Supporting Information for

Synthesis, Structures, and Properties of alkali and alkaline earth coordination polymers based on V-shaped ligand

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Experiments

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Synthesis of [Li_2(OBA)] (1). A reaction mixture of 4,4'-oxybisbenzoic acid ($C_{14}H_{10}O_5$, H_2OBA, 0.2582 g, 1 mmol), LiOH (0.1437 g, 6 mmol), *N*,*N*-dimethylformamide (DMF, 10.0 ml) , and H_2O (1.0 ml) was stirred for 20 min at room temperature forming a homogeneous solution with a pH value of 7.85. The solution was heated at 120 °C for 2 days. Colorless crystals of **1** were filtered off, washed with ethanol (EtOH), dried at 50 °C in an oven, and collected with the yield of 0.2218 g (82.0 %, based on the H_2OBA reagent). Elemental analysis found/calcd.: C, 62.34/62.25; H, 2.69/2.98 % for **1**. IR (KBr, cm^{-1}): 3069(s), 2961(w), 2562(w), 1913(s), 1594(s), 1547(s), 1411(s), 1256(s), 1154(s), 1100(m), 999(w), 863(s), 782(s), 708(w), 565(w), 484(s).

Synthesis of [Na_2(OBA)(H_2O)] (2). A reaction mixture of H_2OBA (0.1291 g, 0.5 mmol), NaOH (0.1200 g, 3 mmol), methanol (10.0 ml), and H_2O (1.0 ml) was stirred for 20 min at room temperature forming a homogeneous solution with a pH value of 13.41. The solution was heated at 120 °C for 2 days. Colorless crystals of **2** were filtered off, washed with EtOH, dried at 50 °C in an oven, and collected with the yield of 0.0911 g (57.0 %, based on H_2OBA). Elemental analysis found/calcd.: C, 52.44/52.51; H, 2.70/3.15 % for **2**. IR (KBr, cm^{-1}): 3258(br), 1688(w), 1594(s), 1540(s), 1400(s), 1255(s), 1147(s), 1087(m), 1005(m), 1022(w), 877(s), 796(s), 704(s), 647(w), 491(s), 430(w).

Synthesis of [K(HOBA)] (3). A reaction mixture of H_2OBA (0.1291 g, 0.5 mmol), KOH (0.0561 g, 1.0 mmol), DMF (10.0 ml), and H_2O (1.0 ml) was stirred for 20 min at room

temperature forming a homogeneous solution with a pH value of 8.10. The solution was heated at 120 °C for 2 days. Colorless crystals of **3** were filtered off, washed with EtOH, dried at 50 °C in an oven, and collected with the yield of 0.1109 g (74.9 %, based on the H_2OBA reagent). Elemental analysis found/calcd.: C, 56.74/56.94; H, 3.32/2.73 % for **3**. IR (KBr, cm^{-1}): 3720(w), 3070(s), 1919(w), 1699(s), 1601(s), 1507(s), 1330(br), 1249(s), 1100(w), 986(m), 870(s), 789(w), 687(w), 613(w), 519(s), 471(w).

Synthesis of [Rb(HOBA)] (4). A reaction mixture of H_2OBA (0.0645 g, 0.25 mmol), RbCl (0.0605 g, 0.5 mmol), DMF (10.0 ml), and H_2O (1.0 ml) was stirred for 20 min at room temperature forming a homogeneous solution with a pH value of 5.87. The solution was heated at 120 °C for 2 days. Colorless crystals of **4** were filtered off, washed with EtOH, dried at 50 °C in an oven, and collected with the yield of 0.075 g (87.5 %, based on H_2OBA). Elemental analysis found/calcd.: C, 49.16/49.21.; H, 2.93/2.36 % for **4**. IR (KBr, cm^{-1}): 3720(w), 3071(s), 1918(w), 1696(s), 1635(s), 1598(s), 1507(s), 1337(s), 1252(s), 1104(w), 986(m), 870(s), 789(w), 691(w), 687(w), 610(w), 518(s), 478(w).

Synthesis of [Cs(HOBA)] (5). A reaction mixture of H_2OBA (0.0645 g, 0.25 mmol), CsCl (0.0842 g, 0.5 mmol), DMF (10.0 ml), and H_2O (1.0 ml) was stirred for 20 min at room temperature forming a homogeneous solution with a pH value of 6.11. The solution was heated at 120 °C for 2 days. Colorless crystals of **5** were filtered off, washed with ethanol (EtOH), dried at 50 °C in an oven, and collected with the yield of 0.097 g (99.0 %, based on H_2OBA). Elemental analysis found/calcd.: C, 43.14/43.21; H, 2.53/2.07 % for **5**. IR (KBr,

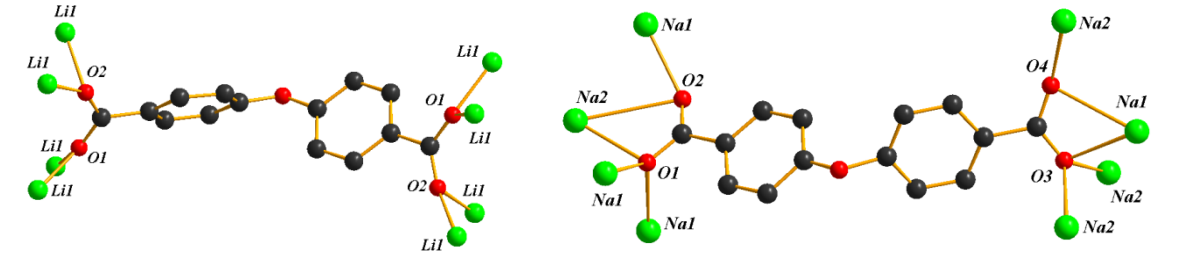
cm^{-1}): 3075(s), 2988(w), 2785(w), 2596(w), 2434(s), 2261(w), 1920(w), 1635(s), 1594(s), 1502(s), 1414(w), 1337(s), 1259(s), 1104(s), 951(br), 867(s), 782(s), 684(s), 610(w), 521(s), 481(s).

Synthesis of [Mg(OBA)$(H_2O)_2$] (6). A reaction mixture of H_2OBA (0.1032 g, 0.4 mmol), $Mg(NO_3)_2 \cdot 6H_2O$ (0.01025 g, 0.4 mmol), ethanol (EtOH, 5.0 ml) , and H_2O (1.0 ml) was stirred for 20 min at room temperature forming a homogeneous solution with a pH value of 3.58. The solution was heated at 150 °C for 2 days. Colorless crystals of **6** were filtered off, washed with EtOH, dried at 50 °C in an oven, and collected with the yield of 0.0684 g (54.0 %, based on H_2OBA). Elemental analysis found/calcd.: C, 52.98/53.12; H, 4.15/3.82 % for **6**. IR (KBr, cm^{-1}): 3614(w), 3204(b), 1598(s), 1536(s), 1410(s), 1254(s), 1159(m), 1105(w), 875(w), 786(m), 700(w), 658(w), 512(w).

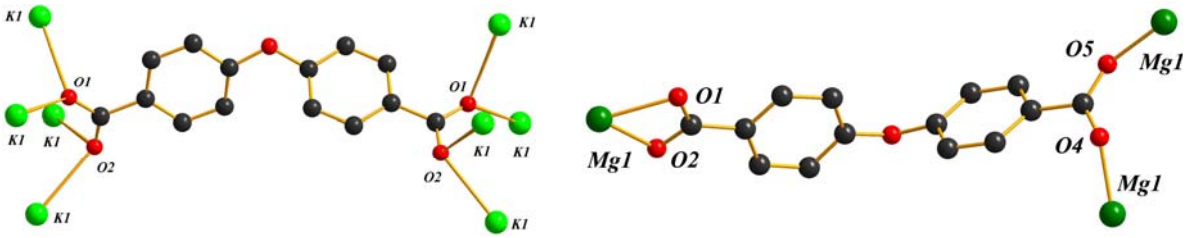
Synthesis of [Ca(OBA)(H_2O)] (7). A reaction mixture of H_2OBA (0.0516 g, 0.2 mmol), $Ca(NO_3)_2 \cdot 4H_2O$ (0.0945 g, 0.4 mmol), DMF (7.0 ml), ethanol (2.0 ml), and H_2O (1.0 ml) was stirred for 20 min at room temperature forming a homogeneous solution with a pH value of 4.41. The solution was heated at 90 °C for 2 days. Colorless crystals of **7** were filtered off, washed with EtOH, dried at 50 °C in an oven, and collected with the yield of 0.051 g (93.7 %, based on H_2OBA). Elemental analysis found/calcd.: C, 53.37/53.49; H, 3.98/3.20 % for **7**. IR (KBr, cm^{-1}): 3337(w), 1602(s), 1539(m), 1399(s), 1357(s), 1254(s), 1162(m), 1099(w), 862(w), 786(s), 697(w), 619(w), 469(w).

