Electronic Supplementary Information for CrystEngComm

Electronic Supplementary Information (ESI)

Structure evolutions and luminescent properties of lithium(I)-sulfonate complexes constructed from multifunctional arenedisulfonic acids

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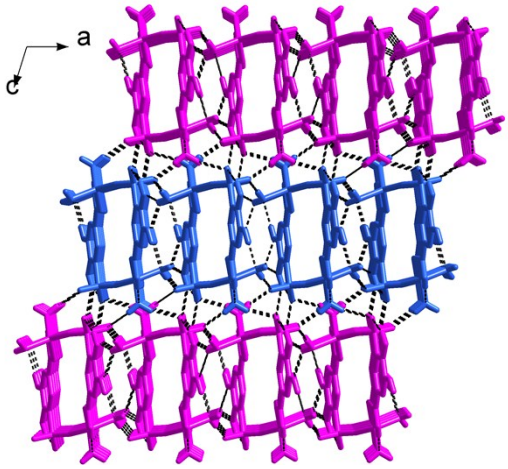

Fig. S1 3-D supramolecular network extended by the hydrogen-bonding interactions (black dashed lines).

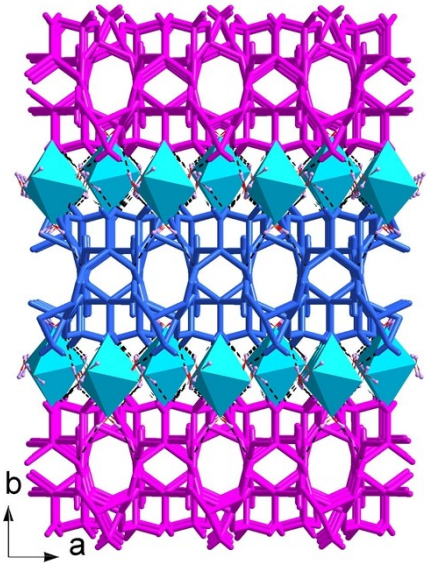

Fig. S2 3-D supramolecular network extended by the $[Li3(H_2O)_5]^+$ cations through the hydrogen-bonding interactions (black dashed lines).

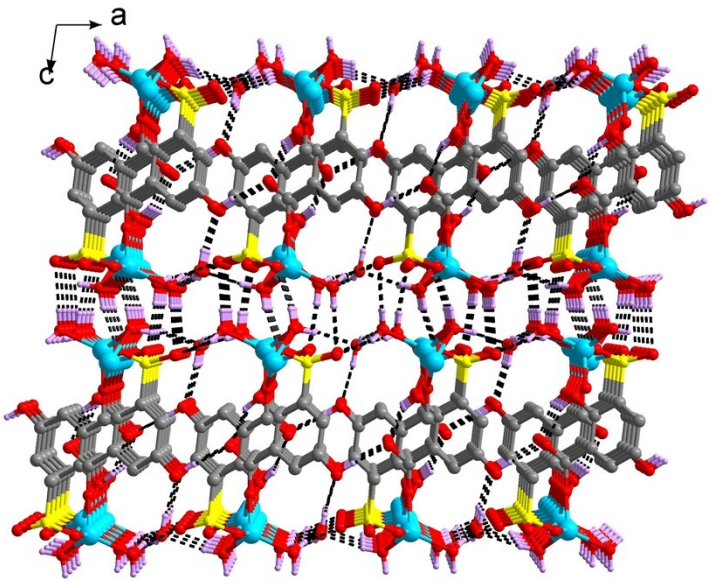

Fig. S3 3-D supramolecular network extended by the hydrogen-bonding interactions (black dashed lines).

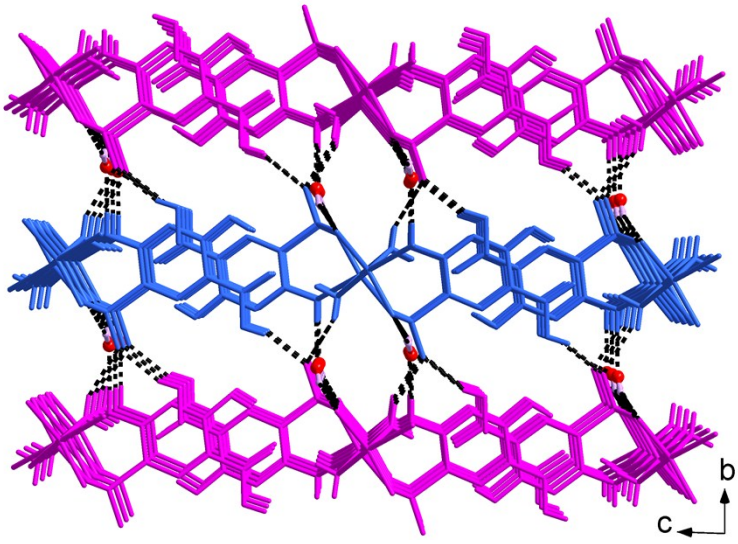

Fig. S4 3-D supramolecular network extended by the free water molecules (O2w) through the hydrogen-bonding interactions (black dashed lines).

