Electronic Supplementary Material (ESI) for CrystEngComm

Supporting Information

Construction of diverse Cd^{II}/Zn^{II} coordination polymers based on 5-(quinolyl)tetrazolate generated via *in situ* hydrothermal synthesis

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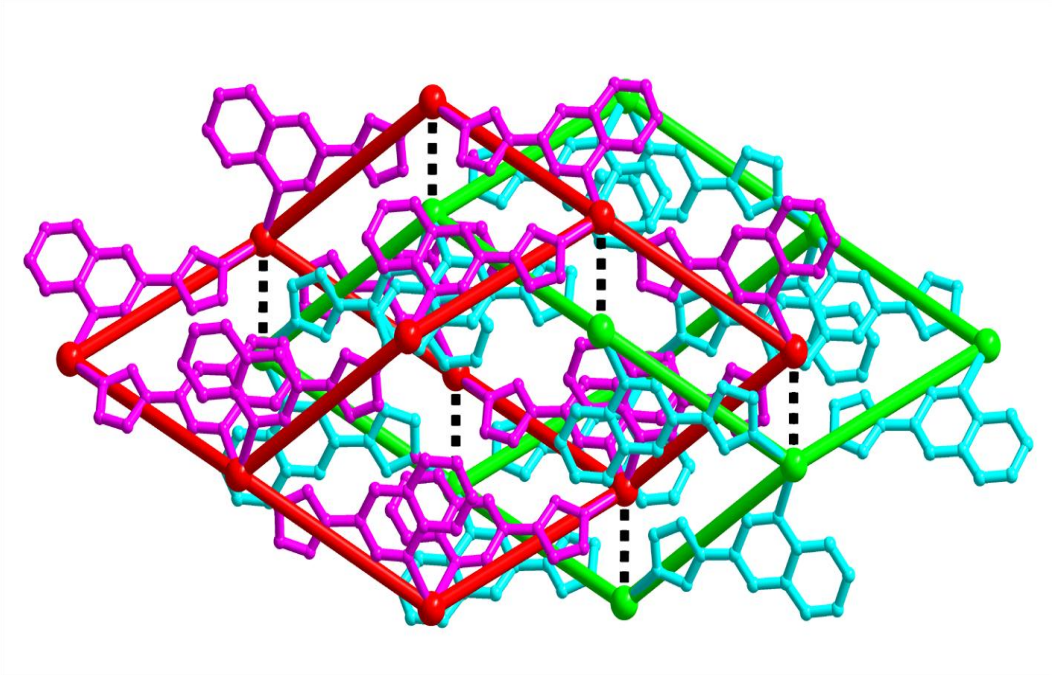

Fig S1. The strong interaction between Cd...Cd in compound **1**.