Synthesis of [Sr(OBA)(H_2O)] (8). A reaction mixture of H_2OBA (0.0516 g, 0.2 mmol), $Sr(NO_3)_2 \cdot 4H_2O$ (0.1692 g, 0.8 mmol), ethanol (5.0 ml), and H_2O (1.0 ml) was stirred for 20 min at room temperature forming a homogeneous solution with a pH value of 4.25. The solution was heated at 120 °C for 2 days. Colorless crystals of **8** were filtered off, washed with EtOH, dried at 50 °C in an oven, and collected with the yield of 0.063 g (87.1 %, based on H_2OBA). Elemental analysis found/calcd.: C, 46.20/46.47; H, 3.04/2.78 % for **8**. IR (KBr, cm^{-1}): 3530(m), 3176(s), 1598(s), 1532(s), 1414(s), 1254(s), 1160(m), 1094(w), 855(m), 786(m), 700(m), 655(m), 612(w), 549(w).

(a) compound **1** (b) compound **2**



(c) compound **3** (d) compound **6**



(e) compound **7** (f) compound **8**

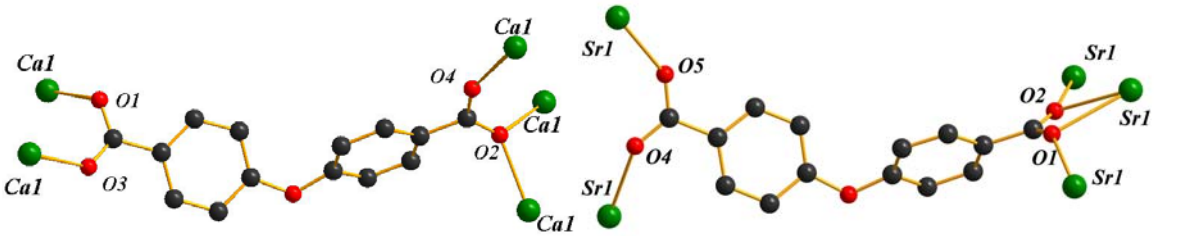
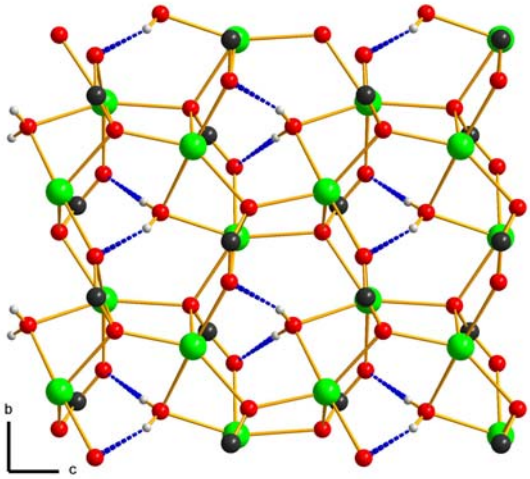
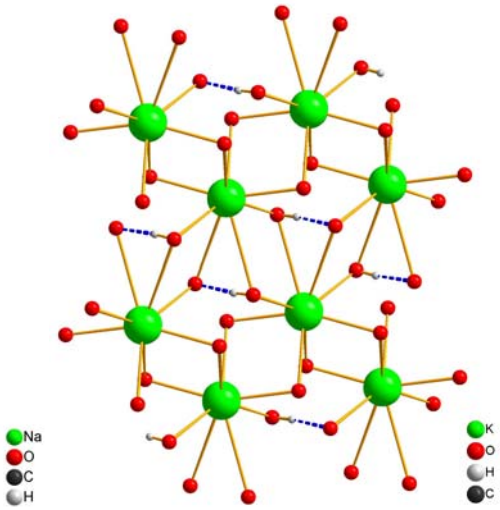


Fig. S1. The coordination models of OBA ligand in **1**–**3** and **6**–**8**.

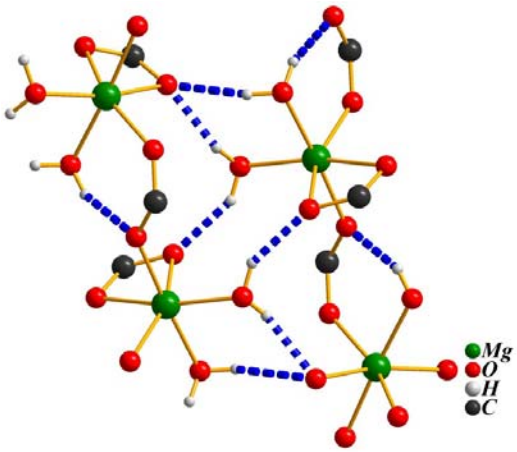
Compound (**2**)



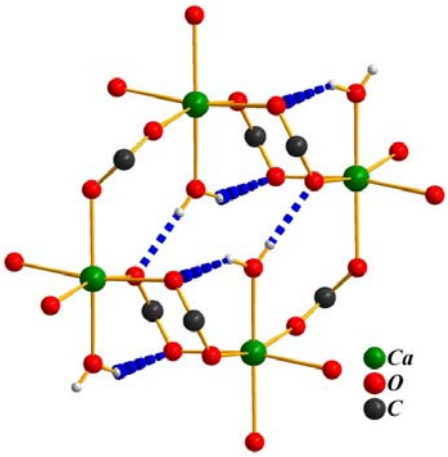
Compound (**3**)



Compound (**6**)



Compound (**7**)



Compound (**8**)

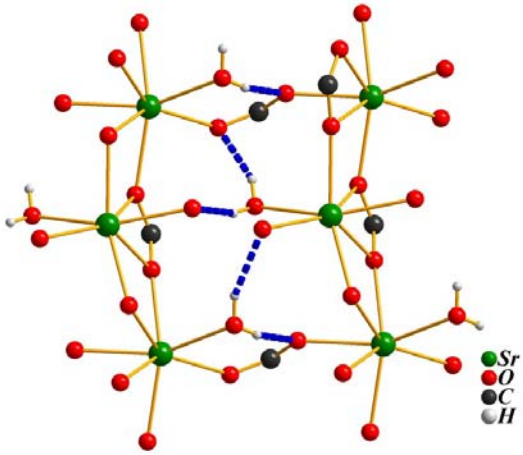
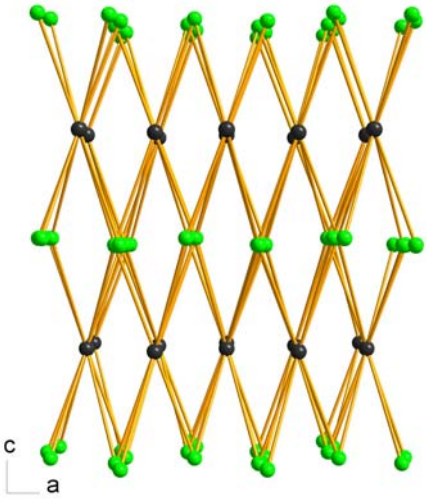
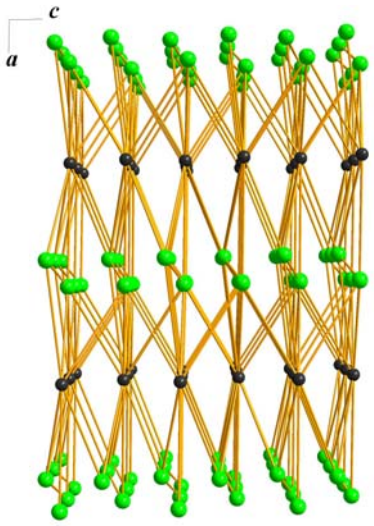


Fig. S2. The diagrams of H-nbonding interactions of **2**–**3** and **6**–**8**.

