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Assembly of Cd(II) Coordination Polymers: Structural Variation, Supramolecular Isomers, and Temperature/Anion-induced Solvent-mediated Structural Transformations

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Supporting information

Table S**1** Selected bond lengths [Å] and angles[°] for the complexes.[a]

Complex **1**			
Cd(1)-N(6)#1	2.284(6)	Cd(1)-N(4)	2.406(7)
Cd(1)-N(6)#2	2.284(6)	Cd(1)-O(1)#3	2.413(6)
Cd(1)-N(4)#3	2.406(7)	Cd(1)-O(1)	2.413(6)
N(6)#1-Cd(1)-N(6)#2	92.0(2)	N(4)#3-Cd(1)-O(1)#3	81.4(2)
N(6)#1-Cd(1)-N(4)#3	88.0(2)	N(4)-Cd(1)-O(1)#3	89.4(2)
N(6)#2-Cd(1)-N(4)#3	88.0(2)	N(6)#1-Cd(1)-O(1)	90.6(2)
N(6)#1-Cd(1)-N(4)	92.0(2)	N(6)#2-Cd(1)-O(1)	81.4(2)
N(6)#2-Cd(1)-N(4)	180.000(1)	N(4)#3-Cd(1)-O(1)	98.6(2)
N(4)#3-Cd(1)-N(4)	90.6(2)	N(4)-Cd(1)-O(1)	180.0(3)
N(6)#1-Cd(1)-O(1)#3	89.4(2)	O(1)#3-Cd(1)-O(1)	121.6
N(6)#2-Cd(1)-O(1)#3	98.6(2)		
Complex **2**			
Cd(1)-N(6)#1	2.275(10)	Cd(1)-N(4)	2.367(10)
Cd(1)-N(12)#2	2.286(11)	Cd(1)-O(2W)	2.355(9)
Cd(1)-N(7)	2.348(10)	Cd(1)-O(1W)	2.513(9)
N(6)#1-Cd(1)-N(12)#2	165.6(4)	N(7)-Cd(1)-O(2W)	165.1(4)
N(6)#1-Cd(1)-N(7)	92.9(4)	N(4)-Cd(1)-O(2W)	93.7(3)
N(12)#2-Cd(1)-N(7)	97.3(4)	N(6)#1-Cd(1)-O(1W)	84.4(3)
N(6)#1-Cd(1)-N(4)	97.0(3)	N(12)#2-Cd(1)-O(1W)	86.1(3)
N(12)#2-Cd(1)-N(4)	91.1(4)	N(7)-Cd(1)-O(1W)	87.1(3)
N(7)-Cd(1)-N(4)	100.3(3)	N(4)-Cd(1)-O(1W)	172.3(3)
N(6)#1-Cd(1)-O(2W)	80.3(3)	O(2W)-Cd(1)-O(1W)	79.0(3)
N(12)#2-Cd(1)-O(2W)	87.3(4)		

Complex **3**			
Cd(1)-N(6)	2.272(10)	Cd(1)-N(6)	2.272(10)
Cd(1)-N(6)#1	2.272(10)	Cd(1)-N(6)#1	2.272(10)
Cd(1)-O(1W)	2.343(11)	Cd(1)-O(1W)	2.343(11)
N(6)-Cd(1)-N(6)#1	180.000(1	O(1W)-Cd(1)-N(2)#2	91.3(4)
N(6)-Cd(1)-O(1W)	84.0(4)	O(1W)#1-Cd(1)-N(2)#2	88.7(4)
N(6)#1-Cd(1)-O(1W)	96.0(4)	N(6)-Cd(1)-N(2)#3	91.7(4)
N(6)-Cd(1)-O(1W)#1	96.0(4)	N(6)#1-Cd(1)-N(2)#3	88.3(4)
N(6)#1-Cd(1)-O(1W)#1	84.0(4)	O(1W)-Cd(1)-N(2)#3	88.7(4)
O(1W)-Cd(1)-O(1W)#1	180.000(1	O(1W)#1-Cd(1)-N(2)#3	91.3(4)
N(6)-Cd(1)-N(2)#2	88.3(4)	N(2)#2-Cd(1)-N(2)#3	180.000(1)
N(6)#1-Cd(1)-N(2)#2	91.7(4)		
Complex **4**			
Cd(1)-N(1)	2.264(5)	Cd(1)-O(1W)#1	2.498(4)
Cd(1)-N(4)	2.358(5)	Cd(1)-Cl(1)	2.5490(16)
Cd(1)-O(1W)	2.464(5)	Cd(1)-Cl(1)#1	2.6396(17)
N(1)-Cd(1)-N(4)	92.70(17	O(1W)-Cd(1)-Cl(1)	79.81(11
N(1)-Cd(1)-O(1W)	90.46(16	O(1W)#1-Cd(1)-Cl(1)	95.58(11
N(4)-Cd(1)-O(1W)	85.03(17	N(1)-Cd(1)-Cl(1)#1	92.38(13
N(1)-Cd(1)-O(1W)#1	161.58(17	N(4)-Cd(1)-Cl(1)#1	102.51(14
N(4)-Cd(1)-O(1W)#1	74.91(16	O(1W)-Cd(1)-Cl(1)#1	171.80(11
O(1W)-Cd(1)-O(1W)#1	101.74(14	O(1W)#1-Cd(1)-Cl(1)	77.47(11
N(1)-Cd(1)-Cl(1)	100.17(13	Cl(1)-Cd(1)-Cl(1)#1	92.11(5)
N(4)-Cd(1)-Cl(1)	160.12(13		
Complex **5**			
Cd(1)-N(6)	2.2325(19)	Cd(1)-Cl(1)	2.4492(6)
Cd(1)-N(1)#1	2.2522(18)	Cd(1)-Cl(1)#3	2.9105(7)
Cd(1)-N(4)#2	2.3565(19)		
N(6)-Cd(1)-N(1)#1	132.40(7)	N(4)#2-Cd(1)-Cl(1)	114.89(5)
N(6)-Cd(1)-N(4)#2	95.56(7)	N(6)-Cd(1)-Cl(1)#3	84.78(5)
N(1)#1-Cd(1)-N(4)#2	82.07(7)	N(1)#1-Cd(1)-Cl(1)#3	80.82(5)
N(6)-Cd(1)-Cl(1)	110.51(5)	N(4)#2-Cd(1)-Cl(1)#3	156.94(5)
N(1)#1-Cd(1)-Cl(1)	113.45(5)	Cl(1)-Cd(1)-Cl(1)#3	86.20(2)
Complex **6**			
Cd(1)-N(6)#1	2.308(10)	Cd(1)-I(1)	3.0146(15)
Cd(1)-N(6)	2.308(10)	Cd(1)-I(1)#2	3.0530(16)
Cd(1)-I(1)#1	3.0146(15)	Cd(1)-I(1)#3	3.0530(16)
N(6)#1-Cd(1)-N(6)	180.0(6)	I(1)#1-Cd(1)-I(1)#2	90.60(5)
N(6)#1-Cd(1)-I(1)#1	90.8(3)	I(1)-Cd(1)-I(1)#2	89.40(5)
N(6)-Cd(1)-I(1)#1	89.2(3)	N(6)#1-Cd(1)-I(1)#3	90.0(3)
N(6)#1-Cd(1)-I(1)	89.2(3)	N(6)-Cd(1)-I(1)#3	90.0(3)
N(6)-Cd(1)-I(1)	90.8(3)	I(1)#1-Cd(1)-I(1)#3	89.40(5)