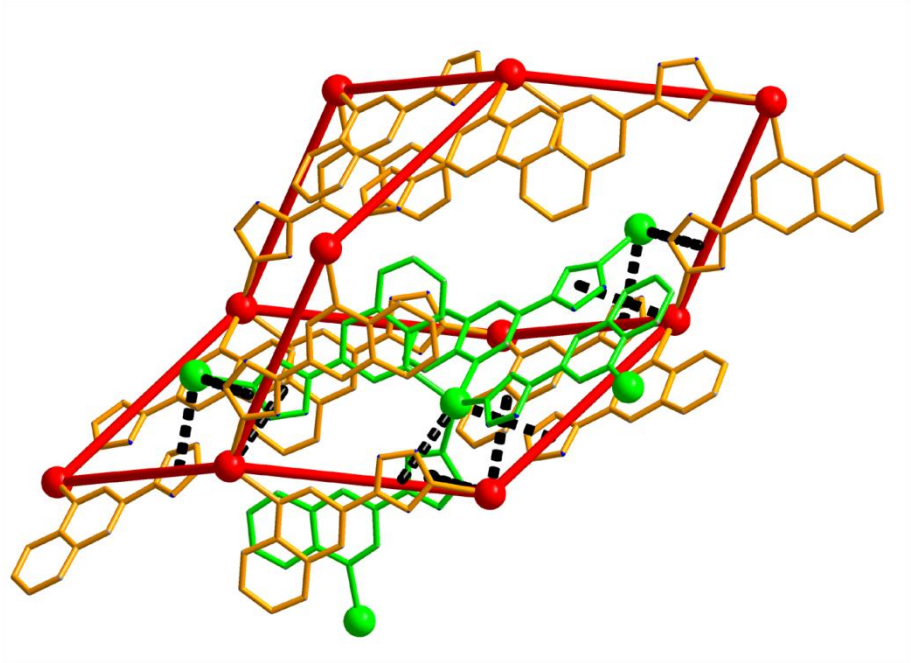

Fig S2. The cation...π interaction between the Cd centers and tetrazole rings in compound **1**.

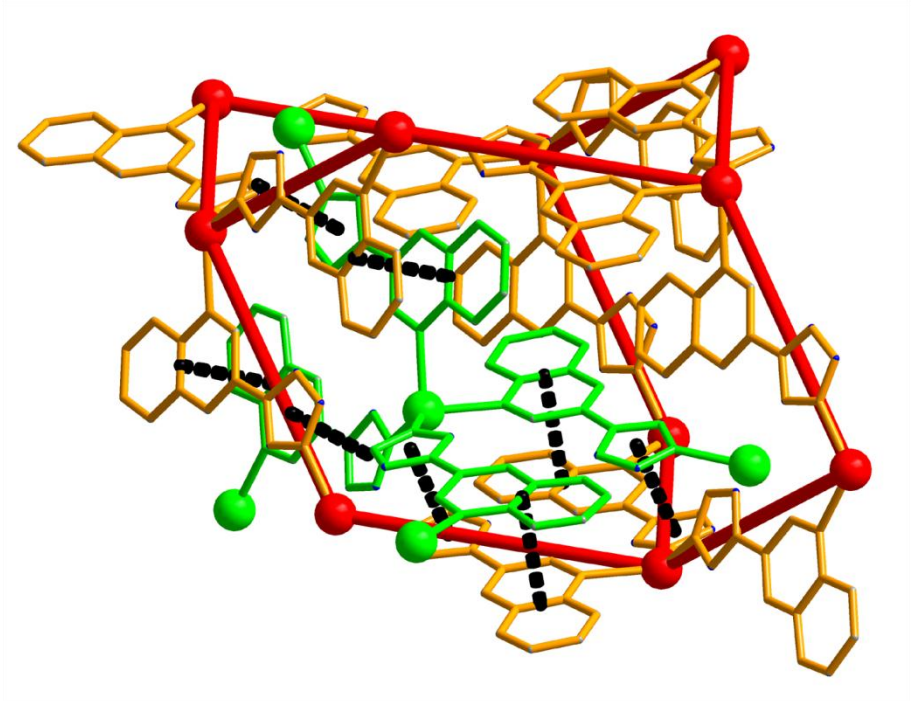

Fig S3. The π...π stacking between quinline ring and tetrazole ring in compound **1**.