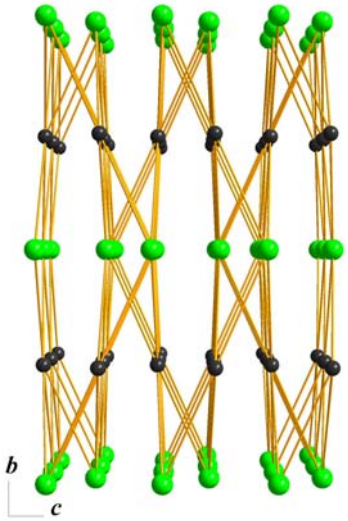
(a) Compound **1**



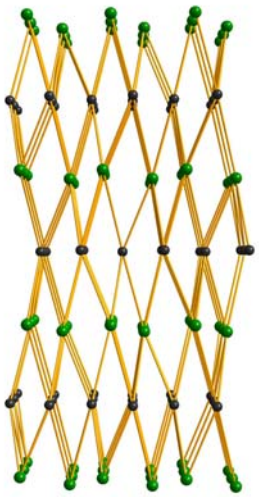
(b) Compound **2**



(a) Compound **3**



(d) Compound **7**



(e) Compound **8**

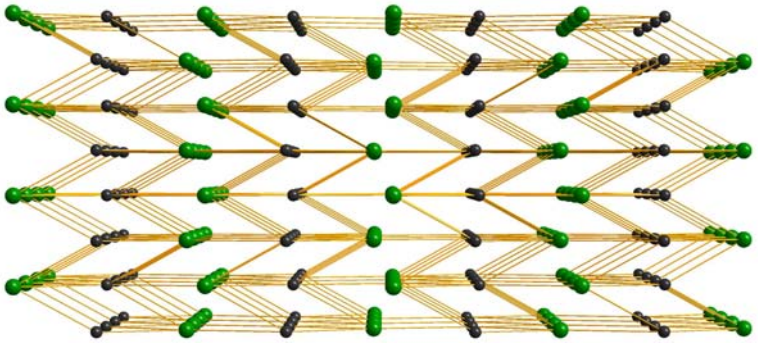


Fig. S3. The schematic descriptions of the 3D topology of **1**–**3** and **7**–**8**.

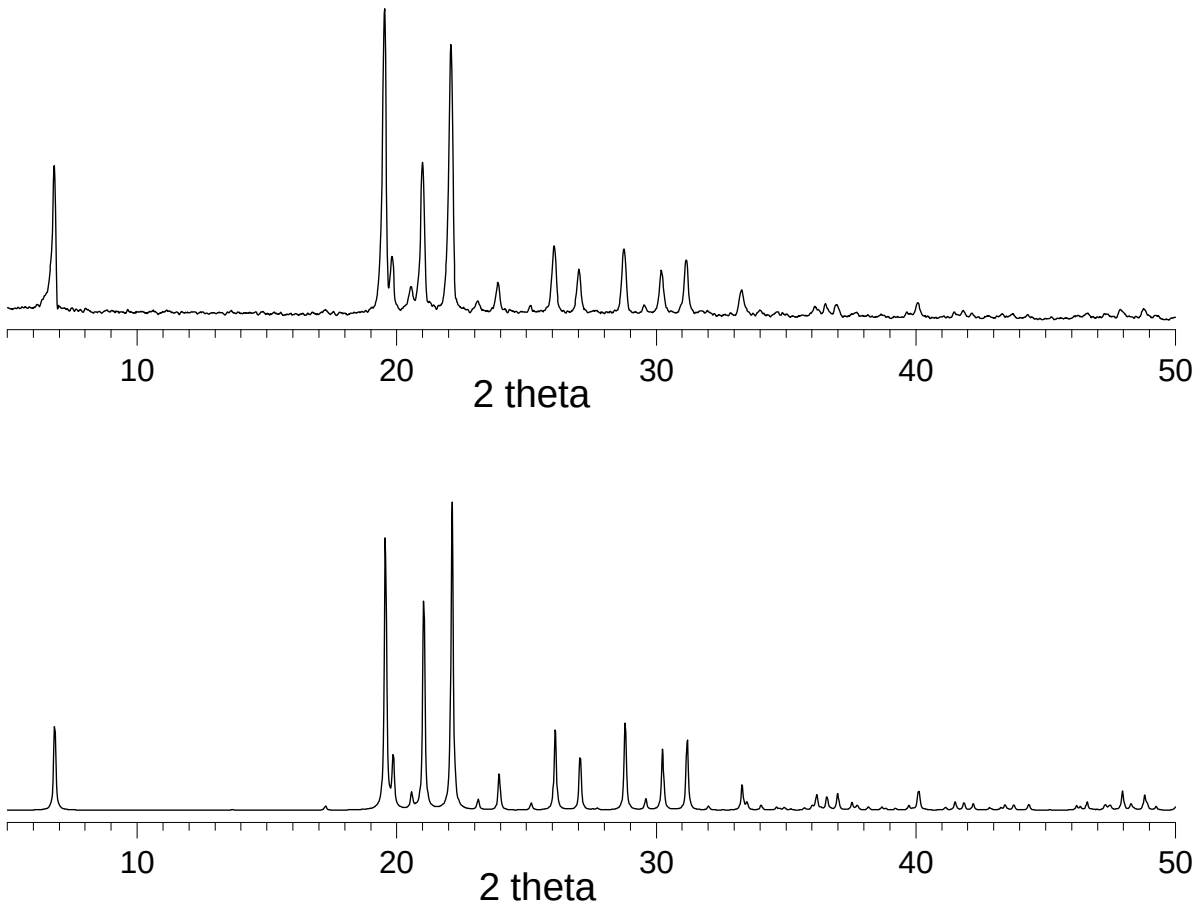


Fig. S4. Powder XRD patterns of **1** (measured, top; calculated, bottom).

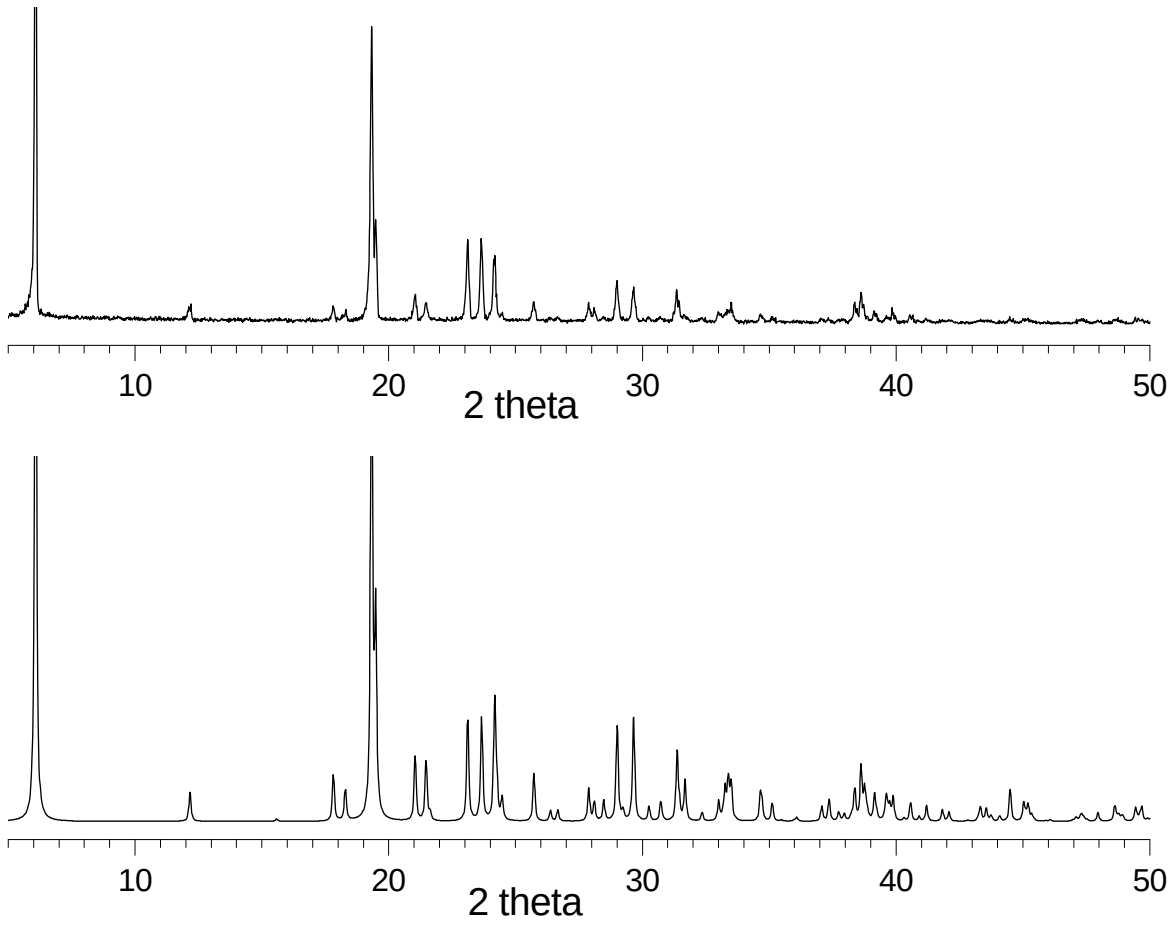


Fig. S5. Powder XRD patterns of **2** (measured, top; calculated, bottom).

