Supporting Information

Single-Crystal-to-Single-Crystal Transformation of an Anion Exchangeable Dynamic Metal-Organic Framework

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Experimental Section:

Materials: All the reagents and solvents were commercially available and used without further purification.

Synthesis of Compound 1: DCM solution of the ligand (21 mg, 1mL) was taken into a glass tube onto which was poured tetrahydrofuran (THF) (1 ml) above which was layered methanolic solution of $Cd(ClO_4)_2$ (31 mg, 1mL). Rod Shaped yellow crystals suitable for X-ray studies were obtained after 15 days in 70 % yield. SQUEEZE routine of PLATON has been used to remove highly disordered guest molecules in compound 1.

Synthesis of Compound 2: When parent crystals are being taken out from the mother liquor and kept in open air for about 2 hrs; it gives rise to another type crystal (confirmed by single x-ray studies).

Elemental analysis (%) calcd for C_{28} H_{32} Cl_2 N_8 $O_{11}Cd_1$: C 40.00, H 3.84, N 13.52. Found: C 40.92, H 3.98, N 13.86.

Anion exchange study: Single crystals of compound **1** were separately dipped in aqueous solutions (1 mmol/10 mL H_2O) of NaN_3 and KSCN for about 7 days at RT which yielded the anion exchanged product. The products were characterized by FT-IR, XPRD.

Anion selectivity study:

Separation of N_3^- and SCN^-: Single crystals of compound 1 were separately dipped in aqueous solution (10 mL) of equimolar NaN_3(1 mmol) and KSCN (1mmol) for about 7 days at RT giving rise to the anion exchange product, characterized by FT-IR spectra.

Physical measurements: Powder X-ray diffraction (PXRD) patterns were measured on Bruker D8 Advanced X-Ray diffractometer at room temperature using Cu-Kα radiation (λ= 1.5406 Å) with a scan speed of 0.5° min^{-1} and a step size of 0.01° in 2 *theta*. Thermogravimetric analysis was recorded on Perkin-Elmer STA 6000, TGA analyser under N_2 atmosphere with heating rate of 10° C/min. The IR-spectra were recorded on a *Thermoscientific*–Nicolet-6700 FT-IR spectrometer. FT-IR spectra were recorded on NICOLET 6700 FT-IR Spectrophotometer using KBr Pellets.

X-ray Structural Studies: Single-crystal X-ray data of compound 1⊃ G and compound 1 were collected at 100 K on a Bruker KAPPA APEX II CCD Duo diffractometer (operated at 1500 W power: 50 kV, 30 mA) using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). Crystal was on nylon CryoLoops (Hampton Research) with Paraton-N (Hampton Research). The data integration and reduction were processed with SAINT[1] software. A multi-scan absorption correction was applied to the collected reflections. The structure was solved by the direct method using SHELXTL[2] and was refined on F^2 by full-matrix least-squares technique using the SHELXL-97[3] program package within the WINGX[4] programme. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were located in successive difference Fourier maps and they were treated as riding atoms using SHELXL default parameters. The structures were examined using the *Adsym* subroutine of PLATON[5] to assure that no additional symmetry could be applied to the models.

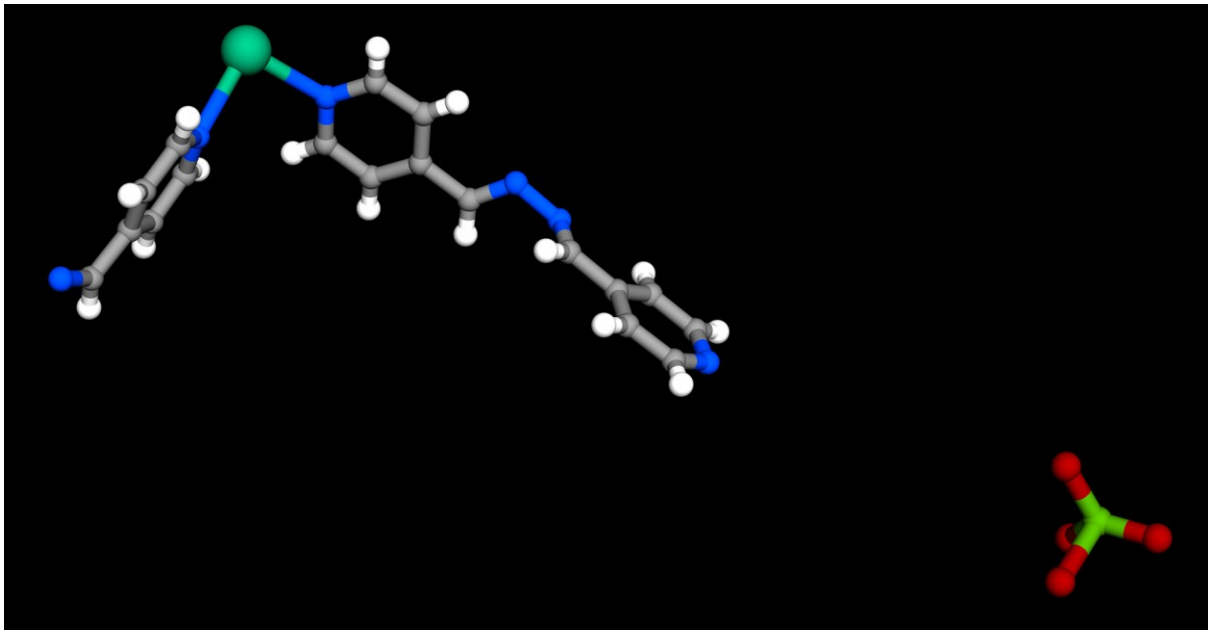

Figure S1: Asymmetric unit of compound 1 (Color code; Carbon: gray, oxygen: red, nitrogen: blue, chlorine: green, cadmium: light green)

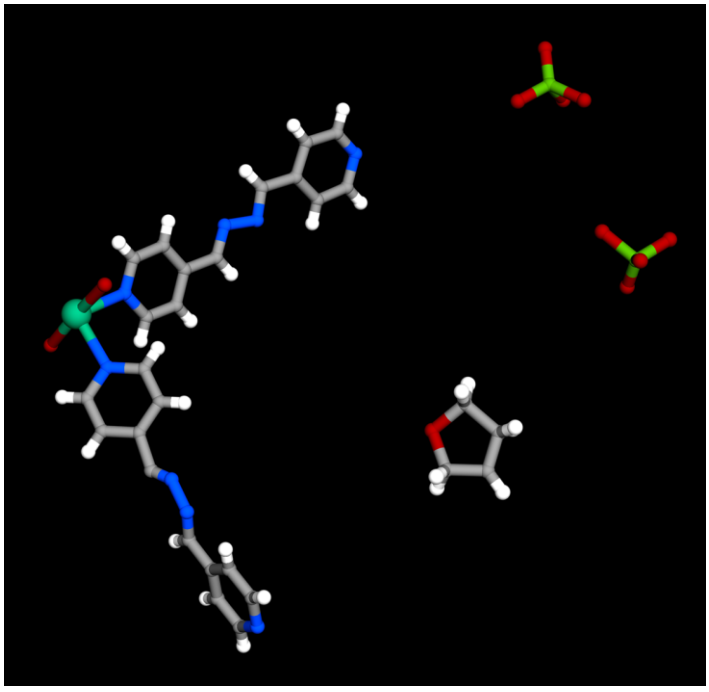

Figure S2: Asymmetric unit of compound 2 (Color code; Carbon: gray, oxygen: red, nitrogen: blue, chlorine: green, cadmium: light green)

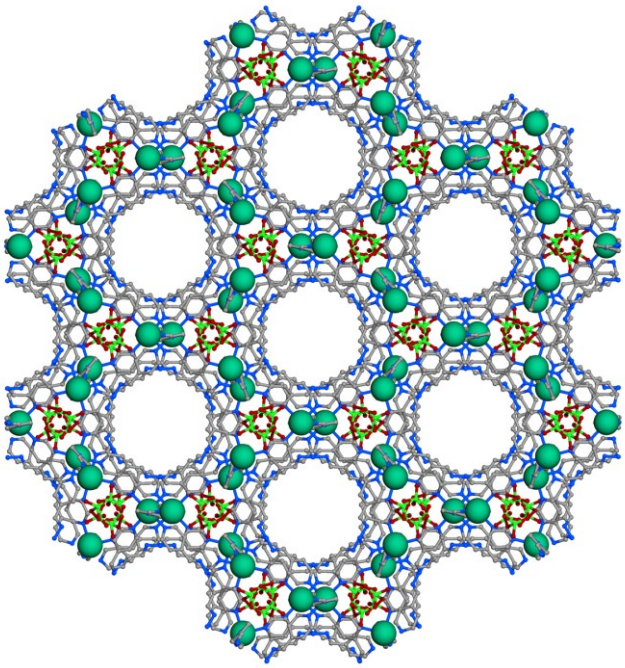

Figure S3: Overall packing of compound 1 along *c* axis (Color code; Carbon: gray, oxygen: red, nitrogen: blue, chlorine: green, cadmium: light green)

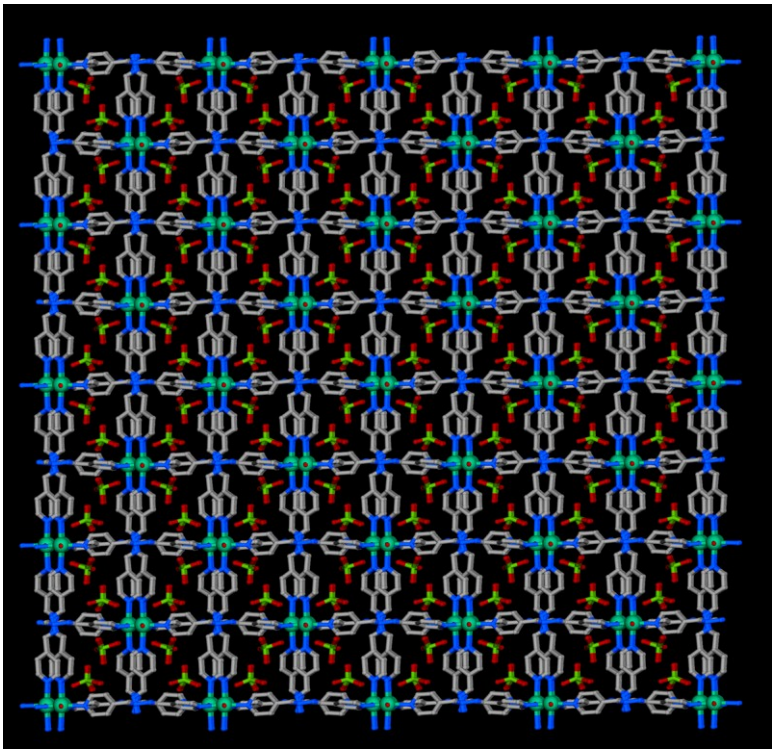

Figure S4: Overall packing of compound 2 along *c* axis (Color code; Carbon: gray, oxygen: red, nitrogen: blue, chlorine: green, cadmium: dark green)

