Electronic Supplementary Information for Dalton Transactions

Supporting Experimental Information

Fixation of Atmospheric Carbon Dioxide by a Cadmium(II) Macrocyclic Complex

Daron E. Janzen, Maikel E. Botros, Donald VanDerveer, Gregory J. Grant

Details of X-ray Structural Analyses

1. Details of Structure 1.

Data collection and Structural Refinement

A crystal (approximate dimensions 0.12 x 0.12 x 0.12 mm^3) was placed onto the tip of a 0.1 mm diameter glass capillary, mounted, and X-ray intensity data were measured at 158(2) K using graphite-monochromated radiation (MoKα, λ = 0.71073Å) on a Rigaku AFC8S diffractometer equipped with a 1 K Mercury CCD detector.[1] The structure was solved using direct methods and refinement was done using full-matrix least-squares techniques (on F^2). Data were corrected for absorption, using semi-empirical methods. Structure, solution, refinement and the calculation of derived results were performed with the SHELXTL package of computer programs.[2] Please refer to Table 1A below for additional crystal and refinement information.

The orthorhombic space group $C222_1$ was determined based on systematic absences and intensity statistics. A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The final full matrix least squares refinement converged to $R1 = 0.0530$ and $wR2 = 0.1428$ (F^2, all data).

Structure description

The structure consists of one Cd(18N2O4) complex cation with all six donors from the macrocycle coordinated to the Cd(II) center. An ORTEP perspective of the cation is shown in Figure S1A.

Two water molecules are also coordinated to give an eight-coordinate complex in a highly distorted geometry. Two perchlorate anions and one quarter of a non-coordinated water molecule are also present in the asymmetric unit. There is a C_2 axis present. We also would note that a second crystal habit was isolated from the reaction mixture. Solving for Space Group *P6₃/m* yielded R1 = 0.085 and GooF = 1.13. However, there were disorder problems within the 18N2O4 ligand with the conformations of the two ethylene straps between O7 and N10. Nevertheless, the partial structure shows a seven-coordinate environment around the Cd(II) center containing a hexadentate 18N2O4 ligand with a single acetonitrile solvent molecule coordinated. A perspective of the partially refined structure is shown in Figure S2A.

Table 1A. Crystal data and structure refinement for **Compound 1**.

Empirical formula	C12 H30.50 Cd Cl2 N2 O14.25	
Formula weight	614.18	
Temperature	158(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$C222_1$	
Unit cell dimensions	a = 9.7500(19) Å	$\alpha = 90°$
	b = 20.124(6) Å	$\beta = 90°$
	c = 11.594(2) Å	$\gamma = 90°$
Volume	2274.8(9) $Å^3$	
Z	4	
Density (calculated)	1.793 Mg/m^3	
Absorption coefficient	1.265 mm^{-1}	
$F(000)$	1250	
Crystal color, morphology	colorless, needle	
Crystal size	0.12 x 0.12 x 0.12 mm^3	
Theta range for data collection	2.91 to 25.04 °	
Index ranges	$-10 \le h \le 11$, $-23 \le k \le 23$, $-13 \le l \le 13$	
Reflections collected	9171	
Independent reflections	2017 [R(int) = 0.0570]	
Completeness to theta = 25.04°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8630 and 0.8630	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2017 / 0 / 162	
Goodness-of-fit on F^2	1.095	
Final R indices [I>2sigma(I)]	$R1$ = 0.0530, $wR2$ = 0.1346	
R indices (all data)	$R1$ = 0.06597, $wR2$ = 0.1428	
Largest diff. peak and hole	1.305 and -0.783 $e.Å^{-3}$	

Table 2A. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **Compound 1.** U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Cd(1)	5000	3418(1)	2500	34(1)
C(1)	5340(11)	1721(4)	3069(8)	54(3)
O(2)	5009(9)	2301(2)	3723(4)	40(1)
C(3)	3718(10)	2228(5)	4322(7)	46(2)
C(4)	2994(10)	2883(5)	4398(7)	44(2)
N(5)	2858(7)	3182(3)	3239(5)	36(2)
C(6)	1907(9)	3749(4)	3210(8)	46(2)
C(7)	2598(9)	4385(5)	3559(8)	46(2)
O(8)	3681(6)	4476(3)	2779(5)	43(2)
C(9)	4459(10)	5075(4)	2958(9)	51(2)
O(1)	6023(7)	3706(3)	4281(5)	51(2)
Cl(1)	0	1936(1)	2500	34(1)
O(9)	425(15)	2564(6)	2066(11)	59(4)
O(10)	532(15)	1549(5)	3391(7)	92(6)
O(11)	1332(14)	1968(11)	1982(11)	118(6)
Cl(2)	3636(4)	0	5000	97(2)
O(12)	3750(40)	286(14)	3607(17)	176(16)
O(13)	4128(17)	558(6)	5372(13)	154(6)
O(14)	2236(14)	0	5000	99(4)
O(15)	5000	-197(9)	2500	22(6)

Table 3A. Bond lengths [Å] and angles [°] for **Compound 1**.

Cd(1)-N(5)#1	2.306(7)	C(9)-C(9)#1	1.497(18)
Cd(1)-N(5)	2.306(7)	Cl(1)-O(10)#2	1.393(7)
Cd(1)-O(1)#1	2.365(6)	Cl(1)-O(10)	1.393(7)
Cd(1)-O(1)	2.365(6)	Cl(1)-O(9)	1.422(12)
Cd(1)-O(8)#1	2.509(5)	Cl(1)-O(9)#2	1.422(12)
Cd(1)-O(8)	2.509(5)	Cl(1)-O(11)	1.432(13)
C(1)-O(2)	1.429(10)	Cl(1)-O(11)#2	1.432(13)
C(1)-C(1)#1	1.48(2)	O(9)-O(9)#2	1.30(3)
O(2)-C(3)	1.445(12)	O(9)-O(11)	1.49(2)
C(3)-C(4)	1.499(13)	Cl(2)-O(13)#3	1.295(11)
C(4)-N(5)	1.478(10)	Cl(2)-O(13)	1.295(11)
N(5)-C(6)	1.471(12)	Cl(2)-O(14)	1.365(14)
C(6)-C(7)	1.503(13)	Cl(2)-O(12)	1.718(16)
C(7)-O(8)	1.402(10)	Cl(2)-O(12)#3	1.718(16)
O(8)-C(9)	1.439(10)		
C(9)-C(9)#1	1.497(18)		

N(5)#1-Cd(1)-N(5)	156.2(3)	N(5)-Cd(1)-O(2)	68.3(2)
N(5)#1-Cd(1)-O(1)#1	96.2(2)	O(1)#1-Cd(1)-O(2)	132.4(2)
N(5)-Cd(1)-O(1)#1	89.6(2)	O(1)-Cd(1)-O(2)	74.9(2)
N(5)#1-Cd(1)-O(1)	89.6(2)	O(2)#1-Cd(1)-O(2)	64.5(2)
N(5)-Cd(1)-O(1)	96.2(2)	O(2)#1-Cd(1)-O(8)	141.7(2)
O(1)#1-Cd(1)-O(1)	151.7(3)	O(2)-Cd(1)-O(8)	130.6(2)
N(5)#1-Cd(1)-O(8)#1	70.3(2)	O(2)#1-Cd(1)-O(8)#1	130.6(2)
N(5)-Cd(1)-O(8)#1	133.4(2)	O(2)-Cd(1)-O(8)#1	141.7(2)
O(1)#1-Cd(1)-O(8)#1	84.0(2)	O(2)#1-Cd(1)-N(5)#1	68.3(2)
O(1)-Cd(1)-O(8)#1	71.9(2)	O(2)-C(1)-C(1)#1	111.9(7)
N(5)#1-Cd(1)-O(8)	133.4(2)	C(1)-O(2)-C(3)	111.6(7)
N(5)-Cd(1)-O(8)	70.3(2)	O(2)-C(3)-C(4)	110.4(7)
O(1)#1-Cd(1)-O(8)	71.9(2)	N(5)-C(4)-C(3)	110.3(7)
O(1)-Cd(1)-O(8)	84.0(2)	C(6)-N(5)-C(4)	113.1(7)
O(8)#1-Cd(1)-O(8)	63.8(3)	C(6)-N(5)-Cd(1)	113.7(5)
N(5)-Cd(1)-O(2)#1	91.2(2)	C(4)-N(5)-Cd(1)	109.9(5)

O(1)#1-Cd(1)-O(2)#1	74.9(2)	N(5)-C(6)-C(7)	111.9(7)
O(1)-Cd(1)-O(2)#1	132.4(2)	O(8)-C(7)-C(6)	105.9(6)
N(5)#1-Cd(1)-O(2)	91.2(2)	C(7)-O(8)-C(9)	114.4(6)
C(7)-O(8)-Cd(1)	111.0(5)	C(9)-O(8)-Cd(1)	117.3(5)
O(8)-C(9)-C(9)#1	105.6(6)	O(10)#2-Cl(1)-O(10)	112.1(8)
O(10)#2-Cl(1)-O(9)	110.1(6)	O(10)-Cl(1)-O(9)	130.5(7)
O(10)#2-Cl(1)-O(9)#2	130.5(7)	O(10)-Cl(1)-O(9)#2	110.1(6)
O(9)-Cl(1)-O(9)#2	54.6(12)	O(10)#2-Cl(1)-O(11)	92.9(10)
O(10)-Cl(1)-O(11)	89.9(9)	O(9)-Cl(1)-O(11)	63.1(10)
O(9)#2-Cl(1)-O(11)	111.9(11)	O(10)#2-Cl(1)-O(11)#2	89.9(9)
O(10)-Cl(1)-O(11)#2	92.9(10)	O(9)-Cl(1)-O(11)#2	111.9(11)
O(9)#2-Cl(1)-O(11)#2	63.1(10)	O(11)-Cl(1)-O(11)#2	174.9(18)
O(9)#2-O(9)-Cl(1)	62.7(6)	O(9)#2-O(9)-O(11)	115.3(9)
Cl(1)-O(9)-O(11)	58.8(8)	Cl(1)-O(11)-O(9)	58.1(7)
O(13)#3-Cl(2)-O(13)	136.5(16)	O(13)#3-Cl(2)-O(14)	111.7(8)
O(13)-Cl(2)-O(14)	111.7(8)	O(13)#3-Cl(2)-O(12)	87.3(14)
O(13)-Cl(2)-O(12)	90.0(10)	O(14)-Cl(2)-O(12)	93.6(12)
O(13)#3-Cl(2)-O(12)#3	90.0(10)	O(13)-Cl(2)-O(12)#3	87.3(14)
O(14)-Cl(2)-O(12)#3	93.6(12)	O(12)-Cl(2)-O(12)#3	173(2)

Symmetry transformations used to generate equivalent atoms:

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

Table 4A. Anisotropic displacement parameters ($Å^2$ x 10^3) for **Compound 1.**

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Cd(1)	31(1)	40(1)	29(1)	0	1(1)	0
C(1)	6	4(9)	45(4)	54(5)	3(4)	7(4)
O(2)	33(2)	48(3)	39(2)	2(2)	1(4)	1(4)
C(3)	50(6)	58(5)	31(4)	11(3)	-1(4)	-8(4)
C(4)	43(5)	59(5)	31(4)	3(4)	7(4)	-9(4)
N(5)	34(4)	41(4)	32(3)	1(3)	-1(3)	0(3)
C(6)	28(4)	45(5)	64(6)	-6(4)	13(4)	-2(4)
C(7)	38(5)	49(5)	51(5)	-12(4)	18(4)	2(4)
O(8)	37(3)	34(3)	57(5)	-10(2)	6(2)	-2(2)
C(9)	45(5)	36(4)	71(6)	-12(4)	15(4)	-2(4)
O(1)	59(4)	54(4)	40(3)	5(3)	-15(3)	-22(3)
Cl(1)	34(1)	38(1)	30(1)	0	-3(2)	0
O(9)	71(12)	49(7)	58(7)	7(5)	-17(6)	-32(7)
O(10)	191(16)	52(5)	33(4)	-8(4)	-64(7)	60(7)
O(11)	65(8)	212(17)	77(8)	-28(10)	27(6)	4(11)
Cl(2)	4(2)	52(2)	204(6)	-51(3)	0	0
O(12)	290(40)	180(20)	63(11)	78(14)	-73(16)	-160(20)
O(13)	173(13)	110(9)	180(13)	-14(9)	-39(10)	-83(9)
O(14)	69(8)	102(10)	127(11)	-33(9)	0	0
O(15)	31(14)	24(10)	10(9)	0	49(14)	0

Table 5A. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **Compound 1**.