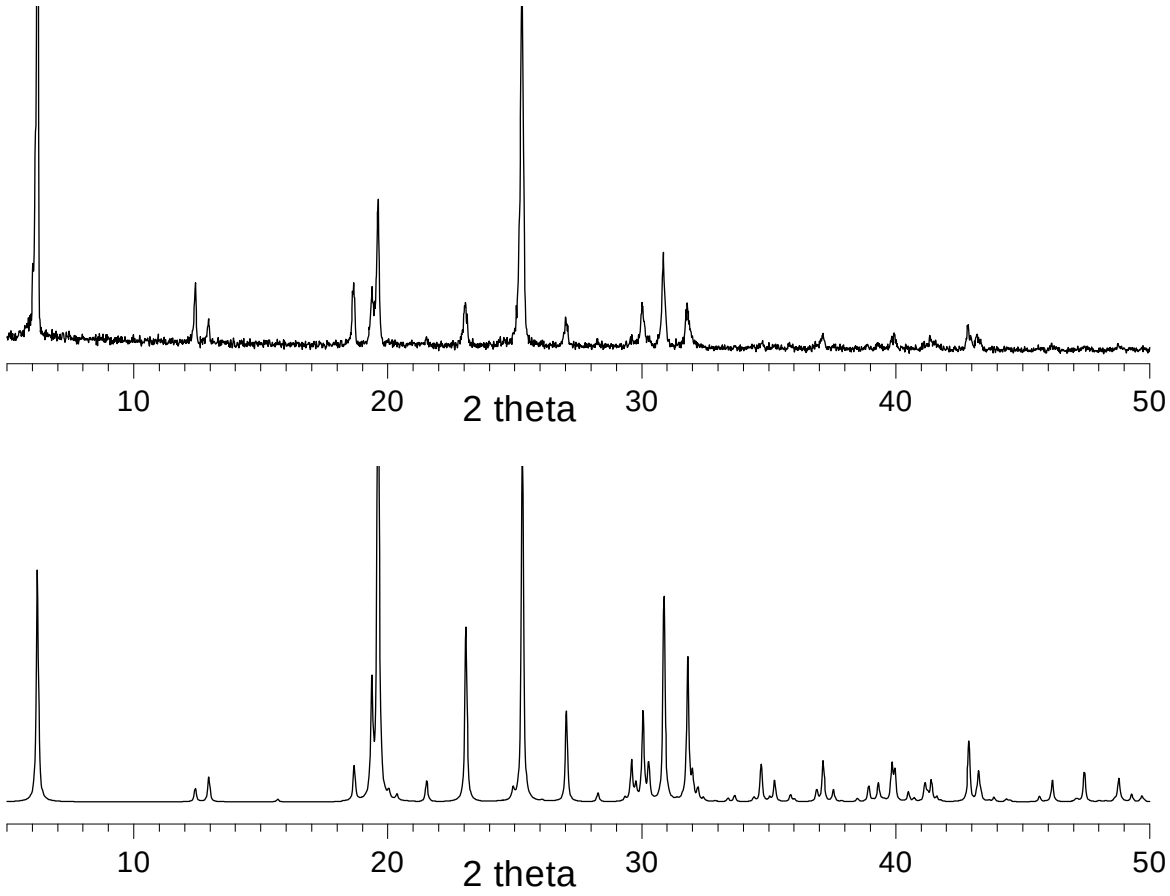


Fig. S6. Powder XRD patterns of **3** (measured, top; calculated, bottom).

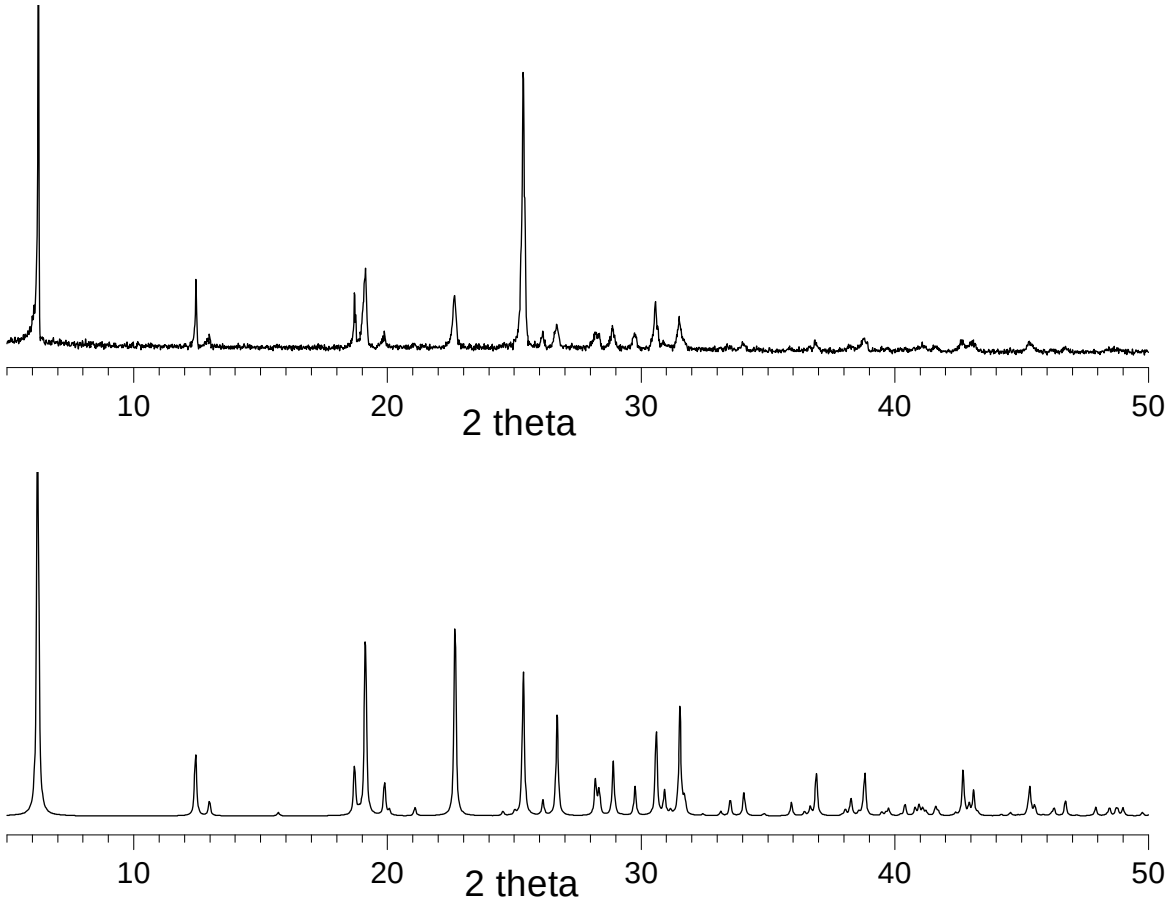


Fig. S7. Powder XRD patterns of **4** (measured, top; calculated, bottom).

