

Supplementary Information for

Synthesis and characterization of a novel 2-fold interpenetrated cadmium-organic framework with trimesic acid and 1,2-bis(4-pyridyl)ethane which exhibits single-crystal-to-single-crystal transformation into the desolvated form with liquid and gas sorption properties

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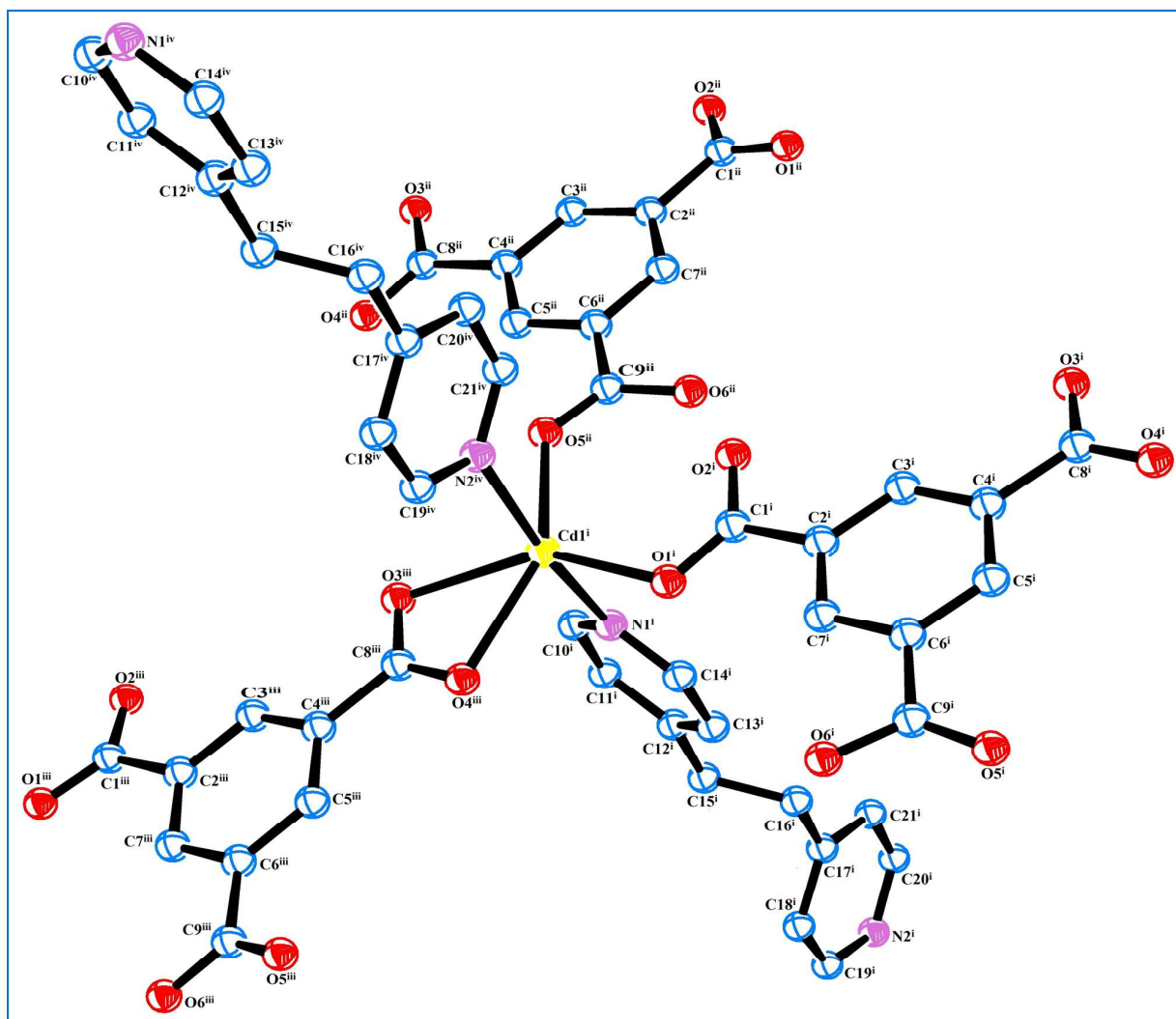


Figure S1. Ortep diagram of compound **2**. Disordered atoms and H-atoms have been omitted for clarity. Symmetry transformations used to generate equivalent atoms: (i) x, y, z (ii) $x-1/2, 3/2-y, -z$ (iii) $x, 3/2-y, 1/2+z$ (iv) $x, 1+y, z$