I(1)#1-Cd(1)-I(1)	180.00(4)	I(1)-Cd(1)-I(1)#3	90.60(5)
N(6)#1-Cd(1)-I(1)#2	90.0(3)	I(1)#2-Cd(1)-I(1)#3	180.00(4)
N(6)-Cd(1)-I(1)#2	90.0(3)	N(3)#2-Zn(2)-O(1)#4	94.4(3)
Complex **7**			
I(1)-Cd(1)	2.6901(4)	Cd(1)-N(1)#1	2.237(3)
Cd(1)-N(6)	2.222(3)	Cd(1)-N(4)#2	2.294(3)
N(6)-Cd(1)-N(1)#1	122.19(10)	N(6)-Cd(1)-I(1)	107.58(7)
N(6)-Cd(1)-N(4)#2	101.64(9)	N(1)#1-Cd(1)-I(1)	117.43(6)
N(1)#1-Cd(1)-N(4)#2	85.34(9)	N(4)#2-Cd(1)-I(1)	120.74(7)
Complex **8**			
Cd(1)-N(2)	2.3466(16)	Cd(2)-N(6)#6	2.2940(17)
Cd(1)-N(2)#1	2.3466(16)	Cd(2)-N(6)#7	2.2940(17)
Cd(1)-N(2)#2	2.3466(16)	Cd(2)-N(6)	2.2940(17)
Cd(1)-N(2)#3	2.3466(16)	Cd(2)-N(3)#8	2.3266(17)
Cd(1)-N(2)#4	2.3466(16)	Cd(2)-N(3)#9	2.3267(17)
Cd(1)-N(2)#5	2.3466(16)	Cd(2)-N(3)#10	2.3267(17)
N(2)-Cd(1)-N(2)#1	88.06(6)	N(6)#6-Cd(2)-N(6)#7	90.98(7)
N(2)-Cd(1)-N(2)#2	180.00(11)	N(6)#6-Cd(2)-N(6)	90.98(7)
N(2)#1-Cd(1)-N(2)#2	91.94(6)	N(6)#7-Cd(2)-N(6)	90.98(7)
N(2)-Cd(1)-N(2)#3	88.06(6)	N(6)#6-Cd(2)-N(3)#8	95.17(6)
N(2)#1-Cd(1)-N(2)#3	88.06(6)	N(6)#7-Cd(2)-N(3)#8	86.56(7)
N(2)#2-Cd(1)-N(2)#3	91.94(6)	N(6)-Cd(2)-N(3)#8	173.41(6)
N(2)-Cd(1)-N(2)#4	91.94(6)	N(6)#6-Cd(2)-N(3)#9	86.56(7)
N(2)#1-Cd(1)-N(2)#4	91.94(6)	N(6)#7-Cd(2)-N(3)#9	173.41(6)
N(2)#2-Cd(1)-N(2)#4	88.06(6)	N(6)-Cd(2)-N(3)#9	95.17(6)
N(2)#3-Cd(1)-N(2)#4	180	N(3)#8-Cd(2)-N(3)#9	87.57(6)
N(2)-Cd(1)-N(2)#5	91.94(6)	N(6)#6-Cd(2)-N(3)#10	173.41(6)
N(2)#1-Cd(1)-N(2)#5	180.00(5)	N(6)#7-Cd(2)-N(3)#10	95.17(6)
N(2)#2-Cd(1)-N(2)#5	88.06(6)	N(6)-Cd(2)-N(3)#10	86.56(7)
N(2)#3-Cd(1)-N(2)#5	91.94(6)	N(3)#8-Cd(2)-N(3)#10	87.57(6)
N(2)#4-Cd(1)-N(2)#5	88.06(6)	N(3)#9-Cd(2)-N(3)#10	87.57(6)

[a]Symmetry transformations used to generate equivalentatoms:#1 –x + 1, -y + 1, -z + 1, #2 x - 1, y + 1, z - 1, #3 -x, -y + 2, -z, #4 x + 1, y - 1, z + 1 for complex **1**; #1 x, y + 1, z, #2 x, -y + 3/2, z + 1/2, #3 x, y - 1, z, #4 x, -y + 3/2, z - 1/2 for complex **2**; #1 -x, -y, -z + 1, #2 –x + 1/2, y - 1/2, -z + 3/2, #3 x - 1/2, -y + 1/2, z - 1/2, #4 –x + 1/2, y + 1/2, -z + 3/2 for complex **3**; #1 x, -y + 1/2, z - 1/2, #2 x, -y + 1/2, z + 1/2, #3 –x + 2, y + 1/2, -z + 3/2, #4 –x + 2, y - 1/2, -z + 3/2 for complex **4**; #1 –x + 1, -y, -z, #2 x - 1, -y + 1/2, z - 1/2, #3 -x, -y, -z, #4 x + 1, -y + 1/2, z + 1/2 for complex **5**; #1 -x, -y, -z, #2 x - 1, y, z, #3 –x + 1, -y, -z, #4 x + 1, y, z for complex **6**. #1 –x + 1, -y, -z, #2 x - 1, -y + 1/2, z - 1/2, #3 x + 1, -y + 1/2, z + 1/2 for complex **7**, #1 –x + y, -x, z, #2 -x, -y, -z, #3 -y, x -y, z, #4 y, -x + y, -z, #5 x – y, x, - z, #6 –y + 1, x – y + 1, z, #7 –x + y, -x + 1, z, #8 –y + 1/3, x – y + 2/3, z - 1/3, #9 x + 1/3, y + 2/3, z - 1/3, #10 –x + y + 1/3, -x + 2/3, z - 1/3, #11 x - 1/3, y - 2/3, z + 1/3 for complex **8**.

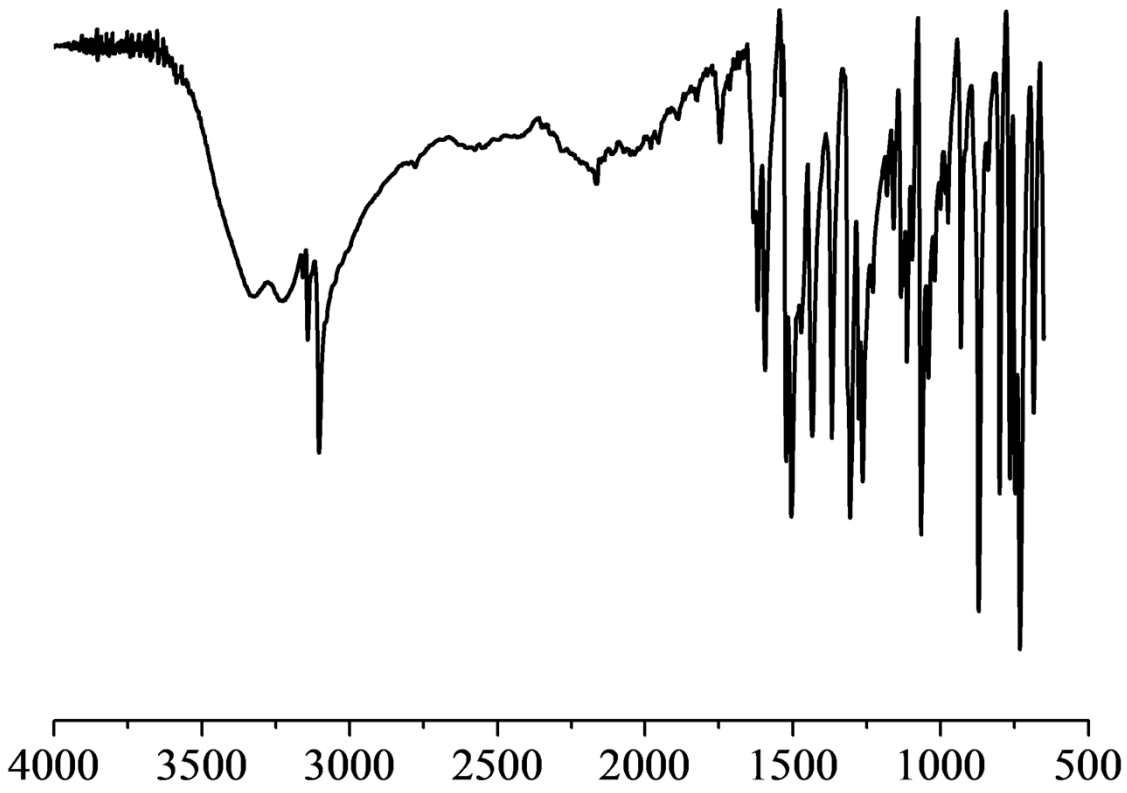

Figure S1. The IR spectrum of compound **1**.

