Construction of metal-organic coordination networks with various metal-linker secondary building units: structures and properties

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Table S1. Selected bond distances (Å) and angles (°) for 1−3[a]

1			
Zn(1)-O(4)	1.967(3)	Zn(1)-O(2)$^{\#1}$	1.969(3)
Zn(1)-N(2)	2.030(3)	Zn(1)-O(5)	2.155(3)
Zn(1)-O(7)	2.190(3)	Zn(2)-O(8)$^{\#2}$	1.979(2)
Zn(2)-O(8)$^{\#3}$	1.979(2)	Zn(2)-O(6)	1.979(3)
Zn(2)-O(6)$^{\#4}$	1.979(3)	Zn(3)-N(1)$^{\#5}$	2.014(3)
Zn(3)-N(1)	2.014(3)	Zn(3)-O(3)$^{\#5}$	2.183(3)
Zn(3)-O(3)	2.183(3)	Zn(3)-O(1)$^{\#5}$	2. 183(3)
Zn(3)-O(1)	2. 183(3)		
O(4)-Zn(1)-O(2)$^{\#1}$	97.73(11)	O(4)-Zn(1)-N(2)	132.77(11)
O(2)$^{\#1}$-Zn(1)-N(2)	129.50(11)	O(4)-Zn(1)-O(5)	98.99(12)
O(2)$^{\#1}$-Zn(1)-O(5)	98.93(12)	N(2)-Zn(1)-O(5)	76.31(11)
O(4)-Zn(1)-O(7)	99.56(12)	O(2)$^{\#1}$-Zn(1)-O(7)	99.85(12)
N(2)-Zn(1)-O(7)	75.17(10)	O(5)-Zn(1)-O(7)	151.46(10)
O(8)$^{\#2}$-Zn(2)-O(8)$^{\#2}$	116.95(16)	O(8)$^{\#2}$-Zn(2)-O(6)$^{\#4}$	97.06(11)
O(8)$^{\#3}$-Zn(2)-O(6)$^{\#4}$	116.00(12)	O(8)$^{\#2}$-Zn(2)-O(6)	116.00(12)
O(8)$^{\#3}$-Zn(2)-O(6)	97.06(11)	O(6)$^{\#4}$-Zn(2)-O(6)	115.07(17)
N(1)-Zn(3)-N(1)$^{\#5}$	178.02(17)	N(1)-Zn(3)-O(3)	76.57(11)
N(1)$^{\#5}$-Zn(3)-O(3)	104.83(11)	N(1)-Zn(3)-O(3)$^{\#5}$	104.83(11)
N(1)$^{\#5}$-Zn(3)-O(3)$^{\#5}$	76.57(11)	O(3)-Zn(3)-O(3)$^{\#5}$	93.47(16)
N(1)-Zn(3)-O(1)	76.45(11)	N(1)$^{\#5}$-Zn(3)-O(1)	102.15(11)
O(3)-Zn(3)-O(1)	153.02(9)	O(3)$^{\#5}$-Zn(3)-O(1)	92.93(12)
N(1)-Zn(3)-O(1)$^{\#5}$	102.15(11)	N(1)$^{\#5}$-Zn(3)-O(1)$^{\#5}$	76.46(11)
O(3)-Zn(3)-O(1)$^{\#5}$	92.93(12)	O(3)$^{\#5}$-Zn(3)-O(1)$^{\#5}$	153.02(9)
O(1)-Zn(3)-O(1)$^{\#5}$	93.15(16)		
2			
Pb(1)-N(1)	2.493(7)	Pb(1)-O(3)	2.536(6)
Pb(1)-O(1)	2.605(6)	Pb(1)-O(1)$^{\#6}$	2.620(6)
Pb(1)-O(2)$^{\#6}$	2.628(8)	Pb(1)-O(3)$^{\#7}$	2.683(6)
Ca(1)-O(4)$^{\#8}$	2.372(6)	Ca(1)-O(4)$^{\#9}$	2.372(6)
Ca(1)-O(4)$^{\#10}$	2.372(6)	Ca(1)-O(4)$^{\#11}$	2.372(6)
Ca(1)-O(4)	2.372(6)	Ca(1)-O(4)$^{\#12}$	2.372(6)
N(1)-Pb(1)-O(3)	64.2(2)	N(1)-Pb(1)-O(1)	64.3(2)
O(3)-Pb(1)-O(1)	127.7(2)	N(1)-Pb(1)-O(1)$^{\#6}$	74.9(2)
O(3)-Pb(1)-O(1)$^{\#6}$	72.4(2)	O(1)-Pb(1)-O(1)$^{\#6}$	102.7(3)
N(1)-Pb(1)-O(2)$^{\#6}$	100.9(3)	O(3)-Pb(1)-O(2)$^{\#6}$	121.6(2)
O(1)-Pb(1)-O(2)$^{\#6}$	77.3(2)	O(1)$^{\#6}$-Pb(1)-O(2)$^{\#6}$	49.5(2)
N(1)-Pb(1)-O(3)$^{\#7}$	128.8(2)	O(3)-Pb(1)-O(3)$^{\#7}$	66.2(3)
O(1)-Pb(1)-O(3)$^{\#7}$	166.1(2)	O(1)$^{\#6}$-Pb(1)-O(3)$^{\#6}$	78.9(2)
O(2)$^{\#6}$-Pb(1)-O(3)$^{\#7}$	94.0(2)	O(4)$^{\#8}$-Ca(1)-O(4)$^{\#9}$	88.0(2)
O(4)$^{\#8}$-Ca(1)-O(4)$^{\#10}$	179.999(1)	O(4)$^{\#9}$-Ca(1)-O(4)$^{\#10}$	92.0(2)
O(4)$^{\#8}$-Ca(1)-O(4)$^{\#11}$	88.0(2)	O(4)$^{\#9}$-Ca(1)-O(4)$^{\#11}$	88.0(2)