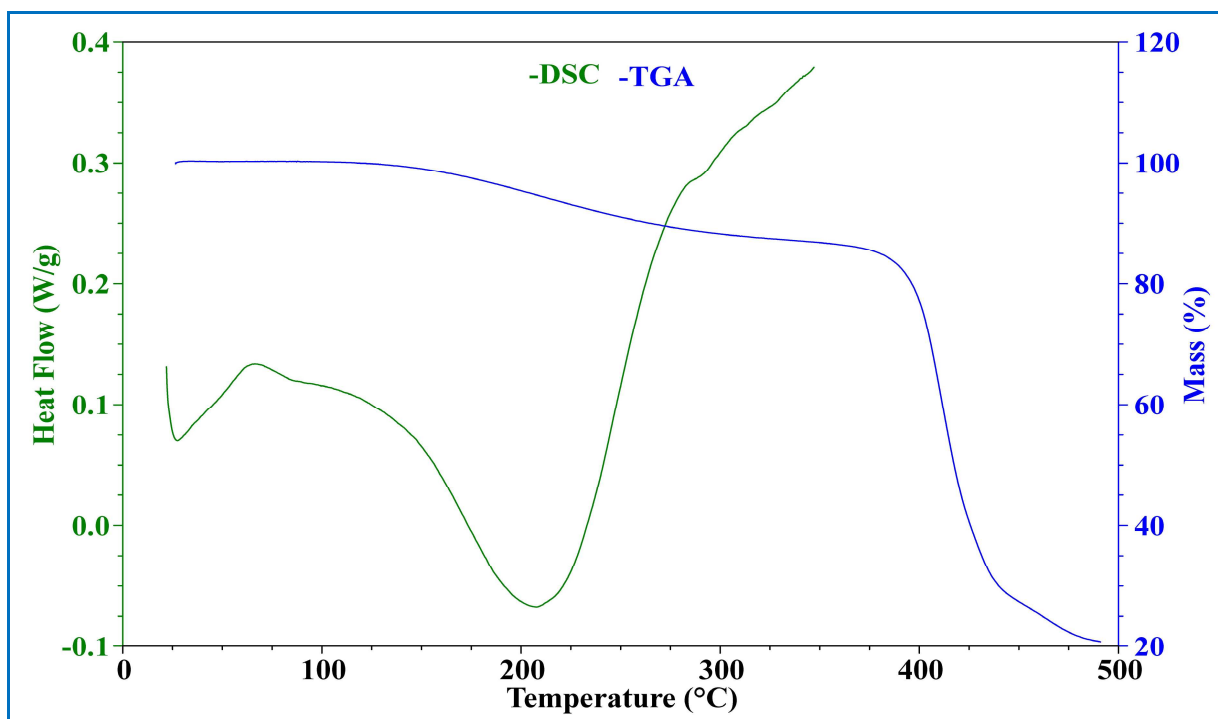


Figure S2. TGA (blue) and DSC (green) curves for compound 1.