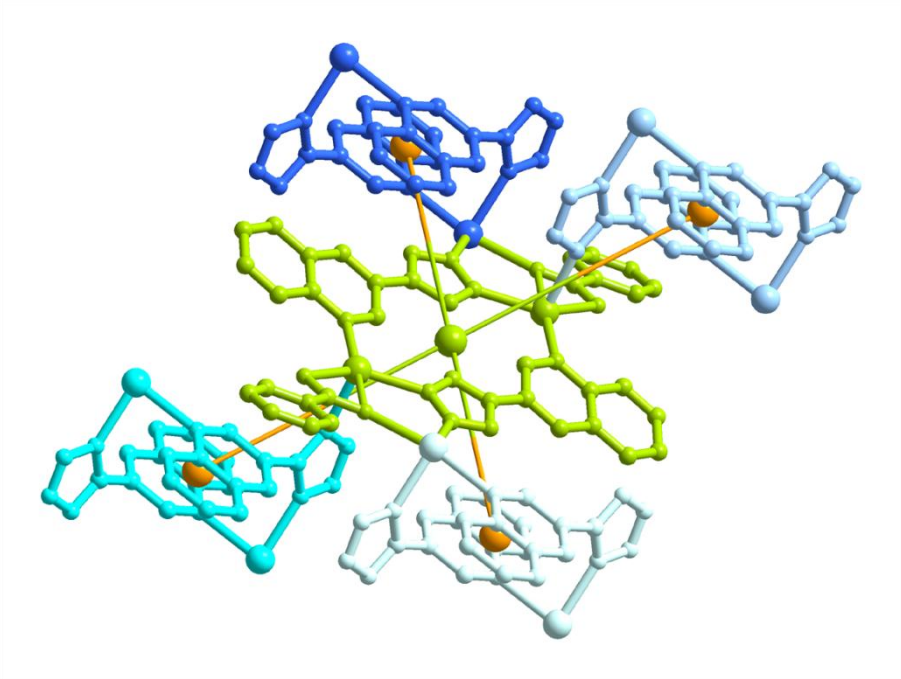

Fig S4. The four connected node simplified by $Cd_4(QTZ)_2(IN)_2$ subunit (show in green) in compound **4**.

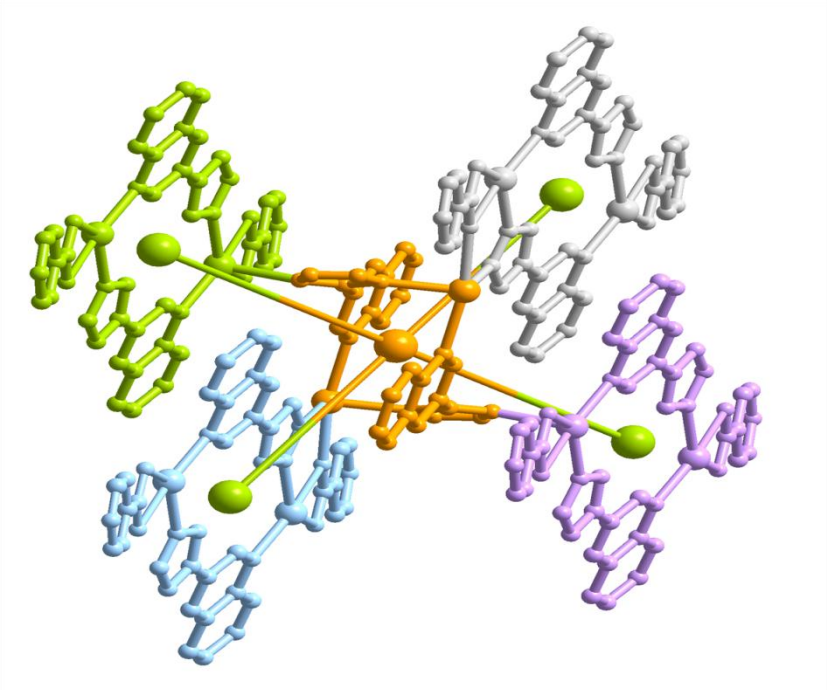

Fig S5. Another four connected node simplified by $Cd_2(QTZ)_2$ subunit (show in orange) in compound **4**.

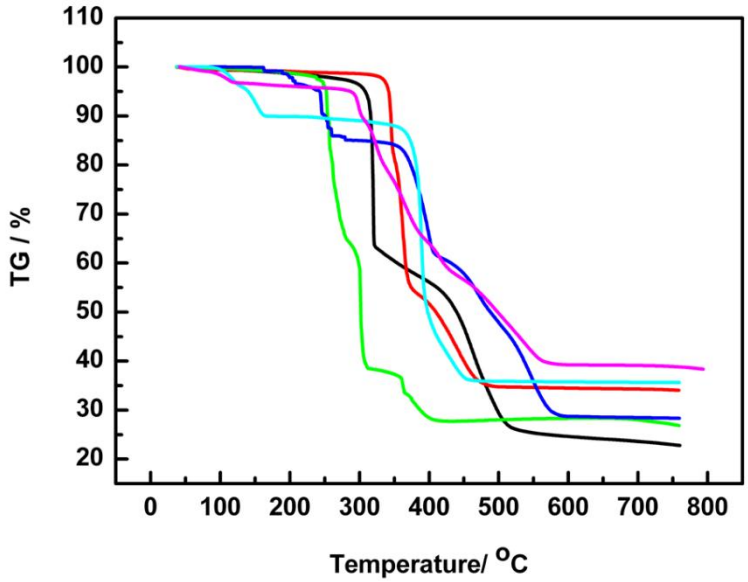

Fig S6. The TGA curves of compound **1** (black), compound **2** (red), compound **3** (green), compound **4** (blue), compound **5** (cyan), compound **6** (magenta).