	x	y	z	U(eq)
H(1A)	5063	1333	3491	65
H(1B)	6315	1699	2962	65
H(3A)	3880	2059	5084	56
H(3B)	3151	1915	3919	56
H(4A)	2101	2821	4729	53
H(4B)	3502	3178	4890	53
H(5)	2485	2860	2771	43
H(6A)	1153	3663	3721	55
H(6B)	1545	3796	2444	55
H(7A)	1966	4750	3518	55
H(7B)	2940	4354	4334	55
H(9A)	4868	5076	3711	61
H(9B)	3881	5459	2886	61

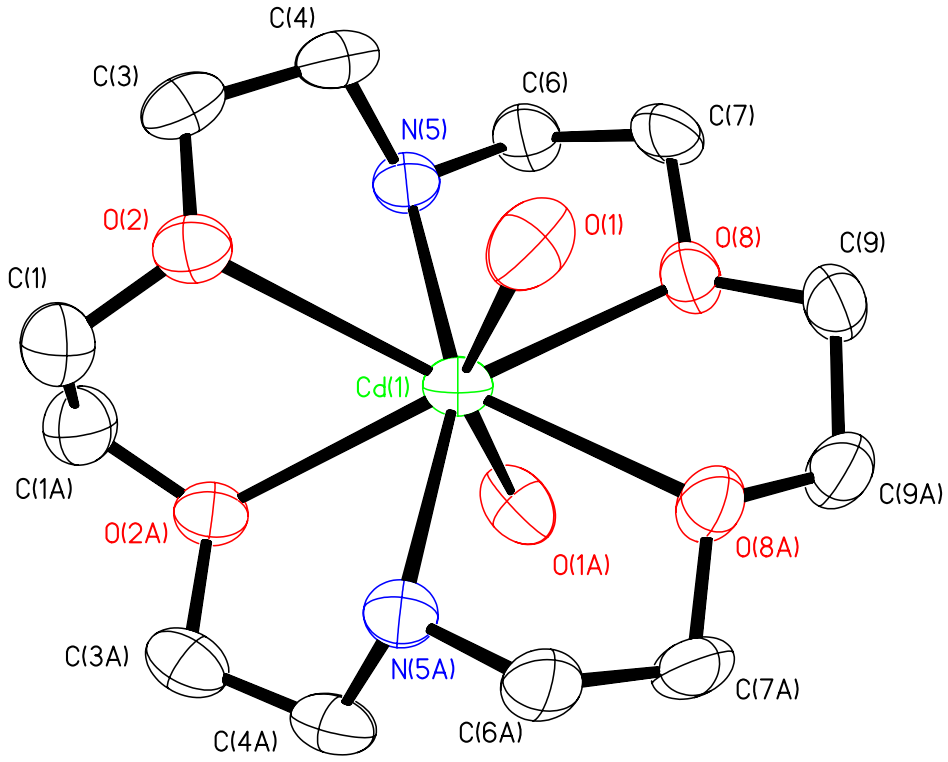


Figure S1A. Thermal ellipsoid perspective of cation in **Compound 1**. 50% Probability.

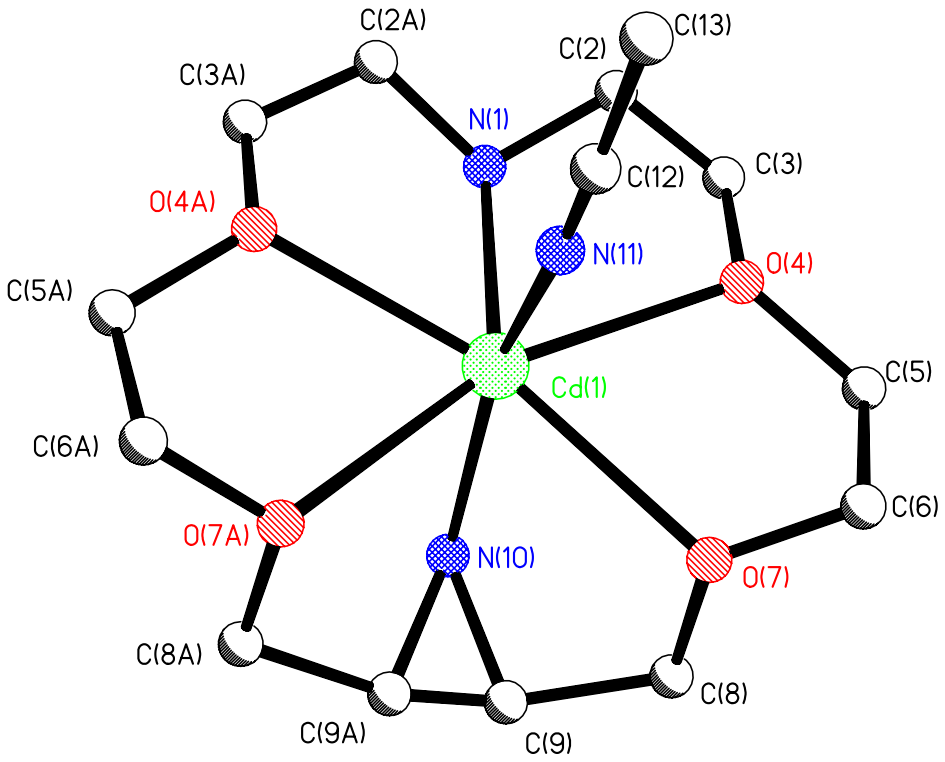


Figure S2A. Partial structure of cation in acetonitrile complex analog of **Compound 1**.

2. Details of X-ray Structural Analysis of Compound 2.

Data collection and Structural Refinement.

A crystal (approximate dimensions 0.55 x 0.24 x 0.06 mm^3) was placed onto the tip of a 0.1 mm diameter glass capillary, mounted, and X-ray intensity data were measured at 163(2) K using graphite-monochromated radiation (MoKα, λ = 0.71073Å) on a Rigaku AFC8S diffractometer equipped with a 1 K Mercury CCD detector.[1] A preliminary set of cell constants was calculated from reflections harvested from a few frames. The structure was solved using direct methods and refinement was done using full-matrix least-squares techniques (on F^2). Data were corrected for absorption, using semi-empirical methods. Structure, solution, refinement and the calculation of derived results were performed with the SHELXTL package of computer programs.[2] Please refer to Table 1B below for additional crystal and refinement information.

The orthorhombic space group *P-1* was determined based on systematic absences and intensity statistics. A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The final full matrix least squares refinement converged to $R1 = 0.0498$ and $wR2 = 0.1262$ (F^2, all data).

Structure description

The structure is not as expected and unusual. The structure consists of 3 unique $[Cd(18N2O4)]^{2+}$ complexes triply bridged by a carbonate unit. Four perchlorate anions complete the charge balance ($3*Cd^{2+} + CO_3^{2-} + 4ClO_4^- = 0$). Two acetonitrile solvate molecules and 0.5 water molecules are also present in the asymmetric unit. However unexpectedly, the Cd trimer is triply bridged by a single carbonate ion in μ_3 fashion. The C-O bond lengths and O-C-O bond angles of the triply bridging carbonate in this structure are very similar to those previously observed here (O13-C37 1.272(6) Å, O14-C37 1.284(5) Å, O15-C37 1.293(5) Å; O13-C37-O14 120.5(4)°, O13-C37-O15 119.6(4)°, O14-C37-O15 119.9(4) °). Additionally, the average C-O bond length in triply bridged carbonate Group 12 complexes is 1.28 Å while the average nitrate N-O bond length for the analogous search in the Cambridge Crystallographic Data Base (4 complexes) is 1.25 Å.[3] Also, in previous Cd complexes of this type, the trinuclear 4+ cation has crystallographic 3-fold symmetry, whereas in this structure though the geometry at each Cd center is very similar, there is no

crystallographic 3-fold symmetry.[4]

Even though each Cd has one short Cd-O bond, there is also a second longer Cd-O interaction, giving an asymmetric bidentate carbonate coordination at each Cd center. The formal Cd-O bonds are Cd(1)-O(13) 2.176(3)Å, Cd(2)-O(14) 2.173(3) Å, Cd(3)-O(15) 2.173(3) Å. The longer interactions are at Cd1-O15 2.7337(33) Å, Cd2-O13 2.8439(34) Å, Cd3-O14 2.7903(35) Å. These longer interactions are all less than the sum of Cd and O VDW radii (Cd 1.58 + O 1.52 = 3.1Å).[5] There are also some longer and shorter Cd-O bonds to the 18N2O4 ligands. The Cd bonds to the 18N2O4 ligands are as follows: (Cd1-N1 2.341(4) Å, Cd1-N2 2.328(4) Å, Cd1-O1 2.543(4) Å, Cd1-O2 2.607(4) Å, Cd1-O3 2.6947(38) Å, Cd1-O4 2.507(3) Å) , (Cd2-N3 2.338(5) Å, Cd2-N4 2.322(4) Å, Cd2-O5 2.521(4) Å, Cd2-O6 2.601(4) Å, Cd2-O7 2.6776(38) Å, Cd2-O8 2.500(4)) Å, (Cd3-N5 2.325(4) Å, Cd3-N6 2.336(5) Å, Cd3-O9 2.544(5) Å, Cd3-O10 2.632(5) Å, Cd3-O11 2.597(4) Å, Cd3-O12 2.515(4) Å). Each Cd-O distance is at least the van der Waals radii sum for Cd and O minus 0.4 Å.[5] Thus, each Cd can be described as eight coordinate. Also, at each Cd center, one of the nitrogen donors is almost perfectly trans to the longer Cd-O bond of the carbonate (see figures). The short carbonate Cd-O bond neatly bisects the N-Cd-N angle and has no trans atom coordinated. The 4 oxygen atoms of each 18N2O4 ligand are coordinated in a plane around each Cd center with small mean deviations from least-squares planes (Cd1, O1-O4 0.025, Cd2, O5-O8 0.082, Cd3, O9-O12 0.039). The angles between these least-squares planes are almost 60 (Cd1 plane-Cd2 plane 58.7°, Cd2 plane-Cd3 plane 61.6°, Cd3 plane-Cd1 plane 59.8°). Also, all these least-squares planes are essentially 90° to the Cd carbonate coordinated nitrogens' plane (Cd1,O1-O4 plane-Cd1,N1,N2, O13,O15 plane 88.7°, Cd2,O5-O8 plane-Cd2,N3,N4, O13,O14 plane 88.8°, Cd3,O9-O12 plane-Cd3,N5,N6, O14,O15 plane 88.2°).

As search of the Cambridge Crystallographic Data Base reveals two other related structures with similar 18-membered macrocyclic rings bound to Cd(II). These are [Cd(18N2O4)I_2] (CDTXZO) and a Cd cluster complex (WOZSOT) which uses a N,N'-bis(phosphonomethyl)-1,10-diaza-18-crown-6 ligand. Both involve 18N2O4 and have 8 coordinate Cd centers.[6,7] The structure [Cd(18N2O4)I_2] has *trans* iodides with the 6 coordinated atoms of 18N2O4 in a plane (N-Cd-N angle 180°). The structure of WOZSOT incorporates *cis* oxygens of the phosphonomethyl groups but the coordinated nitrogens of 18N2O4 are still roughly *trans* (N-Cd-N angle 152°).

The coordination environment at each Cd center is remarkably similar. A least-squares overlay of atom positions of Cd and coordinated N and O atoms (8 ligated atoms for each Cd) displays this similarity (Cd1-Cd2 RMS difference 0.123, Cd1-Cd3 0.117, Cd2-Cd3 0.087). See figures for more detail. The 18O4N2 conformation is very similar at each Cd center also with the exception

of one set of ethylene straps next to N6 of Cd3. The ethylene strap orientations are slightly different than for Cd1 and Cd2. If the ethylene straps are also included in the calculated RMS differences in the structure overlays, the results show this clearly. The RMS difference in atom positions for Cd and all C, N, and O atoms of 18O4N2 and the coordinated O atoms of carbonate for pair-wise comparisons are Cd2-Cd3 0.404, Cd1-Cd2 0.129, Cd1-Cd3 0.414. For each Cd center, the coordinated nitrogen atoms of the 18N2O4 ligand are in the same plane as for the bidentate carbonate coordination. This makes the nitrogen donors of each 18N2O4 ligand *cis* as seen by the N-Cd-N angles (N2-Cd1-N1 97.47(15)°, N4-Cd2-N3 98.63(19)°, N5-Cd3-N6 98.32(18)°). The mean deviation from a least-squares plane containing the Cd centers, the coordinated N atoms of the 18N2O4 ligands and the triply bridging carbonate is only 0.078 Å (least-squares plane formed by atoms Cd1-Cd3, N1-N6, C37, O13-O15).