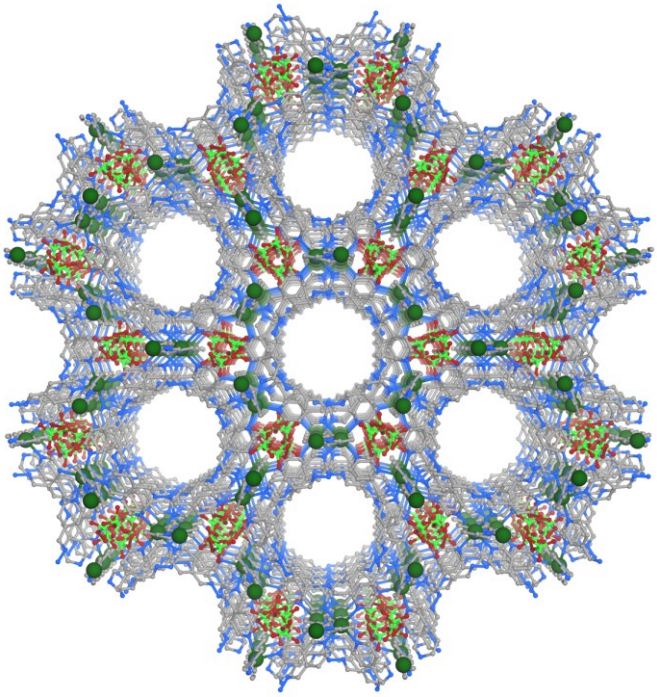

Figure S5: Perspective view of overall packing of compound 1 along *c* axis (free guests omitted for clarity; color code; Carbon: gray, oxygen: red, nitrogen: blue, chlorine: green, cadmium: dark green)

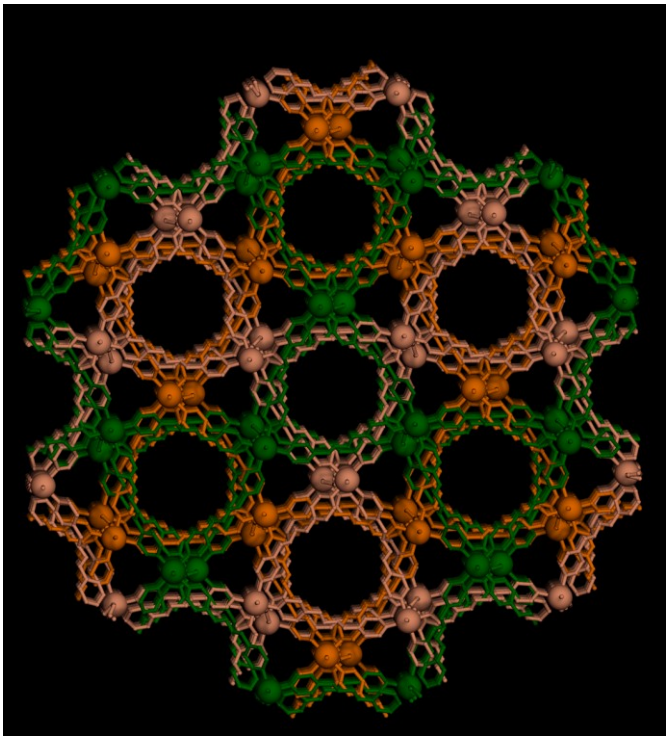

Figure S6: Three fold interpenetration of compound 1 along *c* axis (three nets shown in different colors)

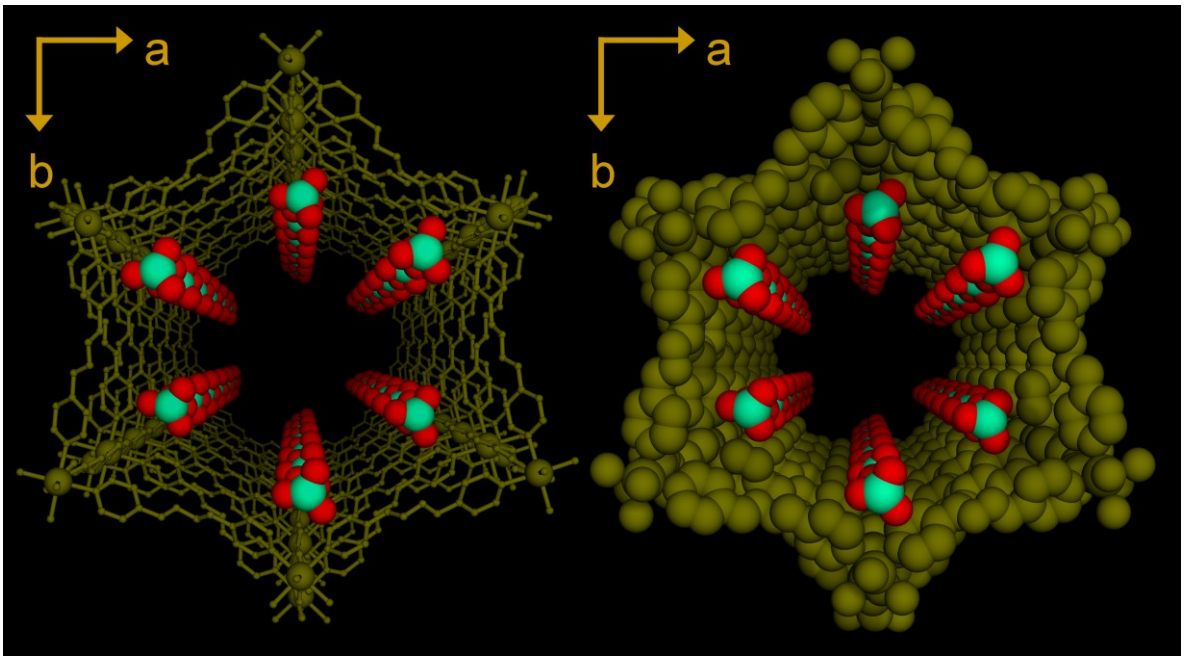

Figure S7: Perspective view of single net packing of compound 1 along *c* axis (left: ball and stick model ; right: CPK model)

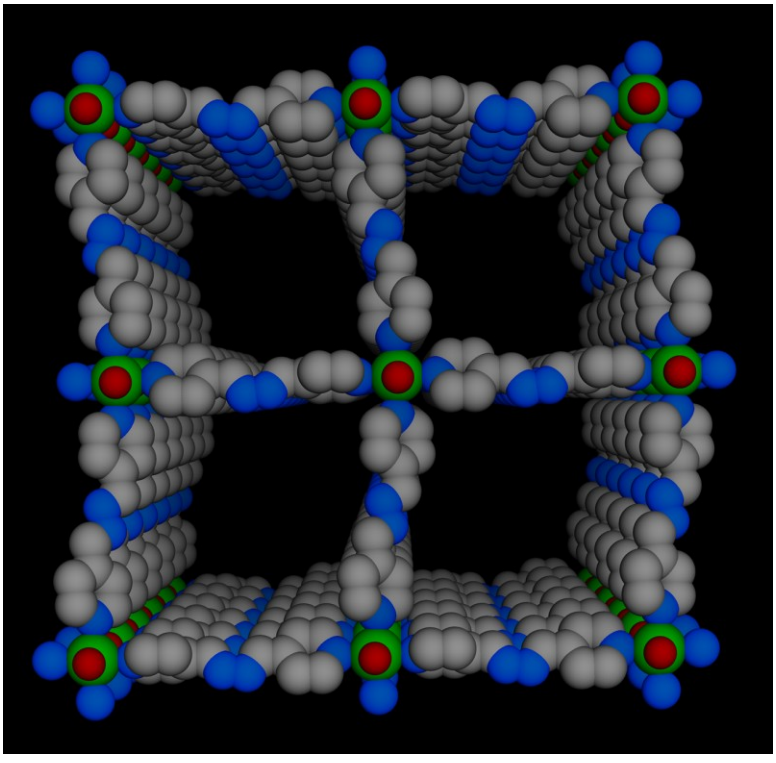

Figure S8: Perspective view of cationic single net packing of compound 2 along *c* axis (anions omitted for clarity; color code; Carbon: gray, oxygen: red, nitrogen: blue, cadmium: green)

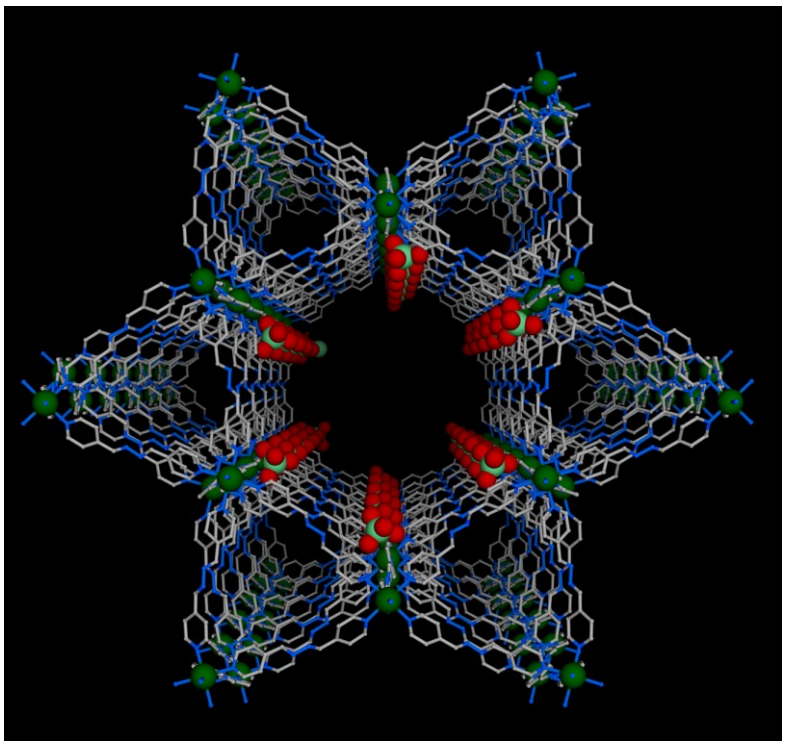

Figure S8: Perspective view of single net packing of compound 1 along *c* axis (Color code; Carbon: gray, oxygen: red, nitrogen: blue, chlorine: green, cadmium: dark green)