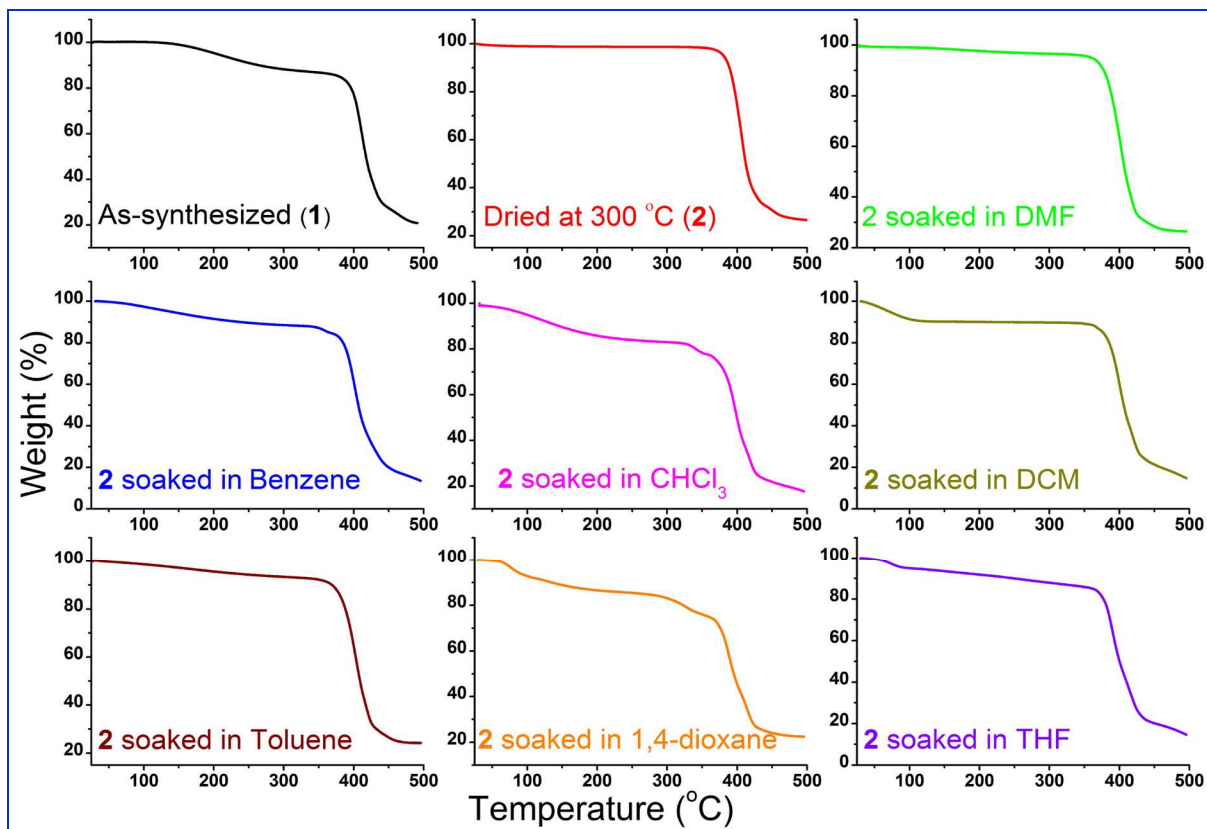


Figure S3. TGA of 2 soaked in various solvents indicating solvent sorption.

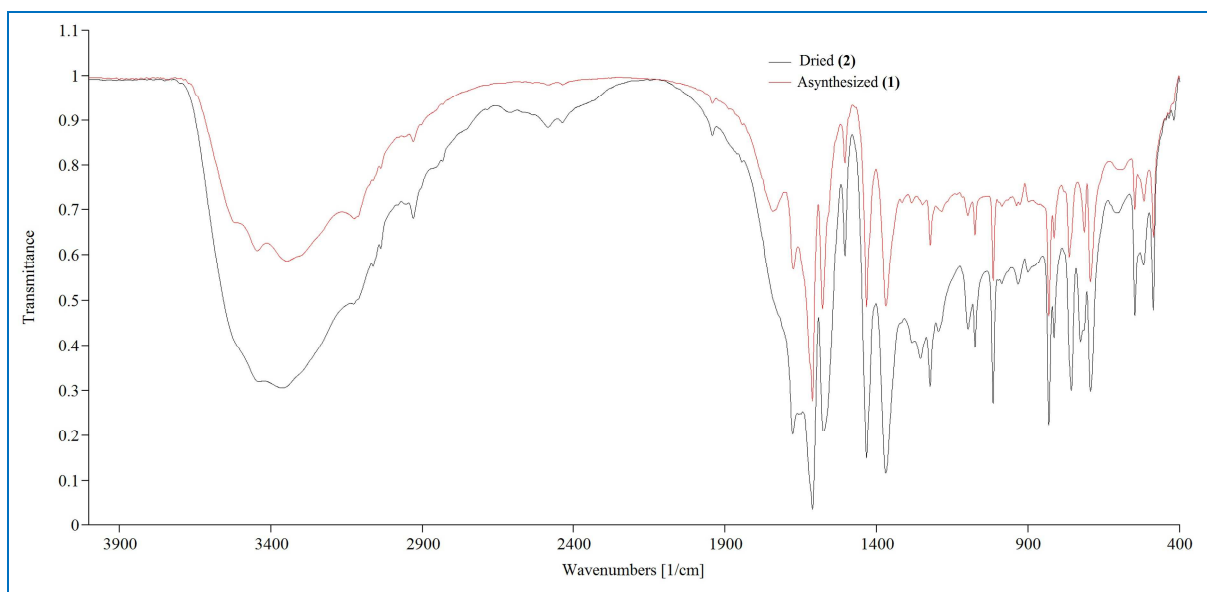


Figure S4. IR spectra of **1** and **2**.