The water molecule is disordered over an inversion center at 0.5,0.5,0.5 and is in a region where H-bonding to the perchlorates anions is possible. Refining the structure without the water molecule results in a solvent accessible void of 64 $Å^3$ and electron density of 6e- at this location (0.5,0.5,0.5) (SQUEEZE)and results in poorer refinement statistics. Spatial disorder was modeled for one of the perchlorate anions over two very similar positions with occupancies of 68%/32% for the two sets of atoms Cl4, O28-O31 and Cl4', O28'-O31'. The thermal displacement parameters were constrained to be the same for pair-wise atoms Cl4, Cl4'; O28,O28'; O29,O29'; O30,O30'; and O31,O31'. A few additional pair-wise constraints were made on the thermal displacement parameters of C18,C19; C28,C29; and C30,C31. The hydrogens of the water molecule were geometrically placed by fixing the O-H distances at 0.85Å and the H-O-H angle at 113.6° by fixing the H-H distance at 1.39 Å. The ideally placed hydrogens of the methyl groups of the acetonitrile molecules (fixed lengths of 0.98 Å) were allowed to refine the torsion angle with the preceding carbon to best place these hydrogens. Hydrogen atoms of the nitrogens of the 18O4N2 ligand were placed in ideal positions at distances of 0.93 Å. Hydrogen atoms of the carbons of the 18O4N2 ligand were placed in ideal positions at distances of 0.99 Å.

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, Clemson University. All calculations were performed using Pentium computers using the current SHELXTL suite of programs.

Table 1B. Crystal data and structure refinement for **Compound 2**.

Empirical formula	C82 H170 Cd6 Cl8 N16 O63	
Formula weight	3346.34	
Temperature	163(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 12.627(3) Å	α = 92.93(3)°
	b = 13.415(3) Å	β = 96.77(3)°
	c = 21.981(4) Å	γ = 117.74(3)°
Volume	3248.4(16) Å^3	
Z	1	
Density (calculated)	1.711 Mg/m^3	
Absorption coefficient	1.229 mm^{-1}	
F(000)	1702	
Crystal color, morphology	colorless, plate	
Crystal size	0.55 x 0.24 x 0.06 mm^3	
Theta range for data collection	2.56 to 26.02°	
Index ranges	$-15 \le h \le 15$, $-16 \le k \le 16$, $-23 \le l \le 27$	
Reflections collected	28278	
Independent reflections	12649 [R(int) = 0.0369]	
Observed reflections	10006	
Completeness to theta = 26.02°	98.6%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9299 and 0.5514	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12649 / 13 / 788	
Goodness-of-fit on F^2	1.063	
Final R indices [I>2sigma(I)]	R1 = 0.0498, wR2 = 0.1178	
R indices (all data)	R1 = 0.0693, wR2 = 0.1262	
Largest diff. peak and hole	1.265 and -0.716 e.Å^{-3}	

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

	x	y	z	U_{eq}
Cd1	3344(1)	10122(1)	2422(1)	25(1)
Cd2	1020(1)	6363(1)	3187(1)	28(1)
Cd3	4004(1)	6932(1)	1794(1)	30(1)
O13	2391(3)	8449(3)	2720(2)	28(1)
O15	3542(3)	8229(3)	2095(2)	26(1)
O4	5348(3)	10657(3)	3066(2)	31(1)
O8	2285(3)	7564(3)	4170(2)	38(1)
O14	2354(3)	6784(3)	2571(2)	28(1)
O1	2467(3)	9696(3)	1279(2)	38(1)
O12	4877(3)	6657(3)	2821(2)	41(1)
O2	1104(3)	9709(3)	2130(2)	37(1)
O6	-60(3)	4615(3)	2346(2)	50(1)
O7	2535(3)	5723(3)	3783(2)	38(1)
N2	3153(4)	11724(3)	2695(2)	30(1)
O5	-509(4)	6391(4)	2349(2)	50(1)
O10	3854(5)	7781(4)	754(2)	60(1)
N1	4898(3)	10970(3)	1835(2)	29(1)
O11	6125(3)	8539(4)	2304(2)	50(1)
C34	6051(5)	7426(6)	3141(3)	52(2)
O3	3505(3)	10580(3)	3648(2)	34(1)
C10	5588(5)	10931(4)	3723(2)	35(1)
N3	128(4)	7392(4)	3578(2)	40(1)
O9	2075(4)	5790(4)	1018(2)	61(1)
C5	1065(5)	10764(5)	2168(3)	44(1)
C8	3735(5)	11718(4)	3816(3)	40(1)
C12	6007(4)	10918(5)	2098(3)	36(1)
N4	-3(4)	4709(4)	3631(3)	50(1)
N5	3193(4)	5013(4)	1904(2)	41(1)
C7	4009(5)	12382(4)	3264(3)	40(1)
C9	4394(5)	10301(4)	3948(2)	35(1)
C3	1263(5)	9458(6)	1056(3)	47(2)

Cl1	1400(1)	8788(1)	9105(1)	38(1)
C37	2760(4)	7821(4)	2466(2)	24(1)
O19	2670(4)	9254(5)	9298(3)	71(2)
C11	6356(4)	11342(5)	2769(3)	37(1)
C1	4533(5)	10457(5)	1184(3)	40(1)
N6	5495(5)	7084(5)	1213(3)	56(2)
C6	1898(5)	11458(5)	2740(3)	41(1)
O18	1044(5)	9624(4)	9243(3)	79(2)
O17	786(5)	7866(5)	9448(4)	92(2)
C24	976(6)	8358(5)	4044(3)	52(2)
C13	-412(6)	7787(6)	3065(4)	55(2)
C4	531(5)	8993(5)	1559(3)	41(1)
C22	3120(5)	7332(5)	4550(3)	45(1)
C2	3338(5)	10366(5)	912(3)	43(1)
C21	3537(5)	6709(5)	4130(3)	42(1)
C23	1661(6)	8018(5)	4504(3)	52(2)
Cl2	9591(1)	1092(1)	3771(1)	47(1)
O23	10751(4)	2056(4)	3909(3)	67(1)
C20	1912(5)	4821(5)	4144(3)	46(2)
O22	9177(5)	1052(5)	3122(3)	80(2)
O21	8765(6)	1183(6)	4094(4)	103(2)
C25	1916(6)	4315(5)	1580(4)	57(2)
O20	9711(6)	115(5)	3831(4)	98(2)
C19	698(6)	4720(5)	4227(4)	60(1)
C26	1745(7)	4606(6)	958(4)	64(2)
Cl3	7210(1)	4894(1)	3980(1)	46(1)
C35	4508(6)	5497(5)	2886(3)	50(2)
O27	8391(5)	5450(7)	4327(3)	108(3)
O26	6411(6)	4132(6)	4303(3)	129(3)
C18	-355(6)	3657(5)	3180(4)	60(1)
C36	3260(6)	4810(5)	2555(3)	48(2)
C17	-910(7)	3682(6)	2577(4)	66(2)
C15	-1255(7)	5447(7)	1888(4)	71(2)
O16	1105(7)	8458(8)	8468(3)	125(3)
C29	4553(9)	7606(7)	329(4)	79(2)
C14	-1218(6)	6841(6)	2577(4)	59(2)

O25	7187(7)	4360(7)	3393(3)	131(3)
C32	7066(6)	8508(8)	2023(4)	72(2)
C33	6294(6)	8567(6)	2969(3)	55(2)
C16	-543(7)	4901(7)	1771(4)	70(2)
C28	2620(9)	7424(7)	530(4)	79(2)
C31	6616(9)	8177(8)	1366(5)	90(2)
C27	1873(9)	6183(7)	437(4)	82(3)
C30	4997(9)	6780(8)	556(5)	90(2)
O24	7006(10)	5754(8)	3832(5)	161(4)
N8	6271(5)	8993(5)	4627(3)	60(2)
C38	8323(6)	8000(6)	-140(3)	51(2)
C41	7031(6)	8773(6)	4700(3)	52(2)
C39	8295(8)	7217(6)	262(4)	71(2)
C40	8005(8)	8478(9)	4785(4)	87(3)
N7	8278(13)	6576(8)	578(4)	151(5)
O32	5720(18)	5770(19)	5220(5)	197(10)
Cl4	5178(7)	3901(5)	1390(3)	39(1)
O28	5920(7)	3418(7)	1277(5)	76(3)
O29	4170(30)	3224(17)	1660(20)	133(5)
O30	5856(9)	5044(7)	1694(5)	61(3)
O31	4557(9)	3965(9)	835(4)	103(3)
Cl4'	5038(17)	3718(12)	1481(8)	39(1)
O28'	5317(17)	3250(16)	979(9)	76(3)
O29'	3890(50)	3090(40)	1640(50)	133(5)
O30'	5470(20)	4901(15)	1481(12)	61(3)
O31'	5610(20)	3529(18)	2014(8)	103(3)

Table 3B. Bond lengths [Å] and angles [°] for **Compound 2**.

Cd(1)-O(13)	2.176(3)	O(7)-C(21)	1.429(7)
Cd(1)-N(2)	2.328(4)	O(7)-C(20)	1.439(6)
Cd(1)-N(1)	2.341(4)	N(2)-C(6)	1.470(7)
Cd(1)-O(4)	2.507(3)	N(2)-C(7)	1.480(7)
Cd(1)-O(1)	2.543(4)	N(2)-H(2C)	0.9300
Cd(1)-O(2)	2.607(4)	O(5)-C(14)	1.412(8)
Cd(2)-O(14)	2.173(3)	O(5)-C(15)	1.432(9)
Cd(2)-N(4)	2.322(4)	O(10)-C(28)	1.415(10)
Cd(2)-N(3)	2.338(5)	O(10)-C(29)	1.439(10)
Cd(2)-O(8)	2.500(4)	N(1)-C(1)	1.477(7)
Cd(2)-O(5)	2.521(4)	N(1)-C(12)	1.485(6)
Cd(2)-O(6)	2.601(4)	N(1)-H(1C)	0.9300
Cd(3)-O(15)	2.173(3)	O(11)-C(32)	1.418(8)
Cd(3)-N(5)	2.325(4)	O(11)-C(33)	1.448(8)
Cd(3)-N(6)	2.336(5)	C(34)-C(33)	1.493(10)
Cd(3)-O(12)	2.515(4)	C(34)-H(34A)	0.9900
Cd(3)-O(9)	2.544(5)	C(34)-H(34B)	0.9900
Cd(3)-O(11)	2.597(4)	O(3)-C(8)	1.434(6)
Cd(3)-O(10)	2.632(5)	O(3)-C(9)	1.442(6)
O(13)-C(37)	1.272(6)	C(10)-C(9)	1.504(7)
O(15)-C(37)	1.293(5)	C(10)-H(10A)	0.9900
O(4)-C(10)	1.431(6)	C(10)-H(10B)	0.9900
O(4)-C(11)	1.435(6)	N(3)-C(24)	1.479(8)
O(8)-C(22)	1.425(7)	N(3)-C(13)	1.495(8)
O(8)-C(23)	1.437(7)	N(3)-H(3C)	0.9300
O(14)-C(37)	1.284(5)	O(9)-C(26)	1.435(8)
O(1)-C(3)	1.418(6)	O(9)-C(27)	1.445(9)
O(1)-C(2)	1.427(6)	C(5)-C(6)	1.487(9)
O(12)-C(34)	1.419(7)	C(5)-H(5A)	0.9900
O(12)-C(35)	1.422(7)	C(5)-H(5B)	0.9900
O(2)-C(4)	1.427(7)	C(8)-C(7)	1.519(8)
O(2)-C(5)	1.437(7)	C(8)-H(8A)	0.9900
O(6)-C(17)	1.386(8)	C(8)-H(8B)	0.9900
O(6)-C(16)	1.484(9)	C(12)-C(11)	1.491(8)