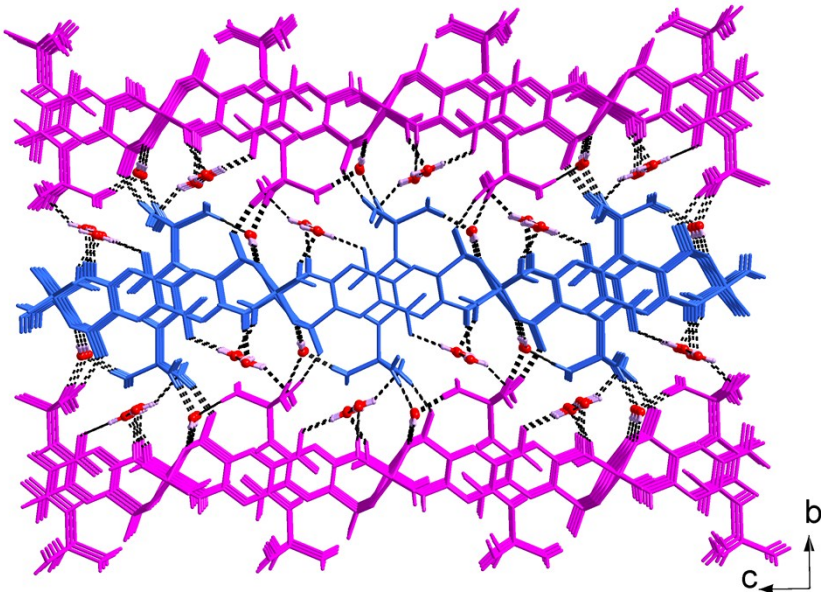

Fig. S5 3-D supramolecular network extended by the free water molecules through the hydrogen-bonding interactions (black dashed lines).

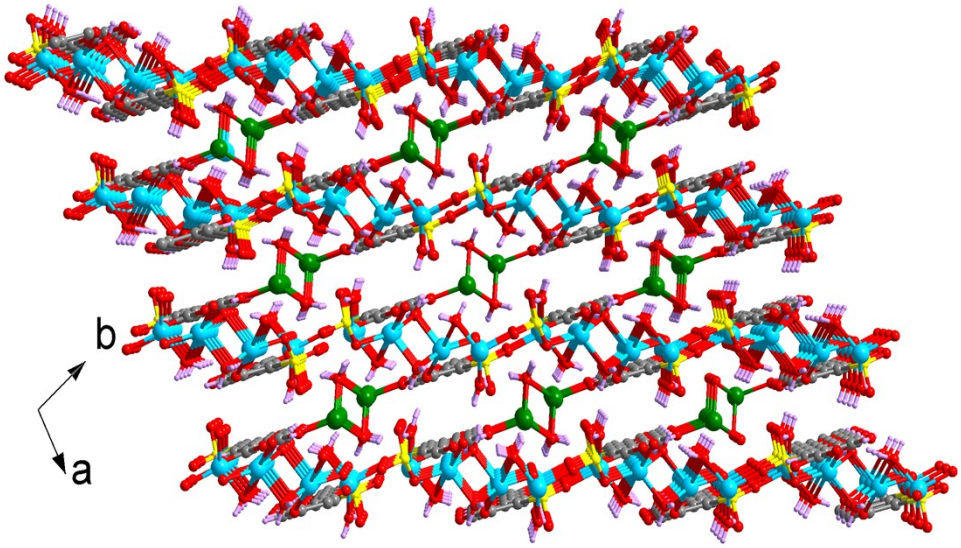

Fig. S6 3-D network of complex **8** with the Li3 cations being denoted as green balls.

Electronic Supplementary Information for CrystEngComm

Powder X-ray diffraction (PXRD)

Powder X-ray diffraction (PXRD) patterns for solid samples of complexes **1-8** were measured at room temperature as illustrated in Fig. S7. The patterns are highly similar to their simulated ones (based on the single-crystal X-ray diffraction data), indicating that the single-crystal structures are really representative of the bulk of the corresponding samples.