Table S1. Bond angles [°] for **1**, **2** and **3**.

(1)		(2)		(3)	
O(1)-Cd(1)-O(3)#1	91.2(2)	O(1)-C(1)-O(2)	124.2(3)	O(4)#1-Cd(1)-N(10)	85.2(8)
O(1)-Cd(1)-O(5)#2	149.6(2)	O(4)-C(8)-O(3)	123.0(3)	O(4)#2-Cd(1)-N(10)	94.8(8)
O(3)#1-Cd(1)-O(5)#2	119.3(2)	O(5)-C(9)-O(6)	124.3(3)	N(10)-Cd(1)-N(10)#3	172.2(3)
O(1)-Cd(1)-N(1)	92.88(16)	O(1)-Cd(1)-N(1)	91.04(8)	O(4)#1-Cd(1)-O(2)	146.3(3)
O(3)#1-Cd(1)-N(1)	89.03(17)	O(1)-Cd(1)-N(2)#4	91.73(8)	N(10)-Cd(1)-O(2)	92.16(14)
O(5)#2-Cd(1)-N(1)	87.98(18)	N(1)-Cd(1)-N(2)#4	171.45(9)	O(4)#1-Cd(1)-O(6)#4	121.9(2)
O(1)-Cd(1)-N(1)#3	92.88(16)	O(1)-Cd(1)-O(3)#5	145.85(7)	N(10)-Cd(1)-O(6)#4	86.71(13)
O(3)#1-Cd(1)-N(1)#3	89.04(17)	N(1)-Cd(1)-O(3)#5	88.67(8)	O(2)-Cd(1)-O(6)#4	91.3(2)
O(5)#2-Cd(1)-N(1)#3	87.98(18)	N(2)#4-Cd(1)-O(3)#5	93.57(8)	O(4)#1-Cd(1)-O(1)	91.0(2)
N(1)-Cd(1)-N(1)#3	174.0(3)	O(1)-Cd(1)-O(4)#5	90.40(8)	N(10)-Cd(1)-O(1)	93.90(13)
O(1)-Cd(1)-O(2)	55.50(19)	N(1)-Cd(1)-O(4)#5	92.83(8)	O(2)-Cd(1)-O(1)	55.57(19)
O(3)#1-Cd(1)-O(2)	146.7(2)	N(2)#4-Cd(1)-O(4)#5	95.24(8)	O(6)#4-Cd(1)-O(1)	146.90(19)
O(5)#2-Cd(1)-O(2)	94.1(2)	O(3)#5-Cd(1)-O(4)#5	55.52(7)	O(1)-C(1)-O(2)	122.3(7)
N(1)-Cd(1)-O(2)	92.38(15)	O(1)-Cd(1)-O(5)#6	121.72(7)	O(6)-C(8)-O(5)	125.1(8)
N(1)#3-Cd(1)-O(2)	92.38(15)	N(1)-Cd(1)-O(5)#6	85.12(8)	O(4)-C(9)-O(3)	124.0(11)
O(2)-C(1)-O(1)	123.0(8)	N(2)#4-Cd(1)-O(5)#6	86.54(8)		
O(3)-C(5)-O(4)	124.1(9)	O(3)#5-Cd(1)-O(5)#6	92.29(7)		
O(5)-C(8)-O(6)	125.4(8)	O(4)#5-Cd(1)-O(5)#6	147.81(7)		
Symmetry transformations used to generate equivalent atoms:					
#1 -x+1,y+1/2,z	#2 x+1,y,z	#1 x,-y+3/2,z-1/2	#2 x,y-1,z	#1 x+1,y,-z+1/2	#2 x+1,y,z
#3 x,y,-z+1/2	#4 x,y,-z+3/2	#3 x+1/2,-y+3/2,-z		#3 x,y,-z+1/2	#4 -x+2,y-1/2,z
#5 -x+1,y-1/2,z	#6 x-1,y,z	#4 x,y+1,z	#5 x,-y+3/2,z+1/2	#5 x-1,y,z	#6 -x+2,y+1/2,z
		#6 x-1/2,-y+3/2,-z		#7 x,y,-z-1/2	