O(4)$^{\#10}$-Ca(1)-O(4)$^{\#11}$	92.0(2)	O(4)$^{\#8}$-Ca(1)-O(4)	92.0(2)
O(4)$^{\#9}$-Ca(1)-O(4)	179.998(1)	O(4)$^{\#10}$-Ca(1)-O(4)	88.0(2)
O(4)$^{\#11}$-Ca(1)-O(4)	92.0(2)	O(4)$^{\#8}$-Ca(1)-O(4)$^{\#12}$	92.0(2)
O(4)$^{\#9}$-Ca(1)-O(4)$^{\#12}$	92.0(2)	O(4)$^{\#10}$-Ca(1)-O(4)$^{\#12}$	88.0(2)
O(4)$^{\#11}$-Ca(1)-O(4)$^{\#12}$	179.998(1)	O(4)-Ca(1)-O(4)$^{\#12}$	88.0(2)
3			
Ce(1)-O(1)$^{\#13}$	2.5027(18)	Ce(1)-O(1)$^{\#14}$	2.5027(18)
Ce(1)-O(1)$^{\#15}$	2.5027(18)	Ce(1)-O(1)	2.5027(18)
Ce(1)-O(1)$^{\#16}$	2.5027(18)	Ce(1)-O(1)$^{\#17}$	2.5027(18)
Ce(1)-N(1)$^{\#15}$	2.605(3)	Ce(1)-N(1)	2.605(3)
Ce(1)-N(1)$^{\#17}$	2.605(3)	Mg(1)-O(2)	2.0798(16)
Mg(1)-O(2)$^{\#18}$	2.0798(16)	Mg(1)-O(2)$^{\#19}$	2.0798(16)
Mg(1)-O(2)$^{\#20}$	2.0798(16)	Mg(1)-O(1W)	2.113(2)
Mg(1)-O(1W)$^{\#18}$	2.113(2)		
O(1)$^{\#13}$-Ce(1)-O(1)$^{\#14}$	81.31(7)	O(1)$^{\#13}$-Ce(1)-O(1)$^{\#15}$	124.22(8)
O(1)$^{\#14}$-Ce(1)-O(1)$^{\#15}$	83.82(10)	O(1)$^{\#13}$-Ce(1)-O(1)	147.91(9)
O(1)$^{\#14}$-Ce(1)-O(1)	124.22(8)	O(1)$^{\#15}$-Ce(1)-O(1)	81.31(7)
O(1)$^{\#13}$-Ce(1)-O(1)$^{\#16}$	81.32(7)	O(1)$^{\#14}$-Ce(1)-O(1)$^{\#16}$	81.32(7)
O(1)$^{\#15}$-Ce(1)-O(1)$^{\#16}$	147.91(9)	O(1)-Ce(1)-O(1)$^{\#16}$	83.82(10)
O(1)$^{\#13}$-Ce(1)-O(1)$^{\#17}$	83.82(10)	O(1)$^{\#14}$-Ce(1)-O(1)$^{\#17}$	147.91(9)
O(1)$^{\#15}$-Ce(1)-O(1)$^{\#17}$	81.32(7)	O(1)-Ce(1)-O(1)$^{\#17}$	81.32(7)
O(1)$^{\#16}$-Ce(1)-O(1)$^{\#17}$	124.22(8)	O(1)$^{\#13}$-Ce(1)-N(1)$^{\#15}$	62.11(4)
O(1)$^{\#14}$-Ce(1)-N(1)$^{\#15}$	73.96(4)	O(1)$^{\#15}$-Ce(1)-N(1)$^{\#15}$	62.11(4)
O(1)-Ce(1)-N(1)$^{\#15}$	138.09(5)	O(1)$^{\#16}$-Ce(1)-N(1)$^{\#15}$	138.09(5)
O(1)$^{\#17}$-Ce(1)-N(1)$^{\#15}$	73.95(4)	O(1)$^{\#13}$-Ce(1)-N(1)	138.09(5)
O(1)$^{\#14}$-Ce(1)-N(1)	62.11(4)	O(1)$^{\#15}$-Ce(1)-N(1)	73.96(4)
O(1)-Ce(1)-N(1)	62.11(4)	O(1)$^{\#16}$-Ce(1)-N(1)	73.96(4)
O(1)$^{\#17}$-Ce(1)-N(1)	138.09(5)	N(1)$^{\#15}$-Ce(1)-N(1)	120.0
O(1)$^{\#13}$-Ce(1)-N(1)$^{\#17}$	73.96(4)	O(1)$^{\#14}$-Ce(1)-N(1)$^{\#17}$	138.09(5)
O(1)$^{\#15}$-Ce(1)-N(1)$^{\#17}$	138.09(5)	O(1)-Ce(1)-N(1)$^{\#17}$	73.96(4)
O(1)$^{\#16}$-Ce(1)-N(1)$^{\#17}$	62.11(4)	O(1)$^{\#17}$-Ce(1)-N(1)$^{\#17}$	62.11(4)
N(1)$^{\#15}$-Ce(1)-N(1)$^{\#17}$	120.0	N(1)-Ce(1)-N(1)$^{\#17}$	120.0
O(2)-Mg(1)-O(2)$^{\#18}$	180.0	O(2)-Mg(1)-O(2)$^{\#19}$	93.07(10)
O(2)$^{\#18}$-Mg(1)-O(2)$^{\#19}$	86.93(10)	O(2)-Mg(1)-O(2)$^{\#20}$	86.93(10)
O(2)$^{\#18}$-Mg(1)-O(2)$^{\#20}$	93.07(10)	O(2)$^{\#19}$-Mg(1)-O(2)$^{\#20}$	180.0
O(2)-Mg(1)-O(1W)	91.71(6)	O(2)$^{\#18}$-Mg(1)-O(1W)	88.29(6)
O(2)$^{\#19}$-Mg(1)-O(1W)	88.29(6)	O(2)$^{\#20}$-Mg(1)-O(1W)	91.71(6)
O(2)-Mg(1)-O(1W)$^{\#18}$	88.29(6)	O(2)$^{\#18}$-Mg(1)-O(1W)$^{\#18}$	91.71(6)
O(2)$^{\#19}$-Mg(1)-O(1W)$^{\#18}$	91.71(6)	O(2)$^{\#20}$-Mg(1)-O(1W)$^{\#18}$	88.29(6)
O(1W)-Mg(1)-O(1W)$^{\#18}$	180.0		