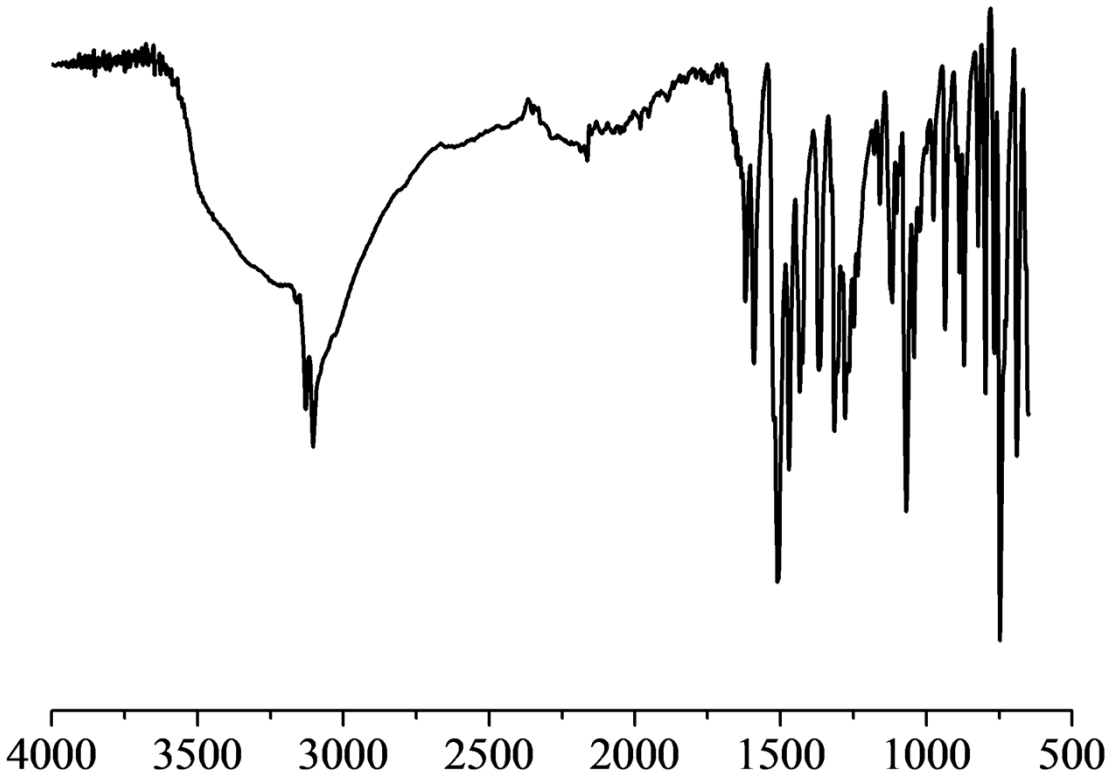

Figure S2. The IR spectrum of compound **2**.

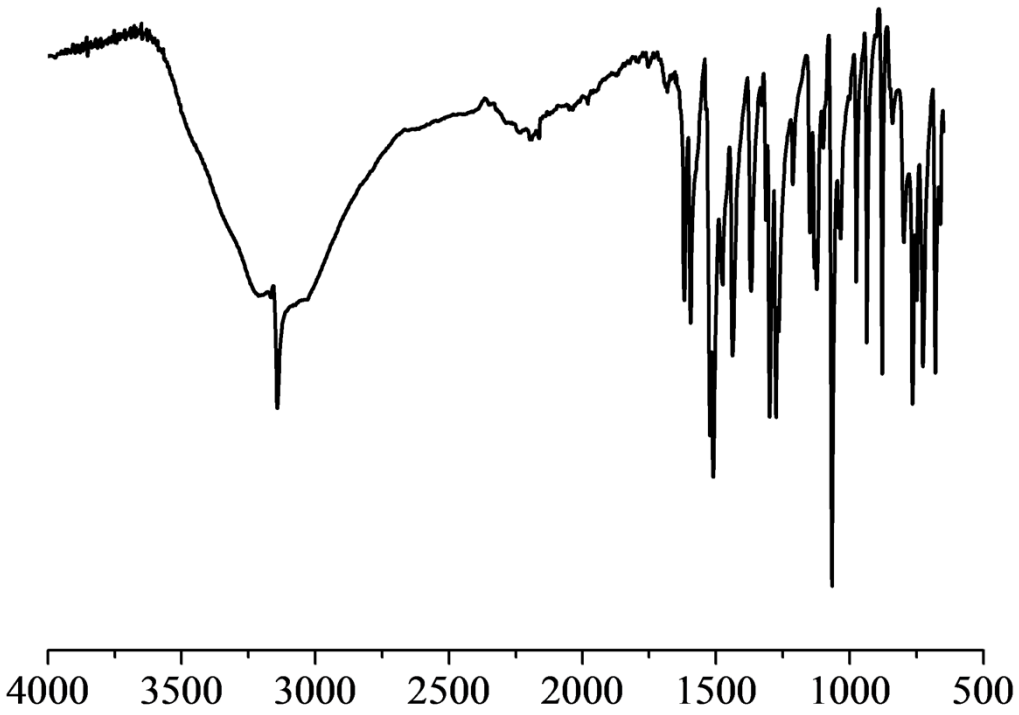

Figure S3. The IR spectrum of compound **3**.

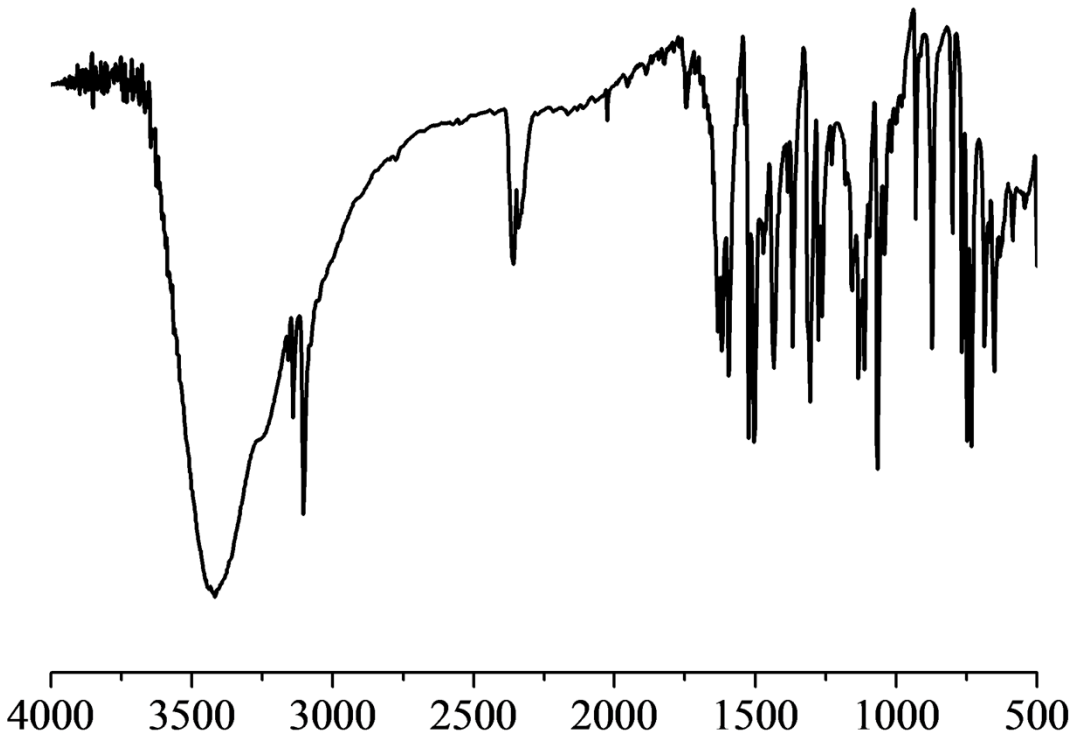

Figure S4. The IR spectrum of compound **4**.

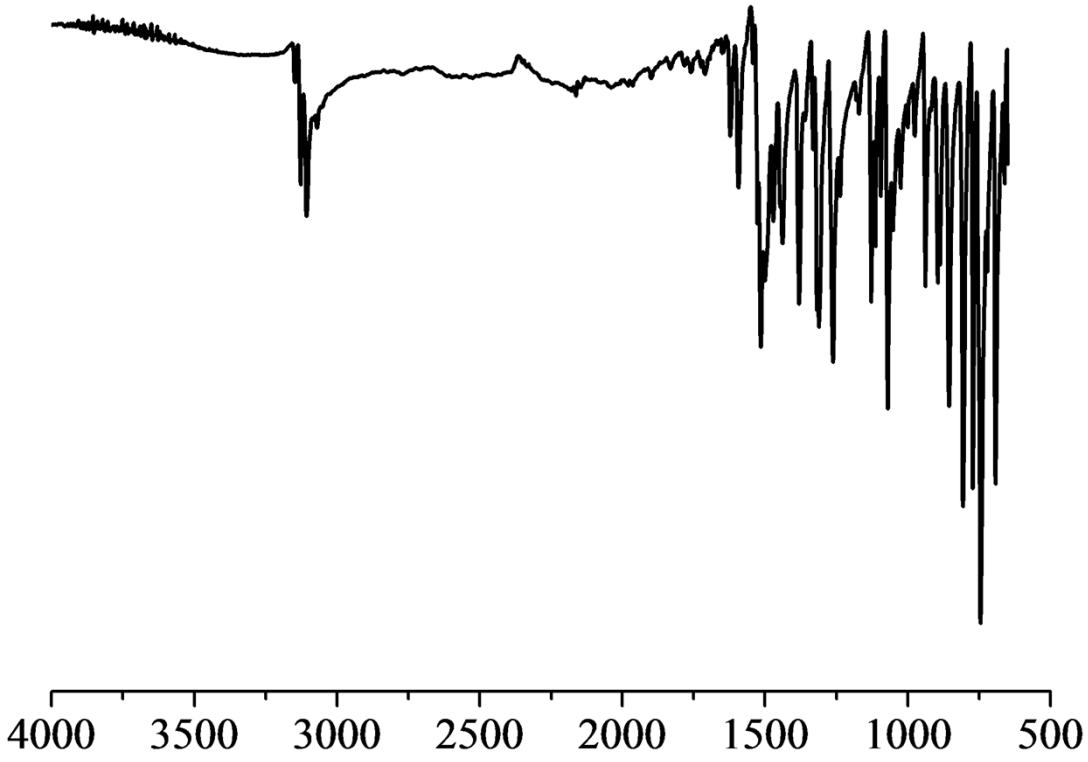

Figure S5. The IR spectrum of compound **5**.