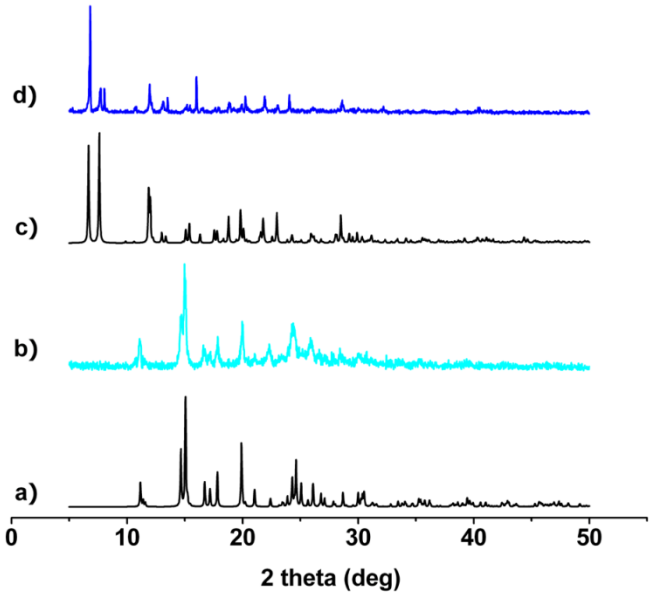

Fig S7. PXRD patterns (a) simulated based on the X-ray single-crystal diffraction date of **3**, (b) for as-synthesized **3**, (c) simulated based on X-ray single-crystal diffraction date of **4**, and (d) for as-synthesized **4**.

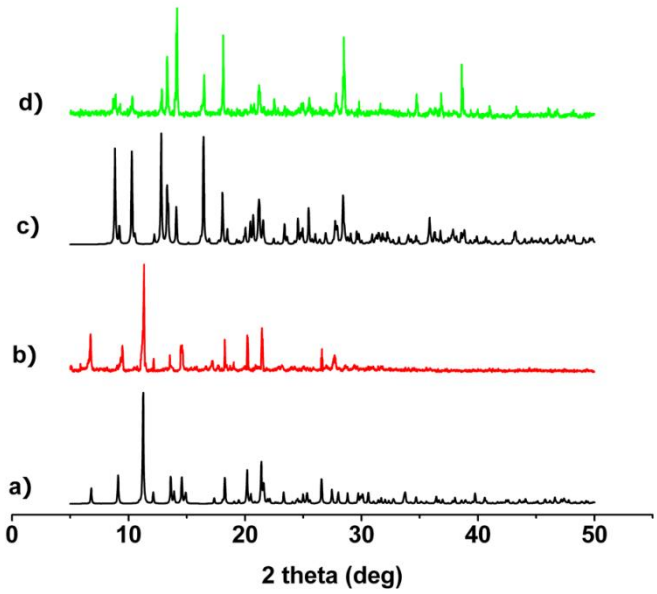

Fig S8. PXRD patterns (a) simulated based on the X-ray single-crystal diffraction date of **5**, (b) for as-synthesized **5**, (c) simulated based on X-ray single-crystal diffraction date of **6**, and (d) for as-synthesized **6**.