[a]Symmetry transformations used to generate equivalent atoms: #1 x+1/2, y-1/2, z; #2 -x+1/2, y+1/2, -z+1/2; #3 x+1/2, y+1/2, z; #4 -x+1, y, -z+1/2; #5 -x, y, -z+1/2; #6 x-y+2/3, x+1/3, -z+1/3; #7 -x-1/3, -y+4/3, -z+1/3; #8 x-y+1/3, x+2/3, -z+2/3; #9 -x-2/3, -y+2/3, -z+2/3; #10

-x+y-1, -x, z; #11 y-2/3, -x+y-1/3, -z+2/3; #12 -y, x-y+1, z; #13 -x+y-1, y, -z-1/2; #14 -y, -x, -z-1/2; #15 -x+y-1, -x, z; #16 x, x-y+1, -z-1/2; #17 -y, x-y+1, z; #18 -x, -y+1, -z; #19 -x, -y+1, z; #20 x, y, -z.

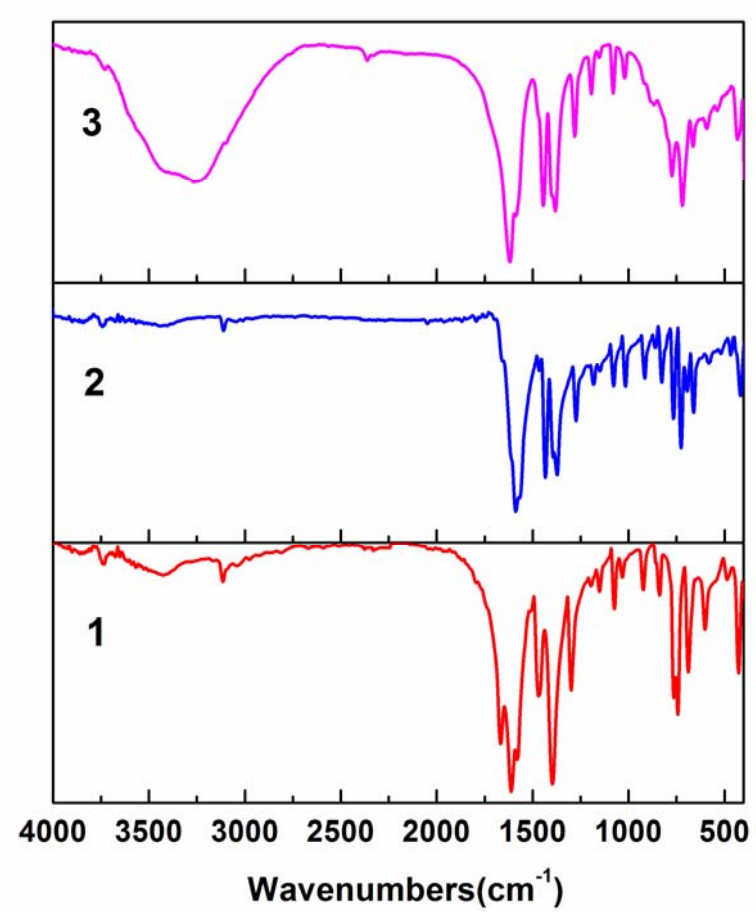

Fig. S1 The IR spectra of complexes **1**–**3**.