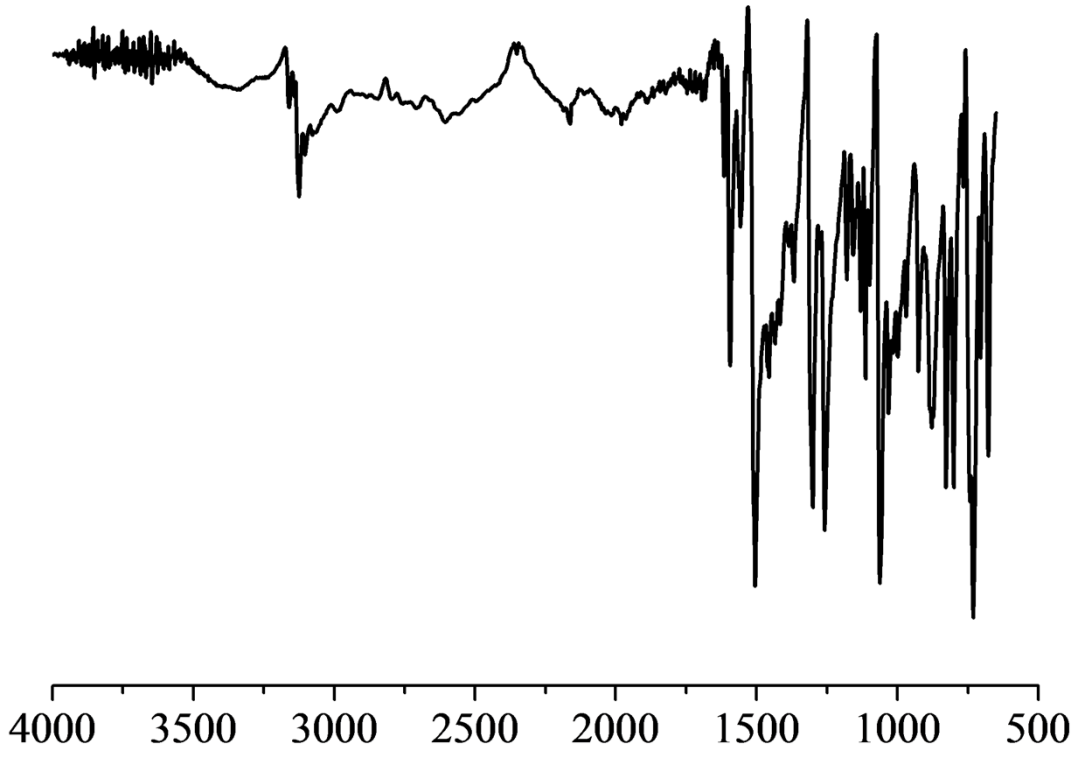

Figure S6. The IR spectrum of compound **6**.

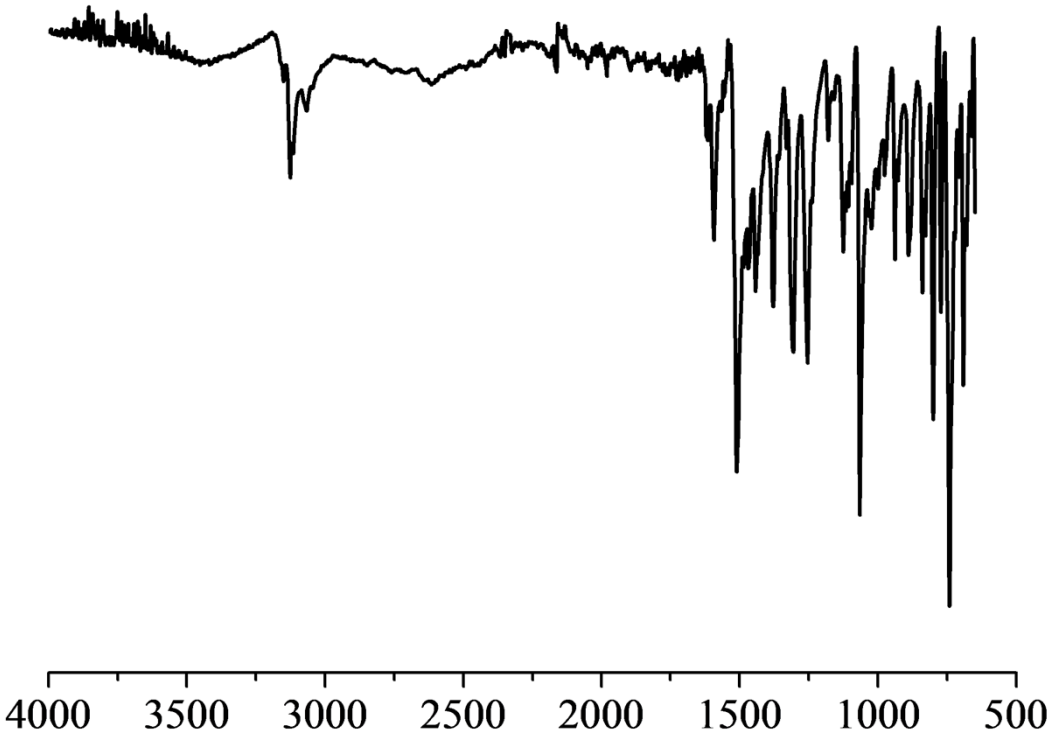

Figure S7. The IR spectrum of compound **7**.

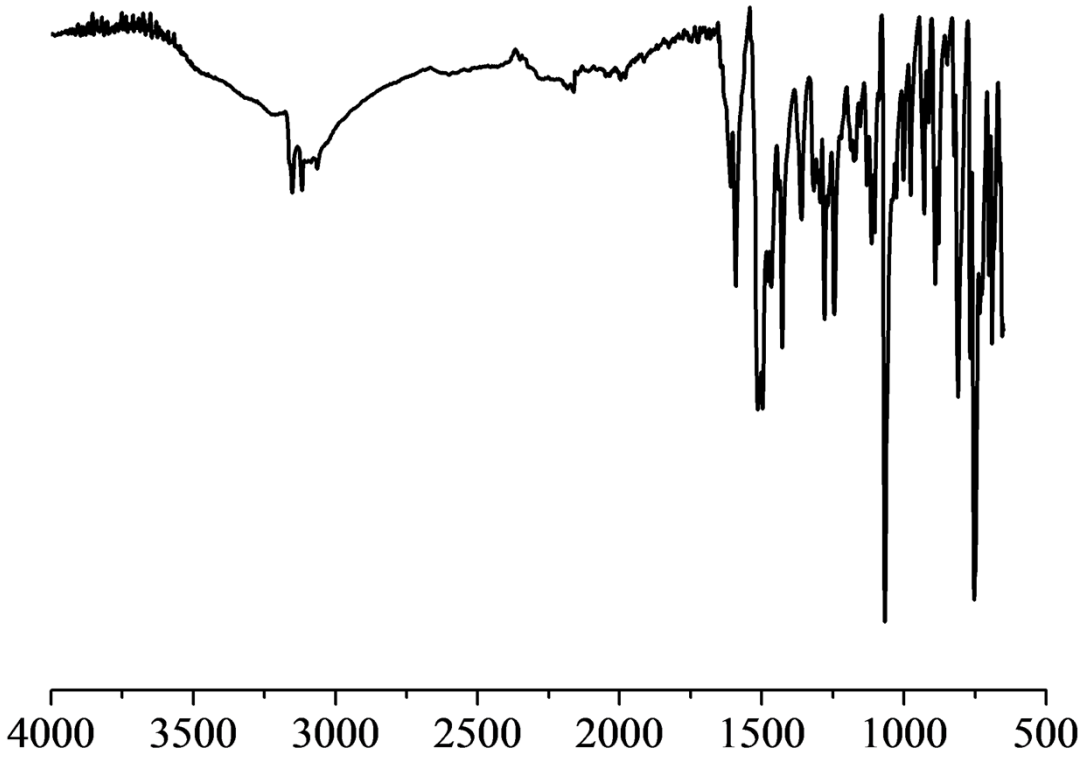

Figure S8. The IR spectrum of compound **8**.

