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Bis(μ-4-chlorobenzoato)bis[(4-chlorobenzoato)bis(1*H*-imidazole-κN^3)cadmium(II)] dihydrate

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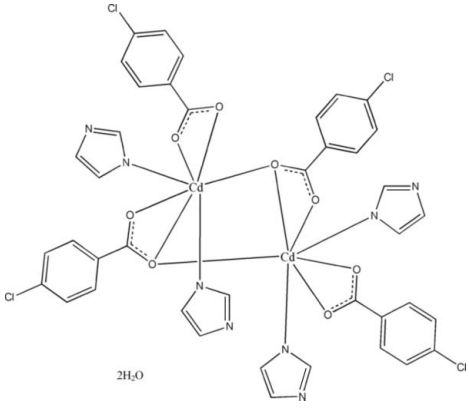
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.034; wR factor = 0.079; data-to-parameter ratio = 16.9.

In the centrosymmetric title complex, $[Cd_2(C_7H_4ClO_2)_4(C_3H_4N_2)_4]\cdot 2H_2O$, each Cd^{II} atom is coordinated by five carboxylate O atoms from three 4-chlorobenzoate ligands and two N atoms from two imidazole ligands, displaying a distorted pentagonal–bipyramidal geometry. The dinuclear molecules, with a Cd···Cd separation of 3.868 (3) Å, form a supramolecular network *via* intermolecular hydrogen bonds and π–π stacking interactions. The face-to-face distance between parallel 4-chlorobenzoic acids of neighboring complexes [at $(x, y, z-1)$] is 3.563 (3) Å. There are also π–π stacking interactions of imidazoles [at $(2-x, -y, 1-z)$], with a centroid-centroid distance of 3.623 (3) Å.

Related literature

For related literature, see: Burrows *et al.* (1997); Gu et al. (2004); Iglesias et al. (2003); Kim et al. (2003); Moulton & Zaworotko (2001)..



Experimental

Crystal data

$[Cd_2(C_7H_4ClO_2)_4(C_3H_4N_2)_4]\cdot 2H_2O$
M_r = 1155.37
Triclinic, $P\overline{1}$
a = 9.7468 (1) Å
b = 10.3997 (1) Å
c = 12.3424 (1) Å
α = 106.862 (1)°
β = 99.363 (1)°
γ = 96.840 (1)°
V = 1162.87 (2) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.21 mm^{-1}
T = 293 (2) K
0.20 × 0.18 × 0.15 mm

Data collection

Bruker APEX II area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.794, T_{max} = 0.840
9372 measured reflections
5392 independent reflections
4500 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.079
S = 1.02
5392 reflections
320 parameters
57 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N4*B*—H4*C*···O5*B*	0.86	1.94	2.781 (12)	165
N4*A*—H4*B*···O5*A*	0.86	1.95	2.789 (11)	167
N3—H3*B*···O3^{i}	0.86	1.98	2.799 (3)	160
O5*B*—H5*D*···O5*A*^{ii}	0.845 (10)	2.25 (5)	3.000 (7)	148 (8)
O5*B*—H5*C*···O1^{iii}	0.846 (10)	2.11 (6)	2.716 (9)	128 (6)
O5*A*—H5*B*···O3^{iii}	0.851 (10)	1.93 (3)	2.707 (7)	151 (5)

Symmetry codes: (i) $-x+2, -y, -z+1$; (ii) $-x, -y+1, -z+1$; (iii) $-x+1, -y+1, -z+1$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2013).