Thermogravimetric analysis

To examine the thermal stability of the complexes, in this study, their stabilities were analyzed on crystalline samples by thermogravimetric analyses (TGA) from room temperature to 900 °C at a rate of 10 °C min^{-1}, under N_2 atmosphere. As shown in Fig. S8, the TGA curve indicates that complex **1** loses the coordinated water molecules from 90 to 135 °C with the observed weight loss of 12.73% (calcd 13.05%). Then, one sharp step corresponding to the loss of the organic components occurs in the temperature range 135-710 °C. Complex **2** loses the free and coordinated water molecules from 85 to 164 °C with the observed weight loss of 18.94% (calcd 18.76%). The organic components are then removed progressively from 164 to 630 °C. The sharp weight loss in complex **3** between 50 and 160 °C corresponds to the removal of the free and coordinated water molecules (obsd 22.45%, calcd 22.65%). Then, the organic components are removed progressively from 245 to 480 °C. Complex **4** loses the free and coordinated water molecules from 76 to 122 °C with the observed weight loss of 9.88% (calcd 10.00%). The organic components are then removed progressively from 255 to 465 °C. The sharp weight loss in complex **5** between 86 and 150 °C corresponds to the removal of the free and coordinated water molecules (obsd 13.19%, calcd 13.05%). Then, the organic components are removed progressively from 150 to 775 °C. For complex **6**, the first sharp step between 60 and 170 °C corresponds to the release of free and coordinated water molecules with the observed weight loss of 33.38% (calcd 33.89%). Then, the following weight loss with the decomposing of organic components occurs in the temperature range 340-660 °C. Complex **7** loses the free and coordinated water molecules from 55 to 190 °C with the observed weight loss of 28.88% (calcd 28.71%). The organic components are then removed progressively from 190 to 623 °C. Complex **8** begins to lose the free and coordinated water molecules from 60 to 133 °C (obsd 17.88%, calcd 17.96%). The following gradually weight loss from 133 to 605 °C corresponds to the loss of the organic components.

