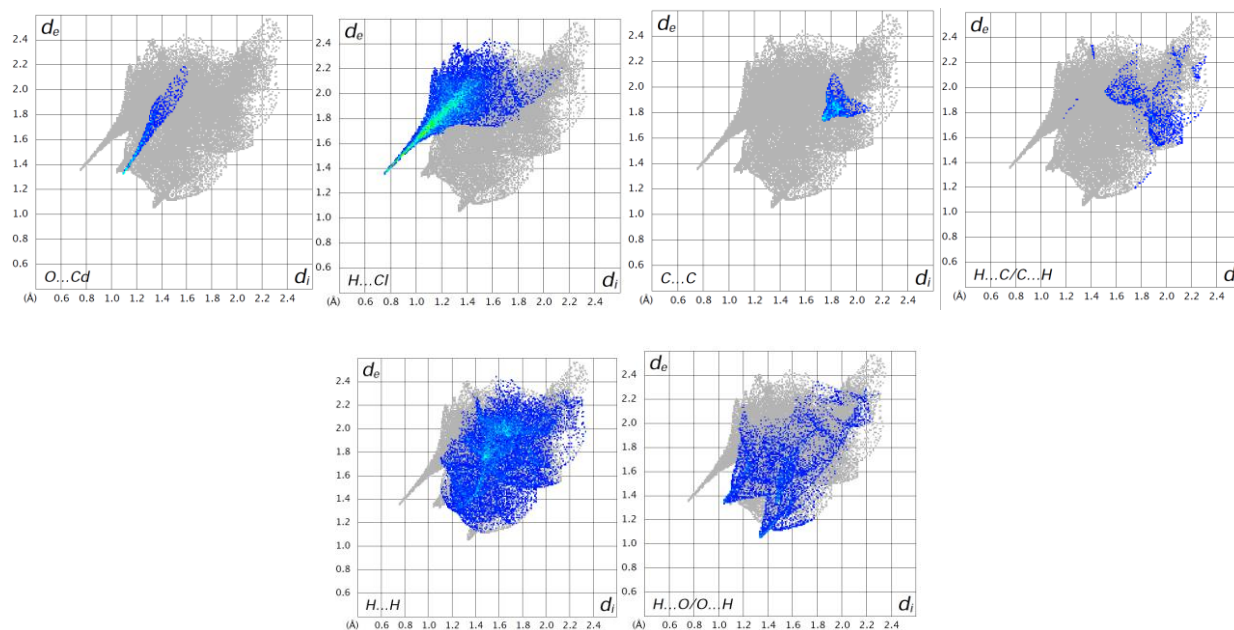


Compound (I)



Compound (II)

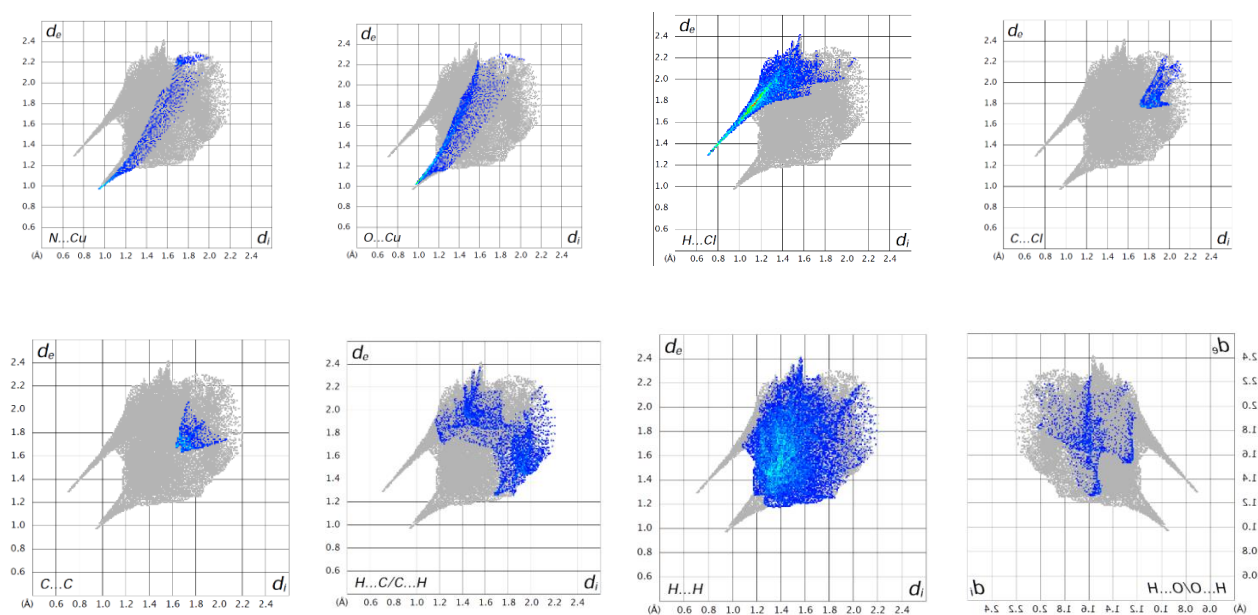


Figure S1. The 2D fingerprint plots of the maincontacts around the ligand for both compounds.

