

Table S1. Characteristics of hydrogen bonds in structure 2

D-H...A	Distance, Å			DHA angle, deg	Transformation of atom A
	D...A, Å	D-H, Å	H...A, Å		
O1W-H2O1...O5	2.826(6)	1.07	1.76	173	-x,1-y,1-z
O1W-H1O1...O6W	2.740(7)	0.83	2.03	162	x,y,z
O2W-H1O2...O3W	2.928(7)	0.88	2.14	148	1-x,2-y,1-z
O2W-H2O2...O1	2.849(6)	0.89	2.00	160	x,1+y,z
O3W-H1O3...O6W	2.751(7)	0.83	1.93	172	-x,1-y,1-z
O3W-H2O3...O7	2.820(7)	0.85	2.03	155	1-x,2-y,1-z
O4W-H1O4...O7W	2.804(8)	0.91	2.01	145	-x-1,1-y,2-z
O5W-H1O5...O2	2.849(6)	0.95	1.90	172	x,1+y,z
O5W-H2O5...O2	2.943(6)	0.92	2.09	154	-x,1-y,2-z
O6W-H2O6...O5W	3.079(7)	0.90	2.20	166	x,y-1,z
O6W-H1O6...O9W	2.682(7)	0.90	1.93	140	x,y,z
O7W-H1O7...O7	3.026(7)	0.90	2.49	119	-x,1-y,2-z
O7W-H2O7...O8W	2.890(7)	0.90	2.00	170	x-1,y,z
O8W-H1O8...O2	2.838(7)	0.90	2.06	159	x,y,z
O8W-H2O8...O4	2.876(6)	0.90	2.12	168	-x,-y,2-z
O9W-H1O9...O4	2.734(7)	0.90	1.83	176	x,y,z
O9W-H2O9...O8W	2.790(7)	0.90	1.90	167	x-1,y,z

Table S2. Characteristics of hydrogen bonds in structure 3

D-H...A	Distance, Å			DHA angle, deg	Transformation of atom A
	D...A, Å	D-H, Å	H...A, Å		
O1W-H2O1...O4W	2.732(2)	0.89	1.85	167	1-x,1-y,2-z
O1W-H1O1...O1	2.727(2)	0.89	1.85	169	1-x,1-y,2-z
O2W-H1O2...O5	2.735(2)	0.88	1.86	172	x,y,z-1

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O2W-H2O2...O6	2.816(2)	0.89	1.98	156	1-x,2-y,2-z
O3W-H2O3... O8W	2.756(2)	0.90	1.89	161	x,y,z
O3W-H1O3...O1W	3.065(2)	0.89	2.25	151	-x,-y,-z-1
O4W-H2O4...O6W	2.816(2)	0.89	1.93	172	x,y,z
O4W-H1O4...O2W	2.752(2)	0.90	1.87	166	1-x,1-y,1-z
O5W-H1O5...O4	3.050(2)	0.90	2.41	129	-x,1-y,1-z
O5W-H2O5...O8	2.741(2)	0.91	1.85	168	1-x,2-y,2-z
O6W-H2O6...O8	2.695(2)	0.90	1.90	157	1-x,1-y,2-z
O6W-H1O6...O7W	2.770(3)	0.89	1.91	162	-x,-y,1-z
O7W-H2O7...O6W	2.846(2)	0.90	2.00	157	x,y,z
O7W-H1O7 ..O6	2.762(3)	0.90	1.92	153	x,y-1,z-1
O8W-H2O8...O7W	2.843(2)	0.89	1.96	173	x,y,z
O8W-H1O8...O8	3.020(2)	0.88	2.23	149	x-1,y-1,z-1

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Fig. S2. Fragment of the crystal structure of compound 3.

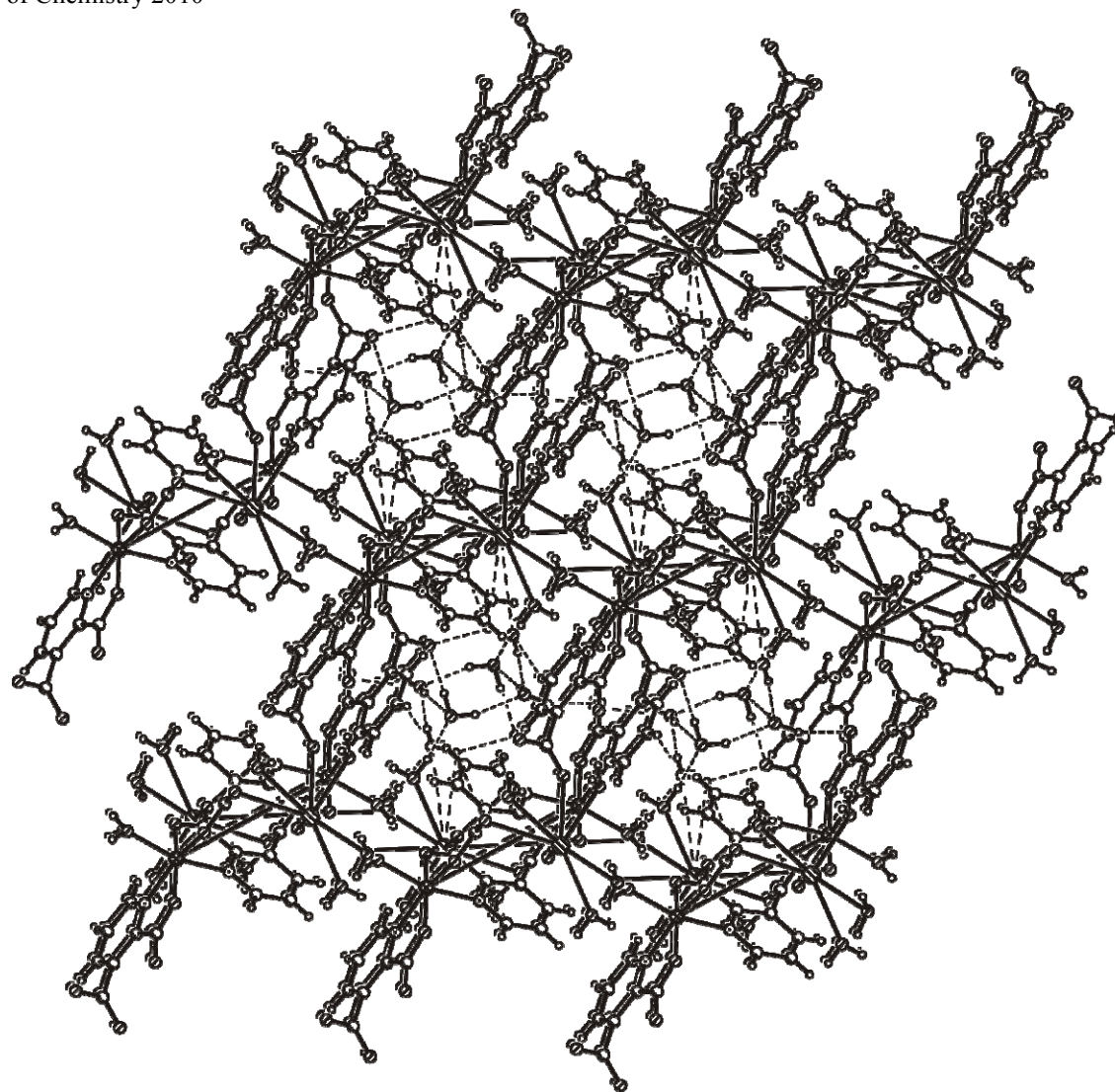


Fig. S1. Fragment of the crystal structure of compound 2.