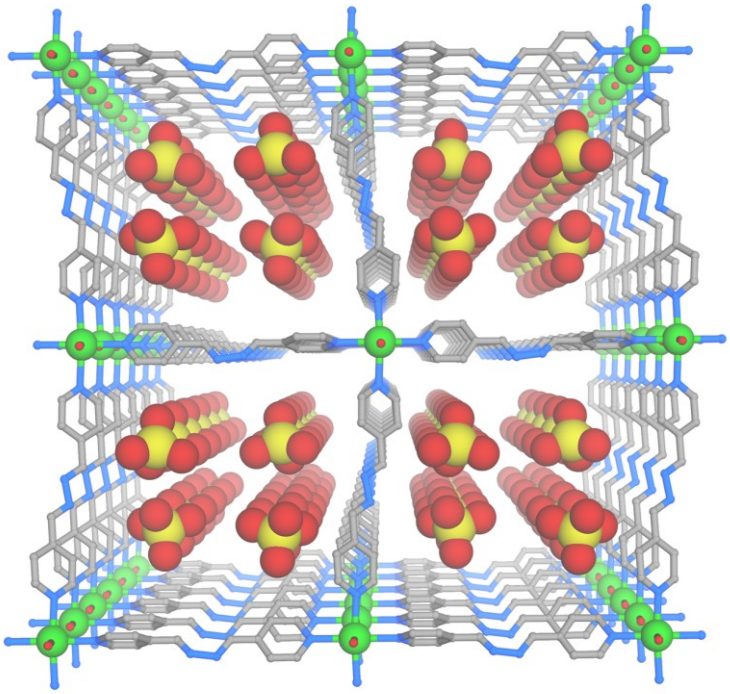

Figure S9: Perspective view of similar net packing of compound 2 along *c* axis (Color code; Carbon: gray, oxygen: red, nitrogen: blue, chlorine: dark yellow, cadmium: dark green)

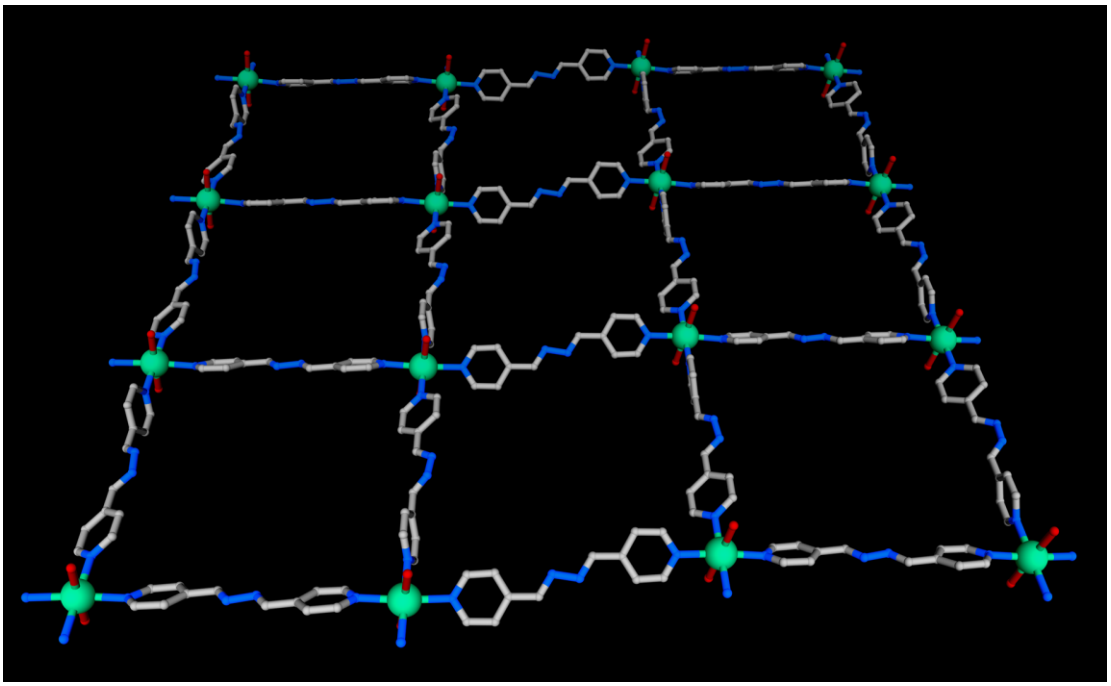

Figure S10: Single 2D sheet of compound 2 (Color code; Carbon: gray, oxygen: red, nitrogen: blue, cadmium: dark green)

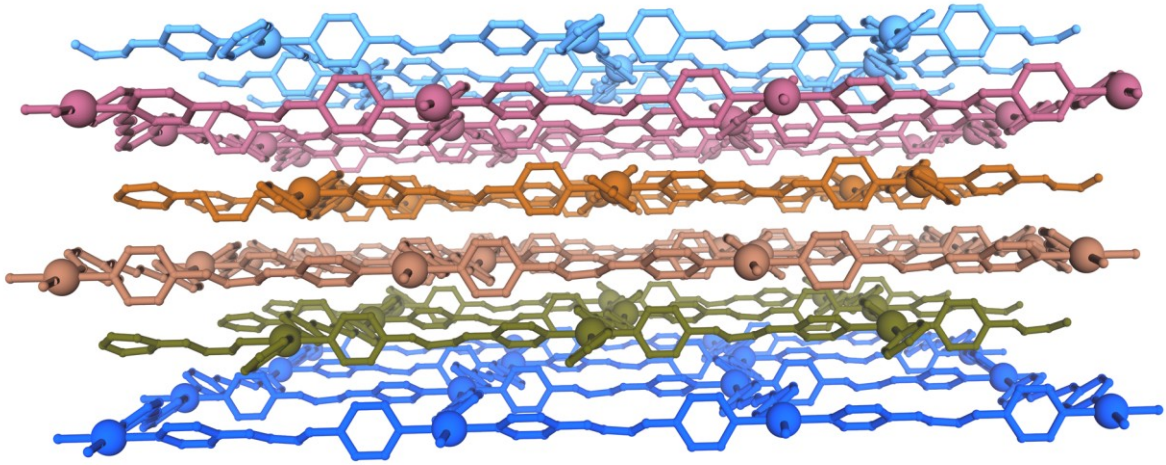

Figure S11: Various 2D sheets of compound 2 shown in different colors

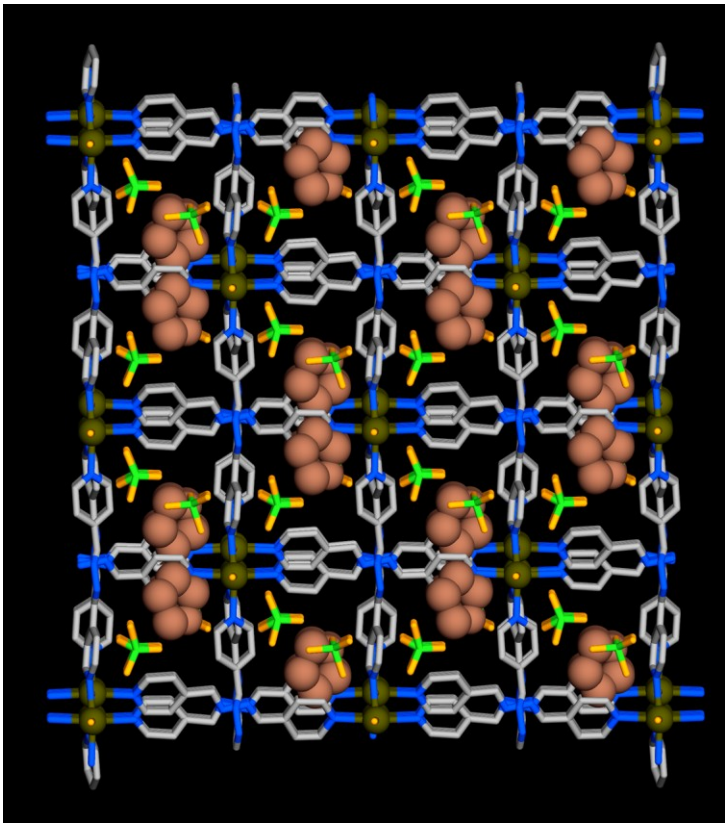

Figure S12: Overall packing of compound 2 along *c* axis with free tetrahydrofuran as guests shown in CPK model (color code; Carbon: grey, oxygen: orange, nitrogen: blue, chlorine: green, cadmium: dark yellow)

