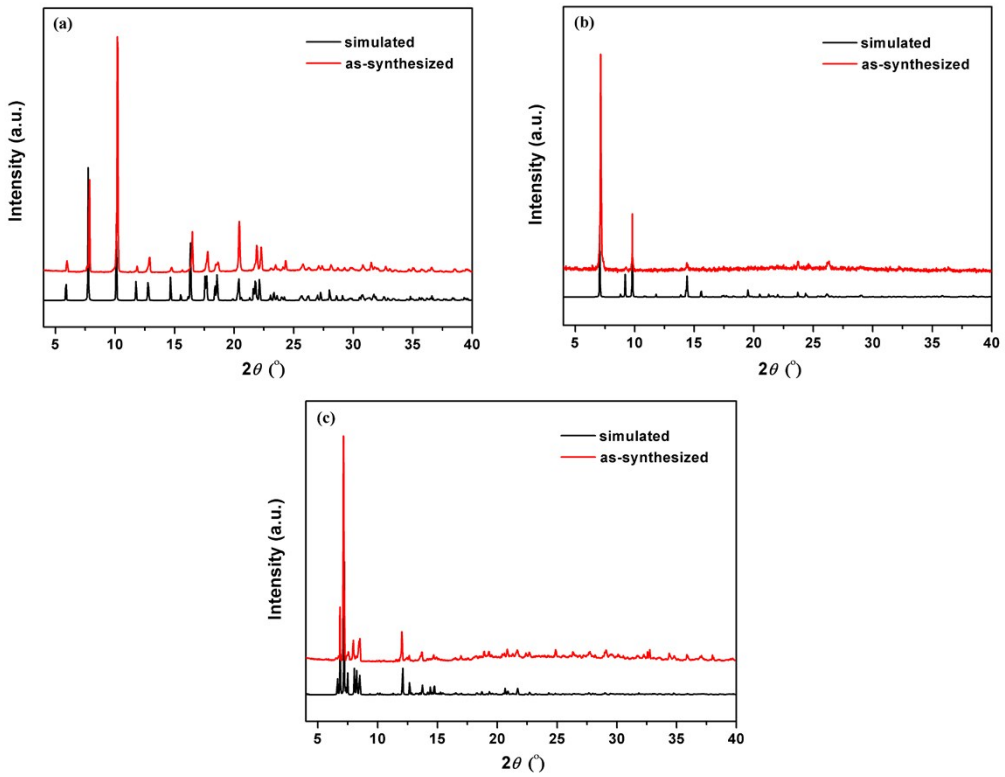

Figure S2. Experimental and simulated PXRD patterns of (a) compound 1, (b) compound 2 and (c) compound 3.