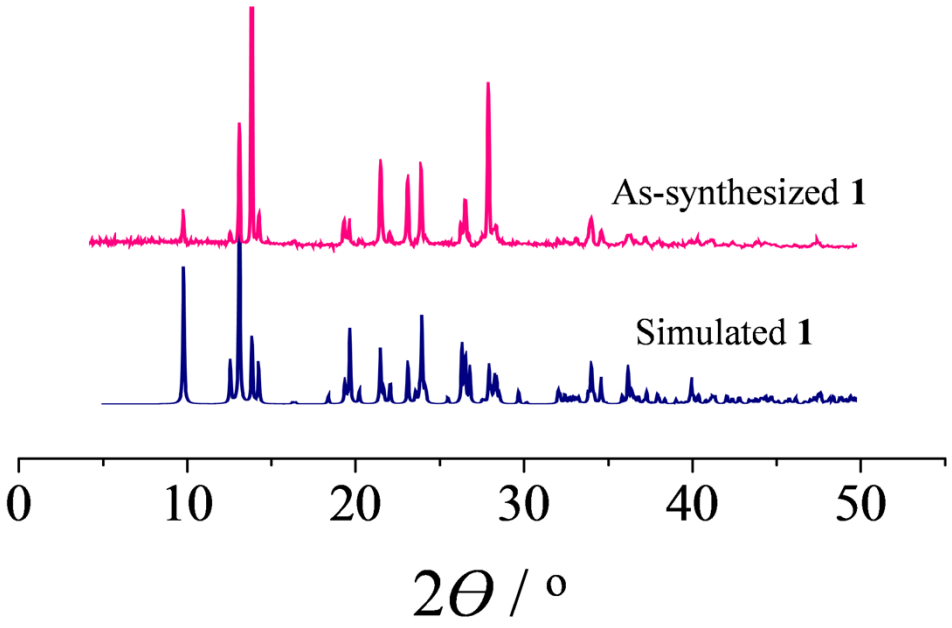

Figure S9. Powder X-ray diffraction patterns of as-synthesized **1** and simulated **1**.

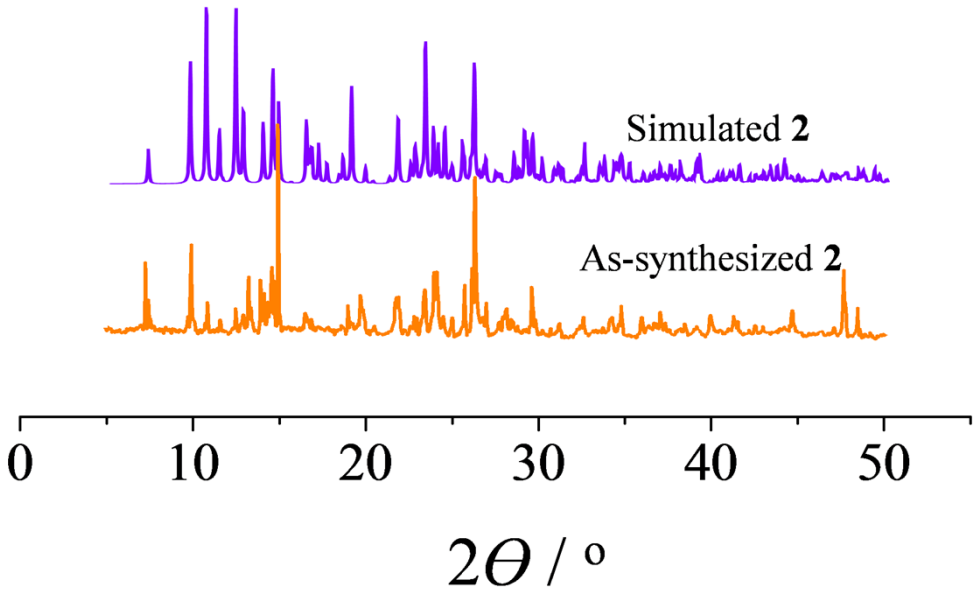

Figure S10. Powder X-ray diffraction patterns of as-synthesized **2** and simulated **2**.

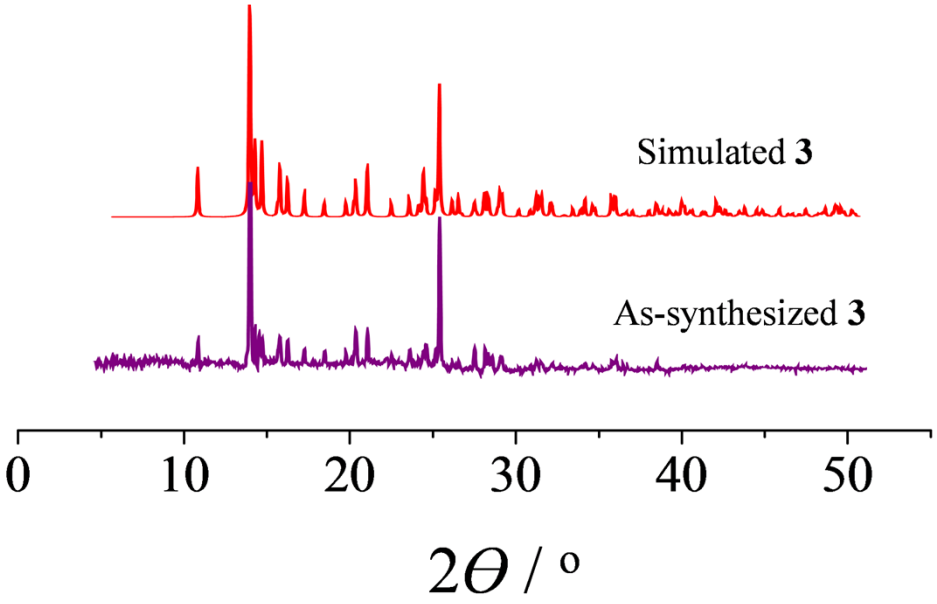

Figure S11. Powder X-ray diffraction patterns of as-synthesized **3** and simulated **3**.

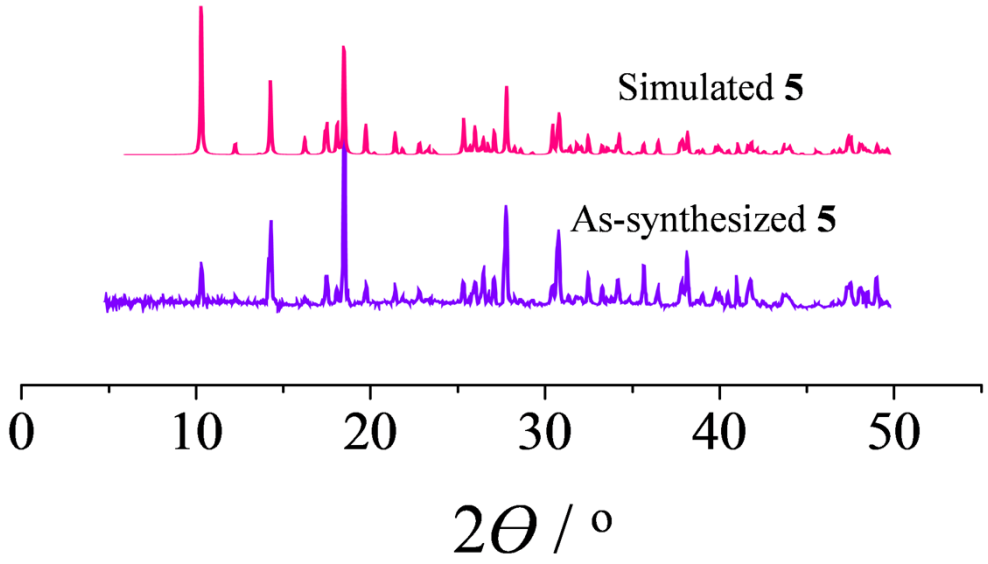

Figure S12. Powder X-ray diffraction patterns of as-synthesized **5** and simulated **5**.