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supplementary materials

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Bis(μ-4-chlorobenzoato)bis[(4-chlorobenzoato)bis(1*H*-imidazole-κN^3)cadmium(II)] dihydrate

X.-X. Guo, J.-B. Yan and W.-D. Song

Comment

Molecular self-assembly of supramolecular architectures has received much attention during recent decades (Kim *et al.*, 2003; Iglesias *et al.*, 2003; Moulton & Zaworotko, 2001). The structures and properties of such systems depend on the coordination and geometric preferences of both the central metals ions and bridging building blocks as well as the influence of weaker non-covalent interactions, such as hydrogen bonds and π-π stacking interactions. 4-Chlorobenzoic acid and imidazole are excellent candidates for the construction of supramolecular complexes, since they not only have multiple coordination modes but also can form regular hydrogen bonds by functioning as both hydrogen-bond donor and acceptor (Gu *et al.*, 2004). Recently, we obtained the title novel polymer cadmium complex (I) by the reaction of cadmium nitryl, 4-chlorobenzoic acid and imidazole in an aqueous solution, and its crystal structure is reported here.

As illustrated in Fig. 1, in the asymmetric unit of (I) each Cd^{II} centre is coordinated by five carboxyl O atoms from three 4-chlorobenzoic acid ligands, two N atoms from two imidazole ligands, and displaying a distorted pentagonal-bipyramidal geometry (Table 1). Via a Cd···Cd interaction between symmetrically related moieties the compound forms dinuclear structures with a Cd···Cd separation of 3.868 (3)Å that are further extended to a supramolecular network through intermolecular hydrogen bonds (Table 2) and *via* π-π stacking interactions. The face-to-face distance between parallel 4-chlorobenzoic acids of neighboring complexes is 3.563 (3) Å. There is also π-π stacking interactions of imidazoles with a centroid-centroid distance of 3.623 (3) Å. The interstitial water molecules are arranged in hydrogen bonded pairs around a center of inversion. The H bonds between the water molecules are incompatible with the inversion symmetry of the unit cell thus inducing a disorder of the water molecule as well as the imidazole ligand H-bonded to it (see refinement section for details).

Experimental

The title complex was prepared by the addition of a stoichiometric amount of cadmium nitryl (20 mmol) and imidazole (20 mmol) to a hot aqueous solution of 4-chlorobenzoic acid (30 mmol). The Ph was then adjusted to 7.0 to 8.0 with NaOH (30 mmol). The resulting solution was filtered, and colorless crystals were obtained at room temperature on slow evaporation of the solvent over several days.

Refinement

The water molecules are arranged as symmetry related pairs around a center of inversion. Each of the water molecules showed significantly elongated thermal ellipsoids indicating disorder over two positions. The most likely cause for this behavior seems to be asymmetric hydrogen bonding between the pairs of water molecules which are separated by about three Å. The disorder of the water molecule also translates to the imidazole ligand hydrogen bonded to it as indicated by the asymmetric anisotropic displacement parameters when compared to the other imidazole ligand. Based on these observations both the water molecule as well as the imidazole ligand were refined as being disordered over two sites in a one to one ratio. Due to the significant overlap of the disordered atoms the following restraints

were applied: The adps of the disordered atoms were restrained to be close to isotropic and those of equivalent atoms were set to be identical. In the imidazole ring equivalent bond distances were restrained to be the same.

Carbon-bound H atoms were placed at calculated positions and were treated as riding on the parent C atoms with C—H = 0.93 Å, N—H = 0.86 Å and with U_{iso}(H) = 1.2 U_{eq}(C, N). Water H atoms were tentatively located in difference Fourier maps and were refined with distance restraints of O–H = 0.85 Å and H···H = 1.39 Å, each within a standard deviation of 0.01 Å; other H-atoms.

Figures

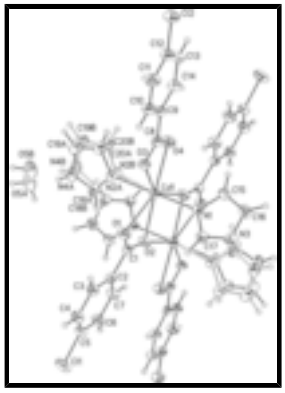
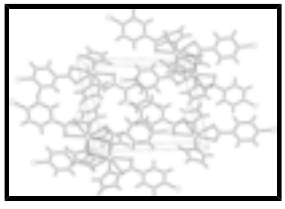


Figure 1 The structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Unlabelled atoms are related to the labelled atoms by the symmetry operator (2 − *x*, 1 − *y*, −*z*).