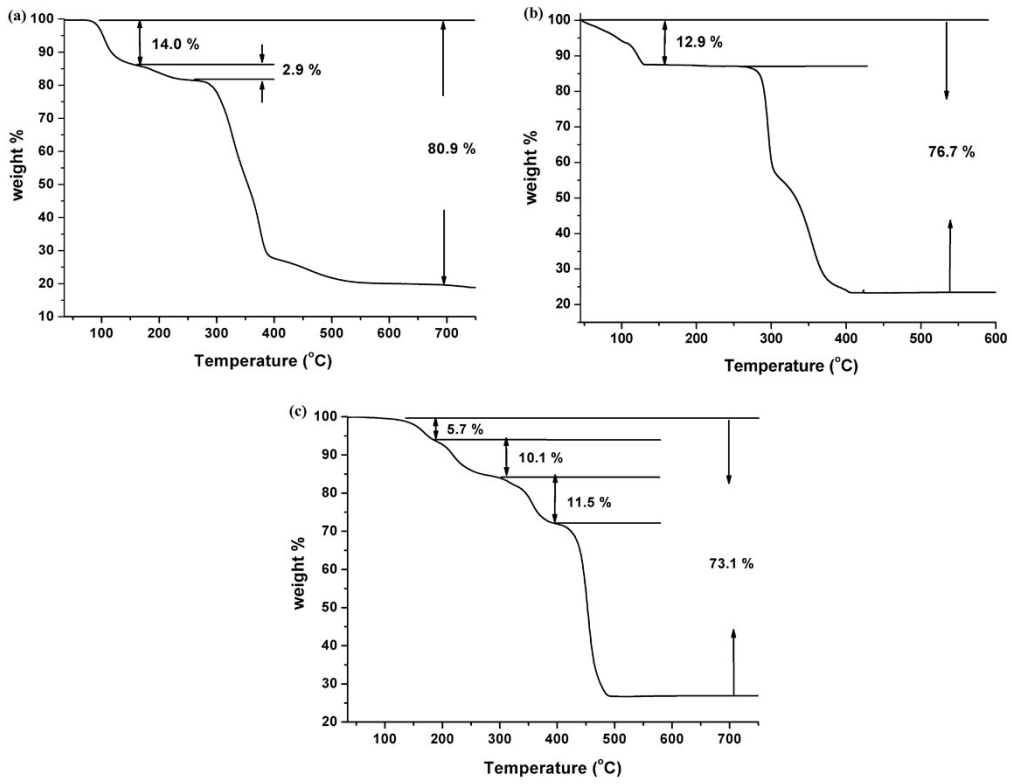

Figure S3. TGA curves of (a) compound 1, (b) compound 2 and (c) compound 3.

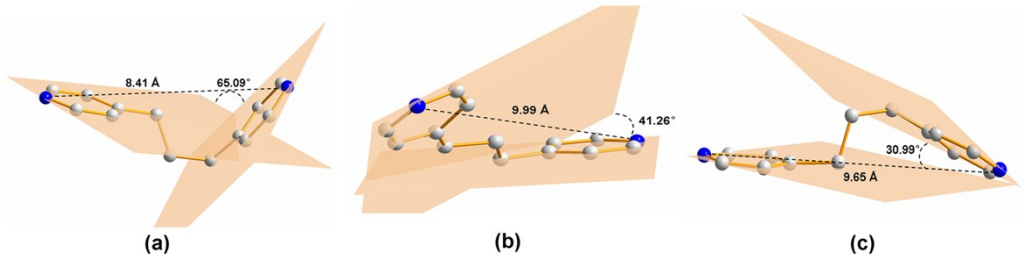

Figure S4. Schematic illustrations of the dihedral angle of the two pyridyl rings, φ and the N-N distance, ***d*** of (a) compound 1, (b) compound 2 and (c) compound 3.

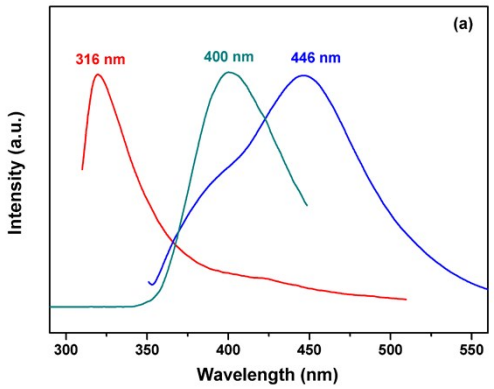

Figure S5. Solid-state photoluminescence spectra of free ligands: H_2OBA (red/left)**,** 4-H_3OIP (blue/right)**,** H_2BPDC (green/middle) at room temperature.

Table S1. Selected bond lengths (Å) for compound 1, compound 2 and compound 3.