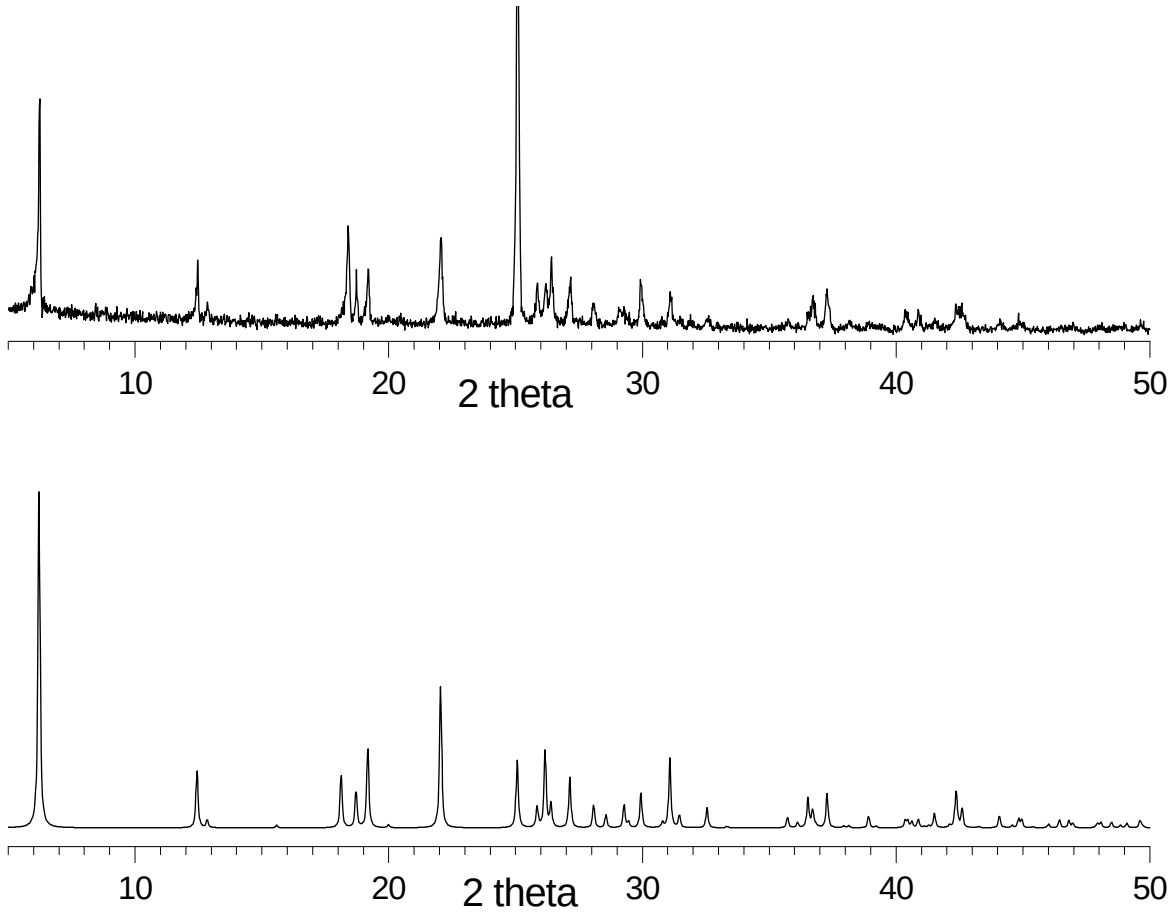


Fig. S8. Powder XRD patterns of **5** (measured, top; calculated, bottom).

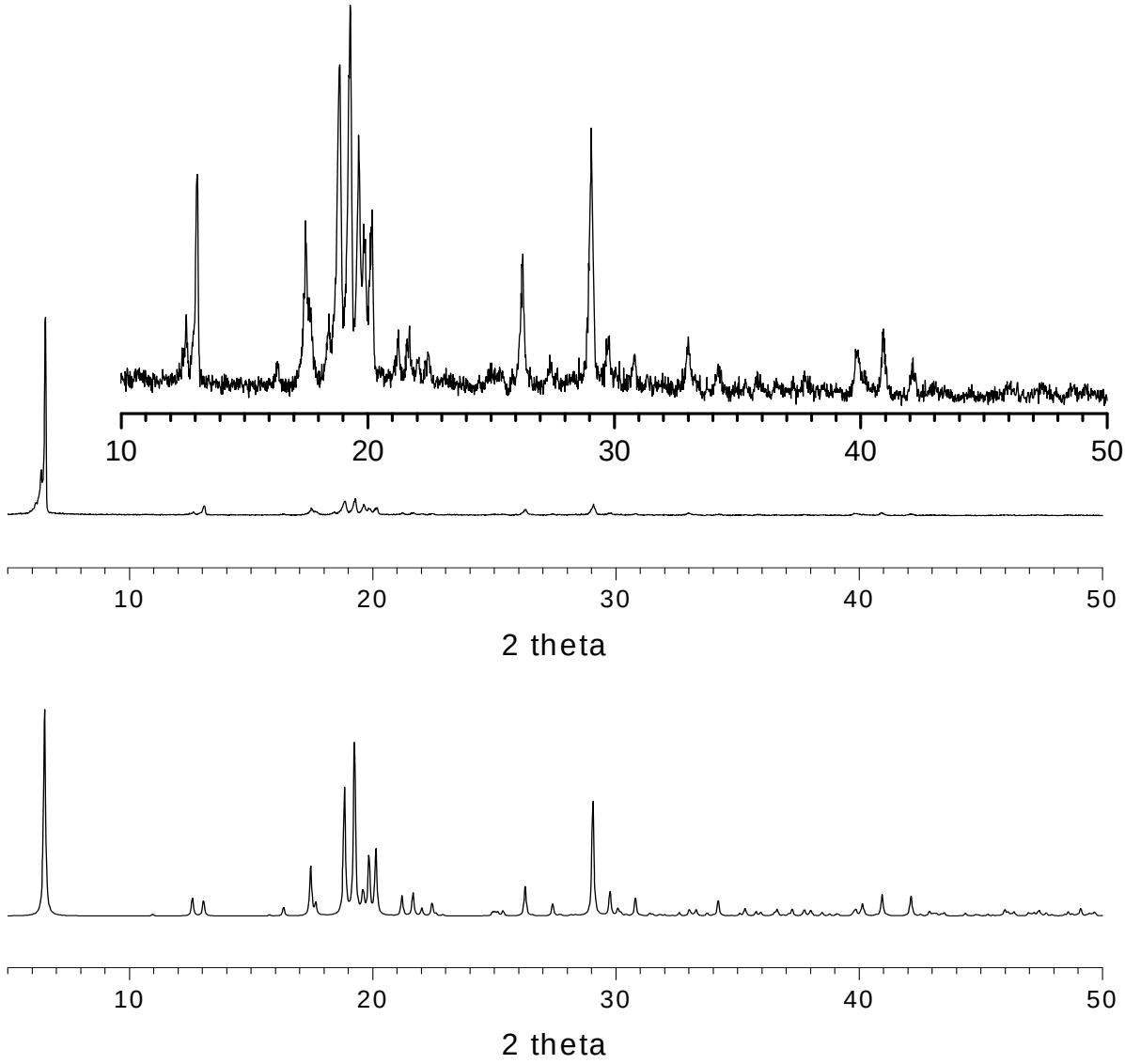


Fig. S9. Powder XRD patterns of **6** (measured, top; calculated, bottom).

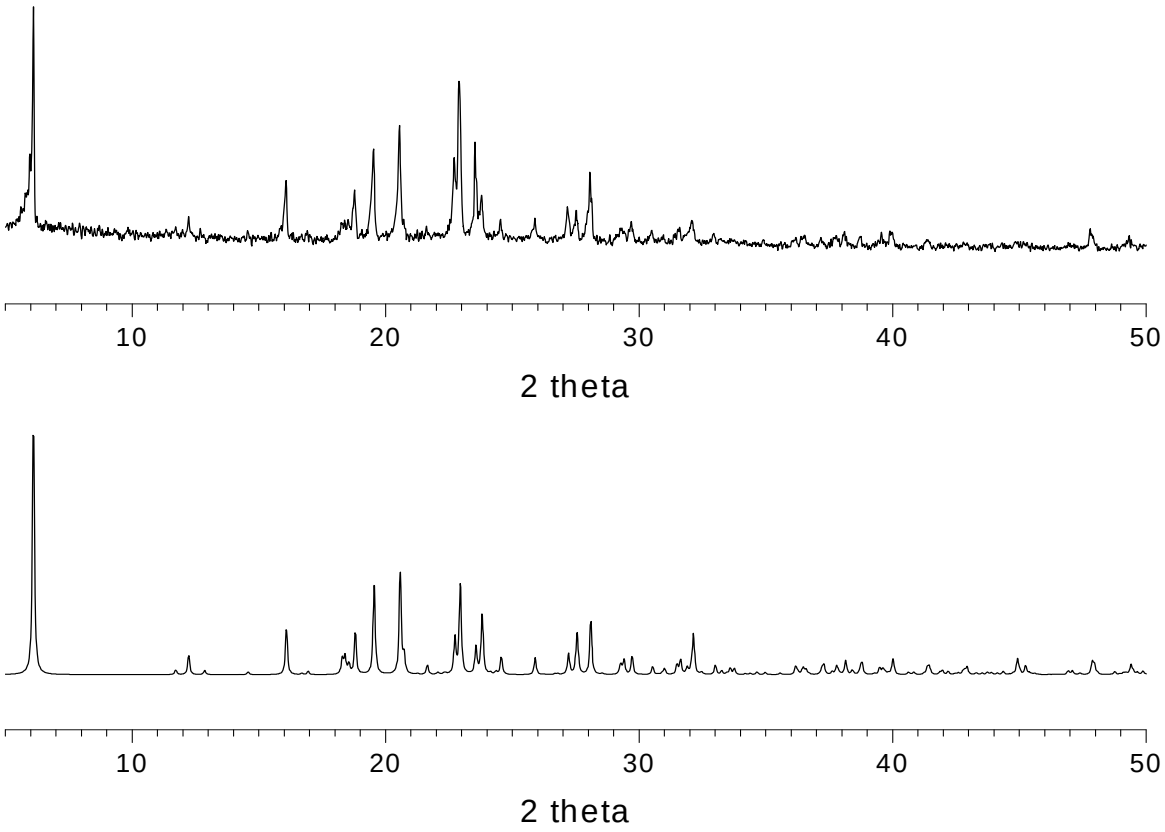


Fig. S10. Powder XRD patterns of **7** (measured, top; calculated, bottom).