Table S1. Selected bond angles (°) for compounds **1-6**

Compound **1** [a]			
N(4)#1-Cd(1)-N(4)#2	127.63(8)	N(4)#1-Cd(1)-N(1)	110.79(6)
N(4)#2-Cd(1)-N(1)#3	110.79(6)	N(4)#2-Cd(1)-N(1)	106.36(6)
N(1)-Cd(1)-N(1)#3	87.69(8)	N(4)#1-Cd(1)-N(1)#3	106.36(6)
Compound **2** [b]			
N(6)#1-Cd(1)-N(3)#3	84.26(9)	N(6)#1-Cd(1)-O(1)	159.96(8)
N(6)-Cd(1)-N(3)#3	157.21(10)	N(6)-Cd(1)-O(1)	80.83(9)
N(4)#2-Cd(1)-N(3)#3	93.00(9)	N(4)#2-Cd(1)-O(1)	96.55(9)
O(1)-Cd(1)-N(3)#3	77.13(8)	N(6)#1-Cd(1)-N(1)	87.00(9)
N(1)-Cd(1)-N(3)#3	91.82(9)	N(6)-Cd(1)-N(1)	92.48(9)
N(6)#1-Cd(1)-N(6)	118.31(10)	N(4)#2-Cd(1)-N(1)	174.87(9)
N(6)#1-Cd(1)-N(4)#2	91.72(9)	O(1)-Cd(1)-N(1)	86.25(8)
N(6)-Cd(1)-N(4)#2	83.75(9)		
Compound **3** [c]			
N(3)#1-Zn(1)-Cl(1)	119.90(13)	N(3)#1-Zn(1)-N(5)#2	101.25(17)
N(5)#2-Zn(1)-Cl(1)	105.68(13)	N(3)#1-Zn(1)-N(1)	108.87(16)
N(1)-Zn(1)-Cl(1)	112.67(14)	N(5)#2-Zn(1)-N(1)	107.06(16)
Compound **4** [d]			
N(10)#1-Cd(2)-N(8)	103.31(10)	N(11)#1-Cd(1)-N(3)#2	101.46(10)
O(1)-Cd(2)-N(8)	118.62(10)	O(4)-Cd(1)-N(3)#2	93.46(11)
N(10)#1-Cd(2)-N(7)#3	95.57(11)	O(2)-Cd(1)-N(3)#2	169.21(10)
O(1)-Cd(2)-N(7)#3	88.30(10)	N(4)-Cd(1)-O(3)	168.13(11)
N(8)-Cd(2)-N(7)#3	96.99(10)	N(11)#1-Cd(1)-O(3)	82.14(11)
N(10)#1-Cd(2)-N(2)#4	91.55(11)	O(4)-Cd(1)-O(3)	54.65(11)
O(1)-Cd(2)-N(2)#4	81.53(10)	O(2)-Cd(1)-O(3)	100.11(12)
N(8)-Cd(2)-N(2)#4	88.41(11)	N(3)#2-Cd(1)-O(3)	89.10(12)
N(4)-Cd(1)-N(3)#2	85.51(10)	N(10)#1-Cd(2)-O(1)	137.11(10)
N(4)-Cd(1)-N(11)#1	109.29(10)	N(7)#3-Cd(2)-N(2)#4	169.81(11)
N(4)-Cd(1)-O(4)	115.07(11)	N(10)#1-Cd(2)-O(2)	83.23(10)
N(11)#1-Cd(1)-O(4)	134.05(11)	O(1)-Cd(2)-O(2)	53.92(9)
N(4)-Cd(1)-O(2)	84.39(10)	N(8)-Cd(2)-O(2)	168.32(10)
N(11)#1-Cd(1)-O(2)	85.49(10)	N(7)#3-Cd(2)-O(2)	91.92(10)
O(4)-Cd(1)-O(2)	87.40(11)	N(2)#4-Cd(2)-O(2)	81.68(11)
Compound **5** [e]			
O(6)#3-Cd(2)-N(3)#4	119.67(10)	N(2)-Cd(1)-O(5)#2	85.86(11)
O(4)-Cd(2)-N(3)#4	93.73(11)	O(1W)-Cd(1)-O(5)#2	171.87(8)
O(6)#3-Cd(2)-O(2W)	89.40(6)	N(5)#1-Cd(1)-O(5)#2	101.03(11)
O(4)-Cd(2)-O(2W)	89.87(10)	O(2)-Cd(1)-O(1)	53.38(9)
N(3)#4-Cd(2)-O(2W)	90.95(10)	N(2)-Cd(1)-O(1)	82.78(10)
O(6)#3-Cd(2)-O(1)#4	82.50(8)	O(1W)-Cd(1)-O(1)	89.70(8)
O(4)-Cd(2)-O(1)#4	102.01(11)	N(5)#1-Cd(1)-O(1)	173.72(10)