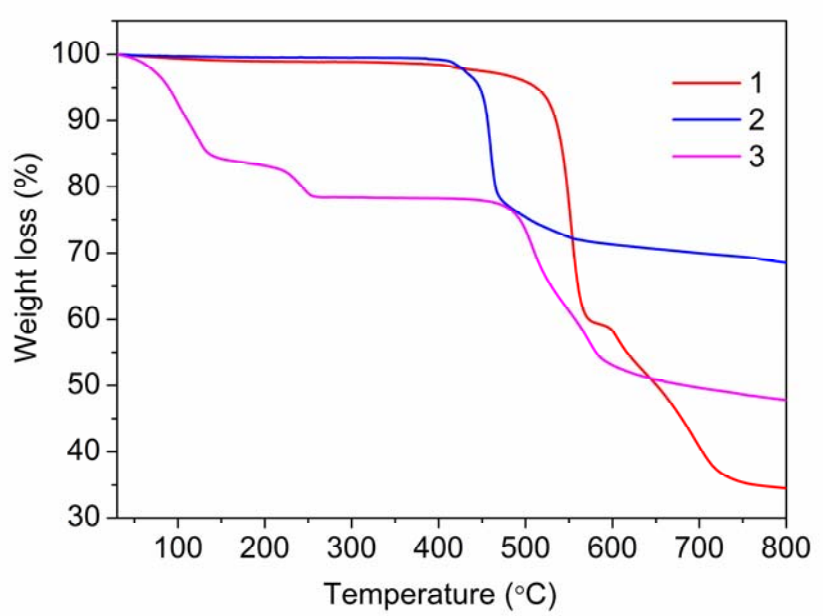

Fig. S2 TGA plots of complexes **1**–**3**.