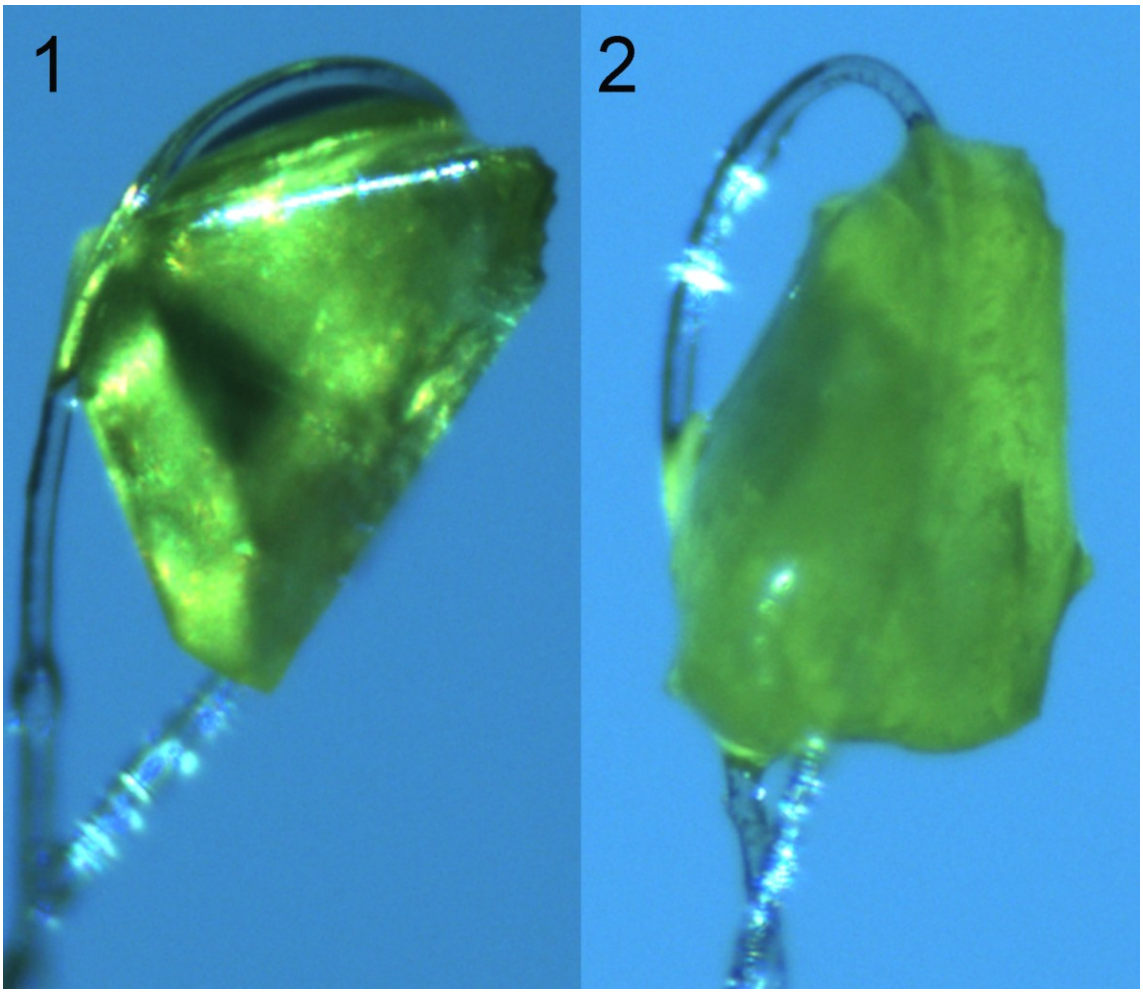

Figure S13: Crystals image of compound 1 and 2 respectively (crystals have taken from the same batch reaction).