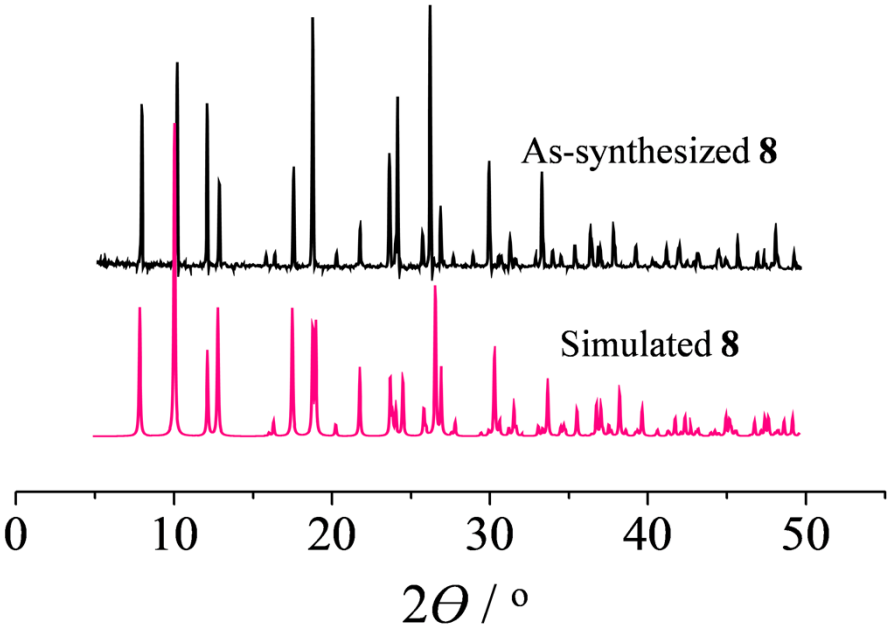

Figure S13. Powder X-ray diffraction patterns of as-synthesized **5** and simulated **5**.

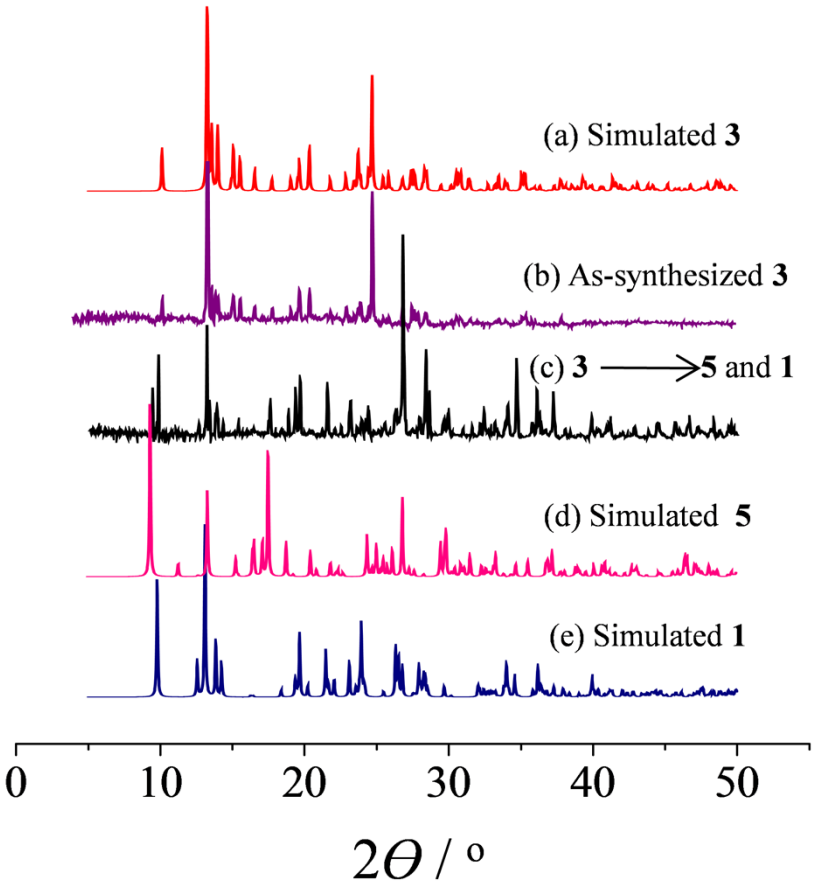

Figure S14. Powder X-ray diffraction patterns of (a) simulated **3**. (b) as-synthesized **3**. (c) after the reaction of **3** in NaCl solution at 170 ºC. (d) simulated **5**. (e) simulated **1**.

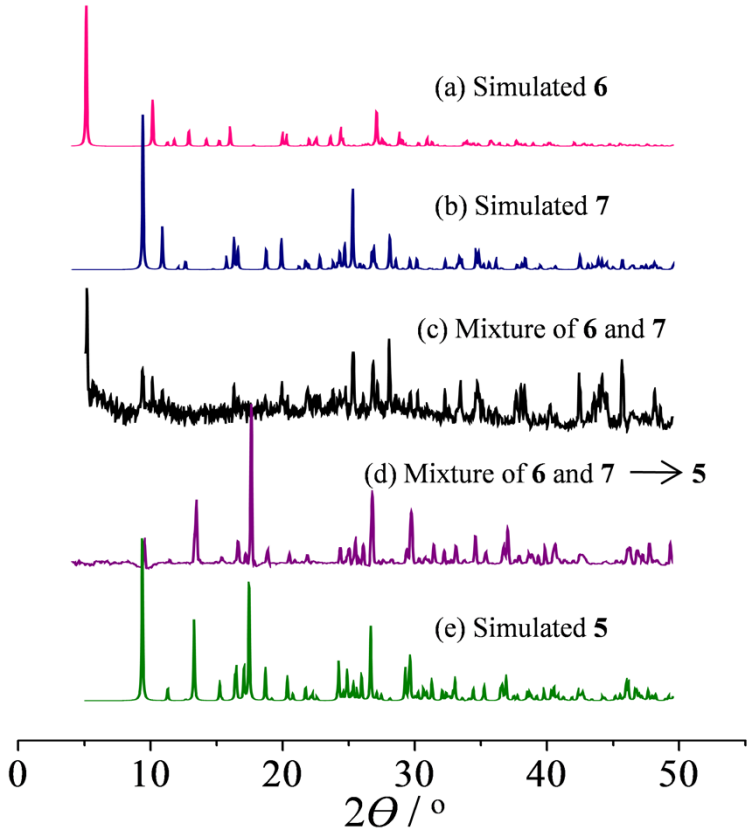

Figure S15. Powder X-ray diffraction patterns of (a) simulated **6**. (b) simulated **7**. (c) as-synthesized mixture of **6** and **7**. (d) after the reaction of mixture of **6** and **7** in NaCl solution at 170 °C. (e) simulated **5**.

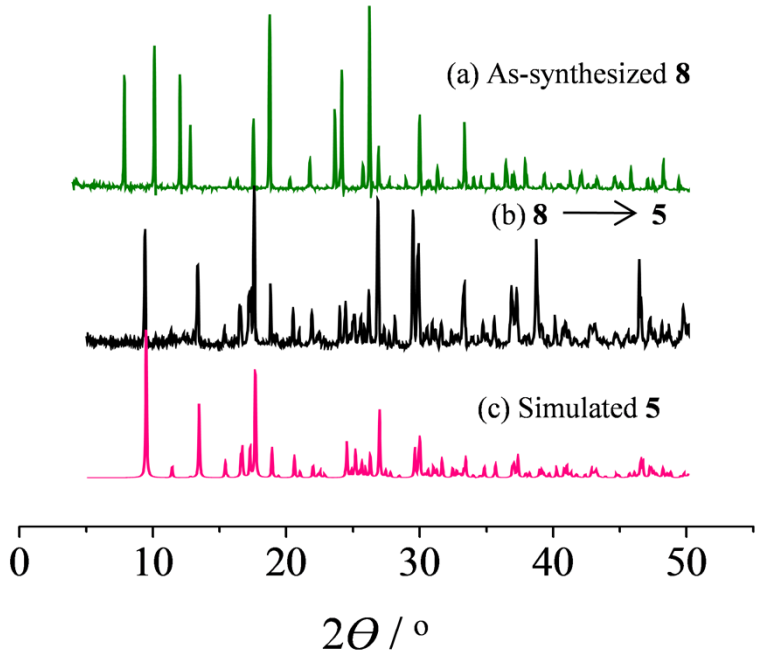

Figure S16. Powder X-ray diffraction patterns of (a) as-synthesized **8**. (d) after the reaction of **8** in NaCl solution at 170 °C. (e) simulated **5**.