compound 1			
Cd(1)-O(1)	2.224(3)	Cd(1)-N(1)	2.289(3)
Cd(1)-O(4)	2.290(3)	Cd(1)-N(2)	2.371(4)
Cd(1)-O(7)	2.384(3)	Cd(1)-O(5)	2.460(3)
compound 2 [a]			
Cd(1)-O(4)#1	2.272(6)	Cd(1)-O(3)#2	2.276(6)
Cd(1)-N(2)	2.305(7)	Cd(1)-N(1)	2.315(7)
Cd(1)-O(2)	2.392(6)	Cd(1)-O(1)	2.432(7)
O(3)-Cd(1)#3	2.276(6)		
compound 3 [b]			
Cd(1)-O(14)	2.190(5)	Cd(1)-O(1)	2.277(5)
Cd(1)-O(6)	2.304(5)	Cd(1)-O(10)	2.349(5)
Cd(1)-O(9)	2.410(5)	Cd(1)-O(2)	2.470(5)
Cd(1)-O(5)	2.730(6)	Cd(2)-O(22)	2.189(5)
Cd(2)-O(13)	2.211(4)	Cd(2)-O(17)	2.214(5)
Cd(2)-O(5)	2.304(5)	Cd(2)-O(11)	2.310(4)
Cd(2)-O(9)	2.329(5)	Cd(3)-O(21)	2.251(5)
Cd(3)-N(1)	2.285(5)	Cd(3)-O(18)	2.303(5)

Cd(3)-O(11)	2.363(5)	Cd(3)-O(29)	2.438(5)
Cd(3)-O(12)	2.479(5)	Cd(3)-O(17)	2.809(6)
Cd(4)-O(20)#3	2.231(5)	Cd(4)-O(7)	2.307(5)
Cd(4)-O(4)#4	2.351(5)	Cd(4)-O(3)#4	2.343(5)
Cd(4)-O(28)#2	2.364(5)	Cd(4)-O(27)#2	2.518(5)
Cd(4)-O(8)	2.546(5)	Cd(5)-O(19)#5	2.202(4)
Cd(5)-O(23)	2.244(4)	Cd(5)-O(15)#3	2.279(4)
Cd(5)-O(27)	2.280(5)	Cd(5)-O(26)	2.292(4)
Cd(5)-O(8)#1	2.298(4)	Cd(6)-N(2)#6	2.281(6)
Cd(6)-O(24)	2.286(4)	Cd(6)-O(26)	2.337(4)
Cd(6)-O(16)#3	2.345(5)	Cd(6)-O(30)	2.437(6)
Cd(6)-O(15)#3	2.506(5)	Cd(6)-O(25)	2.595(6)

[a] Symmetry transformations used to generate equivalent atoms: #1 -x, -y, -z, #2 x+1/2, y+1/2, z, #3 x-1/2, y-1/2, z; [b] Symmetry transformations used to generate equivalent atoms: #1 x, y-1, z, #2 x, y+1, z, #3 x-1/2, -y+3/2, z-1/2, #4 x-1/2, y+1/2, z, #5 x-1/2, -y+1/2, z-1/2, #6 x, -y+1, z-1/2.

Table S2. Selected bond angles (°) for (a) compound 1, (b) compound 2 and (c) compound 3.

compound 1			
O(1)-Cd(1)-N(1)	110.29(12)	O(1)-Cd(1)-O(4)	101.45(11)
N(1)-Cd(1)-O(4)	148.21(11)	O(1)-Cd(1)-N(2)	86.67(12)
N(1)-Cd(1)-N(2)	92.95(13)	O(4)-Cd(1)-N(2)	90.45(13)
O(1)-Cd(1)-O(7)	86.97(11)	N(1)-Cd(1)-O(7)	86.10(12)
O(4)-Cd(1)-O(7)	94.11(12)	N(2)-Cd(1)-O(7)	172.81(12)
O(1)-Cd(1)-O(5)	156.66(11)	N(1)-Cd(1)-O(5)	93.04(11)
O(4)-Cd(1)-O(5)	55.20(10)	N(2)-Cd(1)-O(5)	93.03(13)
O(7)-Cd(1)-O(5)	94.13(11)		
compoun 2 [a]			
O(4)#1-Cd(1)-O(3)#2	127.5(2)	O(4)#1-Cd(1)-N(2)	89.5(3)
O(3)#2-Cd(1)-N(2)	91.2(2)	O(4)#1-Cd(1)-N(1)	88.8(3)
O(3)#2-Cd(1)-N(1)	87.9(2)	N(2)-Cd(1)-N(1)	177.0(2)
O(4)#1-Cd(1)-O(2)	90.7(2)	O(3)#2-Cd(1)-O(2)	141.7(2)