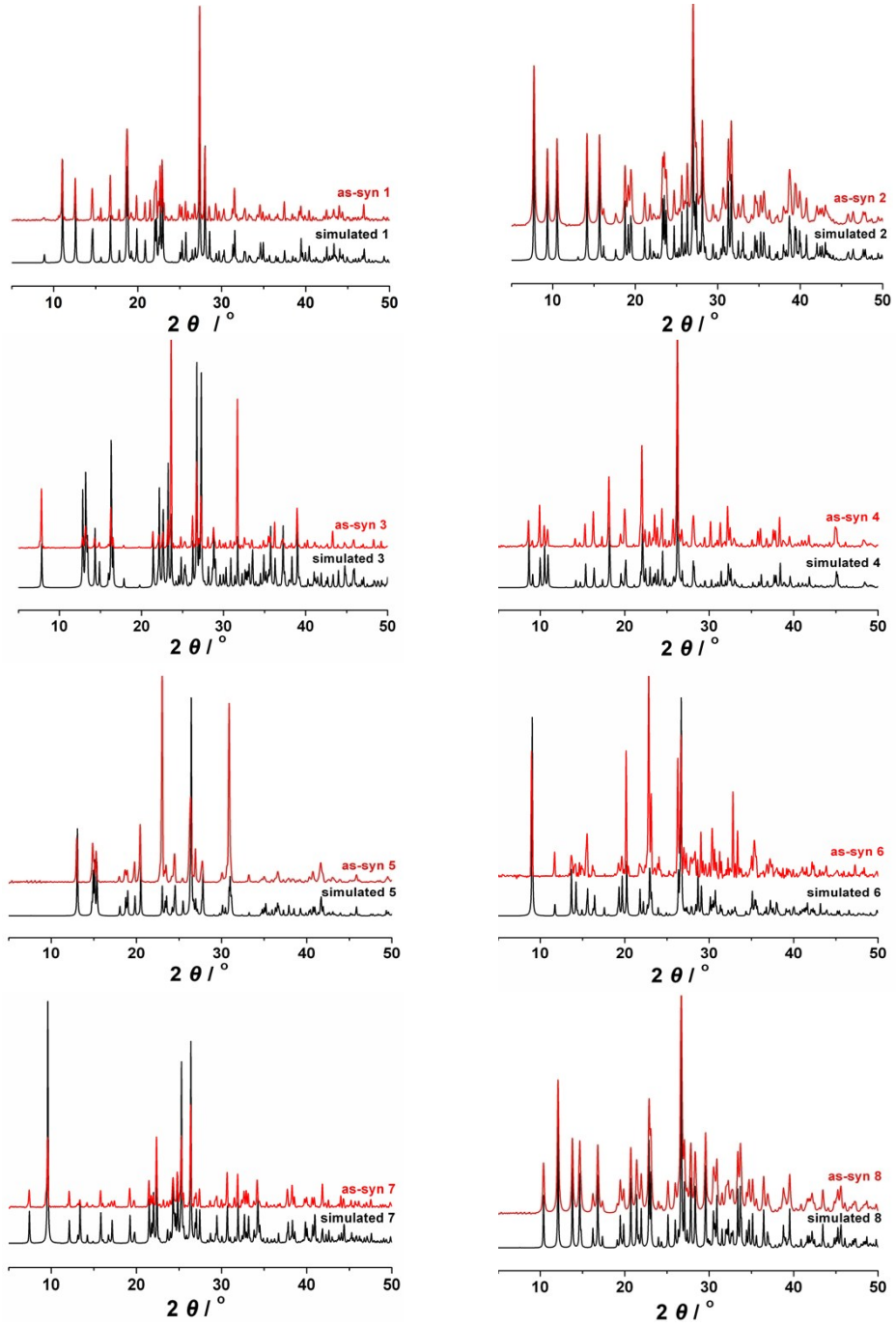

Fig. S7 PXRD patterns for complexes **1-8**.

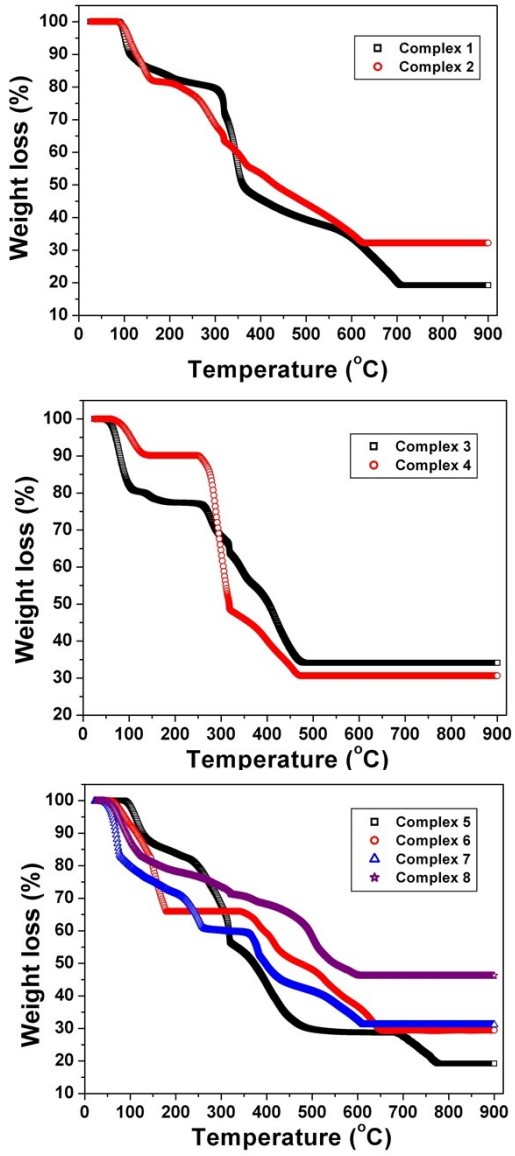

Fig. S8 TG curves of complexes **1-8**.

Table S1 Selected Bond Distances (Å) for Complexes **1-8**[a]

Complex **1**			
Li(1)-O(1)^{i}	1.867(5)	Li(1)-O(6)	1.954(5)
Li(1)-O(1W)	1.949(5)	Li(1)-O(2W)	1.986(5)
Complex **2**			
Li(1)-O(3)^{i}	2.010(8)	Li(2)-O(5)^{i}	2.608(3)
Li(1)-O(1W)	2.015(8)	Li(2)-O(5)^{iv}	2.608(3)
Li(1)-O(4)^{i}	2.033(8)	Li(3)-O(5W)^{ii}	2.106(3)
Li(1)-O(6)	2.054(9)	Li(3)-O(5W)	2.106(3)
Li(1)-O(6)^{ii}	2.192(12)	Li(3)-O(4W)	2.143(16)
Li(1)-Li(1)^{ii}	2.575(2)	Li(3)-O(3W)	2.150(6)
Li(2)-O(2W)	1.900(13)	Li(3)-O(3W)^{ii}	2.150(6)
Li(2)-O(7)^{iii}	1.905(7)	Li(2)-O(7)	1.905(7)
Complex **3**			
Li(1)-O(6)	1.905(12)	Li(2)-O(3)	2.016(11)
Li(1)-O(1)^{i}	1.917(12)	Li(2)-O(6)^{ii}	2.095(11)
Li(1)-O(2W)	1.950(11)	Li(2)-O(4)	2.105(10)
Li(1)-O(1W)	1.980(12)	Li(2)-O(2W)^{ii}	2.176(10)
Li(1)-Li(2)^{ii}	2.769(2)	Li(2)-Li(1)^{ii}	2.769(2)
Li(2)-O(3W)	1.949(12)		
Complex **4**			
Li(1)-O(1W)	1.921(11)	Li(2)-O(3)	2.048(10)
Li(1)-O(9)	1.940(11)	Li(2)-O(10)^{ii}	2.094(10)
Li(1)-O(7)^{i}	2.009(10)	Li(2)-Li(2)^{ii}	3.025(19)