Table S1. Bond lengths and angles for compound (I) and compound (II).

Compound (I)			
Bond	<i>d</i> (Å)	Bond	<i>d</i> (Å)
Cd1—Cl3 ⁱ	2.6372 (2)	N1—C6	1.3517 (13)
Cd1—Cl3	2.6153 (2)	C2—C1	1.5029 (12)
Cd1—Cl1	2.5948 (2)	C2—C3	1.3796 (13)
Cd1—Cl1 ⁱⁱ	2.6047 (2)	C5—C4	1.3876 (14)
Cd1—Cl2	2.5777 (2)	C5—C6	1.3733 (15)
Cd1—O1	2.4214 (7)	C4—C3	1.3891 (13)
O1—C1	1.4200 (11)	C6—C7	1.455 (4)
N1—C2	1.3488 (11)	O3—C7	1.415 (4)
C8—O2	1.426 (4)	C6—C8	1.571 (4)
Angles (°)	ω (°)	Angles (°)	ω (°)
Cl3—Cd1—Cl3 ⁱ	167.972(4)	C6—C5—C4	119.17(9)
Cl1—Cd1—Cl3 ⁱ	84.090(7)	C5—C4—C3	120.37(9)
Cl1 ² —Cd1—Cl3 ⁱ	89.977(6)	O1—C1—C2	112.56(7)
Cl1 ² —Cd1—Cl3	84.331(7)	N1—C6—C5	118.84(8)
Cl1—Cd1—Cl3	99.587(7)	N1—C6—C8	111.33(17)
Cl1—Cd1—Cl1 ²	168.469(3)	N1—C6—C7	121.45(15)
Cl2—Cd1—Cl3 ⁱ	95.087(7)	C5—C6—C8	129.54(18)
Cl2—Cd1—Cl3	96.125(7)	C5—C6—C7	119.70(15)
Cl2—Cd1—Cl1 ²	97.128(7)	C7—C6—C8	11.94(18)
Cl2—Cd1—Cl1	93.248(7)	C2—C3—C4	119.38(9)
O1—Cd1—Cl3	80.281(17)	O2—C8—C6	113.6(3)
O1—Cd1—Cl3 ⁱ	88.834(17)	O3—C7—C6	107.2(3)
O1—Cd1—Cl1	83.368(17)	C1—O1—Cd1	120.50(5)
O1—Cd1—Cl1 ²	86.643(17)	C2—N1—C6	123.89(8)
O1—Cd1—Cl2	174.545(18)	N1—C2—C1	117.01(8)
Cd1—Cl3—Cd1 ²	94.156(6)	N1—C2—C3	118.35(8)
Cd1—Cl1—Cd1 ¹	95.420(7)	C3—C2—C1	124.60(8)
(i) $-x+1, y-1/2, -z+1/2$; (ii) $-x+1, y+1/2, -z+1/2$.			
Compound (II)			
Bond (Å)	<i>d</i> (Å)	Bond	<i>d</i> (Å)
Cu1—Cl1	2.2228 (4)	N1—C6	1.3437 (19)
Cu1—Cl2	2.5062 (4)	N1—C2	1.3438 (18)
Cu1—O1	2.0120 (12)	C6—C7	1.505 (2)
Cu1—O2	2.0305 (12)	C6—C5	1.383 (2)
Cu1—N1	1.9356 (12)	C4—C3	1.394 (2)
O1—C1	1.4379 (19)	C4—C5	1.394 (2)
O2—C7	1.4309 (19)	C1—C2	1.504 (2)
C3—C2	1.389 (2)		
Angles (°)	ω (°)	Angles (°)	ω (°)
C3—C4—C5	119.94 (13)	O2—Cu1—Cl1	97.66 (3)
O1—C1—C2	107.41 (11)	O2—Cu1—Cl2	98.03 (4)
C2—C3—C4	118.37 (13)	N1—Cu1—Cl1	162.48 (4)
O2—C7—C6	108.03 (12)	N1—Cu1—Cl2	97.31 (4)
C6—C5—C4	118.76 (14)	N1—Cu1—O1	79.11 (5)
N1—C2—C1	114.82 (12)	N1—Cu1—O2	79.09 (5)
N1—C2—C3	120.84 (13)	C1—O1—Cu1	115.24 (9)
C3—C2—C1	124.35 (13)	C7—O2—Cu1	117.01 (9)