N(2)-Cd(1)-O(2)	90.9(2)	N(1)-Cd(1)-O(2)	91.5(3)
O(4)#1-Cd(1)-O(1)	144.5(2)	O(3)#2-Cd(1)-O(1)	87.7(2)
N(2)-Cd(1)-O(1)	95.4(3)	N(1)-Cd(1)-O(1)	87.4(3)
O(2)-Cd(1)-O(1)	54.1(2)		
compond 3 [b]			
O(14)-Cd(1)-O(1)	102.8(3)	O(14)-Cd(1)-O(6)	117.5(3)
O(1)-Cd(1)-O(6)	86.9(3)	O(14)-Cd(1)-O(10)	144.1(3)
O(1)-Cd(1)-O(10)	104.5(3)	O(6)-Cd(1)-O(10)	87.0(3)
O(14)-Cd(1)-O(9)	91.3(2)	O(1)-Cd(1)-O(9)	152.6(3)
O(6)-Cd(1)-O(9)	107.5(3)	O(10)-Cd(1)-O(9)	54.8(2)
O(14)-Cd(1)-O(2)	87.2(3)	O(1)-Cd(1)-O(2)	54.2(2)
O(6)-Cd(1)-O(2)	138.8(3)	O(10)-Cd(1)-O(2)	90.1(3)
O(9)-Cd(1)-O(2)	104.2(3)	O(14)-Cd(1)-O(5)	76.7(2)
O(1)-Cd(1)-O(5)	125.0(2)	O(6)-Cd(1)-O(5)	50.1(2)
O(10)-Cd(1)-O(5)	105.4(2)	O(9)-Cd(1)-O(5)	80.9(2)
O(2)-Cd(1)-O(5)	163.4(2)	O(22)-Cd(2)-O(13)	170.4(2)
O(22)-Cd(2)-O(17)	97.0(3)	O(13)-Cd(2)-O(17)	90.2(3)
O(22)-Cd(2)-O(5)	86.6(3)	O(13)-Cd(2)-O(5)	87.1(2)
O(17)-Cd(2)-O(5)	172.7(3)	O(22)-Cd(2)-O(11)	87.1(2)
O(13)-Cd(2)-O(11)	100.4(2)	O(17)-Cd(2)-O(11)	81.5(3)
O(5)-Cd(2)-O(11)	92.4(2)	O(22)-Cd(2)-O(9)	83.0(3)
O(13)-Cd(2)-O(9)	90.1(2)	O(17)-Cd(2)-O(9)	94.4(3)
O(5)-Cd(2)-O(9)	92.4(3)	O(11)-Cd(2)-O(9)	168.7(2)
O(21)-Cd(3)-N(1)	106.8(3)	O(21)-Cd(3)-O(18)	95.5(3)
N(1)-Cd(3)-O(18)	85.7(3)	O(21)-Cd(3)-O(11)	100.7(2)
N(1)-Cd(3)-O(11)	145.3(3)	O(18)-Cd(3)-O(11)	112.5(3)
O(21)-Cd(3)-O(29)	81.6(3)	N(1)-Cd(3)-O(29)	83.0(3)
O(18)-Cd(3)-O(29)	166.9(3)	O(11)-Cd(3)-O(29)	80.6(3)
O(21)-Cd(3)-O(12)	150.2(2)	N(1)-Cd(3)-O(12)	94.2(3)
O(18)-Cd(3)-O(12)	107.2(3)	O(11)-Cd(3)-O(12)	53.0(2)
O(29)-Cd(3)-O(12)	80.2(3)	O(21)-Cd(3)-O(17)	85.1(3)
N(1)-Cd(3)-O(17)	133.2(3)	O(18)-Cd(3)-O(17)	47.7(2)