Li(1)-O(3)	2.032(10)	Li(3)-O(2W)	1.884(11)
Li(1)-Li(2)	3.367(12)	Li(3)-O(1)	1.923(10)
Li(2)-O(10)	1.964(10)	Li(3)-O(6)^{iii}	1.980(11)
Li(2)-O(4)	1.991(10)	Li(3)-O(13)^{iv}	1.997(10)
Li(2)-O(11)^{ii}	2.040(11)		

Complex **5**

Li(1)-O(2)^{i}	1.966(6)	Li(1)-O(1W)	2.102(7)
Li(1)-O(1)	1.983(6)	Li(1)-O(4)	2.459(7)
Li(1)-O(1W)^{ii}	2.062(6)	Li(1)-Li(1)^{ii}	3.115(1)

Complex **6**

Li(1)-O(3)	1.962(7)	Li(1)-Li(1)^{ii}	3.064(1)
Li(1)-O(2)^{i}	1.970(7)	Li(2)-O(4W)	1.881(6)
Li(1)-O(1W)^{ii}	2.074(8)	Li(2)-O(2W)	1.908(7)
Li(1)-O(1W)	2.084(7)	Li(2)-O(5)	1.946(6)
Li(1)-O(4)	2.463(7)	Li(2)-O(3W)	1.966(7)

Complex **7**

Li(1)-O(4)	1.928(7)	Li(2)-O(2)^{iii}	2.021(6)
Li(1)-O(3)^{i}	1.947(7)	Li(2)-O(2W)	2.096(7)
Li(1)-O(1W)	2.005(7)	Li(2)-O(3W)	2.102(7)
Li(1)-O(6)^{ii}	2.092(7)	Li(2)-O(1W)^{iii}	2.181(7)
Li(1)-O(2)	2.219(7)	Li(2)-Li(1)^{iii}	3.116(9)
Li(1)-Li(2)^{iii}	3.116(9)	Li(2)-Li(2)^{iii}	3.490(9)
Li(2)-O(1)	1.982(7)		

Complex **8**

Li(1)-O(3)	2.029(6)	Li(2)-O(3W)	1.960(6)
Li(1)-O(4)	2.041(6)	Li(2)-O(7)	1.974(5)
Li(1)-O(1W)	2.074(6)	Li(2)-Li(1)^{iv}	3.227(8)

Li(1)-O(1W)^{i}	2.078(6)	Li(3)-O(5W)	1.887(9)
Li(1)-O(3W)^{ii}	2.349(6)	Li(3)-O(5)	1.935(6)
Li(1)-Li(1)^{i}	2.855(10)	Li(3)-O(4W)	2.040(7)
Li(1)-Li(2)^{ii}	3.227(8)	Li(3)-O(4W)^{v}	2.047(7)
Li(2)-O(2W)	1.906(6)	Li(3)-Li(3)^{v}	2.855(13)
Li(2)-O(2)^{iii}	1.906(5)		

[a] Symmetry transformations used to generate equivalent atoms: (i) -x+2,-y+2,-z+1 for **1**; (i) x,-y+1,z-1/2; (ii) -x,y,-z+1/2; (iii) -x+1,y,-z+1/2; (iv) -x+1,-y+1,-z+1 for **2**; (i) -x+2,-y+1,-z+1; (ii) -x+2,-y,-z+1 for **3**; (i) -x,-y,-z+1; (ii) -x+1,-y+1,-z+1; (iii) -x+1,-y,-z+1; (iv) x-1,y-1,z-1 for **4**; (i) -x+1,-y+1,-z; (ii) -x+2,-y+1,-z for **5**; (i) -x,-y+1,-z; (ii) -x-1,-y+1,-z for **6**; (i) -x+2,y,-z+3/2; (ii) x+1/2,-y+1/2,z+1/2; (iii) -x+1,y,-z+3/2 for **7**; (i) -x+1,-y+2,-z; (ii) x,y,z-1; (iii) -x,-y+1,-z+1; (iv) x,y,z+1; (v) -x+1,-y+3,-z+1 for **8**.

