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Conformational control of the self-assembly of triple helicates and [2 x 2]-grids from Zinc(II) and 3,6-di(2-pyridyl)pyridazine based ligands

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	H3	H4	H5	H6	H9
L_1	8.71	8.00	7.52	8.77	8.67
1	8.61	8.45	7.91	8.02	9.05
CIS[b]	-0.1	+0.45	+0.39	-0.75	+0.38

[a] For deuterated acetonitrile solutions. [b] CIS= δcomplex-δligand.

Table S1: ^{1}H-NMR Chemical shifts[a] and Coordination Induced Shifts[b] of complex **1**

	H3	H4	H5	H6	H10	H11
L_2	8.51	7.98	7.47	8.76	3.49	2.14[c]
3	8.46	8.39	7.83	7.96	3.60	2.87[c]
CIS[b]	-0.05	+0.41	+0.36	-0.80	+0.11	+0.73

[a] For deuterated acetonitrile solutions. [b] CIS= δcomplex-δligand. [c] Solvent overlap.

Table S2: ^{1}H-NMR Chemical shifts[a] and Coordination Induced Shifts[b] of complex **3**

	H3	H4	H5	H6	H10	H11
L_4	7.88	7.98	7.48	8.72	2.94	1.80
4	8.43	8.31	7.81	8.47	3.18/3.32	1.62/2.13
CIS[b]	+0.55	+0.33	+0.33	-0.25	+0.25/+0.38	-0.18/+0.33

[a] For deuterated acetonitrile solutions. [b] CIS= δcomplex-δligand.

Table S3: ^{1}H-NMR Chemical shifts[a] and Coordination Induced Shifts[b] of complex **4**

	H3	H4	H5	H6	H10	H11	H12[c]
L_5	7.86	7.98	7.49	8.73	3.00	1.71	1.89[c]
5	8.12	8.32	7.82	8.42	3.32	1.87/1.76	2.00[c]
CIS[b]	+0.26	+0.34	+0.33	-0.31	+0.32	+0.16/+0.05	+0.11[c]

[a] For deuterated acetonitrile solutions. [b] CIS= δcomplex-δligand. [c] Solvent overlap.

Table S4: ^{1}H-NMR Chemical shifts[a] and Coordination Induced Shifts[b] of complex **5**

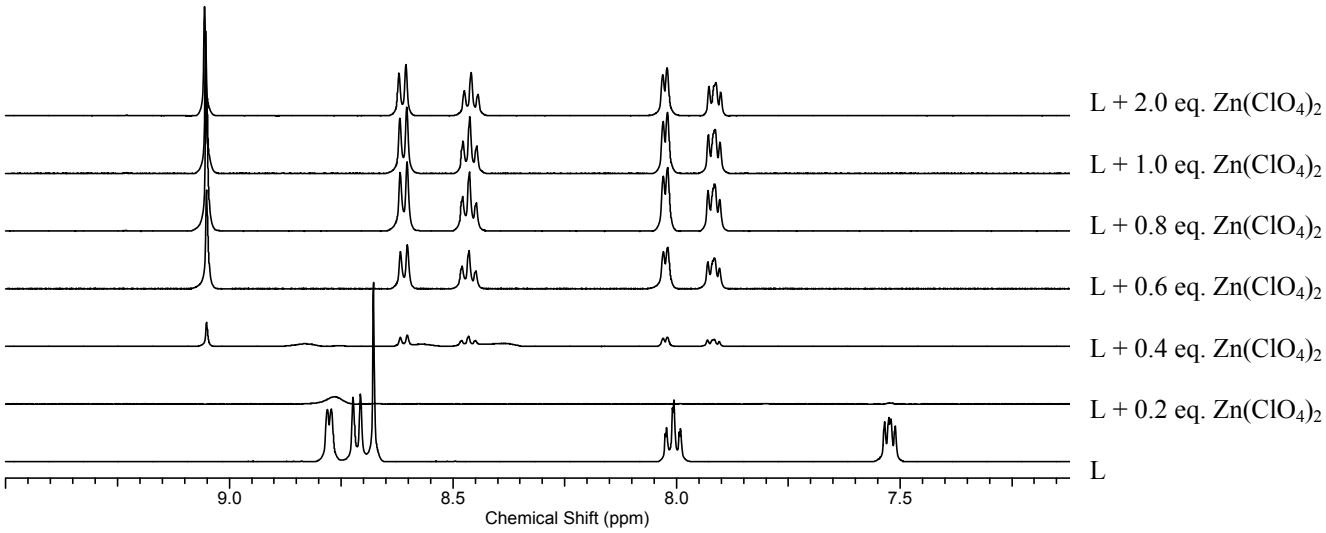

Figure S1: ^{1}H-NMR titration to form complex **1**, aromatic region shown.