C(12)-H(12A)	0.9900	C(4)-H(4B)	0.9900
C(12)-H(12B)	0.9900	C(22)-C(21)	1.508(9)
N(4)-C(19)	1.487(8)	C(22)-H(22A)	0.9900
N(4)-C(18)	1.531(9)	C(22)-H(22B)	0.9900
N(4)-H(4C)	0.9300	C(2)-H(2A)	0.9900
N(5)-C(36)	1.471(8)	C(2)-H(2B)	0.9900
N(5)-C(25)	1.496(8)	C(21)-H(21A)	0.9900
N(5)-H(5C)	0.9300	C(21)-H(21B)	0.9900
C(7)-H(7A)	0.9900	C(23)-H(23A)	0.9900
C(7)-H(7B)	0.9900	C(23)-H(23B)	0.9900
C(9)-H(9A)	0.9900	Cl(2)-O(21)	1.375(6)
C(9)-H(9B)	0.9900	Cl(2)-O(20)	1.399(5)
C(3)-C(4)	1.498(9)	Cl(2)-O(23)	1.415(5)
C(3)-H(3A)	0.9900	Cl(2)-O(22)	1.450(6)
C(3)-H(3B)	0.9900	C(20)-C(19)	1.509(10)
Cl(1)-O(16)	1.398(6)	C(20)-H(20A)	0.9900
Cl(1)-O(18)	1.421(5)	C(20)-H(20B)	0.9900
Cl(1)-O(19)	1.422(5)	C(25)-C(26)	1.459(11)
Cl(1)-O(17)	1.427(5)	C(25)-H(25A)	0.9900
C(11)-H(11A)	0.9900	C(25)-H(25B)	0.9900
C(11)-H(11B)	0.9900	C(19)-H(19A)	0.9900
C(1)-C(2)	1.502(8)	C(19)-H(19B)	0.9900
C(1)-H(1A)	0.9900	C(26)-H(26A)	0.9900
C(1)-H(1B)	0.9900	C(26)-H(26B)	0.9900
N(6)-C(30)	1.459(12)	Cl(3)-O(24)	1.342(7)
N(6)-C(31)	1.473(11)	Cl(3)-O(26)	1.361(6)
N(6)-H(6C)	0.9300	Cl(3)-O(27)	1.414(5)
C(6)-H(6A)	0.9900	Cl(3)-O(25)	1.432(7)
C(6)-H(6B)	0.9900	C(35)-C(36)	1.473(9)
C(24)-C(23)	1.478(10)	C(35)-H(35A)	0.9900
C(24)-H(24A)	0.9900	C(35)-H(35B)	0.9900
C(24)-H(24B)	0.9900	C(18)-C(17)	1.433(10)
C(13)-C(14)	1.483(11)	C(18)-H(18A)	0.9900
C(13)-H(13A)	0.9900	C(18)-H(18B)	0.9900
C(13)-H(13B)	0.9900	C(36)-H(36A)	0.9900
C(4)-H(4A)	0.9900	C(36)-H(36B)	0.9900

C(17)-H(17A)	0.9900	C(27)-H(27B)	0.9900
C(17)-H(17B)	0.9900	C(30)-H(30A)	0.9900
C(15)-C(16)	1.435(12)	C(30)-H(30B)	0.9900
C(15)-H(15A)	0.9900	N(8)-C(41)	1.126(9)
C(15)-H(15B)	0.9900	C(38)-C(39)	1.397(10)
C(29)-C(30)	1.537(12)	C(38)-H(38C)	0.9800
C(29)-H(29A)	0.9900	C(38)-H(38B)	0.9800
C(29)-H(29B)	0.9900	C(38)-H(38A)	0.9800
C(14)-H(14A)	0.9900	C(41)-C(40)	1.453(11)
C(14)-H(14B)	0.9900	C(39)-N(7)	1.128(11)
C(32)-C(31)	1.452(13)	C(40)-H(40C)	0.9800
C(32)-H(32A)	0.9900	C(40)-H(40B)	0.9800
C(32)-H(32B)	0.9900	C(40)-H(40A)	0.9800
C(33)-H(33A)	0.9900	O(32)-H(32E)	0.8527
C(33)-H(33B)	0.9900	O(32)-H(32F)	0.8554
C(16)-H(16A)	0.9900	Cl(4)-O(29)	1.396(10)
C(16)-H(16B)	0.9900	Cl(4)-O(31)	1.399(12)
C(28)-C(27)	1.470(11)	Cl(4)-O(28)	1.402(9)
C(28)-H(28A)	0.9900	Cl(4)-O(30)	1.438(8)
C(28)-H(28B)	0.9900	Cl(4')-O(29')	1.399(16)
C(31)-H(31A)	0.9900	Cl(4')-O(28')	1.400(15)
C(31)-H(31B)	0.9900	Cl(4')-O(31')	1.40(2)
C(27)-H(27A)	0.9900	Cl(4')-O(30')	1.418(14)

O(13)-Cd(1)-N(2)	127.50(14)	O(15)-Cd(3)-O(9)	95.61(15)
O(13)-Cd(1)-N(1)	134.88(14)	N(5)-Cd(3)-O(9)	69.85(17)
N(2)-Cd(1)-N(1)	97.47(15)	N(6)-Cd(3)-O(9)	101.8(2)
O(13)-Cd(1)-O(4)	95.68(12)	O(12)-Cd(3)-O(9)	135.82(14)
N(2)-Cd(1)-O(4)	99.72(14)	O(15)-Cd(3)-O(11)	79.38(13)
N(1)-Cd(1)-O(4)	70.29(13)	N(5)-Cd(3)-O(11)	126.67(16)
O(13)-Cd(1)-O(1)	100.87(13)	N(6)-Cd(3)-O(11)	68.84(19)
N(2)-Cd(1)-O(1)	100.98(14)	O(12)-Cd(3)-O(11)	63.13(14)
N(1)-Cd(1)-O(1)	69.88(13)	O(9)-Cd(3)-O(11)	161.03(15)
O(4)-Cd(1)-O(1)	136.94(12)	O(15)-Cd(3)-O(10)	79.29(14)
O(13)-Cd(1)-O(2)	79.46(12)	N(5)-Cd(3)-O(10)	125.57(17)
N(2)-Cd(1)-O(2)	69.33(13)	N(6)-Cd(3)-O(10)	67.06(19)
N(1)-Cd(1)-O(2)	126.50(13)	O(12)-Cd(3)-O(10)	160.40(15)
O(4)-Cd(1)-O(2)	159.94(12)	O(9)-Cd(3)-O(10)	63.39(16)
O(1)-Cd(1)-O(2)	63.00(12)	O(11)-Cd(3)-O(10)	97.65(16)
O(14)-Cd(2)-N(4)	130.11(17)	C(37)-O(13)-Cd(1)	107.4(3)
O(14)-Cd(2)-N(3)	131.24(14)	C(37)-O(15)-Cd(3)	108.5(3)
N(4)-Cd(2)-N(3)	98.63(19)	C(10)-O(4)-C(11)	113.4(4)
O(14)-Cd(2)-O(8)	102.03(13)	C(10)-O(4)-Cd(1)	123.5(3)
N(4)-Cd(2)-O(8)	95.93(17)	C(11)-O(4)-Cd(1)	112.6(3)
N(3)-Cd(2)-O(8)	69.95(15)	C(22)-O(8)-C(23)	114.4(5)
O(14)-Cd(2)-O(5)	91.54(14)	C(22)-O(8)-Cd(2)	123.5(3)
N(4)-Cd(2)-O(5)	106.16(16)	C(23)-O(8)-Cd(2)	112.6(3)
N(3)-Cd(2)-O(5)	70.37(17)	C(37)-O(14)-Cd(2)	110.3(3)
O(8)-Cd(2)-O(5)	136.83(14)	C(3)-O(1)-C(2)	114.3(4)
O(14)-Cd(2)-O(6)	78.56(13)	C(3)-O(1)-Cd(1)	123.0(3)
N(4)-Cd(2)-O(6)	69.43(18)	C(2)-O(1)-Cd(1)	112.1(3)
N(3)-Cd(2)-O(6)	125.37(15)	C(34)-O(12)-C(35)	114.5(5)
O(8)-Cd(2)-O(6)	159.22(13)	C(34)-O(12)-Cd(3)	123.6(4)
O(5)-Cd(2)-O(6)	63.43(14)	C(35)-O(12)-Cd(3)	112.9(3)
O(15)-Cd(3)-N(5)	132.76(15)	C(4)-O(2)-C(5)	115.4(4)
O(15)-Cd(3)-N(6)	128.89(16)	C(4)-O(2)-Cd(1)	112.0(3)
N(5)-Cd(3)-N(6)	98.32(18)	C(5)-O(2)-Cd(1)	109.1(3)
O(15)-Cd(3)-O(12)	99.54(13)	C(17)-O(6)-C(16)	114.3(5)
N(5)-Cd(3)-O(12)	69.42(16)	C(17)-O(6)-Cd(2)	110.9(4)
N(6)-Cd(3)-O(12)	100.29(18)	C(16)-O(6)-Cd(2)	111.2(4)

C(21)-O(7)-C(20)	114.4(4)	C(24)-N(3)-Cd(2)	113.0(3)
C(6)-N(2)-C(7)	112.6(4)	C(13)-N(3)-Cd(2)	110.4(4)
C(6)-N(2)-Cd(1)	112.9(3)	C(24)-N(3)-H(3C)	107.5
C(7)-N(2)-Cd(1)	110.4(3)	C(13)-N(3)-H(3C)	107.5
C(6)-N(2)-H(2C)	106.8	Cd(2)-N(3)-H(3C)	107.5
C(7)-N(2)-H(2C)	106.8	C(26)-O(9)-C(27)	113.2(6)
Cd(1)-N(2)-H(2C)	106.8	C(26)-O(9)-Cd(3)	110.9(4)
C(14)-O(5)-C(15)	109.6(6)	C(27)-O(9)-Cd(3)	121.7(5)
C(14)-O(5)-Cd(2)	112.5(4)	O(2)-C(5)-C(6)	106.3(4)
C(15)-O(5)-Cd(2)	122.9(4)	O(2)-C(5)-H(5A)	110.5
C(28)-O(10)-C(29)	117.1(6)	C(6)-C(5)-H(5A)	110.5
C(28)-O(10)-Cd(3)	108.8(4)	O(2)-C(5)-H(5B)	110.5
C(29)-O(10)-Cd(3)	112.6(4)	C(6)-C(5)-H(5B)	110.5
C(1)-N(1)-C(12)	108.8(4)	H(5A)-C(5)-H(5B)	108.7
C(1)-N(1)-Cd(1)	112.6(3)	O(3)-C(8)-C(7)	110.1(4)
C(12)-N(1)-Cd(1)	111.7(3)	O(3)-C(8)-H(8A)	109.6
C(1)-N(1)-H(1C)	107.8	C(7)-C(8)-H(8A)	109.6
C(12)-N(1)-H(1C)	107.8	O(3)-C(8)-H(8B)	109.6
Cd(1)-N(1)-H(1C)	107.8	C(7)-C(8)-H(8B)	109.6
C(32)-O(11)-C(33)	114.6(5)	H(8A)-C(8)-H(8B)	108.2
C(32)-O(11)-Cd(3)	111.8(5)	N(1)-C(12)-C(11)	110.9(4)
C(33)-O(11)-Cd(3)	111.5(3)	N(1)-C(12)-H(12A)	109.5
O(12)-C(34)-C(33)	105.6(5)	C(11)-C(12)-H(12A)	109.5
O(12)-C(34)-H(34A)	110.6	N(1)-C(12)-H(12B)	109.5
C(33)-C(34)-H(34A)	110.6	C(11)-C(12)-H(12B)	109.5
O(12)-C(34)-H(34B)	110.6	H(12A)-C(12)-H(12B)	108.1
C(33)-C(34)-H(34B)	110.6	C(19)-N(4)-C(18)	112.3(5)
H(34A)-C(34)-H(34B)	108.7	C(19)-N(4)-Cd(2)	111.6(3)
C(8)-O(3)-C(9)	114.7(4)	C(18)-N(4)-Cd(2)	111.2(4)
O(4)-C(10)-C(9)	106.6(4)	C(19)-N(4)-H(4C)	107.1
O(4)-C(10)-H(10A)	110.4	C(18)-N(4)-H(4C)	107.1
C(9)-C(10)-H(10A)	110.4	Cd(2)-N(4)-H(4C)	107.1
O(4)-C(10)-H(10B)	110.4	C(36)-N(5)-C(25)	109.4(5)
C(9)-C(10)-H(10B)	110.4	C(36)-N(5)-Cd(3)	112.2(3)
H(10A)-C(10)-H(10B)	108.6	C(25)-N(5)-Cd(3)	113.5(4)
C(24)-N(3)-C(13)	110.7(5)	C(36)-N(5)-H(5C)	107.1