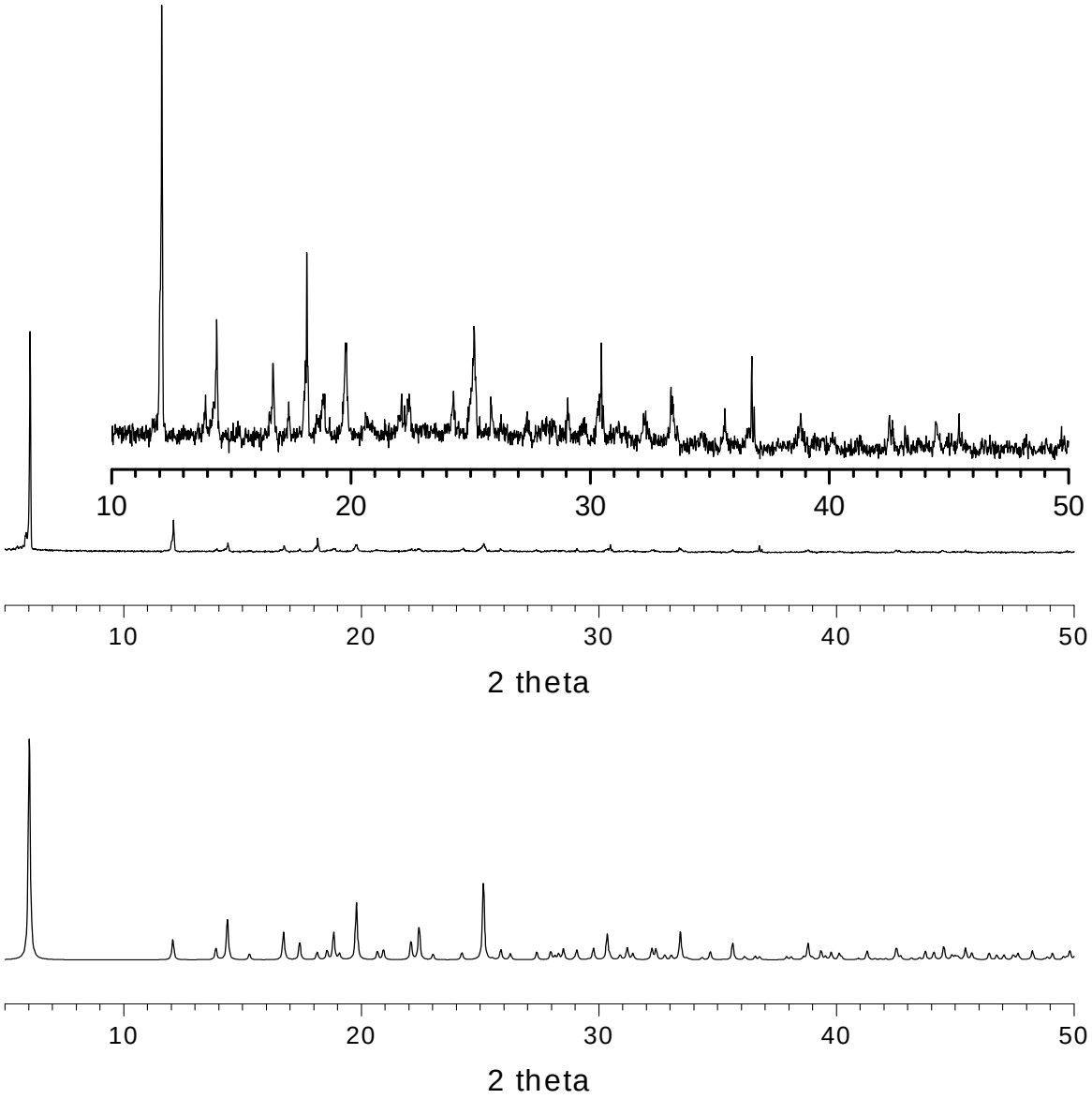
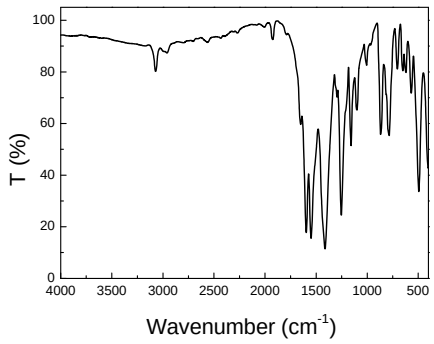
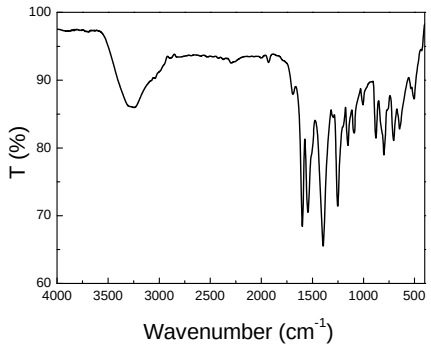


Fig. S11. Powder XRD patterns of **8** (measured, top; calculated, bottom).

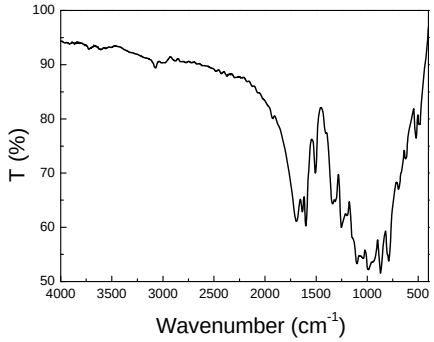
(a) compound **1**



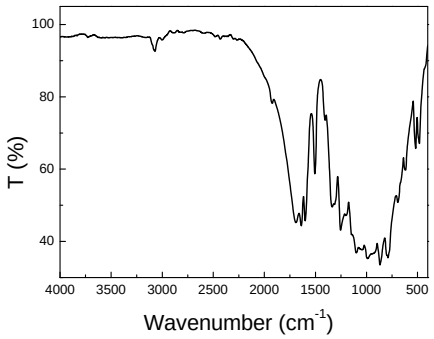
(b) compound **2**



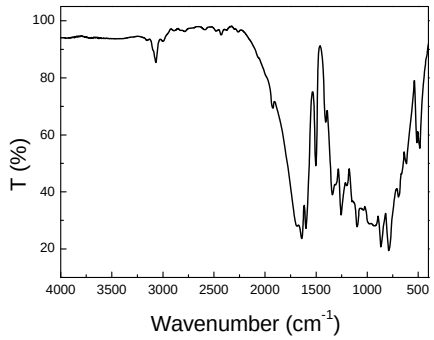
(c) compound **3**



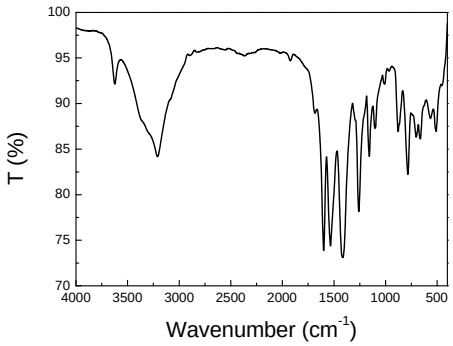
(d) compound **4**



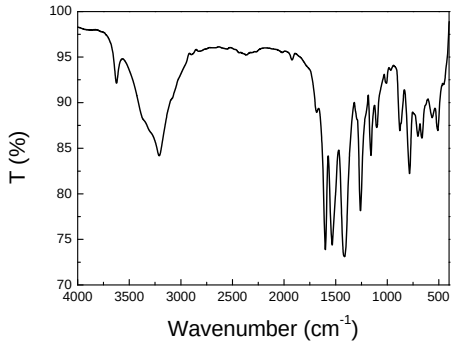
(e) compound **5**



(f) compound **6**



(g) compound **7**



(h) compound **8**

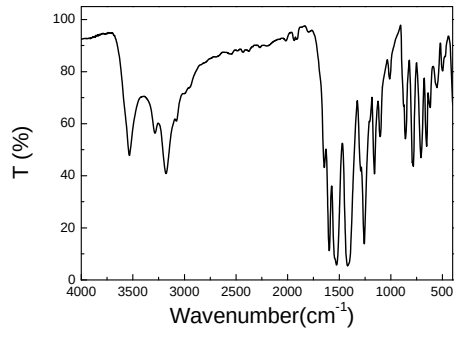
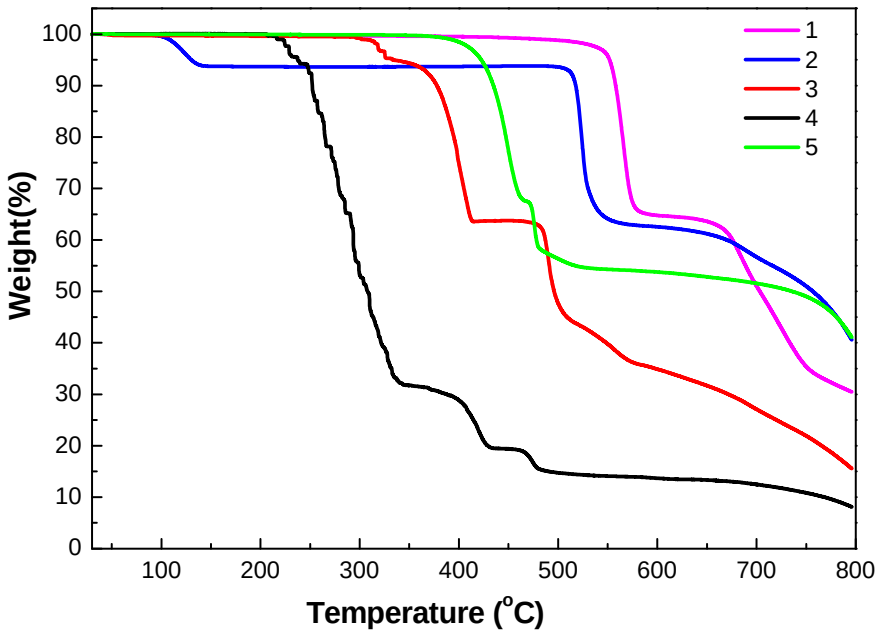


Fig. S12. FT-IR spectra of **1**–**8**.