Table S2 Selected Hydrogen Bond Parameters for Complexes **1-8**[a]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
Complex **1**				
O(1W)-H(1W1)...O(2)^{ii}	0.85(3)	1.949(11)	2.784(3)	169(3)
O(1W)-H(1W2)...O(5)^{iii}	0.85(3)	2.22(2)	2.970(3)	148(3)
O(1W)-H(1W2)...O(4)^{iii}	0.85(3)	2.24(2)	2.895(3)	134(3)
O(2W)-H(2W1)...O(2)^{iv}	0.85(3)	1.935(11)	2.781(3)	172(3)
O(2W)-H(2W2)...O(3)^{v}	0.85(3)	2.102(11)	2.927(3)	165(3)
O(4)-H(4O)...O(1W)^{vi}	0.82	2.03	2.846(3)	176.7
O(5)-H(5O)...O(3)	0.82	1.94	2.674(3)	149.2
O(5)-H(5O)...O(3)^{vii}	0.82	2.47	2.996(3)	123.3
O(7)-H(7O)...O(2W)	0.82	1.87	2.686(3)	170.0
Complex **2**				
O(1W)-H(1W1)...O(3W)^{vi}	0.85(4)	1.970(7)	2.820(4)	175.9(14)
O(2W)-H(2W1)...O(5W)	0.85(4)	2.020(14)	2.858(4)	168(5)
O(3W)-H(3W2)...O(7W)^{i}	0.85(4)	2.005(19)	2.825(4)	161(4)
O(3W)-H(3W1)...O(1)^{vii}	0.85(4)	1.980(17)	2.814(4)	165(5)
O(4)-H(4O)...O(7)^{v}	0.82	1.89	2.647(4)	152.3
O(4)-H(4O)...O(5)	0.82	2.25	2.690(4)	114.2
O(4W)-H(4W1)...O(7)	0.85(5)	2.47(3)	3.196(5)	144(4)
O(5W)-H(5W2)...O(3)^{viii}	0.85(4)	2.20(2)	3.009(4)	158(4)
O(5W)-H(5W2)...O(1W)^{ix}	0.85(4)	2.53(3)	3.117(4)	127(4)
O(5W)-H(5W1)...O(2)	0.86(4)	1.869(19)	2.693(4)	161(5)
O(5)-H(5O)...O(7W)	0.82	1.93	2.752(4)	179.9
O(6W)-H(6W1)...O(6)^{iii}	0.85(4)	2.29(4)	2.988(4)	140(5)
O(7W)-H(7W2)...O(1)^{iv}	0.85(4)	1.981(13)	2.827(4)	173(4)
O(7W)-H(7W1)...O(2)^{x}	0.85(4)	2.20(3)	2.868(5)	136(4)
Complex **3**				
O(4)-H(4O)...O(5)	0.82	1.77	2.504(5)	147.4
O(7)-H(7O)...O(5)^{iii}	0.82	1.81	2.633(5)	175.8
O(3W)-H(3W1)...O(3)^{iv}	0.85(6)	2.092(13)	2.939(6)	174(6)
O(2W)-H(2W2)...O(4W)^{v}	0.85(6)	1.921(15)	2.762(7)	170(6)