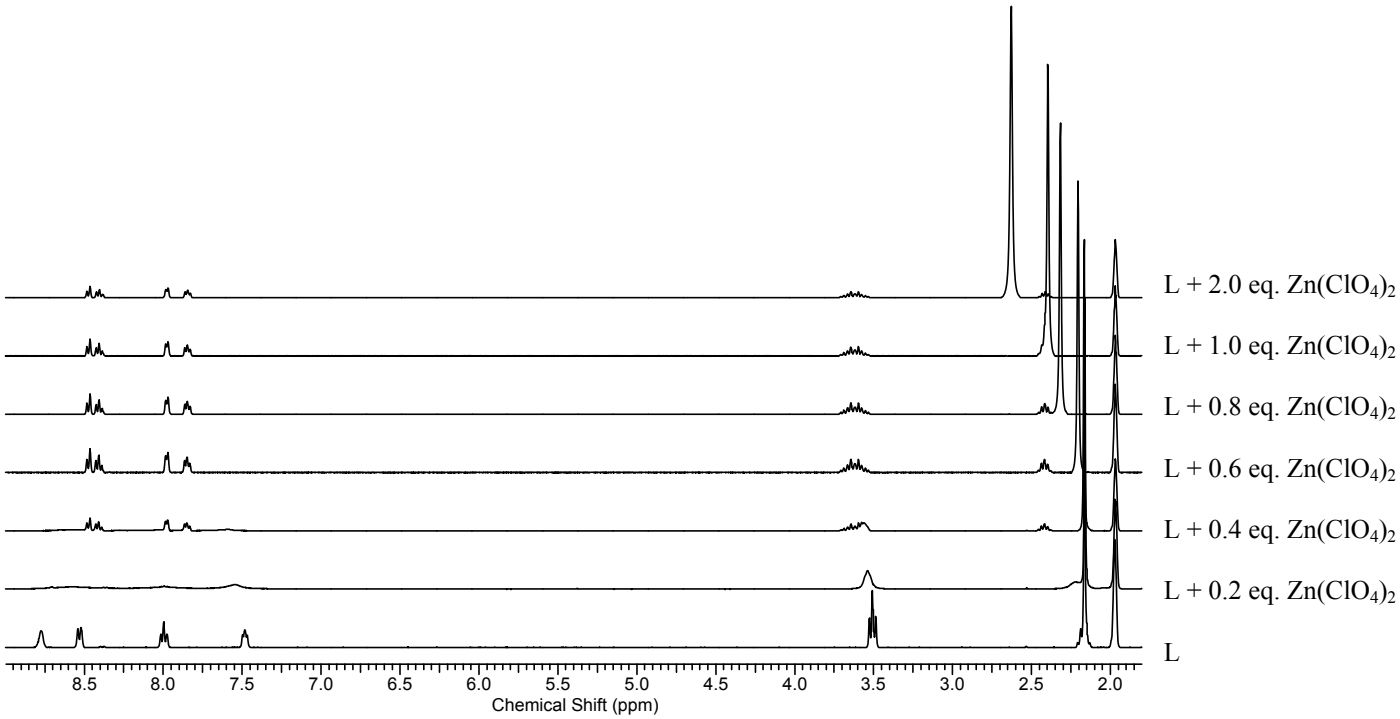

Figure S2: ^{1}H-NMR titration to form complex **3**.