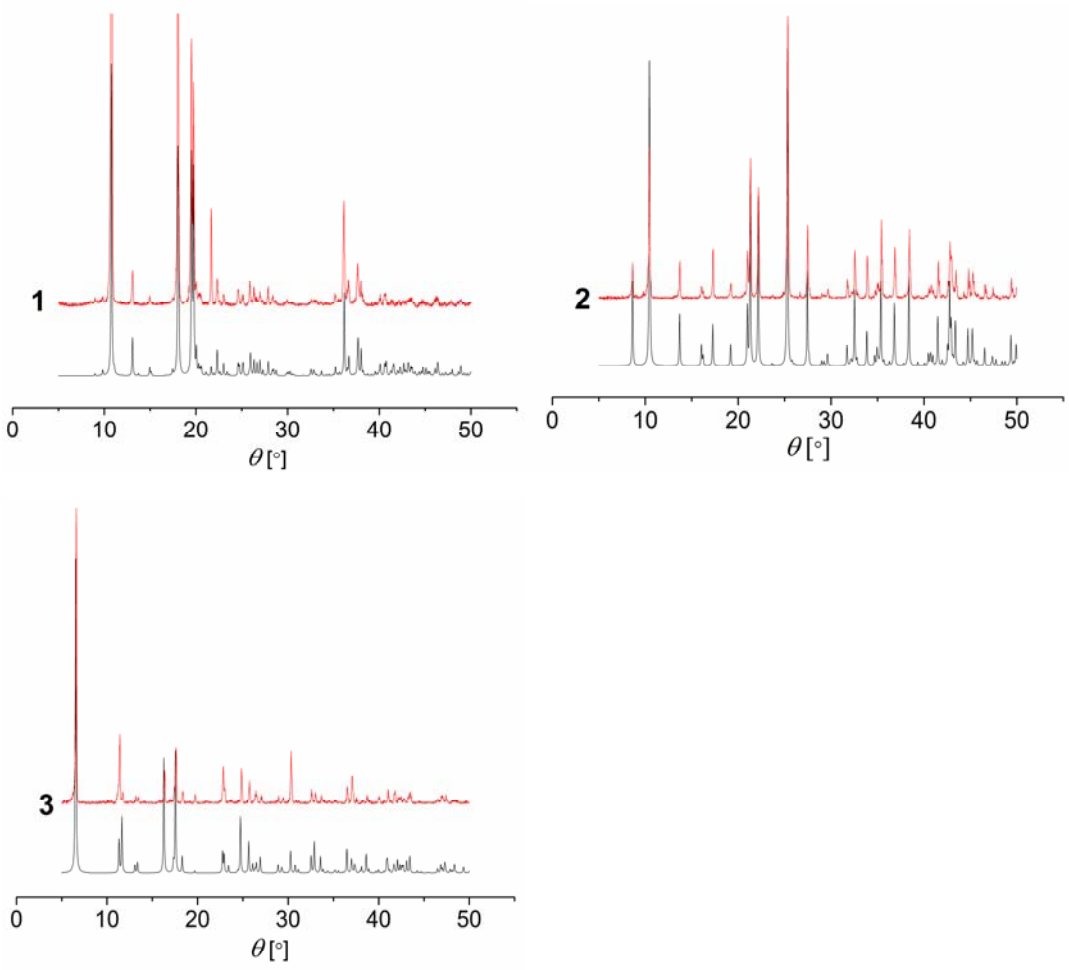

Fig. S3 PXRD patterns of complexes **1**–**3**. Down: calculated from single crystal data; Top: experimental.

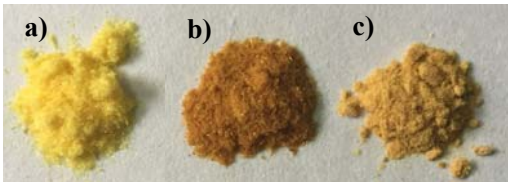

Fig. S4 Photographs of complex **3**: (a) as-synthesized crystalline samples of **3**; (b) after adsorption of iodine; c) after desorption of iodine in the ethanol solution.

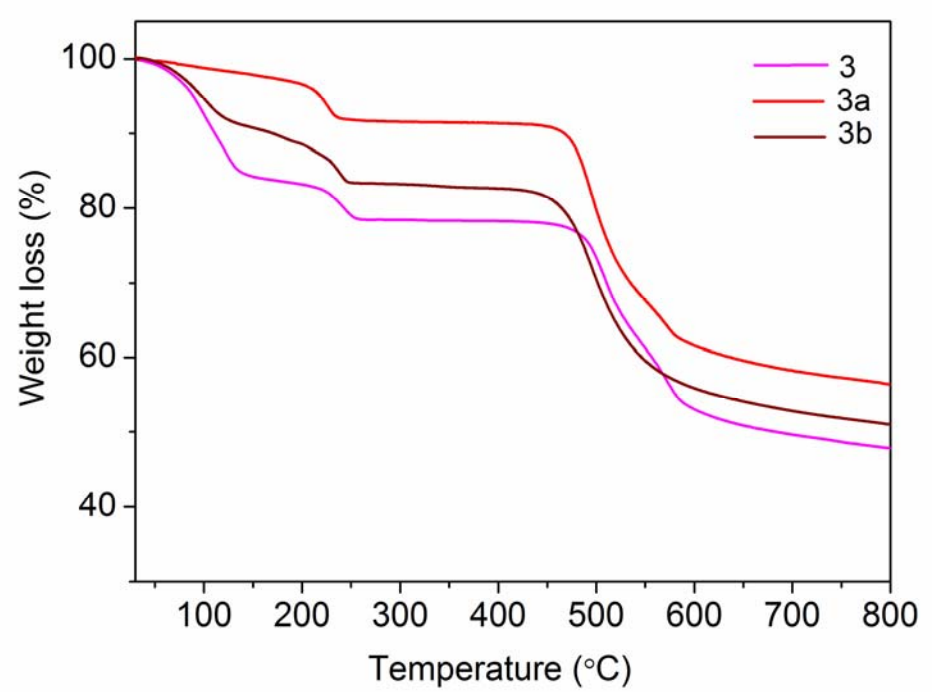

Fig. S5 Thermogravimetric analysis for **3a** shows a weight loss of 8.2% between 30 to 240 °C, which corresponds to the loss of coordinated water molecules and some adsorbed water molecules, implying the guest water molecules in the channels of **3** have been removed after heating in the vacuum oven at 140°C for 12 hours. Thermogravimetric analysis for **3b** shows a weight loss of 8.9% between 30 to 135 °C, which corresponds to the loss of iodine molecules. Upon further heating, a weight loss of 7.4% between 135 to 246 °C occurs due to the removal of coordinated water molecules.