N(3)#4-Cd(2)-O(1)#4	85.08(11)	O(5)#2-Cd(1)-O(1)	82.21(9)
O(2)-Cd(1)-O(5)#2	83.90(10)	O(6)#3-Cd(2)-O(4)	146.60(8)
O(2)-Cd(1)-N(2)	135.90(11)	O(2W)-Cd(2)-O(1)#4	167.68(8)
O(2)-Cd(1)-O(1W)	91.88(9)	O(6)#3-Cd(2)-O(3)	91.65(8)
N(2)-Cd(1)-O(1W)	92.42(10)	O(4)-Cd(2)-O(3)	55.02(10)
O(2)-Cd(1)-N(5)#1	121.31(11)	N(3)#4-Cd(2)-O(3)	148.53(11)
N(2)-Cd(1)-N(5)#1	102.74(12)	O(2W)-Cd(2)-O(3)	92.44(10)
O(1W)-Cd(1)-N(5)#1	87.10(10)	O(1)#4-Cd(2)-O(3)	97.04(11)
Compound **6** [f]			
N(5)#5-Cd(1)-O(2)	88.39(18)	O(3)#2-Cd(2)-N(2)	82.34(13)
O(1)-Cd(1)-O(2)	53.26(16)	O(1W)#3-Cd(2)-N(2)#3	90.89(12)
N(3)-Cd(1)-O(2)	89.9(2)	O(1W)-Cd(2)-N(2)#3	174.15(13)
N(5)#5-Cd(1)-O(3)#2	134.36(14)	O(3)#4-Cd(2)-N(2)#3	82.34(13)
O(1)-Cd(1)-O(3)#2	94.26(18)	O(3)#2-Cd(2)-N(2)#3	90.20(15)
N(3)-Cd(1)-O(3)#2	79.26(13)	N(2)-Cd(2)-N(2)#3	91.19(19)
O(2)-Cd(1)-O(3)#2	137.0(2)	N(5)#5-Cd(1)-O(1)	124.8(2)
N(5)#5-Cd(1)-O(4)#2	102.80(12)	N(5)#5-Cd(1)-N(3)	100.39(12)
O(1)-Cd(1)-O(4)#2	85.55(16)	O(1)-Cd(1)-N(3)	115.4(2)
O(1W)#3-Cd(2)-O(1W)	87.57(16)	N(3)-Cd(1)-O(4)#2	129.97(12)
O(1W)#3-Cd(2)-O(3)#4	84.66(14)	O(2)-Cd(1)-O(4)#2	134.11(17)
O(1W)-Cd(2)-O(3)#4	103.12(12)	O(3)#2-Cd(1)-O(4)#2	53.09(12)
O(1W)#3-Cd(2)-O(3)#2	103.12(12)	N(5)#5-Cd(1)-C(16)#2	121.63(13)
O(1W)-Cd(2)-O(3)#2	84.66(14)	O(1)-Cd(1)-C(16)#2	89.46(14)
O(3)#4-Cd(2)-O(3)#2	169.4(2)	N(3)-Cd(1)-C(16)#2	104.51(14)
O(1W)#3-Cd(2)-N(2)	174.15(13)	O(2)-Cd(1)-C(16)#2	142.43(14)
O(1W)-Cd(2)-N(2)	90.89(12)	O(3)#2-Cd(1)-C(16)#2	26.14(13)
O(3)#4-Cd(2)-N(2)	90.20(15)	O(4)#2-Cd(1)-C(16)#2	26.96(12)