O(11)-Cd(3)-O(17)	69.0(2)	O(29)-Cd(3)-O(17)	143.8(2)
O(12)-Cd(3)-O(17)	95.9(3)	O(20)#3-Cd(4)-O(7)	128.7(3)
O(20)#3-Cd(4)-O(4)#4	92.9(3)	O(7)-Cd(4)-O(4)#4	87.3(3)
O(20)#3-Cd(4)-O(3)#4	98.3(3)	O(7)-Cd(4)-O(3)#4	121.3(3)
O(4)#4-Cd(4)-O(3)#4	54.1(3)	O(20)#3-Cd(4)-O(28)#2	133.3(3)
O(7)-Cd(4)-O(28)#2	85.8(3)	O(4)#6-Cd(4)-O(28)#2	123.6(3)
O(3)#4-Cd(4)-O(28)#2	83.7(3)	O(20)#3-Cd(4)-O(27)#2	81.3(2)
O(7)-Cd(4)-O(27)#2	112.5(2)	O(4)#4-Cd(4)-O(27)#2	158.8(2)
O(3)#4-Cd(4)-O(27)#2	106.9(2)	O(28)#2-Cd(4)-O(27)#2	54.2(2)
O(20)#3-Cd(4)-O(8)	84.4(2)	O(7)-Cd(4)-O(8)	53.1(2)
O(4)#4-Cd(4)-O(8)	120.0(2)	O(3)#4-Cd(4)-O(8)	173.2(2)
O(28)#2-Cd(4)-O(8)	99.1(2)	O(27)#2-Cd(4)-O(8)	79.64(19)
O(19)#5-Cd(5)-O(23)	172.2(2)	O(19)#5-Cd(5)-O(15)#3	99.3(2)
O(23)-Cd(5)-O(15)#3	85.4(2)	O(19)#5-Cd(5)-O(27)	86.7(2)
O(23)-Cd(5)-O(27)	86.6(2)	O(15)#3-Cd(5)-O(27)	95.6(2)
O(19)#5-Cd(5)-O(26)	99.5(2)	O(23)-Cd(5)-O(26)	87.4(2)
O(15)#3-Cd(5)-O(26)	80.2(2)	O(27)-Cd(5)-O(26)	173.0(2)
O(19)#5-Cd(5)-O(8)#1	91.7(2)	O(23)-Cd(5)-O(8)#1	84.4(2)
O(15)#3-Cd(5)-O(8)#1	168.2(2)	O(27)-Cd(5)-O(8)#1	90.2(2)
O(26)-Cd(5)-O(8)#1	92.9(2)	N(2)#6-Cd(6)-O(24)	96.6(3)
N(2)#6-Cd(6)-O(26)	125.8(3)	O(24)-Cd(6)-O(26)	83.8(2)
N(2)#6-Cd(6)-O(16)#3	103.2(3)	O(24)-Cd(6)-O(16)#3	154.8(2)
O(26)-Cd(6)-O(16)#3	96.8(2)	N(2)#6-Cd(6)-O(30)	83.7(3)
O(24)-Cd(6)-O(30)	80.3(2)	O(26)-Cd(6)-O(30)	148.1(2)
O(16)#3-Cd(6)-O(30)	86.4(3)	N(2)#6-Cd(6)-O(15)#3	153.6(3)
O(24)-Cd(6)-O(15)#3	102.4(2)	O(26)-Cd(6)-O(15)#3	74.8(2)
O(16)#3-Cd(6)-O(15)#3	54.1(2)	O(30)-Cd(6)-O(15)#3	81.8(2)
N(2)#6-Cd(6)-O(25)	80.2(3)	O(24)-Cd(6)-O(25)	114.4(3)
O(26)-Cd(6)-O(25)	52.0(2)	O(16)#3-Cd(6)-O(25)	84.6(3)
O(30)-Cd(6)-O(25)	159.2(2)	O(15)#3-Cd(6)-O(25)	107.6(2)

[a] Symmetry transformations used to generate equivalent atoms: #1 -x, -y, -z, #2 x+1/2, y+1/2, z; [b] Symmetry transformations used to generate equivalent atoms: #1 x, y-1, z; #2 x, y+1, z; #3 x-1/2, -y+3/2, z-1/2; #4 x-1/2, y+1/2, z; #5 x-1/2, -y+1/2, z-1/2; #6 x, -y+1, z-1/2.