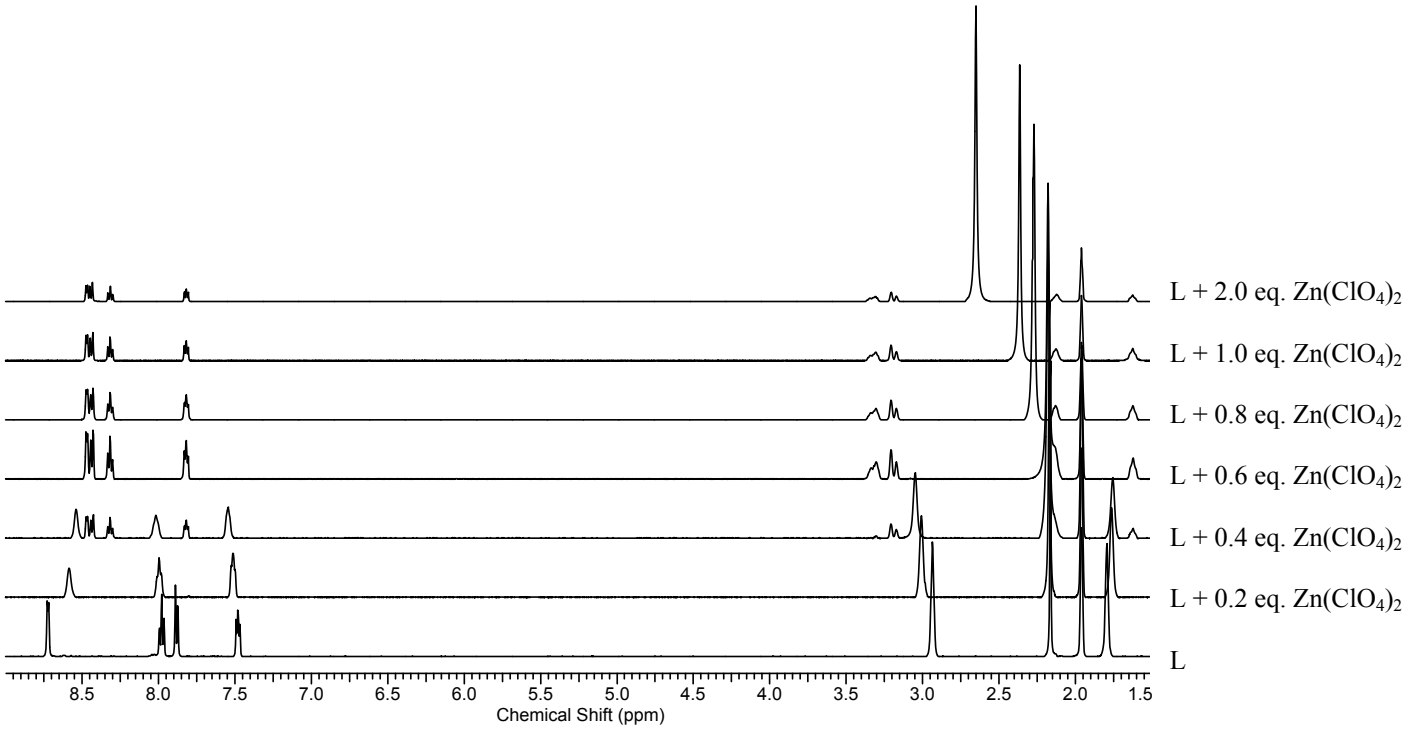

Figure S3: ^{1}H-NMR titration to form complex **4**.