C(25)-N(5)-H(5C)	107.1	N(1)-C(1)-H(1A)	109.4
Cd(3)-N(5)-H(5C)	107.1	C(2)-C(1)-H(1A)	109.4
N(2)-C(7)-C(8)	112.0(4)	N(1)-C(1)-H(1B)	109.4
N(2)-C(7)-H(7A)	109.2	C(2)-C(1)-H(1B)	109.4
C(8)-C(7)-H(7A)	109.2	H(1A)-C(1)-H(1B)	108.0
N(2)-C(7)-H(7B)	109.2	C(30)-N(6)-C(31)	114.6(7)
C(8)-C(7)-H(7B)	109.2	C(30)-N(6)-Cd(3)	110.8(5)
H(7A)-C(7)-H(7B)	107.9	C(31)-N(6)-Cd(3)	113.0(5)
O(3)-C(9)-C(10)	111.1(4)	C(30)-N(6)-H(6C)	105.9
O(3)-C(9)-H(9A)	109.4	C(31)-N(6)-H(6C)	105.9
C(10)-C(9)-H(9A)	109.4	Cd(3)-N(6)-H(6C)	105.9
O(3)-C(9)-H(9B)	109.4	N(2)-C(6)-C(5)	110.8(5)
C(10)-C(9)-H(9B)	109.4	N(2)-C(6)-H(6A)	109.5
H(9A)-C(9)-H(9B)	108.0	C(5)-C(6)-H(6A)	109.5
O(1)-C(3)-C(4)	107.2(4)	N(2)-C(6)-H(6B)	109.5
O(1)-C(3)-H(3A)	110.3	C(5)-C(6)-H(6B)	109.5
C(4)-C(3)-H(3A)	110.3	H(6A)-C(6)-H(6B)	108.1
O(1)-C(3)-H(3B)	110.3	C(23)-C(24)-N(3)	111.5(5)
C(4)-C(3)-H(3B)	110.3	C(23)-C(24)-H(24A)	109.3
H(3A)-C(3)-H(3B)	108.5	N(3)-C(24)-H(24A)	109.3
O(16)-Cl(1)-O(18)	108.3(4)	C(23)-C(24)-H(24B)	109.3
O(16)-Cl(1)-O(19)	110.4(4)	N(3)-C(24)-H(24B)	109.3
O(18)-Cl(1)-O(19)	109.3(4)	H(24A)-C(24)-H(24B)	108.0
O(16)-Cl(1)-O(17)	112.3(5)	C(14)-C(13)-N(3)	111.6(5)
O(18)-Cl(1)-O(17)	107.9(4)	C(14)-C(13)-H(13A)	109.3
O(19)-Cl(1)-O(17)	108.6(3)	N(3)-C(13)-H(13A)	109.3
O(13)-C(37)-O(14)	120.5(4)	C(14)-C(13)-H(13B)	109.3
O(13)-C(37)-O(15)	119.6(4)	N(3)-C(13)-H(13B)	109.3
O(14)-C(37)-O(15)	119.9(4)	H(13A)-C(13)-H(13B)	108.0
O(4)-C(11)-C(12)	107.6(4)	O(2)-C(4)-C(3)	111.2(5)
O(4)-C(11)-H(11A)	110.2	O(2)-C(4)-H(4A)	109.4
C(12)-C(11)-H(11A)	110.2	C(3)-C(4)-H(4A)	109.4
O(4)-C(11)-H(11B)	110.2	O(2)-C(4)-H(4B)	109.4
C(12)-C(11)-H(11B)	110.2	C(3)-C(4)-H(4B)	109.4
H(11A)-C(11)-H(11B)	108.5	H(4A)-C(4)-H(4B)	108.0
N(1)-C(1)-C(2)	111.4(5)	O(8)-C(22)-C(21)	106.6(5)

O(8)-C(22)-H(22A)	110.4	C(26)-C(25)-H(25A)	109.2
C(21)-C(22)-H(22A)	110.4	N(5)-C(25)-H(25A)	109.2
O(8)-C(22)-H(22B)	110.4	C(26)-C(25)-H(25B)	109.2
C(21)-C(22)-H(22B)	110.4	N(5)-C(25)-H(25B)	109.2
H(22A)-C(22)-H(22B)	108.6	H(25A)-C(25)-H(25B)	107.9
O(1)-C(2)-C(1)	107.2(4)	N(4)-C(19)-C(20)	111.5(6)
O(1)-C(2)-H(2A)	110.3	N(4)-C(19)-H(19A)	109.3
C(1)-C(2)-H(2A)	110.3	C(20)-C(19)-H(19A)	109.3
O(1)-C(2)-H(2B)	110.3	N(4)-C(19)-H(19B)	109.3
C(1)-C(2)-H(2B)	110.3	C(20)-C(19)-H(19B)	109.3
H(2A)-C(2)-H(2B)	108.5	H(19A)-C(19)-H(19B)	108.0
O(7)-C(21)-C(22)	111.5(4)	O(9)-C(26)-C(25)	107.1(5)
O(7)-C(21)-H(21A)	109.3	O(9)-C(26)-H(26A)	110.3
C(22)-C(21)-H(21A)	109.3	C(25)-C(26)-H(26A)	110.3
O(7)-C(21)-H(21B)	109.3	O(9)-C(26)-H(26B)	110.3
C(22)-C(21)-H(21B)	109.3	C(25)-C(26)-H(26B)	110.3
H(21A)-C(21)-H(21B)	108.0	H(26A)-C(26)-H(26B)	108.6
O(8)-C(23)-C(24)	107.1(5)	O(24)-Cl(3)-O(26)	116.2(7)
O(8)-C(23)-H(23A)	110.3	O(24)-Cl(3)-O(27)	103.3(6)
C(24)-C(23)-H(23A)	110.3	O(26)-Cl(3)-O(27)	110.9(4)
O(8)-C(23)-H(23B)	110.3	O(24)-Cl(3)-O(25)	103.4(7)
C(24)-C(23)-H(23B)	110.3	O(26)-Cl(3)-O(25)	111.0(5)
H(23A)-C(23)-H(23B)	108.5	O(27)-Cl(3)-O(25)	111.7(5)
O(21)-Cl(2)-O(20)	115.3(5)	O(12)-C(35)-C(36)	108.3(5)
O(21)-Cl(2)-O(23)	112.5(4)	O(12)-C(35)-H(35A)	110.0
O(20)-Cl(2)-O(23)	109.0(4)	C(36)-C(35)-H(35A)	110.0
O(21)-Cl(2)-O(22)	107.3(4)	O(12)-C(35)-H(35B)	110.0
O(20)-Cl(2)-O(22)	106.4(4)	C(36)-C(35)-H(35B)	110.0
O(23)-Cl(2)-O(22)	105.7(4)	H(35A)-C(35)-H(35B)	108.4
O(7)-C(20)-C(19)	111.1(5)	C(17)-C(18)-N(4)	113.7(6)
O(7)-C(20)-H(20A)	109.4	C(17)-C(18)-H(18A)	108.8
C(19)-C(20)-H(20A)	109.4	N(4)-C(18)-H(18A)	108.8
O(7)-C(20)-H(20B)	109.4	C(17)-C(18)-H(18B)	108.8
C(19)-C(20)-H(20B)	109.4	N(4)-C(18)-H(18B)	108.8
H(20A)-C(20)-H(20B)	108.0	H(18A)-C(18)-H(18B)	107.7
C(26)-C(25)-N(5)	112.2(6)	N(5)-C(36)-C(35)	110.5(5)

N(5)-C(36)-H(36A)	109.6	O(11)-C(33)-H(33A)	109.6
C(35)-C(36)-H(36A)	109.6	C(34)-C(33)-H(33A)	109.6
N(5)-C(36)-H(36B)	109.6	O(11)-C(33)-H(33B)	109.6
C(35)-C(36)-H(36B)	109.6	C(34)-C(33)-H(33B)	109.6
H(36A)-C(36)-H(36B)	108.1	H(33A)-C(33)-H(33B)	108.1
O(6)-C(17)-C(18)	106.5(6)	C(15)-C(16)-O(6)	112.0(7)
O(6)-C(17)-H(17A)	110.4	C(15)-C(16)-H(16A)	109.2
C(18)-C(17)-H(17A)	110.4	O(6)-C(16)-H(16A)	109.2
O(6)-C(17)-H(17B)	110.4	C(15)-C(16)-H(16B)	109.2
C(18)-C(17)-H(17B)	110.4	O(6)-C(16)-H(16B)	109.2
H(17A)-C(17)-H(17B)	108.6	H(16A)-C(16)-H(16B)	107.9
O(5)-C(15)-C(16)	106.3(6)	O(10)-C(28)-C(27)	112.9(7)
O(5)-C(15)-H(15A)	110.5	O(10)-C(28)-H(28A)	109.0
C(16)-C(15)-H(15A)	110.5	C(27)-C(28)-H(28A)	109.0
O(5)-C(15)-H(15B)	110.5	O(10)-C(28)-H(28B)	109.0
C(16)-C(15)-H(15B)	110.5	C(27)-C(28)-H(28B)	109.0
H(15A)-C(15)-H(15B)	108.7	H(28A)-C(28)-H(28B)	107.8
O(10)-C(29)-C(30)	110.3(6)	C(32)-C(31)-N(6)	114.4(8)
O(10)-C(29)-H(29A)	109.6	C(32)-C(31)-H(31A)	108.7
C(30)-C(29)-H(29A)	109.6	N(6)-C(31)-H(31A)	108.7
O(10)-C(29)-H(29B)	109.6	C(32)-C(31)-H(31B)	108.7
C(30)-C(29)-H(29B)	109.6	N(6)-C(31)-H(31B)	108.7
H(29A)-C(29)-H(29B)	108.1	H(31A)-C(31)-H(31B)	107.6
O(5)-C(14)-C(13)	107.3(5)	O(9)-C(27)-C(28)	106.3(6)
O(5)-C(14)-H(14A)	110.2	O(9)-C(27)-H(27A)	110.5
C(13)-C(14)-H(14A)	110.2	C(28)-C(27)-H(27A)	110.5
O(5)-C(14)-H(14B)	110.2	O(9)-C(27)-H(27B)	110.5
C(13)-C(14)-H(14B)	110.2	C(28)-C(27)-H(27B)	110.5
H(14A)-C(14)-H(14B)	108.5	H(27A)-C(27)-H(27B)	108.7
O(11)-C(32)-C(31)	107.4(6)	N(6)-C(30)-C(29)	110.3(7)
O(11)-C(32)-H(32A)	110.2	N(6)-C(30)-H(30A)	109.6
C(31)-C(32)-H(32A)	110.2	C(29)-C(30)-H(30A)	109.6
O(11)-C(32)-H(32B)	110.2	N(6)-C(30)-H(30B)	109.6
C(31)-C(32)-H(32B)	110.2	C(29)-C(30)-H(30B)	109.6
H(32A)-C(32)-H(32B)	108.5	H(30A)-C(30)-H(30B)	108.1
O(11)-C(33)-C(34)	110.2(5)	C(39)-C(38)-H(38C)	109.5

C(39)-C(38)-H(38B)	109.5	H(32E)-O(32)-H(32F)	113.7
H(38C)-C(38)-H(38B)	109.5	O(29)-Cl(4)-O(31)	98(2)
C(39)-C(38)-H(38A)	109.5	O(29)-Cl(4)-O(28)	115.3(14)
H(38C)-C(38)-H(38A)	109.5	O(31)-Cl(4)-O(28)	110.5(8)
H(38B)-C(38)-H(38A)	109.5	O(29)-Cl(4)-O(30)	113.4(12)
N(8)-C(41)-C(40)	179.1(9)	O(31)-Cl(4)-O(30)	105.9(7)
N(7)-C(39)-C(38)	178.8(11)	O(28)-Cl(4)-O(30)	112.6(7)
C(41)-C(40)-H(40C)	109.5	O(29')-Cl(4')-O(28')	117(3)
C(41)-C(40)-H(40B)	109.5	O(29')-Cl(4')-O(31')	93(4)
H(40C)-C(40)-H(40B)	109.5	O(28')-Cl(4')-O(31')	106.4(16)
C(41)-C(40)-H(40A)	109.5	O(29')-Cl(4')-O(30')	117(2)
H(40C)-C(40)-H(40A)	109.5	O(28')-Cl(4')-O(30')	112.0(15)
H(40B)-C(40)-H(40A)	109.5	O(31')-Cl(4')-O(30')	109.1(17)

Table 4B. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **Compound 2**. 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}
Cd1	23(1)	22(1)	28(1)	6(1)	6(1)	9(1)
Cd2	24(1)	25(1)	33(1)	9(1)	7(1)	10(1)
Cd3	33(1)	27(1)	29(1)	3(1)	8(1)	14(1)
O13	30(2)	24(2)	33(2)	4(1)	9(1)	14(1)
O15	25(2)	25(2)	28(2)	7(1)	10(1)	10(1)
O4	26(2)	34(2)	27(2)	5(2)	5(1)	9(1)
O8	38(2)	37(2)	33(2)	0(2)	4(2)	13(2)
O14	34(2)	20(2)	33(2)	9(1)	9(2)	14(1)
O1	33(2)	48(2)	31(2)	12(2)	5(2)	17(2)
O12	40(2)	40(2)	41(2)	3(2)	2(2)	20(2)
O2	35(2)	37(2)	39(2)	9(2)	2(2)	18(2)
O6	32(2)	37(2)	67(3)	-3(2)	-1(2)	7(2)
O7	38(2)	34(2)	33(2)	6(2)	2(2)	12(2)
N2	34(2)	21(2)	34(2)	5(2)	8(2)	11(2)
O5	45(2)	45(2)	56(3)	8(2)	-6(2)	21(2)
O10	84(3)	57(3)	41(3)	12(2)	8(2)	35(3)
N1	27(2)	29(2)	32(2)	11(2)	10(2)	12(2)
O11	30(2)	47(2)	76(3)	12(2)	15(2)	19(2)
C34	41(3)	63(4)	53(4)	-5(3)	-11(3)	31(3)
O3	36(2)	26(2)	35(2)	4(2)	5(2)	11(2)
C10	34(3)	33(3)	30(3)	4(2)	0(2)	9(2)
N3	37(2)	34(2)	54(3)	16(2)	21(2)	18(2)
O9	67(3)	52(3)	47(3)	2(2)	-10(2)	20(2)
C5	38(3)	42(3)	57(4)	11(3)	6(3)	25(3)
C8	51(3)	31(3)	39(3)	2(2)	10(3)	21(2)
C12	27(2)	41(3)	44(3)	11(2)	15(2)	16(2)
N4	32(2)	35(2)	71(4)	33(3)	6(2)	4(2)
N5	43(3)	27(2)	55(3)	0(2)	11(2)	18(2)
C7	46(3)	25(2)	41(3)	-1(2)	1(2)	13(2)
C9	41(3)	34(3)	28(3)	9(2)	6(2)	17(2)
C3	38(3)	61(4)	37(3)	6(3)	-9(2)	23(3)