(a)



(b)

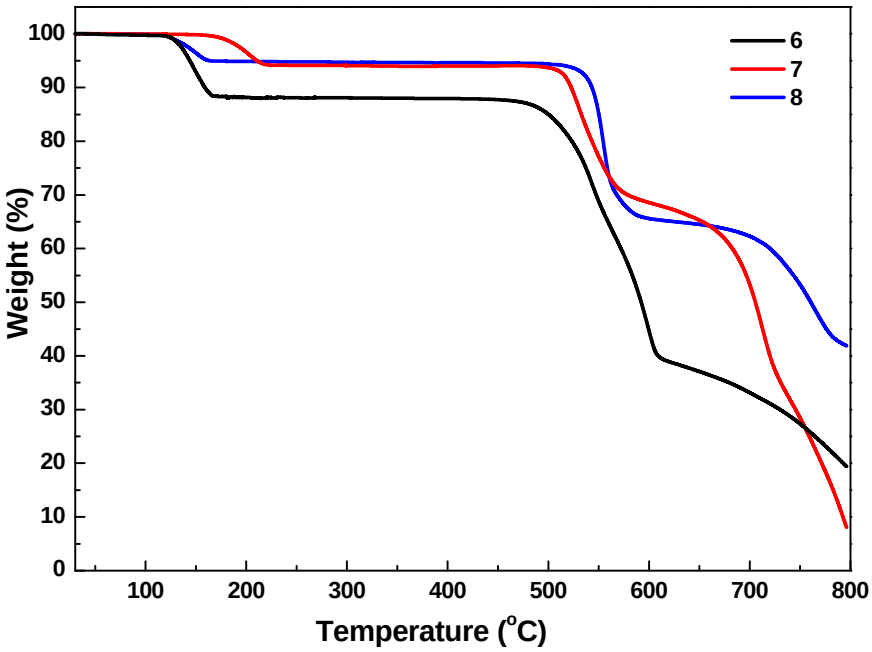


Fig. S13. The TGA curves of (a) **1**–**5**; (b) **6**–**8**.

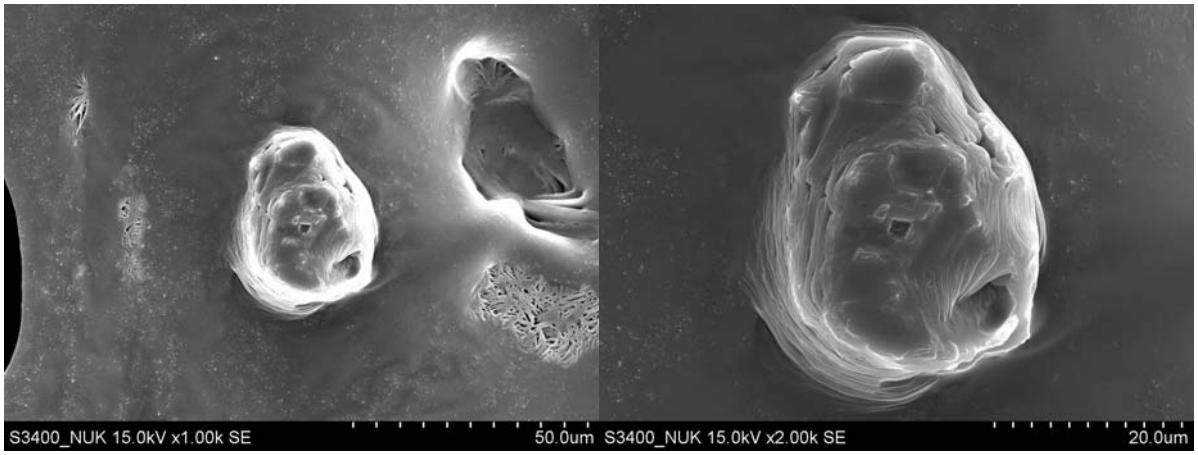
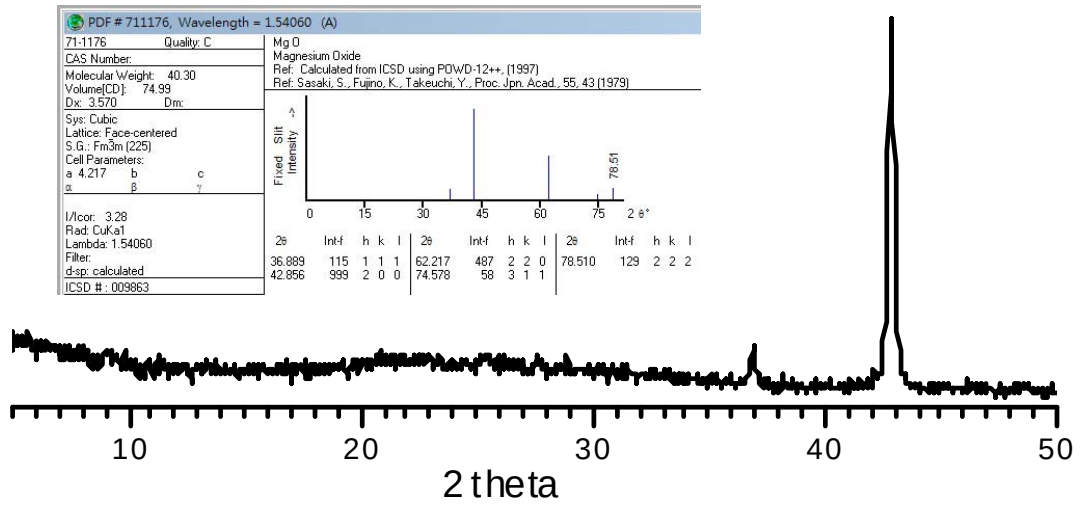
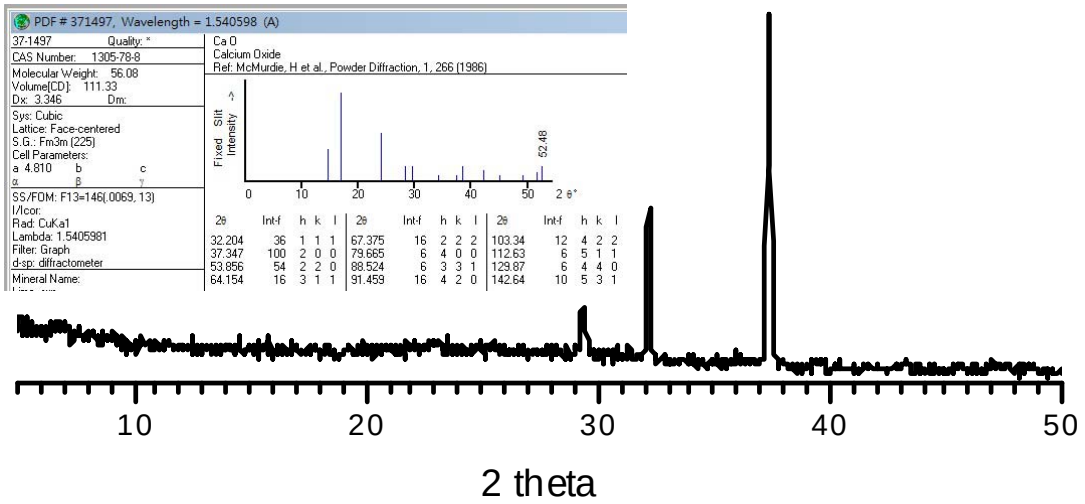


Fig. S14. Scanning electron micrographs for **1**. The particles with sizes ranging from 20 to 30 μm are observed.