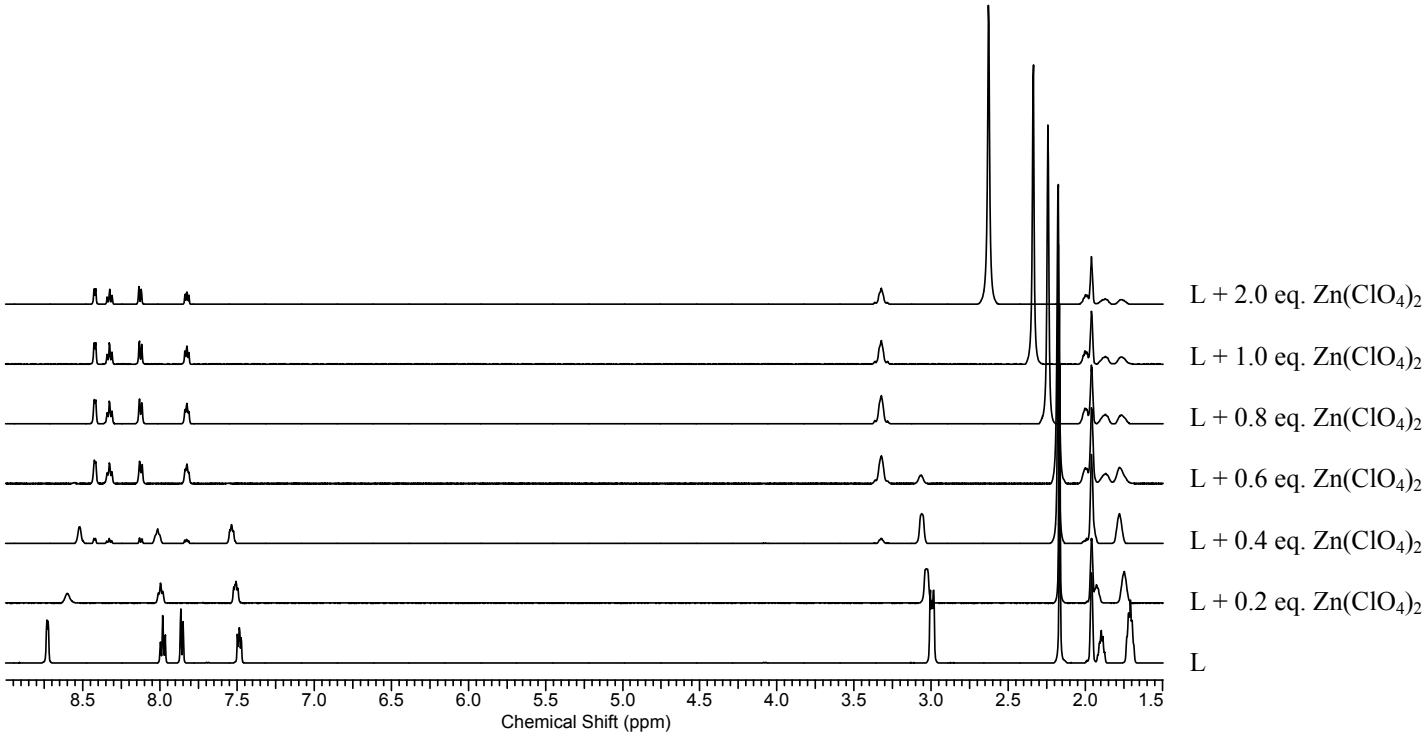

Figure S4: NMR titration to form complex **5**.