Cl1	38(1)	41(1)	34(1)	1(1)	2(1)	19(1)
C37	18(2)	25(2)	24(2)	4(2)	0(2)	7(2)
O19	35(2)	87(4)	77(4)	19(3)	7(2)	19(2)
C11	18(2)	38(3)	47(3)	7(2)	5(2)	7(2)
C1	44(3)	45(3)	30(3)	8(2)	15(2)	17(3)
N6	73(4)	52(3)	64(4)	19(3)	39(3)	39(3)
C6	40(3)	41(3)	50(4)	10(3)	16(3)	24(3)
O18	84(4)	55(3)	110(5)	0(3)	28(3)	42(3)
O17	57(3)	66(3)	154(6)	60(4)	30(4)	23(3)
C24	52(4)	32(3)	77(5)	7(3)	28(3)	21(3)
C13	58(4)	54(4)	86(5)	40(4)	37(4)	46(3)
C4	29(3)	44(3)	42(3)	3(3)	-3(2)	13(2)
C22	34(3)	49(3)	32(3)	-2(3)	0(2)	6(2)
C2	45(3)	50(3)	28(3)	13(3)	8(2)	17(3)
C21	30(3)	44(3)	43(3)	9(3)	2(2)	12(2)
C23	51(4)	46(3)	53(4)	-7(3)	18(3)	17(3)
Cl2	48(1)	34(1)	61(1)	3(1)	4(1)	23(1)
O23	61(3)	52(3)	73(4)	2(2)	-3(3)	18(2)
C20	46(3)	43(3)	38(3)	20(3)	-2(3)	12(3)
O22	80(4)	86(4)	60(4)	-3(3)	-1(3)	31(3)
O21	108(5)	113(5)	112(6)	16(4)	69(4)	59(4)
C25	53(4)	24(3)	79(5)	-5(3)	4(3)	8(3)
O20	129(5)	50(3)	134(6)	16(3)	11(5)	59(4)
C19	49(3)	34(2)	79(4)	24(2)	-1(2)	5(2)
C26	61(4)	41(3)	64(5)	-16(3)	-6(4)	9(3)
Cl3	43(1)	44(1)	40(1)	15(1)	2(1)	10(1)
C35	68(4)	52(4)	48(4)	13(3)	12(3)	42(3)
O27	45(3)	159(6)	55(4)	7(4)	0(3)	-4(3)
O26	93(5)	124(6)	61(4)	34(4)	4(3)	-39(4)
C18	49(3)	34(2)	79(4)	24(2)	-1(2)	5(2)
C36	59(4)	31(3)	58(4)	15(3)	15(3)	24(3)
C17	55(4)	37(3)	85(6)	8(4)	13(4)	4(3)
C15	70(5)	67(5)	62(5)	20(4)	-11(4)	24(4)
O16	146(6)	216(9)	44(4)	-44(4)	-26(4)	128(7)
C29	134(6)	71(4)	41(3)	14(3)	13(3)	57(4)
C14	44(3)	71(5)	75(5)	37(4)	12(3)	35(3)

O25	100(5)	150(7)	66(4)	-38(4)	19(4)	1(5)
C32	40(4)	92(6)	99(7)	30(5)	30(4)	37(4)
C33	41(3)	51(4)	59(4)	-11(3)	-5(3)	14(3)
C16	52(4)	76(5)	52(5)	4(4)	-3(3)	8(4)
C28	134(6)	71(4)	41(3)	14(3)	13(3)	57(4)
C31	102(5)	82(4)	107(6)	24(4)	59(4)	49(4)
C27	106(7)	83(6)	47(5)	-4(4)	-26(4)	47(5)
C30	102(5)	82(4)	107(6)	24(4)	59(4)	49(4)
O24	221(10)	147(8)	177(10)	61(7)	17(8)	139(8)
N8	53(3)	66(4)	53(4)	5(3)	16(3)	20(3)
C38	48(3)	55(4)	46(4)	1(3)	6(3)	22(3)
C41	45(4)	62(4)	33(3)	2(3)	6(3)	13(3)
C39	105(6)	45(4)	50(4)	1(3)	10(4)	26(4)
C40	68(5)	134(8)	67(6)	26(5)	13(4)	53(6)
N7	273(15)	86(6)	67(6)	30(5)	9(7)	65(8)
Cl4	46(2)	33(2)	44(2)	9(1)	20(1)	20(2)
O28	57(5)	55(4)	128(9)	-10(5)	24(5)	35(5)
O29	189(14)	51(6)	188(9)	51(7)	161(14)	50(7)
O30	69(8)	33(3)	75(9)	0(4)	12(5)	20(4)
O31	105(6)	117(7)	67(6)	20(5)	-19(5)	43(6)
Cl4'	46(2)	33(2)	44(2)	9(1)	20(1)	20(2)
O28'	57(5)	55(4)	128(9)	-10(5)	24(5)	35(5)
O29'	189(14)	51(6)	188(9)	51(7)	161(14)	50(7)
O30'	69(8)	33(3)	75(9)	0(4)	12(5)	20(4)
O31'	105(6)	117(7)	67(6)	20(5)	-19(5)	43(6)

Table 5B. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **Compound 2**.

	x	y	z	U(eq)
H2C	3384	12181	2381	36
H1C	5094	11731	1841	35
H34A	6662	7226	3015	62
H34B	6074	7416	3592	62
H10A	5930	11759	3835	42
H10B	6174	10694	3910	42
H3C	-501	6902	3771	48
H5A	230	10628	2189	52
H5B	1333	11156	1802	52
H8A	4431	12094	4156	48
H8B	3017	11704	3963	48
H12A	6681	11384	1878	44
H12B	5860	10125	2037	44
H4C	-719	4682	3718	60
H5C	3662	4750	1725	49
H7A	3965	13091	3353	47
H7B	4846	12592	3197	47
H9A	4098	9474	3864	41
H9B	4510	10498	4399	41
H3A	929	8896	682	56
H3B	1247	10159	948	56
H11A	7081	11281	2942	44
H11B	6547	12147	2834	44
H1A	4469	9692	1158	48
H1B	5162	10927	941	48
H6C	5706	6533	1324	67
H6A	1853	12172	2806	49
H6B	1644	11037	3099	49
H24A	1551	8974	3835	62
H24B	514	8654	4258	62

H13A	-882	8127	3232	66
H13B	246	8382	2884	66
H4A	-284	8925	1443	49
H4B	429	8226	1609	49
H22A	2720	6858	4869	53
H22B	3818	8048	4758	53
H2A	3399	11130	916	51
H2B	3097	10002	479	51
H21A	4009	7223	3842	50
H21B	4076	6482	4379	50
H23A	2250	8682	4800	63
H23B	1102	7437	4736	63
H20A	2413	4971	4553	55
H20B	1791	4096	3936	55
H25A	1700	3502	1555	68
H25B	1363	4432	1823	68
H19A	226	4012	4407	72
H19B	824	5366	4520	72
H26A	2263	4460	702	77
H26B	888	4145	760	77
H35A	4539	5385	3329	60
H35B	5058	5263	2712	60
H18A	380	3585	3142	72
H18B	-924	2977	3351	72
H36A	2997	3996	2581	57
H36B	2706	5010	2752	57
H17A	-1136	2976	2307	79
H17B	-1650	3753	2602	79
H15A	-1486	5710	1507	85
H15B	-2003	4916	2039	85
H29A	5258	8341	290	94
H29B	4048	7294	-84	94
H14A	-1895	6250	2749	71
H14B	-1560	7122	2240	71
H32A	7288	7953	2198	86
H32B	7793	9264	2095	86

H33A	5735	8794	3140	66
H33B	7135	9136	3147	66
H16A	141	5409	1569	84
H16B	-1050	4198	1483	84
H28A	2558	7726	133	94
H28B	2296	7747	827	94
H31A	7253	8131	1162	108
H31B	6465	8776	1195	108
H27A	1006	5969	322	98
H27B	2118	5847	105	98
H30A	4314	5997	486	108
H30B	5628	6804	320	108
H38C	8355	8658	93	62
H38B	7592	7645	-453	62
H38A	9041	8246	-342	62
H40C	7662	7651	4722	104
H40B	8458	8767	5205	104
H40A	8551	8816	4486	104
H32E	5894	5649	4870	236
H32F	5247	6066	5204	236

Table 6B. Torsion angles [°] for **Compound 2**.

N2-Cd1-O13-C37	-179.8(3)	O5-Cd2-O14-C37	71.8(3)
N1-Cd1-O13-C37	-5.2(4)	O6-Cd2-O14-C37	134.3(3)
O4-Cd1-O13-C37	-72.9(3)	O13-Cd1-O1-C3	72.2(4)
O1-Cd1-O13-C37	67.1(3)	N2-Cd1-O1-C3	-59.7(4)
O2-Cd1-O13-C37	126.7(3)	N1-Cd1-O1-C3	-153.8(4)
N5-Cd3-O15-C37	9.7(4)	O4-Cd1-O1-C3	-177.1(4)
N6-Cd3-O15-C37	-172.6(3)	O2-Cd1-O1-C3	0.1(4)
O12-Cd3-O15-C37	-61.0(3)	O13-Cd1-O1-C2	-145.3(4)
O9-Cd3-O15-C37	77.4(3)	N2-Cd1-O1-C2	82.7(4)
O11-Cd3-O15-C37	-121.1(3)	N1-Cd1-O1-C2	-11.3(4)
O10-Cd3-O15-C37	138.9(3)	O4-Cd1-O1-C2	-34.6(4)
O13-Cd1-O4-C10	-72.4(4)	O2-Cd1-O1-C2	142.6(4)
N2-Cd1-O4-C10	57.2(4)	O15-Cd3-O12-C34	-76.5(4)
N1-Cd1-O4-C10	151.7(4)	N5-Cd3-O12-C34	151.3(5)
O1-Cd1-O4-C10	175.0(3)	N6-Cd3-O12-C34	56.2(4)
O2-Cd1-O4-C10	2.3(6)	O9-Cd3-O12-C34	175.2(4)
O13-Cd1-O4-C11	145.2(3)	O11-Cd3-O12-C34	-3.6(4)
N2-Cd1-O4-C11	-85.2(3)	O10-Cd3-O12-C34	8.4(7)
N1-Cd1-O4-C11	9.4(3)	O15-Cd3-O12-C35	138.4(4)
O1-Cd1-O4-C11	32.6(4)	N5-Cd3-O12-C35	6.2(4)
O2-Cd1-O4-C11	-140.1(4)	N6-Cd3-O12-C35	-88.9(4)
O14-Cd2-O8-C22	-72.7(4)	O9-Cd3-O12-C35	30.0(5)
N4-Cd2-O8-C22	60.5(4)	O11-Cd3-O12-C35	-148.7(4)
N3-Cd2-O8-C22	157.5(4)	O10-Cd3-O12-C35	-136.8(5)
O5-Cd2-O8-C22	-178.2(4)	O13-Cd1-O2-C4	-80.6(3)
O6-Cd2-O8-C22	16.7(6)	N2-Cd1-O2-C4	142.4(4)
O14-Cd2-O8-C23	142.8(4)	N1-Cd1-O2-C4	58.5(4)
N4-Cd2-O8-C23	-84.0(4)	O4-Cd1-O2-C4	-158.1(4)
N3-Cd2-O8-C23	13.1(4)	O1-Cd1-O2-C4	27.5(3)
O5-Cd2-O8-C23	37.3(4)	O13-Cd1-O2-C5	150.5(4)
O6-Cd2-O8-C23	-127.7(5)	N2-Cd1-O2-C5	13.4(3)
N4-Cd2-O14-C37	-175.5(3)	N1-Cd1-O2-C5	-70.5(4)
N3-Cd2-O14-C37	6.8(4)	O4-Cd1-O2-C5	73.0(5)
O8-Cd2-O14-C37	-67.0(3)	O1-Cd1-O2-C5	-101.5(4)