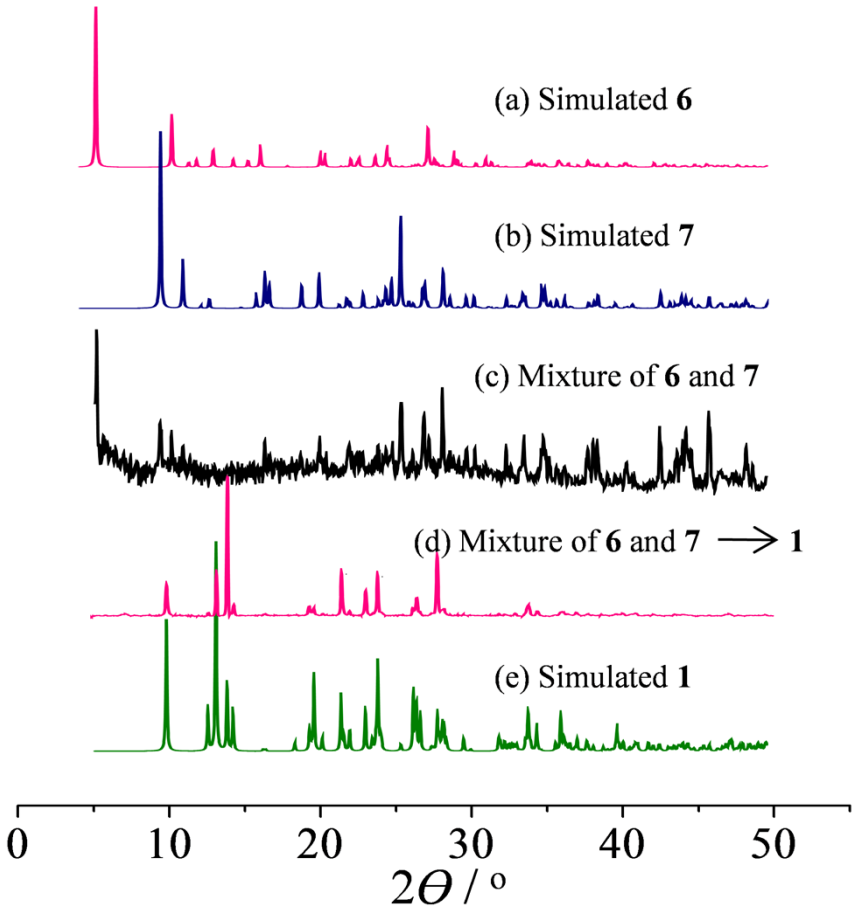

Figure S17. Powder X-ray diffraction patterns of (a) simulated **6**. (b) simulated **7**. (c) as-synthesized mixture of **6** and **7**. (d) after the reaction of mixture of **6** and **7** in water at 170 °C. (e) simulated **1**.

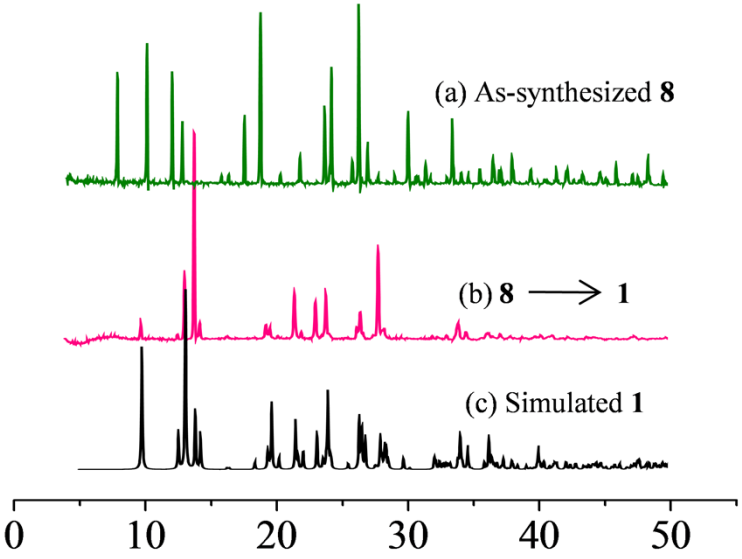

Figure S18. Powder X-ray diffraction patterns of (a) as-synthesized **8**. (d) after the reaction of **8** in water at 170 °C. (e) simulated **1**.

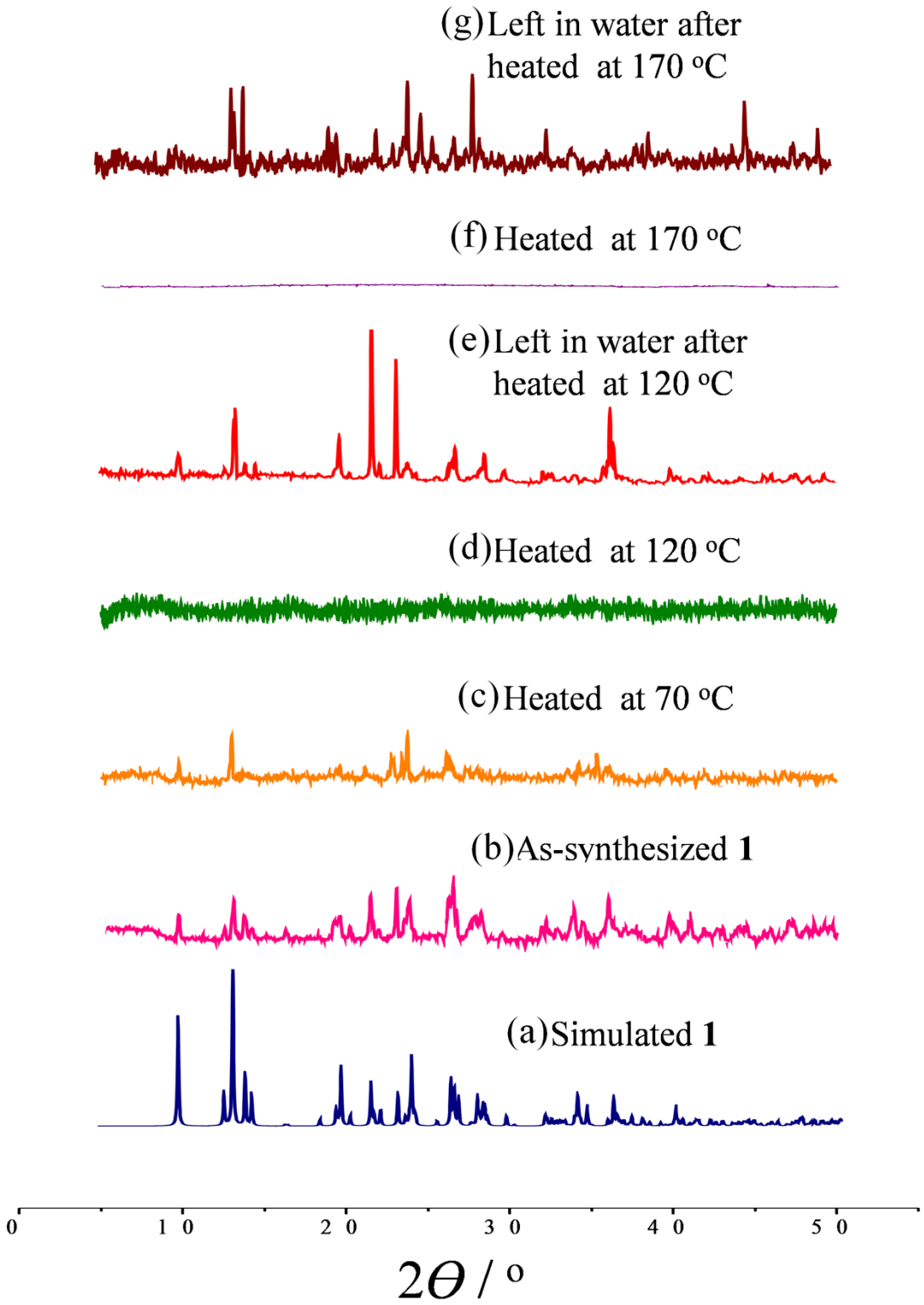

Figure S19. Powder X-ray diffraction patterns of (a) simulated **1**. (b) as-synthesized **1**. (c) heated of **1** at 70 °C. (d) heated of **1** at 120 °C. (e) left in water after heated at 120 °C. (f) heated of **1** at 170 °C. (g) left in water after heated at 170 °C.