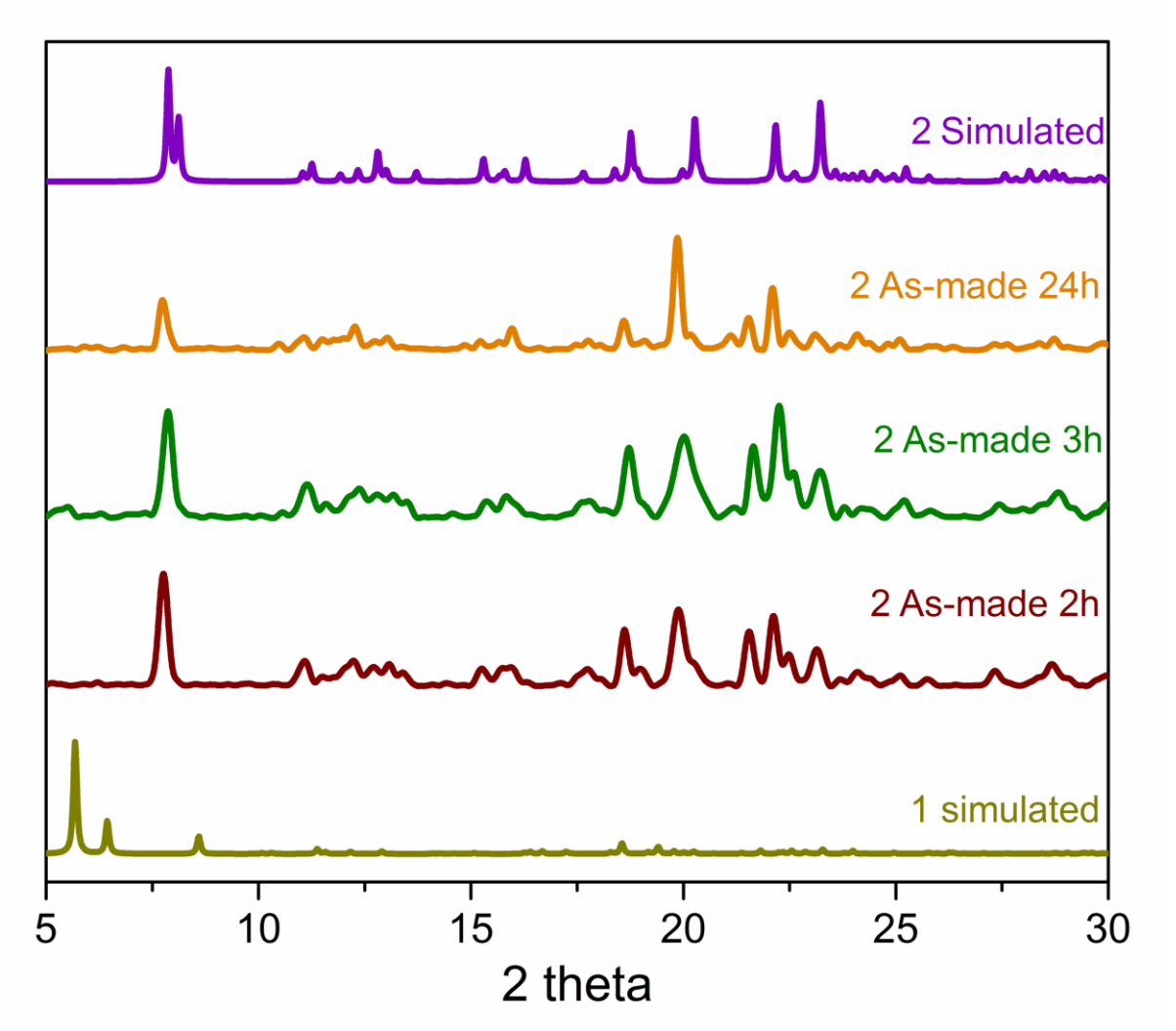

Figure S14: Time dependent PXRD patterns of compound 2

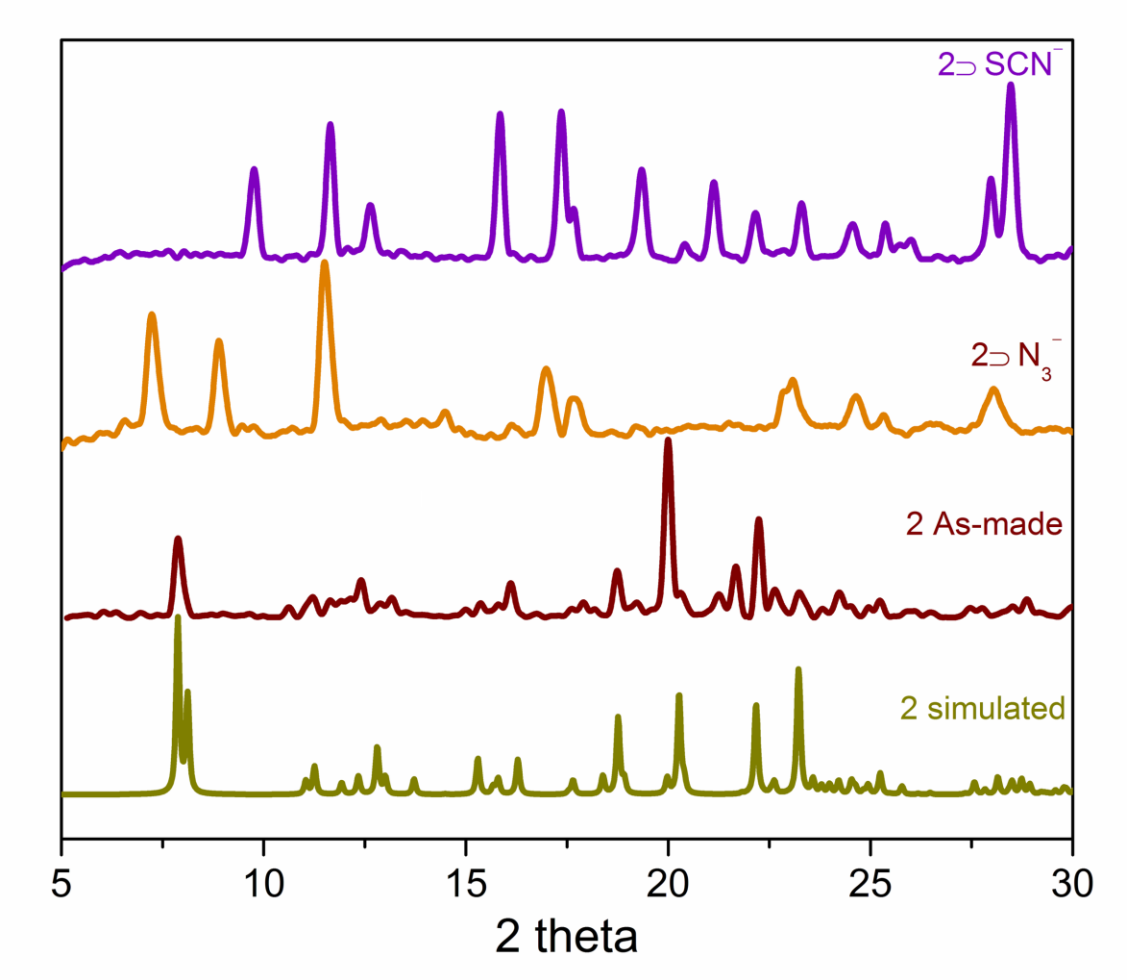

Figure S15: PXRD patterns of various anion exchange solids of compound 2

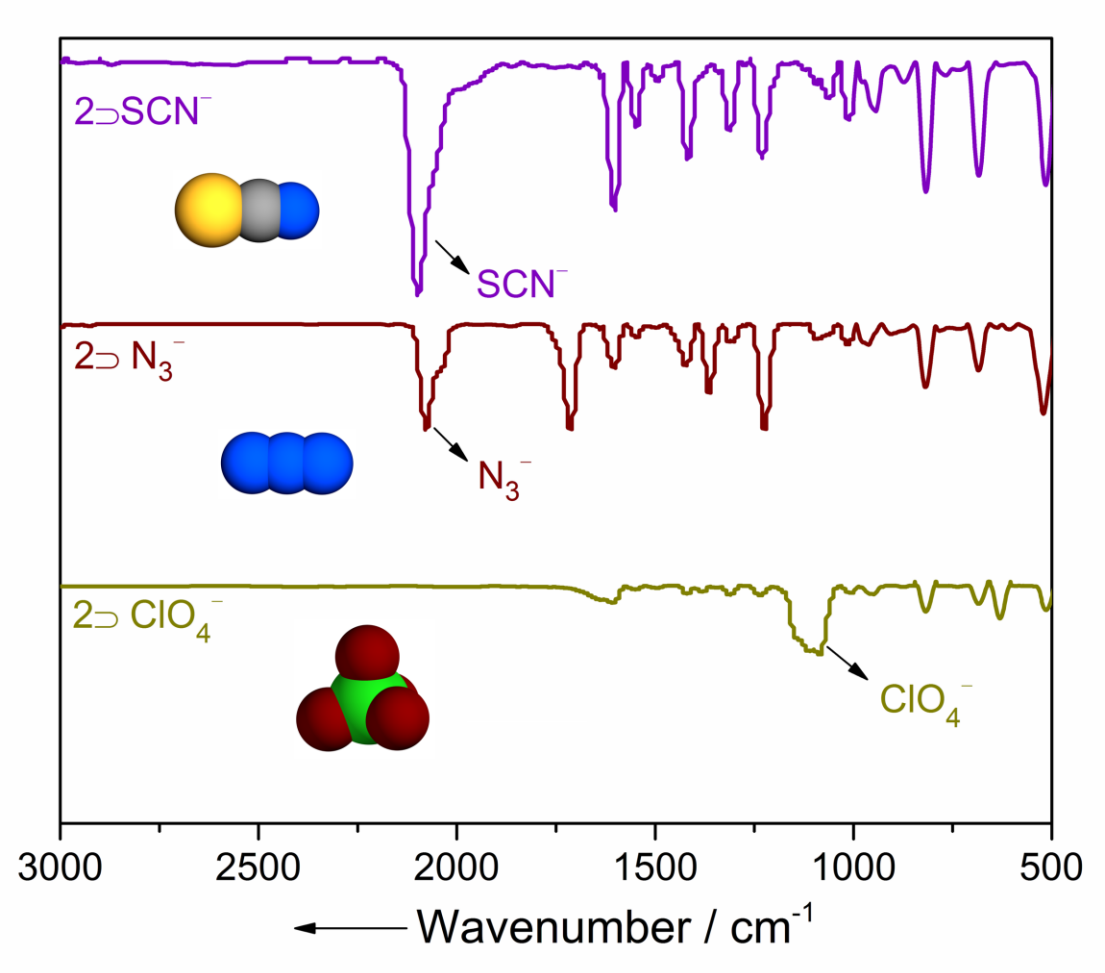

Figure S16: FT-IR spectra of various anion exchange solids of compound 2

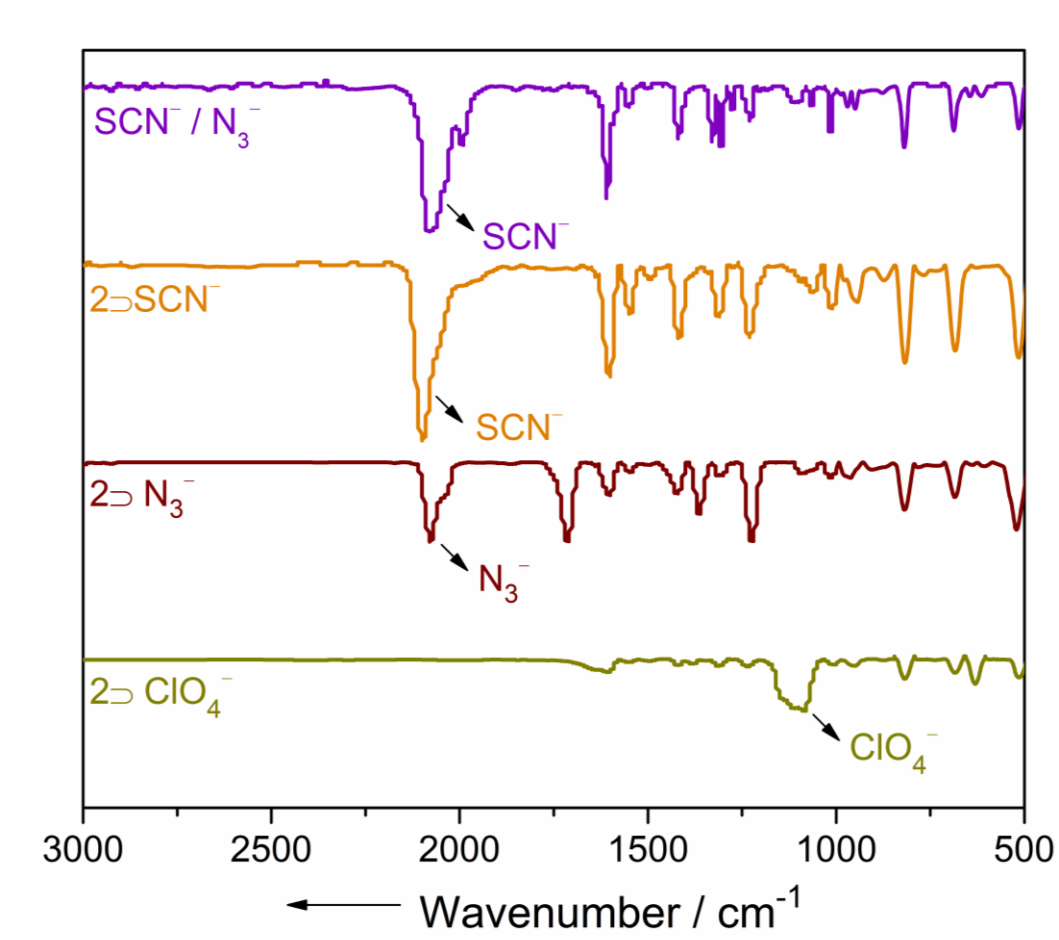

Figure S17: FT-IR spectra of various binary mixtures of anions compound 2

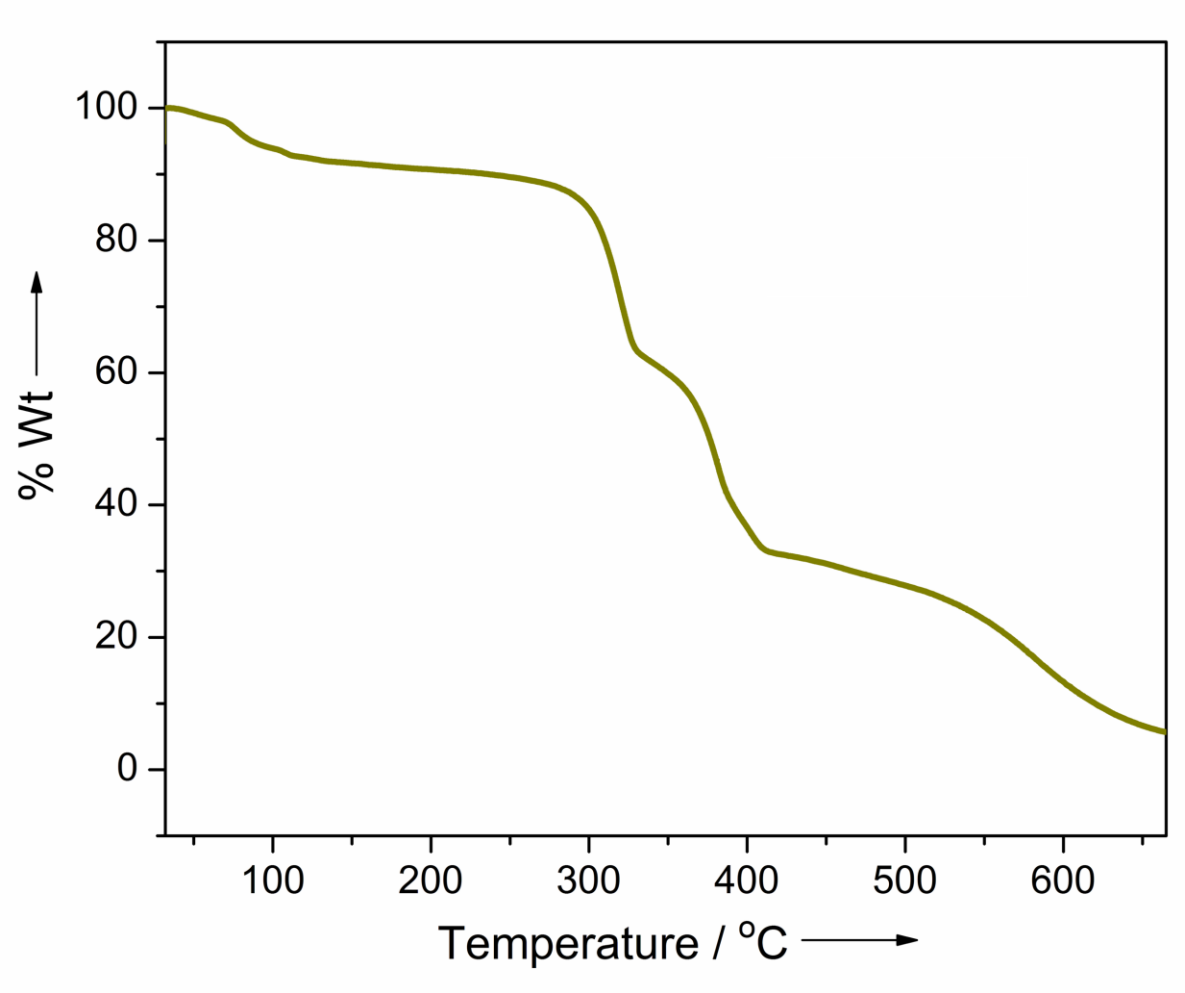

Figure S18: TGA plot of compound 2

Table 1. Crystal data and structure refinement for compound1.