(a)



(b)



(c)

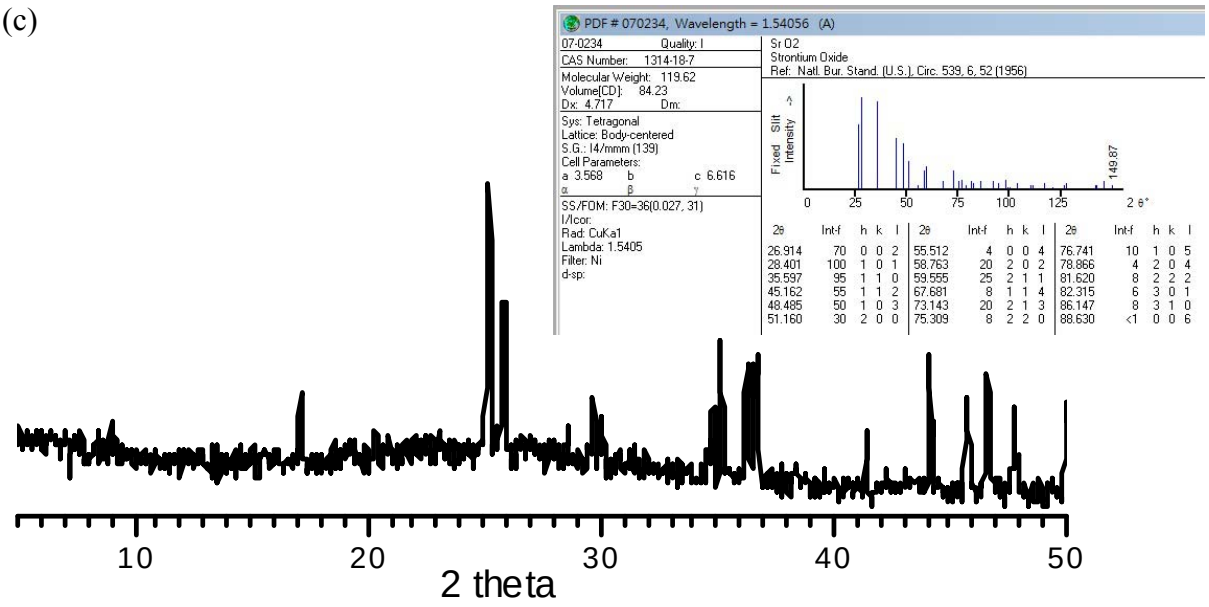


Fig. S15. Powder XRD patterns of residue product of (a) **6**, (b) **7**, and (c) **8** after the TG analysis.

Table S1. Selected bond lengths (Å) for **1**–**8**.

		1	
Li(1)-O(2)#1	1.894(3)	Li(1)-O(1)	2.001(3)
Li(1)-O(1)#2	1.924(3)	Li(1)-O(2)#3	2.006(3)
		2	
Na(1)-O(2)#1	2.3457(15)	Na(1)-O(3)#3	2.4963(14)
Na(1)-O(1W)	2.3889(15)	Na(1)-O(1)	2.5441(16)
Na(1)-O(1)#2	2.4446(15)	Na(1)-O(4)#3	2.7932(16)
Na(2)-O(4)#4	2.2944(15)	Na(2)-O(1)	2.4408(15)
Na(2)-O(3)#3	2.3347(15)	Na(2)-O(3)#6	2.4830(15)
Na(2)-O(1W)#5	2.3689(15)		
		3	
K(1)-O(2)#1	2.7193(11)	K(1)-O(2)#4	2.9993(12)
K(1)-O(2)#2	2.7193(11)	K(1)-O(2)#5	2.9993(12)
K(1)-O(1)#3	2.8683(11)	K(1)-O(1)#6	3.3962(11)
K(1)-O(1)	2.8683(11)	K(1)-O(1)#7	3.3962(11)
		4	
Rb(1)-O(2)#1	2.8821(12)	Rb(1)-O(2)#4	3.0398(13)
Rb(1)-O(2)#2	2.8821(12)	Rb(1)-O(2)#5	3.0398(13)
Rb(1)-O(1)#3	3.0158(14)	Rb(1)-O(1)#6	3.2836(13)
Rb(1)-O(1)	3.0158(14)	Rb(1)-O(1)#7	3.2836(13)
		5	
Cs(1)-O(1)#1	3.0723(16)	Cs(1)-O(2)#4	3.2026(18)
Cs(1)-O(1)#2	3.0723(16)	Cs(1)-O(2)#5	3.2026(18)
Cs(1)-O(1)#3	3.1367(17)	Cs(1)-O(2)#6	3.3122(18)
Cs(1)-O(1)	3.1367(17)	Cs(1)-O(2)#7	3.3122(18)
		6	
Mg(1)-O(1W)	2.002(3)	Mg(1)-O(2)	2.112(3)
Mg(1)-O(5)#1	2.019(3)	Mg(1)-O(2W)	2.120(3)
Mg(1)-O(4)#2	2.064(3)	Mg(1)-O(1)	2.169(3)
		7	
Ca(1)-O(1W)	2.2937(10)	Ca(1)-O(1)	2.3425(9)
Ca(1)-O(4)	2.2994(9)	Ca(1)-O(2)#1	2.3766(8)
Ca(1)-O(2)	2.3424(8)	Ca(1)-O(3)	2.3902(9)
		8	
Sr(1)-O(4)	2.496(2)	Sr(1)-O(1)#2	2.540(3)
Sr(1)-O(5)#1	2.497(3)	Sr(1)-O(2)#3	2.549(3)
Sr(1)-O(1W)	2.543(3)	Sr(1)-O(1)	2.645(3)
Sr(1)-O(2)	2.673(4)		

Symmetry transformations used to generate equivalent atoms: for complex **1**, #1 x-1/2,-y-1/2,-z, #2 -x-1/2,y+1/2,z, #3 -x,-y,-z; for complex **2**, #1 x,-y,z+1/2, #2 x,-y+1,z+1/2, #3 x+1/2,-y+1/2,z+1/2, #4 x+1/2,y+1/2,z, #5 x,-y,z-1/2, #6 x+1/2,y-1/2,z; for complex **3**, #1 x+1,y,z, #2 -x-1/2,-y,z, #3 -x+1/2,-y,z, #4 -x,-y,-z+1, #5 x+1/2,y,-z+1, #6 x+1/2,y,-z, #7 -x,-y,-z; for complex **4**, #1 x+1,y,z, #2 -x-3/2,-y,z, #3 -x-1/2,-y,z, #4 -x-1,-y,-z+1, #5 x+1/2,y,-z+1, #6 x+1/2,y,-z, #7 -x-1,-y,-z; for complex **5**, #1 x+1/2,y,-z+1, #2 -x,-y+1,-z+1, #3 -x+1/2,-y+1,z, #4 x-1/2,y,-z+1, #5 -x+1,-y+1,-z+1, #6 -x+1/2,-y+1,z-1, #7 x,y,z-1; for complex **6**, #1 x+1,y,z+1, #2 x+1,-y+1/2,z+1/2; for complex **7**, #1 -x,-y,-z+1; for complex **8** #1 x,y+1,z #2 -x+1,-y+1,z-1/2 #3 -x+1,-y+1,z+1/2.

Table S2. Hydrogen Bonding Distance (Å) and Angle (deg) Data for **2**–**8**.

D — H ··· A	d(H···A)	d(D···A)	∠DHA	Symmetry Code
		2		
O(1W)-H(1)...O(2)	1.95	2.7998(18)	174.6	[x,y,z+1]
O(1W)-H(2)...O(4)	2.06	2.7910(19)	163.3	[x+1/2,y+1/2,z+1]
		3		
O(1)-H(1)...O(1)	1.65	2.4643(18)	174.2	[-x-1/2,-y,z]
		4		
O(1)-H(1)...O(1)	1.64	2.458(2)	172.3	[-x-3/2,-y,z]
		5		
O(2)-H(2)...O(2)	1.67	2.466(3)	164.8	[-x+1/2,-y+1,z]
		6		
O1W-H1WA…O(2)	1.928	2.664	144.17	[-x+1, y-1/2, -z+1/2]
O1W-H1WB…O(1)	1.948	2.696	146.19	[-x+1, -y, -z]
O2W-H2WA…O(2)	2.479	3.181	140.43	[-x+1, y-1/2, -z+1/2]
O2W-H2WB…O(4)	1.964	2.751	153.56	[x+1, y, z+1]
		7		
O1W-H1…O(3)	2.028	2.789	173.06	[x+1, y, z]
O1W-H2…O(1)	2.054	2.810	148.74	[-x, -y, -z]
		8		
O(1W)-H(1WA)...O(5)	2.31	3.091(4)	153.6	[-x+1,-y+1,z+1/2]
O(1W)-H(1WB)...O(4)	1.95	2.759(3)	159.1	[x,y+1,z]