[a] #1: x-1/4,y-1/4,-z; #2: -x+1/2,y-1/4,z+1/4; #3: -x+1/4,y,-z+1/4; #4: x+1/4,y+1/4,-z; [b] #1: x,-y+1/2,z-1/2; #2: -x,y+1/2,-z+3/2; #3: -x,-y,-z+1; #4: -x,y-1/2,-z+3/2; #5: x,-y+1/2,z+1/2; [c] #1: x,-y+3/2,z+1/2; #2: -x+1,-y+2,-z+2; #3: x,-y+3/2,z-1/2; [d] #1: -x+1,-y+2,-z; #2: -x,-y+1,-z; #3: -x+1,-y+1,-z; #4: -x+1,-y+2,-z+1; [e] #1: -x+1,-y+1,-z+1; #2: -x+2,-y+1,-z; #3: x,y-1,z; #4: -x+2,-y,-z; #5: x,y+1,z; [f] #1: -x+1,y,-z-1/2; #2: -x+1/2,-y+1/2,-z; #3: -x+1,y,-z+1/2; #4: x+1/2,-y+1/2,z+1/2; #5: -x+1,-y,-z.

Table S2. Hydrogen bonds geometries (Å, °) for compounds **1**-**6**

D—H···A	Distance (D···A)	Angle (D—H···A)	D—H···A	Distance (D···A)	Angle (D—H···A)
Compound **1** [a]					
C(1)-H(1)...N(2)	2.913(2)	102			
Compound **2** [b]					
O(1)-H(1A)...N(2)#1	2.907(6)	123	O(1)-H(1B)...N(5)#2	2.862(3)	173
C(1)-H(1)...O(1)	3.239(7)	127			
Compound **3** [c]					
C(1)-H(1)...N(2)	2.805(6)	102	C(1)-H(1)...N(2)#1	3.126(6)	148
C(3)-H(3)...N(4)#2	3.462(6)	153			
Compound **4** [d]					
O1W-H1WA...O4	2.846(14)	164	O1W-H1WB...N1#1	3.021(16)	157
C6-H6...O4	3.189(7)	144	C11-H11...O1#2	3.011(6)	123
C15-H15...N12#3	3.254(6)	156	C18-H18...N1#4	3.393(8)	158
C25-H25...N9	2.921(5)	101	C25-H25...N9#5	3.264(5)	145
C27-H27...O1	3.475(5)	165	C28-H28...O3#6	3.332(7)	146
C30-H30...N6#7	3.397(7)	154			
Compound **5** [e]					
O(1W)-H(1A).O(4W)	2.661(7)	163	O(1W)-H(1B)...O(2)#1	2.753(5)	174
O(2W)-H(2A).O(5)#2	2.813(3)	163	O(2W)-H(2B).O(3W)#3	2.729(7)	174
O(3W)-H(3A)...N(4)#4	2.928(2)	151	O(3W)-H(3B).O(3W)#5	3.160(7)	149
O(4W)-H(4B)..O(6)#1	2.887(2)	119			
Compound **6** [f]					
O(1W)-H(1A)...O(2W)	2.798(9)	156	O(1W)-H(1B)..O(1)#1	3.104(2)	164
O(2W)-H(2A)..O(2W)#2	2.498(8)	133	O(2W)-H(2B)..O(1W)	2.798(9)	141
C(3)-H(3)...N(4)	2.915(6)	100	C(3)-H(3)...N(4)#3	3.236(6)	150
C(5)-H(5)...O(4)#4	3.160(6)	153	C(6)-H(6)...O(2) #5	3.291(9)	149
C(13)-H(13)...O(2)	2.786(7)	100	C(13)-H(13)..O(2)#6	2.786(7)	100

[b] #1: -x,-y,1-z; #2: -x,-y,2-z; [c] #1: 1-x,2-y,2-z; #2: 1-x,-1/2+y,3/2-z; [d] #1: 1-x,1-y,1-z; #2: 1-x,2-y,1-z; #3: -1+x,-1+y,z; #4: -1+x,y,-1+z; #5: 1-x,2-y,-z; #6: 1+x,y,z; #7: 1+x,1+y,z; [e] #1: 1-x,1-y,-z; #2: 2-x,-y,-1-z; #3: x,-1+y,-1+z; #4: x,1+y,z; #5: 2-x,2-y,1-z; [f] #1: 1/2-x,1/2-y,-z; #2: 3/2-x,1/2-y,-z; #3: 1-x,-y,-z; #4: 1/2+x,-1/2+y,z; #5: 2-x,-y,-z; #6: 1-x,y,-1/2-z.