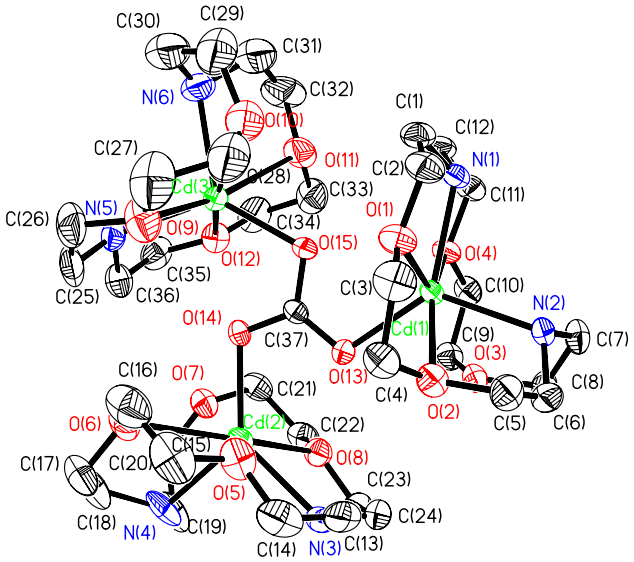
O14-Cd2-O6-C17	156.3(5)	O15-Cd3-O10-C29	155.7(5)
N4-Cd2-O6-C17	15.2(4)	N5-Cd3-O10-C29	-68.7(5)
N3-Cd2-O6-C17	-70.8(5)	N6-Cd3-O10-C29	15.0(5)
O8-Cd2-O6-C17	62.5(6)	O12-Cd3-O10-C29	67.4(7)
O5-Cd2-O6-C17	-106.1(5)	O9-Cd3-O10-C29	-102.4(5)
O14-Cd2-O6-C16	-75.4(4)	O11-Cd3-O10-C29	78.1(5)
N4-Cd2-O6-C16	143.6(4)	O13-Cd1-N1-C1	65.9(4)
N3-Cd2-O6-C16	57.6(5)	N2-Cd1-N1-C1	-118.5(4)
O8-Cd2-O6-C16	-169.1(4)	O4-Cd1-N1-C1	143.8(4)
O5-Cd2-O6-C16	22.2(4)	O1-Cd1-N1-C1	-19.5(3)
O13-Cd1-N2-C6	-38.2(4)	O2-Cd1-N1-C1	-48.7(4)
N1-Cd1-N2-C6	145.7(4)	O13-Cd1-N1-C12	-57.0(4)
O4-Cd1-N2-C6	-143.1(4)	N2-Cd1-N1-C12	118.7(3)
O1-Cd1-N2-C6	74.8(4)	O4-Cd1-N1-C12	21.0(3)
O2-Cd1-N2-C6	19.4(3)	O1-Cd1-N1-C12	-142.3(4)
O13-Cd1-N2-C7	88.8(3)	O2-Cd1-N1-C12	-171.6(3)
N1-Cd1-N2-C7	-87.3(3)	O15-Cd3-O11-C32	-150.1(5)
O4-Cd1-N2-C7	-16.1(3)	N5-Cd3-O11-C32	73.7(5)
O1-Cd1-N2-C7	-158.2(3)	N6-Cd3-O11-C32	-10.8(5)
O2-Cd1-N2-C7	146.4(4)	O12-Cd3-O11-C32	103.4(5)
O14-Cd2-O5-C14	-143.1(4)	O9-Cd3-O11-C32	-73.9(7)
N4-Cd2-O5-C14	84.2(4)	O10-Cd3-O11-C32	-72.5(5)
N3-Cd2-O5-C14	-9.4(4)	O15-Cd3-O11-C33	80.3(4)
O8-Cd2-O5-C14	-33.6(5)	N5-Cd3-O11-C33	-55.9(4)
O6-Cd2-O5-C14	140.5(4)	N6-Cd3-O11-C33	-140.5(4)
O14-Cd2-O5-C15	82.3(5)	O12-Cd3-O11-C33	-26.2(4)
N4-Cd2-O5-C15	-50.4(6)	O9-Cd3-O11-C33	156.4(5)
N3-Cd2-O5-C15	-144.0(6)	O10-Cd3-O11-C33	157.8(4)
O8-Cd2-O5-C15	-168.2(5)	C35-O12-C34-C33	175.4(5)
O6-Cd2-O5-C15	5.9(5)	Cd3-O12-C34-C33	30.7(7)
O15-Cd3-O10-C28	-72.7(4)	C11-O4-C10-C9	169.9(4)
N5-Cd3-O10-C28	62.8(5)	Cd1-O4-C10-C9	27.8(5)
N6-Cd3-O10-C28	146.6(5)	O14-Cd2-N3-C24	-71.5(4)
O12-Cd3-O10-C28	-161.1(5)	N4-Cd2-N3-C24	110.3(4)
O9-Cd3-O10-C28	29.2(4)	O8-Cd2-N3-C24	17.1(4)
O11-Cd3-O10-C28	-150.3(4)	O5-Cd2-N3-C24	-145.5(4)

O6-Cd2-N3-C24	-178.9(4)	O9-Cd3-N5-C36	-138.9(4)
O14-Cd2-N3-C13	53.2(4)	O11-Cd3-N5-C36	51.8(4)
N4-Cd2-N3-C13	-125.1(4)	O10-Cd3-N5-C36	-170.8(4)
O8-Cd2-N3-C13	141.7(4)	O15-Cd3-N5-C25	64.4(5)
O5-Cd2-N3-C13	-20.9(4)	N6-Cd3-N5-C25	-113.8(5)
O6-Cd2-N3-C13	-54.2(4)	O12-Cd3-N5-C25	148.3(5)
O15-Cd3-O9-C26	-149.5(5)	O9-Cd3-N5-C25	-14.2(4)
N5-Cd3-O9-C26	-15.9(5)	O11-Cd3-N5-C25	176.4(4)
N6-Cd3-O9-C26	78.8(5)	O10-Cd3-N5-C25	-46.1(5)
O12-Cd3-O9-C26	-39.7(6)	C6-N2-C7-C8	63.6(6)
O11-Cd3-O9-C26	136.9(5)	Cd1-N2-C7-C8	-63.7(5)
O10-Cd3-O9-C26	135.4(5)	O3-C8-C7-N2	45.0(6)
O15-Cd3-O9-C27	73.3(6)	C8-O3-C9-C10	-68.8(6)
N5-Cd3-O9-C27	-153.0(6)	O4-C10-C9-O3	-56.2(6)
N6-Cd3-O9-C27	-58.4(6)	C2-O1-C3-C4	-167.2(5)
O12-Cd3-O9-C27	-176.8(5)	Cd1-O1-C3-C4	-25.4(6)
O11-Cd3-O9-C27	-0.2(9)	Cd1-O13-C37-O14	179.0(3)
O10-Cd3-O9-C27	-1.7(6)	Cd1-O13-C37-O15	-1.8(5)
C4-O2-C5-C6	-169.5(4)	Cd2-O14-C37-O13	1.2(5)
Cd1-O2-C5-C6	-42.4(5)	Cd2-O14-C37-O15	-178.0(3)
C9-O3-C8-C7	113.8(5)	Cd3-O15-C37-O13	177.4(3)
C1-N1-C12-C11	-175.4(4)	Cd3-O15-C37-O14	-3.4(5)
Cd1-N1-C12-C11	-50.4(5)	C10-O4-C11-C12	176.6(4)
O14-Cd2-N4-C19	87.7(5)	Cd1-O4-C11-C12	-37.2(5)
N3-Cd2-N4-C19	-94.1(5)	N1-C12-C11-O4	58.1(6)
O8-Cd2-N4-C19	-23.5(5)	C12-N1-C1-C2	173.7(4)
O5-Cd2-N4-C19	-166.0(5)	Cd1-N1-C1-C2	49.2(5)
O6-Cd2-N4-C19	141.3(5)	O15-Cd3-N6-C30	-92.5(5)
O14-Cd2-N4-C18	-38.6(5)	N5-Cd3-N6-C30	85.8(5)
N3-Cd2-N4-C18	139.7(4)	O12-Cd3-N6-C30	156.2(5)
O8-Cd2-N4-C18	-149.8(4)	O9-Cd3-N6-C30	14.7(5)
O5-Cd2-N4-C18	67.7(4)	O11-Cd3-N6-C30	-148.0(5)
O6-Cd2-N4-C18	15.0(4)	O10-Cd3-N6-C30	-39.4(5)
O15-Cd3-N5-C36	-60.3(4)	O15-Cd3-N6-C31	37.6(7)
N6-Cd3-N5-C36	121.5(4)	N5-Cd3-N6-C31	-144.1(6)
O12-Cd3-N5-C36	23.6(4)	O12-Cd3-N6-C31	-73.6(6)

O9-Cd3-N6-C31	144.9(6)	C19-N4-C18-C17	-173.3(6)
O11-Cd3-N6-C31	-17.9(6)	Cd2-N4-C18-C17	-47.4(7)
O10-Cd3-N6-C31	90.7(6)	C25-N5-C36-C35	-179.5(5)
C7-N2-C6-C5	-178.0(4)	Cd3-N5-C36-C35	-52.5(5)
Cd1-N2-C6-C5	-52.2(5)	O12-C35-C36-N5	57.0(6)
O2-C5-C6-N2	63.7(6)	C16-O6-C17-C18	-169.6(7)
C13-N3-C24-C23	-171.2(5)	Cd2-O6-C17-C18	-43.0(7)
Cd2-N3-C24-C23	-46.7(6)	N4-C18-C17-O6	61.3(8)
C24-N3-C13-C14	177.1(5)	C14-O5-C15-C16	-168.7(6)
Cd2-N3-C13-C14	51.2(6)	Cd2-O5-C15-C16	-33.1(8)
C5-O2-C4-C3	72.6(6)	C28-O10-C29-C30	-116.7(8)
Cd1-O2-C4-C3	-53.0(5)	Cd3-O10-C29-C30	10.5(9)
O1-C3-C4-O2	50.7(6)	C15-O5-C14-C13	178.1(5)
C23-O8-C22-C21	171.8(4)	Cd2-O5-C14-C13	37.5(6)
Cd2-O8-C22-C21	27.9(6)	N3-C13-C14-O5	-59.4(7)
C3-O1-C2-C1	-175.6(5)	C33-O11-C32-C31	164.9(6)
Cd1-O1-C2-C1	38.5(5)	Cd3-O11-C32-C31	36.9(8)
N1-C1-C2-O1	-58.4(6)	C32-O11-C33-C34	-74.4(7)
C20-O7-C21-C22	-69.9(6)	Cd3-O11-C33-C34	53.8(6)
O8-C22-C21-O7	-55.0(6)	O12-C34-C33-O11	-54.0(7)
C22-O8-C23-C24	172.1(5)	O5-C15-C16-O6	53.5(8)
Cd2-O8-C23-C24	-40.1(5)	C17-O6-C16-C15	75.8(8)
N3-C24-C23-O8	57.3(6)	Cd2-O6-C16-C15	-50.6(7)
C21-O7-C20-C19	106.9(6)	C29-O10-C28-C27	71.8(8)
C36-N5-C25-C26	171.0(6)	Cd3-O10-C28-C27	-57.3(7)
Cd3-N5-C25-C26	44.8(7)	O11-C32-C31-N6	-57.1(10)
C18-N4-C19-C20	65.4(6)	C30-N6-C31-C32	176.4(7)
Cd2-N4-C19-C20	-60.3(6)	Cd3-N6-C31-C32	48.2(9)
O7-C20-C19-N4	48.5(7)	C26-O9-C27-C28	-160.8(7)
C27-O9-C26-C25	-176.1(7)	Cd3-O9-C27-C28	-24.5(10)
Cd3-O9-C26-C25	42.9(7)	O10-C28-C27-O9	54.4(10)
N5-C25-C26-O9	-58.5(8)	C31-N6-C30-C29	-66.6(9)
C34-O12-C35-C36	177.4(5)	Cd3-N6-C30-C29	62.7(8)
Cd3-O12-C35-C36	-34.1(6)	O10-C29-C30-N6	-45.9(10)

Figure S1B. Thermal ellipsoid perspectives of cation in **2.**

a. Numbered perspective (50% probability) of 4+ trinuclear cation.



b. Unlabeled perspective.