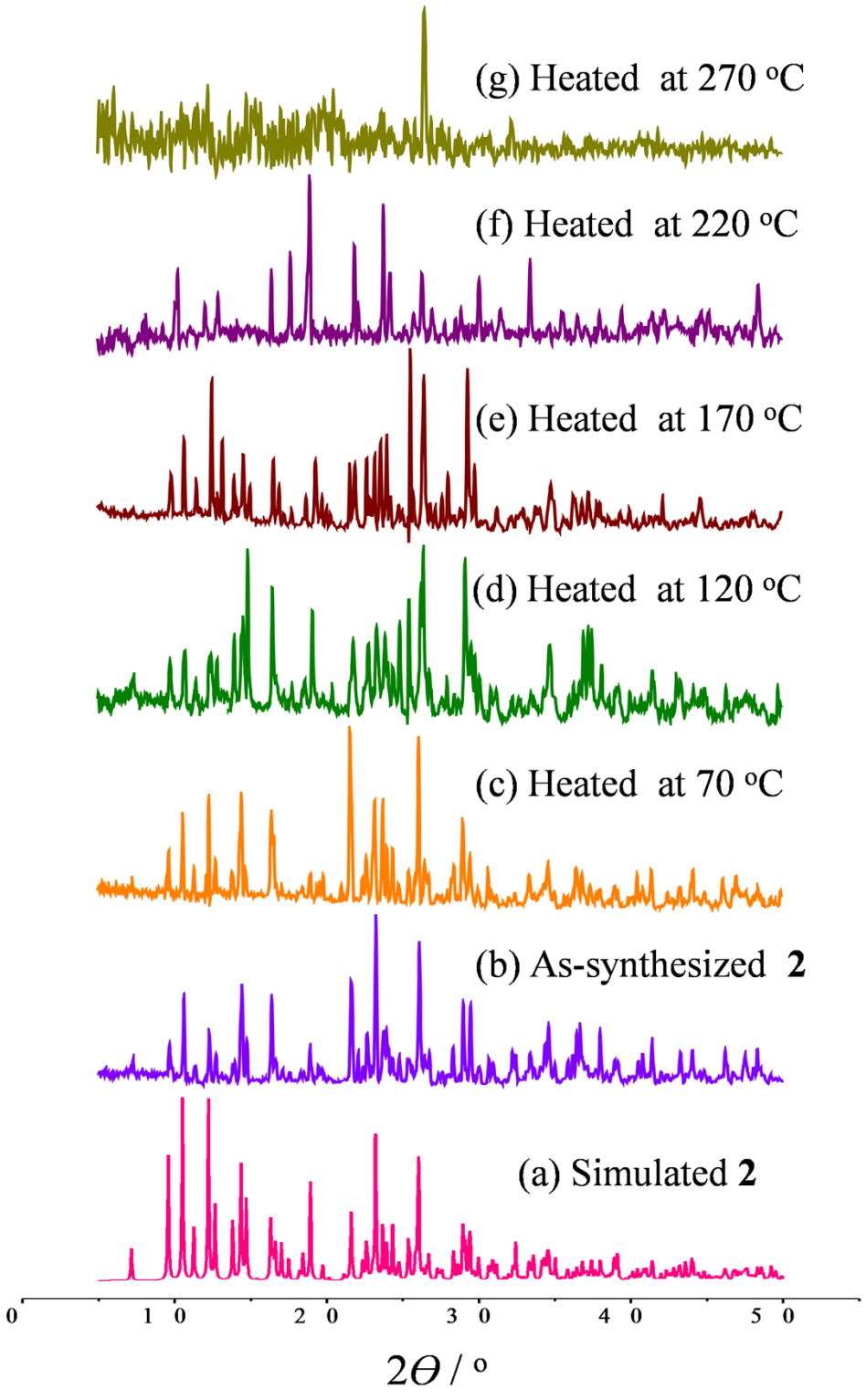

Figure S20. Powder X-ray diffraction patterns of (a) simulated **2**. (b) as-synthesized **2**. (c) heated of **2** at 70 °C. (d) heated of **2** at 120 °C. (e) heated of **2** at 170 °C. (f) heated of **1** at 220 °C. (g) heated of **1** at 270 °C.

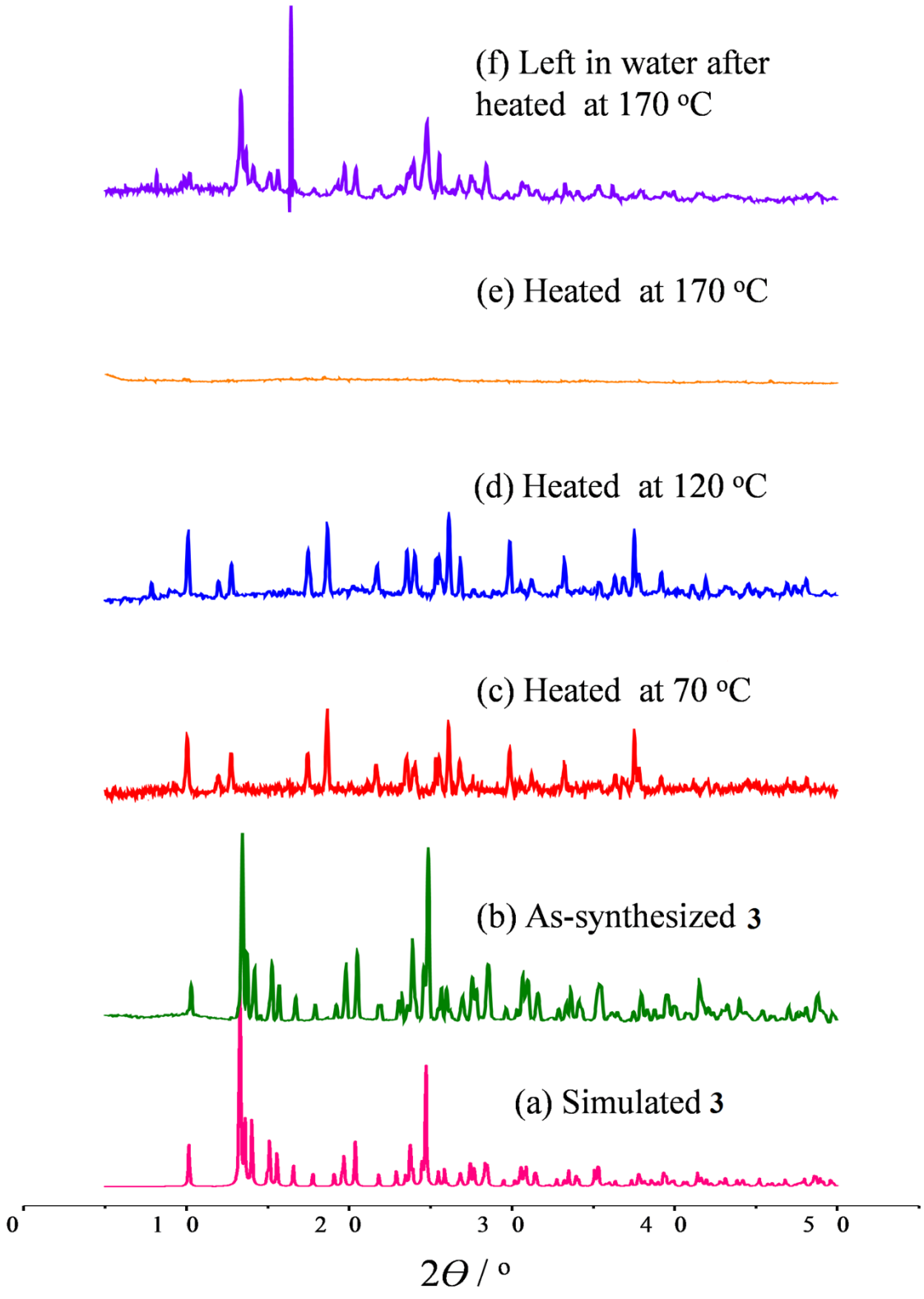

Figure S21. Powder X-ray diffraction patterns of (a) simulated **3**. (b) as-synthesized **3**. (c) heated of **3** at 70 °C. (d) heated of **3** at 120 °C. (e) heated of **1** at 170 °C. (f) left in water after heated at 170 °C.