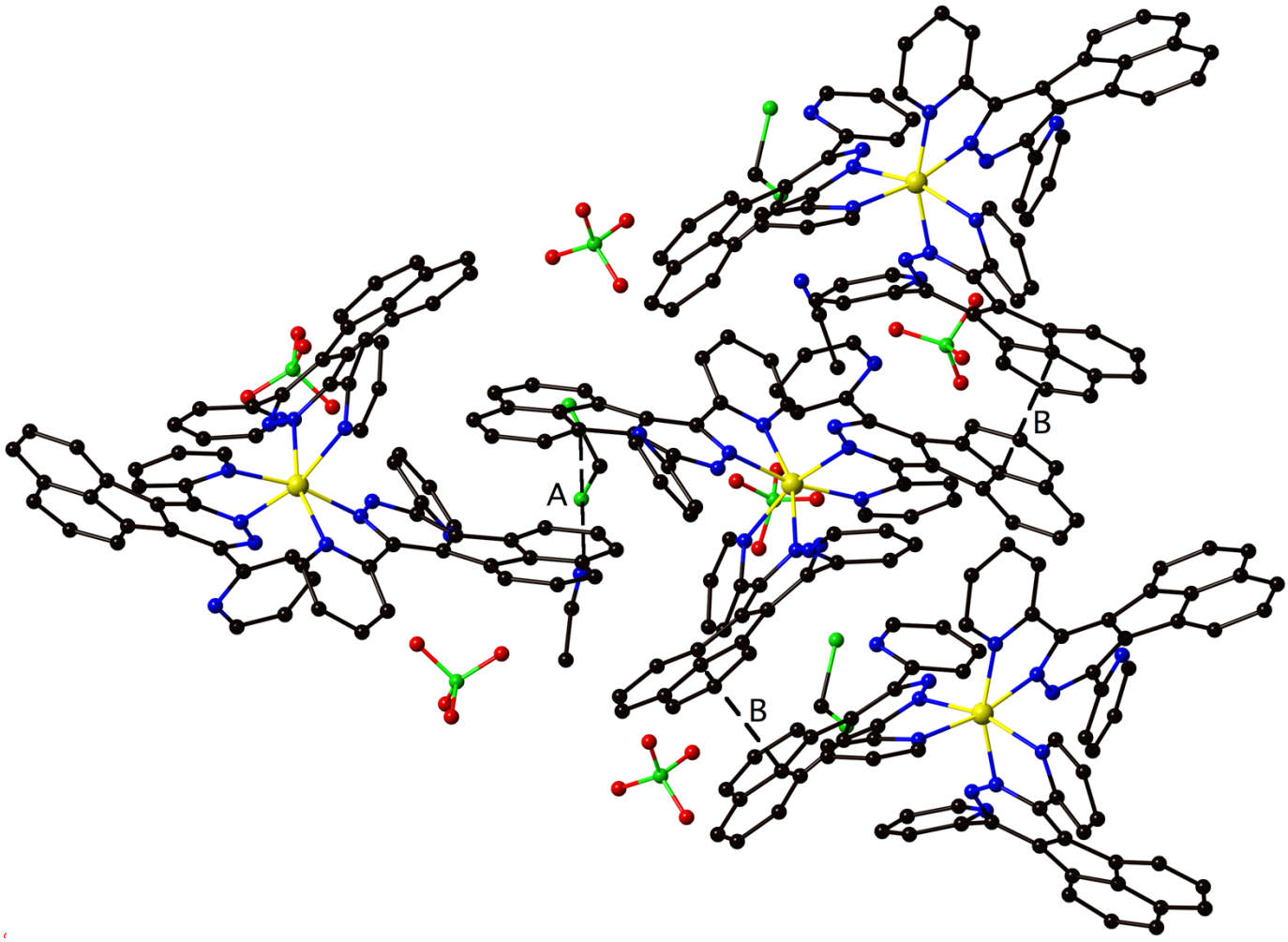

Figure S5: Perspective view of the packing of **2** showing the two independent intramolecular π-π stacks between the coordinated molecules of $\mathbf{L_2}$. The hydrogen atoms have been omitted for clarity, and a layer of solvate molecules and perchlorate counterions is shown. There are two distinct π-π stacking interactions, which can be defined by the stacking of the fluoranthrene sections of the molecules (see Table S5 below).

Stack	interplanare angle (°)	centroid-to-centroid (Å)	centroid-to-plane (Å)	planar offset (Å)
A	0.0(4)	3.815(2)	3.313(2)	1.891(3)
B	6.53(5)	3.607(2)	3.553(2)	0.765(2)

Table S5: π-π stacking interactions in structure of **2**.