O(4W)-H(4W2)...O(7)^{i}	0.85(6)	1.94(2)	2.774(6)	165(7)
O(2W)-H(2W1)...O(1)^{vi}	0.85(6)	1.98(2)	2.792(6)	161(6)
O(3W)-H(3W2)...O(4W)	0.85(6)	1.984(14)	2.832(7)	175(7)
O(4W)-H(4W1)...O(1W)^{i}	0.85(6)	2.15(2)	2.993(7)	169(8)
O(1W)-H(1W2)...O(2)^{vi}	0.85(6)	2.163(14)	3.012(6)	175(6)
O(1W)-H(1W1)...O(2)^{vii}	0.85(6)	2.09(2)	2.912(7)	164(6)
Complex **4**				
O(1W)-H(1W1)...O(5)^{ii}	0.85(6)	1.97(2)	2.809(6)	166(7)
O(1W)-H(1W2)...O(8)^{vi}	0.85(6)	1.891(17)	2.731(5)	169(6)
O(2W)-H(2W1)...O(1W)^{vii}	0.85	2.04	2.866(6)	165.7
O(2W)-H(2W2)...O(3W)^{viii}	0.85	2.40	2.987(7)	126.2
O(3W)-H(3W1)...O(14)^{ix}	0.85(6)	2.20(3)	3.001(6)	157(7)
O(3W)-H(3W2)...O(1)^{iii}	0.85(6)	2.233(18)	3.080(6)	171(7)
O(4)-H(4O)...O(5)	0.82	1.77	2.498(5)	147.7
O(7)-H(7O)...O(3W)	0.82	1.90	2.720(6)	179.3
O(11)-H(11O)...O(13)	0.82	1.87	2.585(5)	145.7
O(12)-H(12O)...O(6)^{x}	0.82	1.72	2.535(5)	173.5
O(14)-H(14O)...O(2)^{i}	0.82	1.93	2.743(5)	170.9
Complex **5**				
O(1W)-H(1W1)...O(3)^{iii}	0.85	2.12	2.903(3)	153.0
O(1W)-H(1W2)...O(6)^{iv}	0.85	1.87	2.707(4)	168.5
O(2W)-H(2W1)...O(2)^{v}	0.85	2.00	2.828(4)	163.7
O(2W)-H(2W2)...O(1)	0.86	1.96	2.794(3)	165.4
O(4)-H(4O)...O(2W)^{vi}	0.82	1.77	2.591(4)	179.1
O(5)-H(5O)...O(6)	0.82	1.91	2.626(4)	146.2
O(7)-H(7O)...O(3)^{vii}	0.82	1.99	2.775(4)	159.5
Complex **6**				
O(1W)-H(1W1)...O(7W)^{iii}	0.85(3)	1.978(18)	2.774(3)	155(3)
O(1W)-H(1W2)...O(6)^{iv}	0.85(3)	1.988(16)	2.806(3)	160(3)
O(2W)-H(2W1)...O(5W)^{v}	0.85(3)	1.842(12)	2.688(4)	174(4)
O(2W)-H(2W2)...O(6W)	0.85(3)	1.982(15)	2.774(4)	155(3)
O(3W)-H(3W1)...O(7)^{iv}	0.85(3)	1.938(11)	2.789(4)	179(4)
O(3W)-H(3W2)...O(1)^{vi}	0.86(3)	1.953(12)	2.787(3)	165(3)
O(4W)-H(4W1)...O(5W)	0.85(3)	1.887(13)	2.728(4)	169(4)
O(4W)-H(4W2)...O(7)^{vii}	0.85(3)	1.960(14)	2.795(4)	169(5)