Identification code	Compound1	
Empirical formula	C36 H30 Cd Cl2 N12 O8	
Formula weight	942.02	
Temperature	100(2) K	
Wavelength	0.71069 Å	
Crystal system	Trigonal	
Space group	R-3c	
Unit cell dimensions	a = 31.070(5) Å	α= 90.000(5)°.
	b = 31.070(5) Å	β= 90.000(5)°.
	c = 31.862(5) Å	γ = 120.000(5)°.
Volume	26637(7) $Å^3$	
Z	18	
Density (calculated)	1.057 Mg/m^3	
Absorption coefficient	0.504 mm^{-1}	
F(000)	8568	
Crystal size	0.17 x 0.15 x 0.12 mm^3	
Theta range for data collection	1.98 to 28.27°.	
Index ranges	-41<=h<=41, -41<=k<=41, -42<=l<=38	
Reflections collected	158511	
Independent reflections	7342 [R(int) = 0.0453]	
Completeness to theta = 28.27°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9420 and 0.9192	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7342 / 4 / 250	
Goodness-of-fit on F^2	1.049	
Final R indices [I>2sigma(I)]	R1 = 0.0622, wR2 = 0.1793	
R indices (all data)	R1 = 0.0664, wR2 = 0.1830	
Extinction coefficient	0.000003(14)	
Largest diff. peak and hole	1.871 and -3.771 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	5808(1)	10603(1)	2716(1)	26(1)
C(2)	6288(1)	10998(1)	2757(1)	31(1)
C(3)	6411(2)	11442(2)	2564(1)	36(1)
C(4)	6055(2)	11469(2)	2322(2)	42(1)
C(5)	5584(1)	11056(1)	2295(1)	34(1)
C(6)	4886(2)	9812(1)	3465(1)	29(1)
C(7)	4917(2)	9814(2)	3899(1)	33(1)
C(8)	4604(2)	9923(2)	4135(1)	33(1)
C(9)	4269(2)	10017(2)	3925(1)	33(1)
C(10)	4267(2)	10013(2)	3487(1)	30(1)
C(11)	4637(2)	9957(2)	4595(1)	38(1)
C(12)	3706(1)	8999(1)	2139(1)	28(1)
C(13)	3262(1)	8556(1)	2125(1)	30(1)
C(14)	2876(1)	8494(1)	2386(1)	28(1)
C(15)	2949(1)	8886(2)	2637(1)	33(1)
C(16)	3404(1)	9318(1)	2634(1)	30(1)
C(17)	2405(1)	8013(1)	2401(1)	34(1)
C(18)	1887(2)	6909(2)	2393(2)	43(1)
Cd(1)	4612(1)	10000	2500	17(1)
Cl(1)	3050(1)	183(1)	3364(1)	117(1)
N(1)	5458(1)	10629(1)	2492(1)	25(1)
N(2)	4570(1)	9916(1)	3258(1)	26(1)
N(3)	5013(2)	9980(2)	4778(1)	42(1)
N(4)	1876(1)	7239(1)	2171(1)	41(1)
N(5)	2324(1)	7683(1)	2131(1)	42(1)
N(6)	3785(1)	9377(1)	2396(1)	25(1)
O(1)	2775(3)	398(3)	3465(3)	154(2)
O(2)	3528(3)	504(3)	3238(3)	154(2)
O(3)	3146(3)	142(3)	3755(2)	154(2)
O(4)	2874(3)	-282(3)	3312(3)	154(2)

Table 3. Bond lengths [Å] and angles [°] for compound1.

C(1)-N(1)	1.337(5)
C(1)-C(2)	1.385(5)
C(2)-C(3)	1.381(6)
C(3)-C(4)	1.383(6)
C(3)-C(18)#1	1.479(5)
C(4)-C(5)	1.385(5)
C(5)-N(1)	1.339(5)
C(6)-N(2)	1.352(5)
C(6)-C(7)	1.383(5)
C(7)-C(8)	1.398(6)
C(8)-C(9)	1.387(6)
C(8)-C(11)	1.468(5)
C(9)-C(10)	1.393(5)
C(10)-N(2)	1.338(5)
C(11)-N(3)	1.277(6)
C(12)-N(6)	1.348(5)
C(12)-C(13)	1.379(5)
C(13)-C(14)	1.395(5)
C(14)-C(15)	1.376(5)
C(14)-C(17)	1.479(5)
C(15)-C(16)	1.380(5)
C(16)-N(6)	1.339(5)
C(17)-N(5)	1.265(6)
C(18)-N(4)	1.258(6)
C(18)-C(3)#2	1.479(5)
Cd(1)-N(6)#3	2.342(3)
Cd(1)-N(6)	2.342(3)
Cd(1)-N(1)#3	2.365(3)
Cd(1)-N(1)	2.365(3)
Cd(1)-N(2)#3	2.425(3)
Cd(1)-N(2)	2.425(3)
Cl(1)-O(4)	1.273(8)
Cl(1)-O(3)	1.3019(10)
Cl(1)-O(1)	1.360(8)
Cl(1)-O(2)	1.370(8)
N(3)-N(3)#4	1.427(6)

N(4)-N(5)	1.392(4)

N(1)-C(1)-C(2)	123.1(3)
C(3)-C(2)-C(1)	118.6(4)
C(2)-C(3)-C(4)	118.7(4)
C(2)-C(3)-C(18)#1	121.9(4)
C(4)-C(3)-C(18)#1	119.4(4)
C(3)-C(4)-C(5)	119.1(4)
N(1)-C(5)-C(4)	122.5(4)
N(2)-C(6)-C(7)	122.9(4)
C(6)-C(7)-C(8)	119.0(4)
C(9)-C(8)-C(7)	118.4(4)
C(9)-C(8)-C(11)	120.0(4)
C(7)-C(8)-C(11)	121.6(4)
C(8)-C(9)-C(10)	118.8(4)
N(2)-C(10)-C(9)	123.3(4)
N(3)-C(11)-C(8)	119.3(4)
N(6)-C(12)-C(13)	123.2(3)
C(12)-C(13)-C(14)	118.6(3)
C(15)-C(14)-C(13)	118.4(3)
C(15)-C(14)-C(17)	121.2(4)
C(13)-C(14)-C(17)	120.4(3)
C(14)-C(15)-C(16)	119.5(4)
N(6)-C(16)-C(15)	122.8(3)
N(5)-C(17)-C(14)	119.6(4)
N(4)-C(18)-C(3)#2	120.9(4)
N(6)#3-Cd(1)-N(6)	93.81(15)
N(6)#3-Cd(1)-N(1)#3	171.25(10)
N(6)-Cd(1)-N(1)#3	88.03(11)
N(6)#3-Cd(1)-N(1)	88.03(11)
N(6)-Cd(1)-N(1)	171.25(10)
N(1)#3-Cd(1)-N(1)	91.44(16)
N(6)#3-Cd(1)-N(2)#3	94.25(11)
N(6)-Cd(1)-N(2)#3	85.74(10)
N(1)#3-Cd(1)-N(2)#3	94.42(10)
N(1)-Cd(1)-N(2)#3	85.60(10)
N(6)#3-Cd(1)-N(2)	85.73(10)
N(6)-Cd(1)-N(2)	94.25(11)

N(1)#3-Cd(1)-N(2)	85.60(10)
N(1)-Cd(1)-N(2)	94.42(10)
N(2)#3-Cd(1)-N(2)	179.97(15)
O(4)-Cl(1)-O(3)	90.2(7)
O(4)-Cl(1)-O(1)	124.5(5)
O(3)-Cl(1)-O(1)	93.0(6)
O(4)-Cl(1)-O(2)	118.9(5)
O(3)-Cl(1)-O(2)	97.6(7)
O(1)-Cl(1)-O(2)	115.4(5)
C(1)-N(1)-C(5)	117.9(3)
C(1)-N(1)-Cd(1)	123.1(2)
C(5)-N(1)-Cd(1)	118.5(2)
C(10)-N(2)-C(6)	117.6(3)
C(10)-N(2)-Cd(1)	121.8(2)
C(6)-N(2)-Cd(1)	120.4(2)
C(11)-N(3)-N(3)#4	111.5(5)
C(18)-N(4)-N(5)	115.9(4)
C(17)-N(5)-N(4)	115.8(4)
C(16)-N(6)-C(12)	117.5(3)
C(16)-N(6)-Cd(1)	124.1(2)
C(12)-N(6)-Cd(1)	117.0(2)

Symmetry transformations used to generate equivalent atoms:

#1 y,x+1,-z+1/2 #2 y-1,x,-z+1/2 #3 x-y+1,-y+2,-z+1/2

#4 -x+1,-y+2,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for compound1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	22(2)	22(2)	30(2)	0(1)	-1(1)	6(1)
C(2)	22(2)	26(2)	35(2)	-1(1)	-4(1)	5(1)
C(3)	25(2)	26(2)	41(2)	3(2)	-3(2)	0(2)
C(4)	32(2)	26(2)	51(2)	12(2)	-5(2)	3(2)
C(5)	26(2)	27(2)	38(2)	7(2)	-5(2)	5(2)
C(6)	34(2)	34(2)	22(2)	1(1)	0(1)	19(2)
C(7)	36(2)	43(2)	23(2)	2(2)	-3(2)	22(2)
C(8)	37(2)	40(2)	19(2)	0(1)	-1(1)	18(2)
C(9)	38(2)	43(2)	21(2)	0(2)	2(1)	23(2)
C(10)	36(2)	36(2)	22(2)	1(1)	-3(1)	21(2)
C(11)	41(2)	53(3)	18(2)	3(2)	3(1)	23(2)
C(12)	26(2)	23(2)	28(2)	-4(1)	3(1)	7(1)
C(13)	28(2)	22(2)	30(2)	-5(1)	-2(1)	6(1)
C(14)	22(2)	21(2)	31(2)	2(1)	-3(1)	3(1)
C(15)	23(2)	34(2)	35(2)	-3(2)	4(1)	8(2)
C(16)	26(2)	28(2)	32(2)	-7(1)	2(1)	10(2)
C(17)	22(2)	27(2)	40(2)	6(2)	-2(2)	2(2)
C(18)	27(2)	29(2)	51(2)	5(2)	-8(2)	-3(2)
Cd(1)	19(1)	13(1)	18(1)	-1(1)	-1(1)	7(1)
Cl(1)	76(1)	49(1)	219(3)	-4(1)	68(2)	26(1)
N(1)	21(1)	20(1)	29(1)	-1(1)	-1(1)	6(1)
N(2)	34(2)	26(1)	19(1)	0(1)	-1(1)	16(1)
N(3)	43(2)	65(3)	16(2)	3(2)	1(1)	25(2)
N(4)	29(2)	26(2)	47(2)	2(1)	-4(2)	-3(1)
N(5)	30(2)	24(2)	48(2)	2(1)	-3(2)	-4(1)
N(6)	22(1)	20(1)	26(1)	-4(1)	0(1)	5(1)
O(1)	126(3)	93(3)	240(5)	4(3)	76(3)	53(2)
O(2)	126(3)	93(3)	240(5)	4(3)	76(3)	53(2)
O(3)	126(3)	93(3)	240(5)	4(3)	76(3)	53(2)
O(4)	126(3)	93(3)	240(5)	4(3)	76(3)	53(2)

Table 5. Crystal data and structure refinement for compound2.