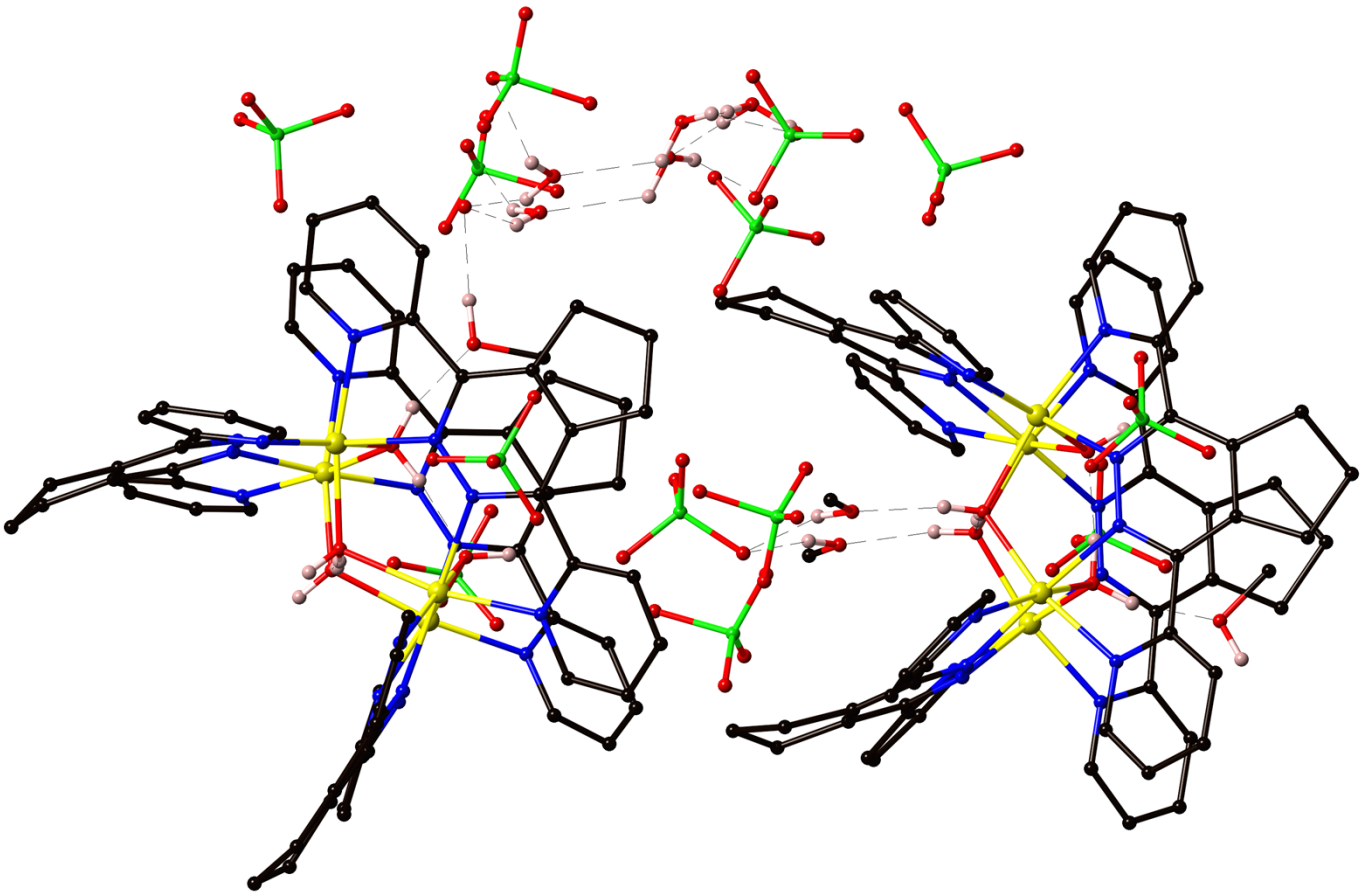

Figure S6: Perspective view of the packing of **6** showing the hydrogen bonding interactions of the solvate molecules and anions. The hydrogen atoms not involved in hydrogen bonds have been omitted for clarity. There are two distinct π-π stacking interactions, which can be defined by the stacking of the fluoranthrene sections of the molecules (see Table S5 below).

Hydrogen Bond	**D**	**H**	**A**	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
Zn-O**H**$_2$…CH_3**O**H	O54	H54	O50	0.828(18)	1.888(19)	2.707(3)	170(4)
Zn-O**H**$_2$… Zn-**O**H	O54	H54A	O54[1]	0.85(2)	1.65(2)	2.487(4)	170(6)
Zn-O**H**$_2$…CH_3**O**H	O55	H55A	O52	0.849(19)	1.72(2)	2.550(5)	164(5)
Zn-O**H**$_2$… Zn-**O**H	O55	H55B	O56	0.851(19)	1.74(2)	2.583(4)	173(5)
Zn-O**H**$_2$…Cl**O**$_4$	O56	H56	O13	0.830(19)	2.21(2)	3.036(5)	175(5)
H$_2$O…Cl**O**$_4$	O60	H60A	O2[2]	0.85	2.13	2.931(6)	157.2
H$_2$O…H$_2$**O**	O60	H60B	O57[3]	0.85	2.12	2.707(8)	125.6
H$_2$O…Cl**O**$_4$	O59	H59A	O9[4]	0.85	2.26	2.965(7)	140.2
H$_2$O…H$_2$**O**	O59	H59B	O60	0.85	1.84	2.686(5)	172.6
CH_3O**H**…H$_2$**O**	O52	H52	O58	0.85(2)	1.84(2)	2.686(7)	176(9)
H$_2$O…H$_2$**O**	O57	H57A	O58	0.85	1.91	2.694(6)	152.6
H$_2$O…Cl**O**$_4$	O57	H57B	O15[2]	0.85	2.07	2.812(6)	145.9
CH_3O**H**…Cl**O**$_4$	O50	H50	O12[5]	0.82	2.07	2.871(4)	165.5

[1]+X,1/2-Y,+Z; [2]1/2-X,-Y,-1/2+Z; [3]-1/2+X,+Y,1/2-Z; [4]+X,+Y,-1+Z; [5]-1/2+X,1/2-Y,3/2-Z

Table S6: Table of hydrogen bonds for **6**, showing the donor and receptor atoms in bold.