O(4)-H(4O)...O(6W)^{iii}	0.82	1.91	2.727(3)	176.2
O(5)-H(5O)...O(6)	0.82	1.72	2.459(3)	148.8
O(5W)-H(5W1)...O(2)^{viii}	0.86(3)	1.878(12)	2.730(3)	173(3)
O(5W)-H(5W2)...O(3)^{vi}	0.85(3)	1.909(11)	2.756(3)	175(4)
O(6W)-H(6W1)...O(3W)	0.85	2.26	2.943(4)	136.9
O(6W)-H(6W2)...O(7W)	0.85	1.88	2.729(4)	178.9
O(7W)-H(7W2)...O(4W)^{ix}	0.85	2.94	3.296(4)	107.1
O(7W)-H(7W1)...O(7)^{x}	0.85	1.86	2.707(3)	177.1
Complex **7**				
O(1W)-H(1W2)...O(5W)^{v}	0.85(4)	2.013(17)	2.830(4)	161(3)
O(1W)-H(1W1)...O(6W)^{vi}	0.85(4)	2.020(13)	2.868(4)	172(4)
O(2W)-H(2W)...O(4W)^{iii}	0.85(4)	1.903(9)	2.754(3)	176(4)
O(3W)-H(3W1)...O(5W)	0.85(4)	1.97(3)	2.751(4)	151(4)
O(3W)-H(3W2)...O(1)^{vii}	0.85(4)	2.13(2)	2.897(3)	150(4)
O(4)-H(4O)...O(7)^{ii}	0.82	1.75	2.548(3)	165.0
O(4W)-H(4W2)...O(5)^{viii}	0.85(4)	1.914(11)	2.757(4)	173(4)
O(4W)-H(4W1)...O(6W)^{ix}	0.85(4)	1.927(14)	2.754(4)	164(4)
O(5)-H(5O)...O(6)	0.82	1.73	2.466(4)	148.8
O(5W)-H(5W1)...O(7)^{vii}	0.85(4)	1.844(14)	2.685(4)	169(5)
O(5W)-H(5W2)...O(4W)^{iii}	0.85(4)	1.884(14)	2.721(4)	167(5)
O(6W)-H(6W1)...O(3)^{x}	0.85(4)	2.057(15)	2.892(4)	168(5)
O(6W)-H(6W2)...O(3W)	0.85(4)	2.000(11)	2.850(4)	177(4)
Complex **8**				
O(1W)-H(1W1)...O(1)^{vi}	0.86(3)	2.024(15)	2.849(3)	162(3)
O(1W)-H(1W2)...O(6)^{ii}	0.86(3)	1.887(12)	2.738(3)	171(3)
O(2W)-H(2W1)...O(1)^{iv}	0.85(4)	1.99(4)	2.828(4)	165(5)
O(2W)-H(2W2)...O(4)^{vii}	0.85(4)	1.85(6)	2.704(3)	176(5)
O(3W)-H(3W1)...O(4)^{viii}	0.85(4)	1.879(17)	2.703(3)	163(4)
O(3W)-H(3W2)...O(6W)	0.85(4)	2.18(2)	2.964(2)	154(4)
O(4W)-H(4W1)...O(7)^{ix}	0.85(4)	2.00(3)	2.842(3)	174(3)
O(4W)-H(4W2)...O(7)^{vii}	0.85(4)	2.040(16)	2.861(3)	164(3)
O(5)-H(5O)...O(6)	0.82	1.77	2.511(3)	148.8
O(5W)-H(5W1)...O(3)^{viii}	0.85	2.32	3.082(5)	149.3
O(5W)-H(5W2)...O(6W)^{ix}	0.85	2.23	2.992(5)	149.3
O(6W)-H(6W1)...O(1)^{iii}	0.85	1.87	2.715(3)	171.1

O(6W)-H(6W2)...O(3)[x]	0.85	2.31	3.156(2)	171.6

[a] Symmetry transformations used to generate equivalent atoms: (ii) -x+1,-y+2,-z+1; (iii) -x+1,-y+1,-z+1; (iv) x,y,z-1; (v) x-1,y,z-1; (vi) x,y-1,z; (vii) -x+2,-y+1,-z+2 for **1**; (i) x,-y+1,z-1/2; (iii) -x+1,y,-z+1/2; (iv) -x+1,-y+1,-z+1; (v) x,-y+1,z+1/2; (vi) x-1/2,y+1/2,z; (vii) x-1/2,-y+1/2,z-1/2; (viii) -x+1/2,-y+1/2,-z+1; (ix) x+1/2,y-1/2,z; (x) -x,-y+1,-z+1 for **2**; (i) -x+2,-y+1,-z+1; (iii) x+1,y+1,z; (iv) -x+2,-y,-z; (v) -x+1,-y,-z+1; (vi) x,y,z+1; (vii) -x+3,-y+1,-z+1 for **3**; (i) -x,-y,-z+1; (ii) -x+1,-y+1,-z+1; (iii) -x+1,-y,-z+1; (vi) -x,-y+1,-z+1; (vii) -x,-y,-z; (viii) x,y,z-1; (ix) -x+1,-y,-z+2; (x) -x+2,-y+1,-z+2 for **4**; (iii) -x+1,-y+2,-z; (iv) x+1,y,z-1; (v) x+1,y,z; (vi) x,y-1,z; (vii) -x,-y+2,-z+1 for **5**; (iii) x,-y+1/2,z-1/2; (iv) -x,-y+1,-z+1; (v) x,-y+1/2,z+1/2; (vi) -x,y-1/2,-z+1/2; (vii) -x+1,-y+1,-z+1; (viii) -x+1,y-1/2,-z+1/2; (ix) x-1,y,z; (x) -x,y-1/2,-z+3/2 for **6**; (ii) x+1/2,-y+1/2,z+1/2; (iii) -x+1,y,-z+3/2; (v) x,-y+1,z+1/2; (vi) x+1,-y+1,z+1/2; (vii) -x+1,-y+1,-z+1; (viii) x-1/2,y+1/2,z; (ix) -x,y,-z+3/2; (x) x-1,y,z for **7**; (ii) x,y,z-1; (iii) -x,-y+1,-z+1; (iv) x,y,z+1; (vi) -x,-y+2,-z; (vii) -x,-y+2,-z+1; (viii) -x+1,-y+2,-z+1; (ix) x,y+1,z; (x) -x+1,-y+1,-z+1 for **8**.