Identification code	Compound2	
Empirical formula	C28 H32 Cd Cl2 N8 O11	
Formula weight	839.92	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	Cc	
Unit cell dimensions	a = 18.938(8) Å	α= 90°.
	b = 16.008(7) Å	β= 123.948(6)°.
	c = 15.549(11) Å	γ = 90°.
Volume	3910(4) $Å^3$	
Z	4	
Density (calculated)	1.427 Mg/m^3	
Absorption coefficient	0.756 mm^{-1}	
F(000)	1704	
Crystal size	0.17 x 0.14 x 0.11 mm^3	
Theta range for data collection	1.82 to 28.29°.	
Index ranges	-25<=h<=25, -21<=k<=21, -20<=l<=20	
Reflections collected	33545	
Independent reflections	9349 [R(int) = 0.0232]	
Completeness to theta = 28.29°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9214 and 0.8822	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9349 / 14 / 421	
Goodness-of-fit on F^2	0.933	
Final R indices [I>2sigma(I)]	R1 = 0.0771, wR2 = 0.2159	
R indices (all data)	R1 = 0.0833, wR2 = 0.2310	
Absolute structure parameter	0.32(4)	
Largest diff. peak and hole	4.394 and -1.292 $e.Å^{-3}$	

Table 6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(5)	9971(3)	1926(1)	2414(4)	25(1)
C(13)	9410(4)	2411(2)	2511(5)	45(2)
C(14)	9464(4)	3277(2)	2516(5)	65(4)
C(15)	10078(4)	3658(1)	2423(6)	85(5)
C(16)	10638(4)	3173(2)	2326(6)	93(7)
C(17)	10585(3)	2307(2)	2321(5)	62(4)
N(8)	9913(3)	-1016(1)	2302(3)	38(2)
C(20)	9779(3)	-1341(2)	1394(3)	48(2)
C(21)	9843(4)	-2197(2)	1299(4)	55(2)
C(22)	10041(4)	-2727(1)	2113(4)	48(2)
C(23)	10175(4)	-2401(1)	3021(4)	57(3)
C(24)	10111(4)	-1546(2)	3116(4)	56(3)
Cd(1)	10016(1)	461(1)	2480(1)	21(1)
O(2)	9950(7)	491(5)	3957(8)	40(3)
O(1)	10064(7)	509(5)	1003(8)	35(2)
Cl(5)	1564(3)	2017(3)	6045(4)	83(2)
N(4)	1481(7)	-411(5)	-1579(9)	24(2)
C(5)	8037(7)	1022(8)	803(7)	37(2)
N(2)	5475(5)	-81(8)	257(7)	45(3)
N(3)	4604(6)	93(6)	-252(7)	36(2)
C(11)	1881(6)	156(6)	-1786(8)	32(2)
N(1)	8515(8)	403(5)	1518(10)	30(3)
C(4)	7184(7)	1043(9)	361(9)	48(3)
C(3)	6791(6)	437(5)	596(9)	33(3)
C(7)	4249(9)	-524(8)	-121(12)	38(3)
C(12)	2755(8)	159(9)	-1348(10)	43(3)
C(2)	7271(6)	-196(8)	1312(8)	33(2)
C(1)	8138(7)	-186(9)	1768(9)	40(2)
C(6)	5899(8)	472(6)	141(10)	28(3)
C(8)	3295(10)	-440(6)	-604(10)	38(4)
C(10)	1977(5)	-952(6)	-863(8)	29(2)
C(9)	2881(5)	-1005(7)	-341(8)	31(2)
O(4)	4081(7)	7287(7)	10067(9)	73(3)

Cl(21)	3536(3)	7038(3)	8997(3)	64(1)
O(6)	2660(8)	6969(8)	8718(10)	98(5)
O(3)	3853(9)	6173(8)	9063(9)	106(5)
O(7)	2363(7)	2031(10)	6209(10)	94(5)
O(9)	969(7)	2288(8)	5108(11)	123(6)
O(10)	1349(6)	2751(6)	6426(7)	72(2)
O(8)	1226(12)	1185(9)	5967(11)	141(8)
O(5)	3301(17)	7066(15)	7950(20)	191(9)
C(28)	8519(4)	8960(6)	8803(6)	38(2)
C(25)	7756(13)	7960(14)	9128(13)	124(10)
O(11)	8347(11)	8040(10)	8756(12)	141(7)
C(27)	7867(11)	9441(11)	8795(16)	105(7)
C(26)	7403(15)	8842(14)	8940(20)	144(11)
C(18)	10182(8)	4561(5)	2294(8)	49(3)
N(7)	10176(12)	5898(5)	2691(11)	76(5)
N(6)	9990(30)	5032(6)	2553(15)	219(15)
C(19)	10093(6)	6373(5)	2015(7)	40(2)

Table 7. Bond lengths [Å] and angles [°] for compound2.

N(5)-C(13)	1.3900
N(5)-C(17)	1.3900
N(5)-Cd(1)	2.347(2)
C(13)-C(14)	1.3900
C(13)-H(13)	0.9300
C(14)-C(15)	1.3900
C(14)-H(14)	0.9300
C(15)-C(16)	1.3900
C(15)-C(18)	1.487(8)
C(16)-C(17)	1.3900
C(16)-H(16)	0.9300
C(17)-H(17)	0.9300
N(8)-C(20)	1.3900
N(8)-C(24)	1.3900
N(8)-Cd(1)	2.375(2)
C(20)-C(21)	1.3900
C(20)-H(20)	0.9300
C(21)-C(22)	1.3900
C(21)-H(21)	0.9300
C(22)-C(23)	1.3900
C(22)-C(19)#1	1.458(9)
C(23)-C(24)	1.3900
C(23)-H(23)	0.9300
C(24)-H(24)	0.9300
Cd(1)-N(4)#2	2.304(11)
Cd(1)-N(1)	2.362(12)
Cd(1)-O(1)	2.350(9)
Cd(1)-O(2)	2.369(11)
Cl(5)-O(9)	1.323(11)
Cl(5)-O(7)	1.387(12)
Cl(5)-O(8)	1.453(13)
Cl(5)-O(10)	1.471(8)
N(4)-C(10)	1.305(14)
N(4)-C(11)	1.332(13)
N(4)-Cd(1)#3	2.304(11)
C(5)-C(4)	1.359(16)

C(5)-N(1)	1.384(15)
C(5)-H(5)	0.9300
N(2)-C(6)	1.272(16)
N(2)-N(3)	1.403(7)
N(3)-C(7)	1.274(16)
C(11)-C(12)	1.395(14)
C(11)-H(11)	0.9300
N(1)-C(1)	1.363(16)
C(4)-C(3)	1.391(16)
C(4)-H(4)	0.9300
C(3)-C(2)	1.400(14)
C(3)-C(6)	1.422(16)
C(7)-C(8)	1.53(2)
C(7)-H(7)	0.9300
C(12)-C(8)	1.407(19)
C(12)-H(12)	0.9300
C(2)-C(1)	1.377(14)
C(2)-H(2)	0.9300
C(1)-H(1)	0.9300
C(6)-H(6)	0.9300
C(8)-C(9)	1.400(15)
C(10)-C(9)	1.430(11)
C(10)-H(10)	0.9300
C(9)-H(9)	0.9300
O(4)-Cl(21)	1.440(13)
Cl(21)-O(5)	1.43(3)
Cl(21)-O(6)	1.465(15)
Cl(21)-O(3)	1.490(12)
C(28)-C(27)	1.449(13)
C(28)-O(11)	1.501(17)
C(28)-H(28A)	0.9700
C(28)-H(28B)	0.9700
C(25)-O(11)	1.524(16)
C(25)-C(26)	1.52(3)
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700
C(27)-C(26)	1.40(2)
C(27)-H(27)	0.9300

C(26)-H(26A)	0.9700
C(26)-H(26B)	0.9700
C(18)-N(6)	1.01(2)
N(7)-C(19)	1.234(15)
N(7)-N(6)	1.417(17)
C(19)-C(22)#4	1.458(9)
C(19)-H(19)	0.9300

C(13)-N(5)-C(17)	120.0
C(13)-N(5)-Cd(1)	124.38(11)
C(17)-N(5)-Cd(1)	115.54(11)
C(14)-C(13)-N(5)	120.0
C(14)-C(13)-H(13)	120.0
N(5)-C(13)-H(13)	120.0
C(15)-C(14)-C(13)	120.0
C(15)-C(14)-H(14)	120.0
C(13)-C(14)-H(14)	120.0
C(14)-C(15)-C(16)	120.0
C(14)-C(15)-C(18)	128.5(7)
C(16)-C(15)-C(18)	111.1(7)
C(17)-C(16)-C(15)	120.0
C(17)-C(16)-H(16)	120.0
C(15)-C(16)-H(16)	120.0
C(16)-C(17)-N(5)	120.0
C(16)-C(17)-H(17)	120.0
N(5)-C(17)-H(17)	120.0
C(20)-N(8)-C(24)	120.0
C(20)-N(8)-Cd(1)	116.61(11)
C(24)-N(8)-Cd(1)	122.59(10)
C(21)-C(20)-N(8)	120.0
C(21)-C(20)-H(20)	120.0
N(8)-C(20)-H(20)	120.0
C(22)-C(21)-C(20)	120.0
C(22)-C(21)-H(21)	120.0
C(20)-C(21)-H(21)	120.0
C(21)-C(22)-C(23)	120.0
C(21)-C(22)-C(19)#1	120.6(4)
C(23)-C(22)-C(19)#1	119.4(4)