Cl1—Cu1—Cl2	100.192 (15)	C6—N1—Cu1	119.75 (10)
O1—Cu1—Cl1	97.81 (4)	N1—C6—C7	115.27 (12)
O1—Cu1—Cl2	102.13 (4)	N1—C6—C5	120.72 (13)
O1—Cu1—O2	151.90 (5)	C6—N1—C2	121.35 (12)
C5—C6—C7	124.01 (13)	C2—N1—Cu1	118.77 (10)

Table S2. Non-covalent interactions in the crystal structure of compound (I) and (II).

Compound (I)				
D—H...A	d(D—H) (Å)	d(H—A) (Å)	d(D—A) (Å)	D—H...A (°)
O1—H1...Cl2 ¹	0.858 (8)	2.289 (8)	3.1294 (7)	166.5 (13)
O2—H2...Cl2 ²	0.84	2.84	3.6676 (19)	163.2
O3—H3A...Cl3 ⁶	0.84	2.26	3.1002 (14)	176.0
C1—H1B...Cl2 ⁴	0.99	2.75	3.5511 (11)	138.3
C1—H1C...Cl3 ²	0.99	2.89	3.4279 (9)	114.8
C1—H1C...Cl2 ²	0.99	2.76	3.6778 (10)	154.6
C3—H3...Cl2 ¹	0.95	2.84	3.7443 (9)	159.0
C5—H5...Cl3 ³	0.95	2.80	3.6630 (9)	150.8
C7—H7A...Cl1 ⁴	0.99	2.87	3.453 (4)	118.8
C7—H7B...Cl2 ⁷	0.99	2.94	3.921 (5)	170.4
C8—H8A...Cl3 ⁶	0.99	2.92	3.832 (5)	153.5
C8—H8B...Cl3 ³	0.99	2.92	3.827 (4)	152.5
C3—H3...O3 ⁵	0.95	2.46	3.0752 (16)	122.1
N1—H1A...Cl2 ²	0.88	2.53	3.3854 (9)	165.8
(1) 1-x, 1/2+y, 1/2-z; (2) 1-x, -1/2+y, 1/2-z; (3) 2-x, 1-y, 1-z; (4) 1+x, y, z; (5) x, 1+y, z; (6) 1+x, -1+y, z; (7) 1+x, 1/2-y, 1/2+z.				
Compound (II)				
D—H...A	d(D—H) (Å)	d(H—A) (Å)	d(D—A) (Å)	D—H...A (°)
O1—H1...Cl2 ¹	0.84	2.16	2.9950 (12)	170.7
O2—H2...Cl2 ²	0.84	2.23	3.0587 (12)	168.4
C1—H1A...Cl1 ¹	0.99	2.76	3.6594 (16)	151.3
C1—H1B...Cl1 ³	0.99	2.89	3.8666 (16)	168.2
C3—H3...Cl2 ³	0.95	2.86	3.7054 (15)	148.6
C5—H5...Cl1 ⁶	0.95	2.90	3.6505 (16)	136.9
C7—H7A...Cl2 ⁴	0.99	2.98	3.9522 (16)	168.7
C7—H7B...Cl2 ⁵	0.99	2.98	3.8659 (16)	149.4
(1) 1-x, -y, 1-z; (2) 2-x, 1-y, 1-z; (3) -1+x, y, z; (4) x, 1+y, z; (5) 2-x, 1-y, 2-z; (6) x, 1+y, 1+z.				

Table S3. Comparison of the IR frequencies of compound (I) and (II).

Assignments	Compound (I)	Compound (II)
$\nu(\text{OH})$	3424	3221
	3380	
$\nu(\text{NH})$	3320	-
	3259	
$\nu(\text{CH})$	3155	3030
	3078	
$\nu(\text{CH}_2)$	2968	2798
	2913	
$\nu(\text{C}=\text{C})$	1627	1599
$\nu(\text{C}=\text{N})$	1429	1519
	1395	
$\delta_{\text{in}}(\text{C}-\text{OH})$	1207	1269
	1157	
$\nu(\text{C}-\text{O})$	1055	1019
$\omega_{\text{op}}(\text{CH})$	795	797