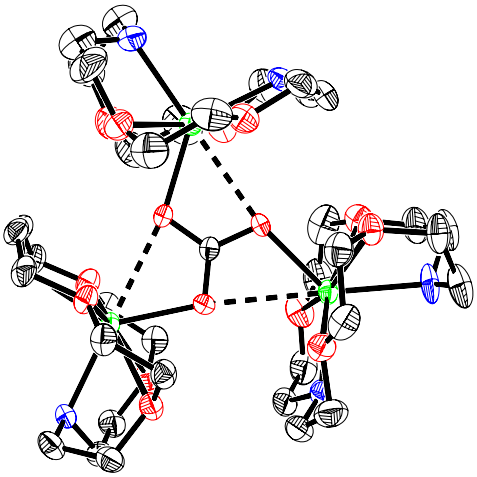
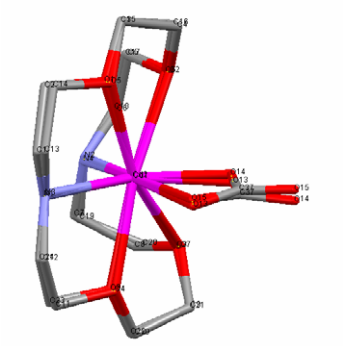
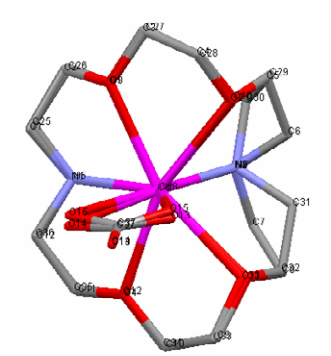


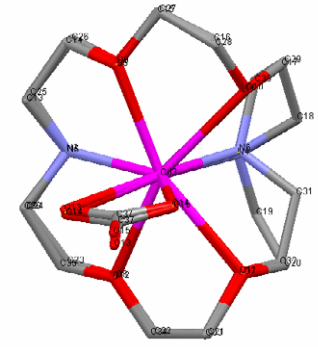
Figure SB2. Cd Coordination Environment Overlays



a. Cd1-Cd2 coordination environment overlay.



b. Cd1-Cd3 coordination environment overlay. Notice how the ethylene straps next to a N atom are in different conformations.



c. Cd2-Cd3 coordination environment overlay. Notice how the ethylene straps next to a N atom are in different conformations.

Figure S3B. Angles between the least-squares planes of the ligated O atoms at each Cd center and neighboring analogous Cd coordination spheres.

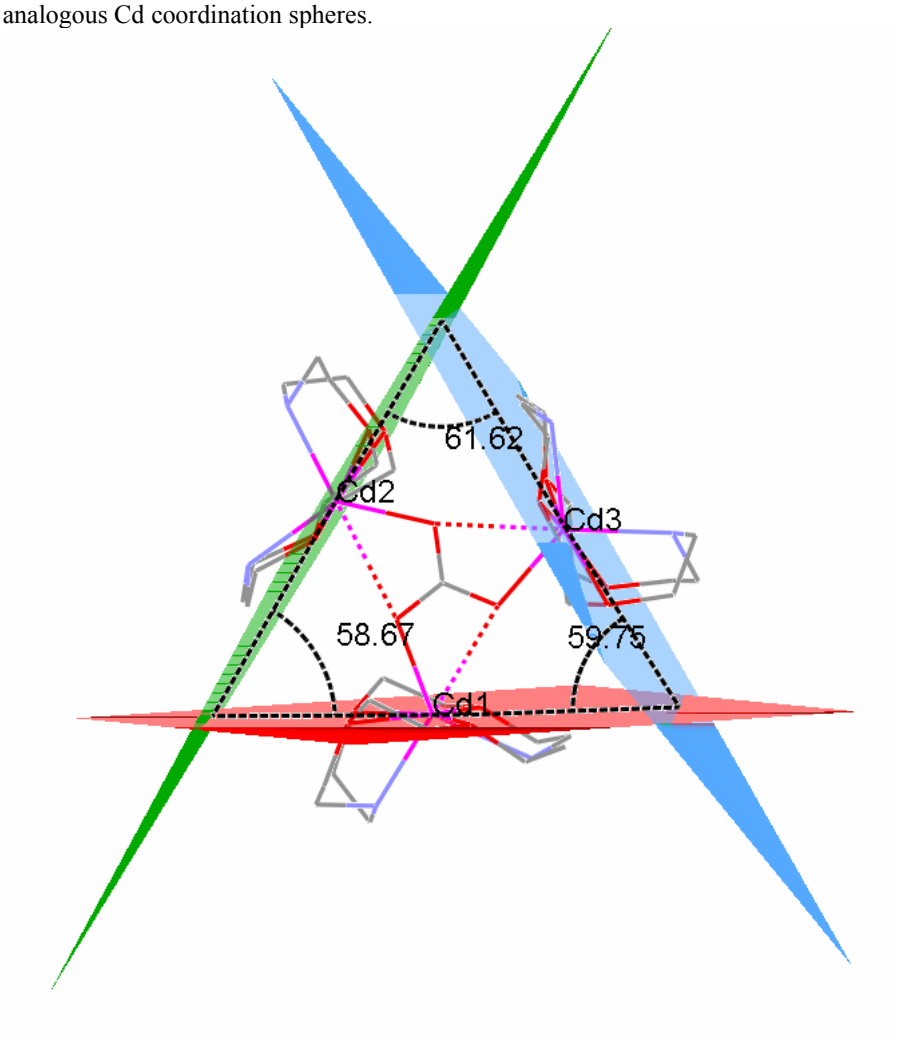


Figure S4B. Angle between least-squares planes formed by the Cd1, O1-O4 plane and the Cd1,N1,N2,O13,O15 plane. The other Cd centers exhibit similar angles between the CdO_4 plane (only O atoms from 18O4N2) and the Cd_3,N_6,CO_3 plane.

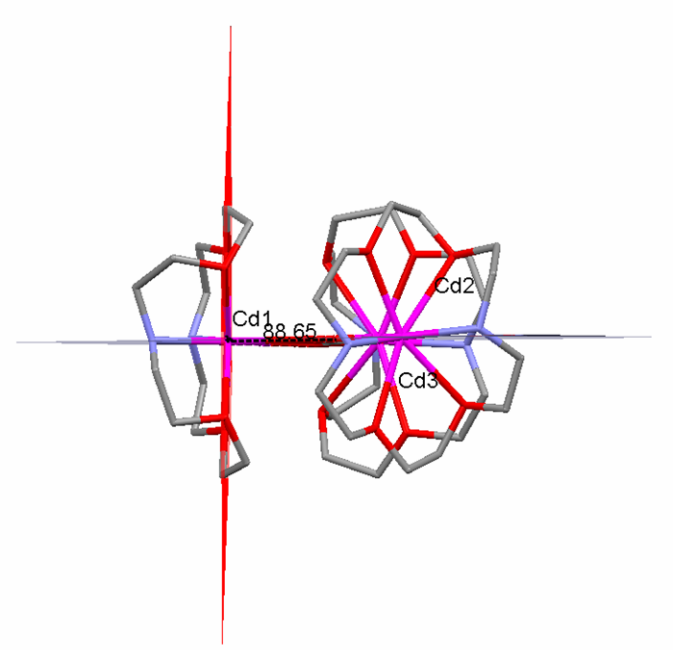


Figure S5B. Environment around carbonate ion in **2.**

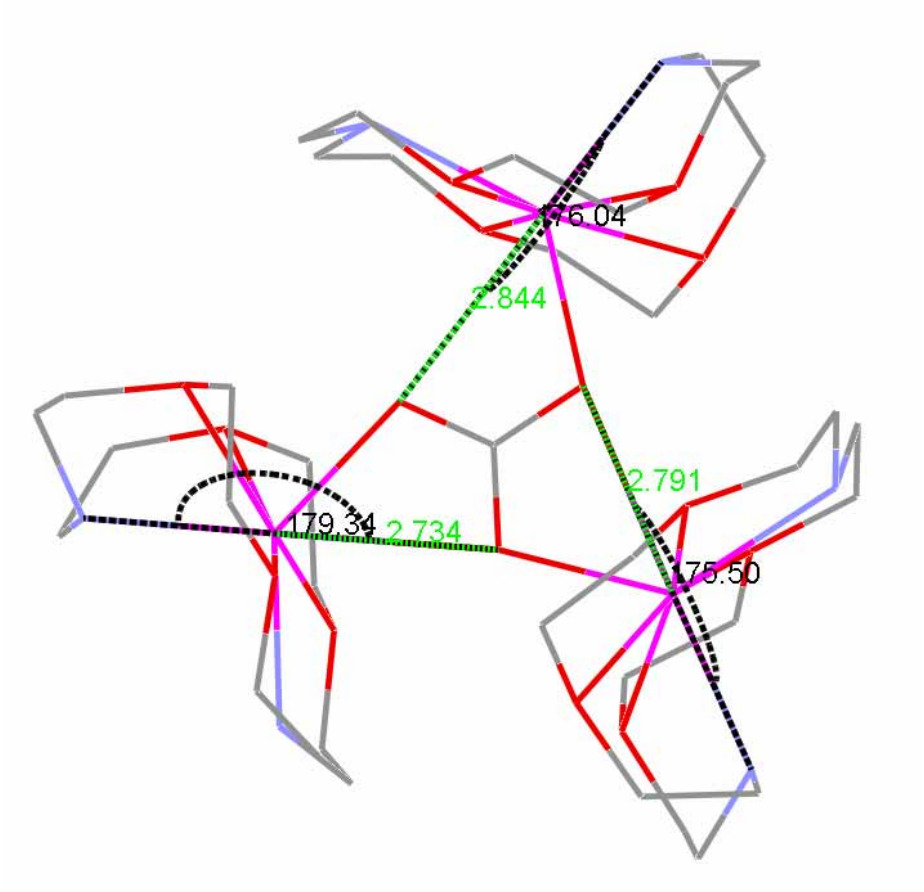
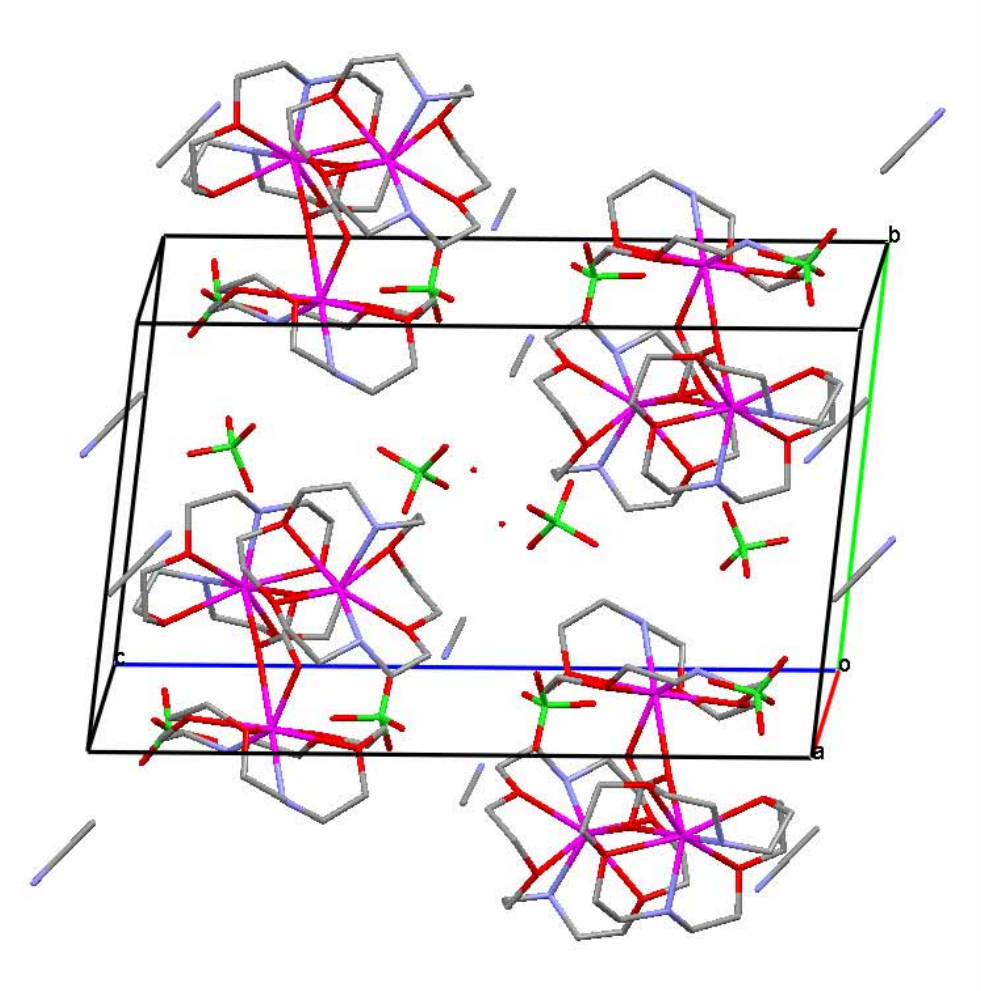


Figure S6B. Packing diagram for **2**. Disordered water over inversion center at center of cell. Perchlorates are close to the disordered water.



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