C(22)-C(23)-C(24)	120.0
C(22)-C(23)-H(23)	120.0
C(24)-C(23)-H(23)	120.0
N(8)-C(24)-C(23)	120.0
N(8)-C(24)-H(24)	120.0
C(23)-C(24)-H(24)	120.0
N(4)#2-Cd(1)-N(5)	93.7(2)
N(4)#2-Cd(1)-N(1)	175.79(16)
N(5)-Cd(1)-N(1)	90.6(2)
N(4)#2-Cd(1)-O(1)	86.1(4)
N(5)-Cd(1)-O(1)	86.8(2)
N(1)-Cd(1)-O(1)	94.1(4)
N(4)#2-Cd(1)-O(2)	94.7(4)
N(5)-Cd(1)-O(2)	90.1(2)
N(1)-Cd(1)-O(2)	85.3(4)
O(1)-Cd(1)-O(2)	176.86(18)
N(4)#2-Cd(1)-N(8)	91.8(2)
N(5)-Cd(1)-N(8)	172.17(18)
N(1)-Cd(1)-N(8)	84.0(2)
O(1)-Cd(1)-N(8)	88.0(2)
O(2)-Cd(1)-N(8)	95.0(2)
O(9)-Cl(5)-O(7)	111.6(10)
O(9)-Cl(5)-O(8)	98.3(7)
O(7)-Cl(5)-O(8)	114.5(12)
O(9)-Cl(5)-O(10)	85.7(9)
O(7)-Cl(5)-O(10)	115.6(7)
O(8)-Cl(5)-O(10)	123.9(11)
C(10)-N(4)-C(11)	115.0(10)
C(10)-N(4)-Cd(1)#3	123.8(7)
C(11)-N(4)-Cd(1)#3	121.0(7)
C(4)-C(5)-N(1)	118.9(12)
C(4)-C(5)-H(5)	120.5
N(1)-C(5)-H(5)	120.5
C(6)-N(2)-N(3)	114.7(9)
C(7)-N(3)-N(2)	108.3(9)
N(4)-C(11)-C(12)	124.3(10)
N(4)-C(11)-H(11)	117.8
C(12)-C(11)-H(11)	117.8

C(1)-N(1)-C(5)	120.8(12)
C(1)-N(1)-Cd(1)	118.9(9)
C(5)-N(1)-Cd(1)	119.8(8)
C(5)-C(4)-C(3)	120.7(12)
C(5)-C(4)-H(4)	119.7
C(3)-C(4)-H(4)	119.7
C(4)-C(3)-C(2)	120.5(10)
C(4)-C(3)-C(6)	120.2(10)
C(2)-C(3)-C(6)	119.2(10)
N(3)-C(7)-C(8)	115.9(11)
N(3)-C(7)-H(7)	122.1
C(8)-C(7)-H(7)	122.1
C(11)-C(12)-C(8)	121.3(12)
C(11)-C(12)-H(12)	119.4
C(8)-C(12)-H(12)	119.4
C(1)-C(2)-C(3)	117.4(11)
C(1)-C(2)-H(2)	121.3
C(3)-C(2)-H(2)	121.3
N(1)-C(1)-C(2)	121.7(13)
N(1)-C(1)-H(1)	119.2
C(2)-C(1)-H(1)	119.2
N(2)-C(6)-C(3)	124.7(11)
N(2)-C(6)-H(6)	117.6
C(3)-C(6)-H(6)	117.6
C(9)-C(8)-C(12)	114.3(12)
C(9)-C(8)-C(7)	120.0(12)
C(12)-C(8)-C(7)	125.6(11)
N(4)-C(10)-C(9)	125.9(10)
N(4)-C(10)-H(10)	117.0
C(9)-C(10)-H(10)	117.0
C(8)-C(9)-C(10)	119.0(10)
C(8)-C(9)-H(9)	120.5
C(10)-C(9)-H(9)	120.5
O(5)-Cl(21)-O(4)	150.9(12)
O(5)-Cl(21)-O(6)	94.8(12)
O(4)-Cl(21)-O(6)	109.0(8)
O(5)-Cl(21)-O(3)	87.9(12)
O(4)-Cl(21)-O(3)	100.2(6)

O(6)-Cl(21)-O(3)	107.2(9)
C(27)-C(28)-O(11)	111.1(10)
C(27)-C(28)-H(28A)	109.4
O(11)-C(28)-H(28A)	109.4
C(27)-C(28)-H(28B)	109.4
O(11)-C(28)-H(28B)	109.4
H(28A)-C(28)-H(28B)	108.0
O(11)-C(25)-C(26)	100.6(13)
O(11)-C(25)-H(25A)	111.7
C(26)-C(25)-H(25A)	111.7
O(11)-C(25)-H(25B)	111.7
C(26)-C(25)-H(25B)	111.7
H(25A)-C(25)-H(25B)	109.4
C(28)-O(11)-C(25)	104.4(12)
C(26)-C(27)-C(28)	103.9(13)
C(26)-C(27)-H(27)	128.0
C(28)-C(27)-H(27)	128.0
C(27)-C(26)-C(25)	114.9(12)
C(27)-C(26)-H(26A)	108.5
C(25)-C(26)-H(26A)	108.5
C(27)-C(26)-H(26B)	108.5
C(25)-C(26)-H(26B)	108.5
H(26A)-C(26)-H(26B)	107.5
N(6)-C(18)-C(15)	124(2)
C(19)-N(7)-N(6)	124.8(11)
C(18)-N(6)-N(7)	133(3)
N(7)-C(19)-C(22)#4	120.3(10)
N(7)-C(19)-H(19)	119.8
C(22)#4-C(19)-H(19)	119.8

Symmetry transformations used to generate equivalent atoms:

#1 x,y-1,z #2 x+1,-y,z+1/2 #3 x-1,-y,z-1/2

#4 x,y+1,z

Table 8. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for compound2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(5)	18(2)	17(2)	31(2)	-6(3)	7(2)	-10(3)
C(13)	56(7)	36(5)	35(4)	-3(3)	20(4)	4(4)
C(14)	73(8)	41(6)	38(5)	-13(4)	4(5)	41(6)
C(15)	61(6)	24(3)	68(6)	-2(6)	-27(5)	-21(6)
C(16)	38(6)	28(5)	116(12)	25(6)	-18(7)	-8(4)
C(17)	24(4)	22(4)	88(8)	22(4)	-1(5)	-21(3)
N(8)	12(3)	26(2)	72(6)	-1(3)	21(4)	2(2)
C(20)	53(5)	21(4)	65(6)	-7(4)	29(5)	-5(3)
C(21)	66(6)	38(5)	60(6)	2(4)	34(5)	0(4)
C(22)	35(5)	59(6)	46(5)	-5(4)	21(4)	-4(4)
C(23)	65(7)	82(8)	36(5)	12(5)	35(5)	7(6)
C(24)	65(7)	37(5)	71(7)	15(5)	41(6)	6(4)
Cd(1)	12(1)	19(1)	30(1)	1(1)	10(1)	0(1)
O(2)	27(6)	56(7)	27(5)	9(3)	9(4)	7(3)
O(1)	28(5)	54(7)	33(5)	-7(3)	23(4)	-1(3)
Cl(5)	75(3)	121(4)	79(3)	-30(2)	58(3)	-14(2)
N(4)	16(5)	30(6)	31(5)	3(3)	16(4)	0(2)
C(5)	28(5)	56(7)	25(4)	7(4)	13(4)	1(4)
N(2)	8(3)	83(9)	36(5)	-7(5)	7(3)	-9(4)
N(3)	22(4)	41(5)	39(5)	-6(4)	15(3)	-6(3)
C(11)	17(4)	24(4)	47(5)	9(4)	12(4)	1(4)
N(1)	12(5)	36(7)	32(5)	-4(3)	7(4)	-9(3)
C(4)	29(5)	70(8)	28(5)	9(5)	6(4)	-15(5)
C(3)	-7(4)	48(8)	32(6)	3(3)	-8(3)	-6(2)
C(7)	9(5)	66(8)	34(6)	3(4)	9(4)	-2(3)
C(12)	31(5)	43(7)	58(7)	-9(6)	26(5)	-19(5)
C(2)	11(4)	48(6)	34(5)	8(5)	10(4)	-1(4)
C(1)	25(5)	61(7)	39(5)	-4(5)	21(4)	-16(5)
C(6)	4(5)	46(6)	27(5)	-8(3)	4(4)	-2(2)
C(8)	49(9)	48(8)	43(7)	-15(4)	41(7)	-14(4)
C(10)	7(3)	35(4)	38(5)	1(3)	8(3)	-9(3)
C(9)	10(4)	41(5)	41(5)	6(4)	13(4)	4(3)
O(4)	47(6)	85(7)	70(6)	21(5)	22(5)	2(5)

Cl(21)	61(2)	77(3)	44(2)	15(1)	23(1)	1(2)
O(6)	51(7)	88(9)	81(8)	37(7)	-8(6)	-15(6)
O(3)	96(9)	113(11)	55(6)	8(7)	8(6)	50(8)
O(7)	34(5)	143(12)	87(8)	-62(8)	24(6)	-7(6)
O(9)	37(6)	92(9)	135(12)	36(8)	-17(6)	25(6)
O(10)	59(5)	87(6)	66(5)	-17(4)	32(4)	18(4)
O(8)	179(17)	123(13)	83(9)	26(9)	50(11)	-79(12)
O(5)	191(9)	192(9)	191(9)	0(1)	107(5)	1(1)
C(28)	5(2)	76(6)	33(3)	15(3)	11(2)	-8(3)
C(25)	142(16)	190(20)	91(10)	-76(12)	97(12)	-132(16)
O(11)	185(14)	172(13)	170(13)	-125(11)	163(13)	-128(11)
C(27)	82(10)	151(15)	153(15)	91(12)	108(12)	71(10)
C(26)	137(18)	132(17)	270(30)	-75(19)	180(20)	-49(14)
C(18)	54(7)	26(4)	34(5)	0(3)	5(4)	-14(3)
N(7)	143(14)	31(4)	101(12)	5(5)	97(12)	2(6)
N(6)	510(40)	28(4)	66(7)	5(7)	128(14)	79(14)
C(19)	49(5)	30(4)	45(4)	-7(3)	28(4)	-2(3)

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