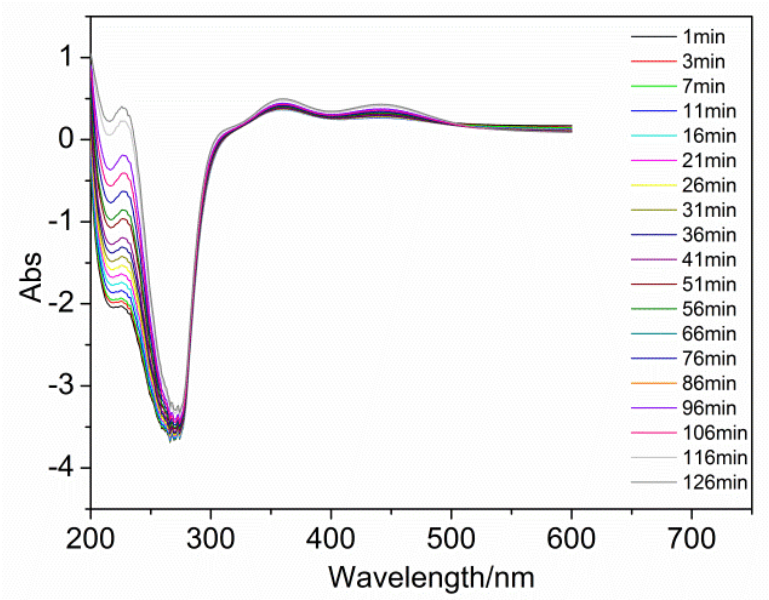

Fig. S6 UV/vis absorption spectra for the release of the I_2 into ethanol solution.

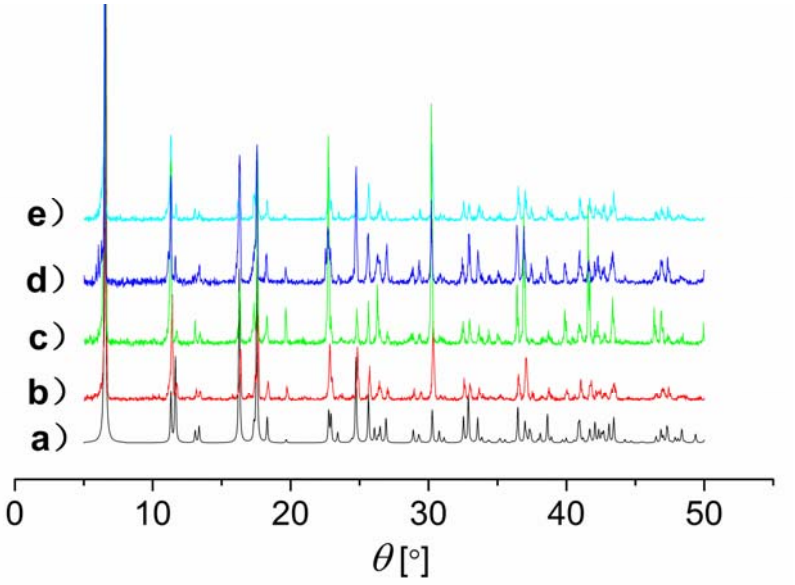

Fig. S7 PXRD patterns monitoring the adsorption and desorption of iodine for complex **3**. a) Calculated from single crystal data; b) as-synthesized bulk crystalline sample; c) after desorption of guest water molecules at 140 °C for 12 h; d) after adsorption of iodine; e) after desorption of iodine in the ethanol solution.