Bis(μ-4-chlorobenzoato)bis[(4-chlorobenzoato)bis(1*H*-imidazole- κN^3)cadmium(II)] dihydrate

Crystal data

$[Cd_2(C_7H_4ClO_2)_4(C_3H_4N_2)_4]\cdot 2H_2O$	Z = 1
M_r = 1155.37	F_{000} = 576
Triclinic, $P\overline{1}$	D_x = 1.650 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 9.74680 (10) Å	Cell parameters from 7500 reflections
b = 10.39970 (10) Å	θ = 1.7–26.0º
c = 12.34240 (10) Å	μ = 1.21 mm^{-1}
α = 106.8620 (10)º	T = 293 (2) K
β = 99.3630 (10)º	Block, colorless
γ = 96.8400 (10)º	0.20 × 0.18 × 0.15 mm
V = 1162.870 (19) Å^3	

Data collection

Bruker APEX II area-detector diffractometer	5392 independent reflections
Radiation source: fine-focus sealed tube	4500 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.023$
$T = 293(2)$ K	$\theta_{max} = 28.0°$
φ and ω scans	$\theta_{min} = 3.1°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -12 \rightarrow 12$
$T_{min} = 0.794$, $T_{max} = 0.840$	$k = -10 \rightarrow 13$
9372 measured reflections	$l = -16 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.034$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.079$	$w = 1/[\sigma^2(F_o^2) + (0.0348P)^2 + 0.3021P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.004$
5392 reflections	$\Delta\rho_{max} = 0.76$ e Å^{-3}
320 parameters	$\Delta\rho_{min} = -0.56$ e Å^{-3}
57 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O5A	0.1480 (8)	0.5478 (7)	0.5065 (6)	0.0916 (19)	0.50
H5A	0.150 (8)	0.522 (3)	0.5668 (17)	0.110*	0.50
H5B	0.173 (8)	0.6341 (13)	0.534 (3)	0.110*	0.50

O5B	0.1396 (8)	0.5423 (7)	0.4559 (7)	0.0916 (19)	0.50
H5C	0.149 (4)	0.6277 (14)	0.469 (7)	0.110*	0.50
H5D	0.0517 (15)	0.512 (3)	0.437 (7)	0.110*	0.50
C1	0.6595 (3)	0.2089 (2)	0.6653 (2)	0.0387 (5)	
C2	0.6679 (3)	0.2823 (2)	0.7909 (2)	0.0400 (6)	
C3	0.7770 (3)	0.3898 (3)	0.8517 (2)	0.0523 (7)	
H3A	0.8445	0.4179	0.8141	0.063*	
C4	0.7861 (4)	0.4558 (3)	0.9683 (2)	0.0627 (9)	
H4A	0.8599	0.5276	1.0093	0.075*	
C5	0.6854 (4)	0.4143 (3)	1.0226 (2)	0.0615 (8)	
C6	0.5759 (4)	0.3090 (3)	0.9639 (2)	0.0629 (8)	
H6	0.5080	0.2821	1.0017	0.075*	
C7	0.5679 (3)	0.2432 (3)	0.8479 (2)	0.0532 (7)	
H7	0.4939	0.1714	0.8076	0.064*	
C8	0.7588 (3)	0.1222 (3)	0.2471 (2)	0.0437 (6)	
C9	0.8245 (3)	0.1342 (3)	0.1478 (2)	0.0431 (6)	
C10	0.9519 (3)	0.2195 (3)	0.1670 (2)	0.0552 (7)	
H10	0.9965	0.2718	0.2421	0.066*	
C11	1.0138 (4)	0.2278 (3)	0.0753 (3)	0.0629 (8)	
H11	1.1003	0.2843	0.0883	0.075*	
C12	0.9448 (3)	0.1506 (3)	−0.0357 (2)	0.0549 (7)	
C13	0.8191 (3)	0.0658 (3)	−0.0569 (2)	0.0576 (8)	
H13	0.7743	0.0144	−0.1322	0.069*	
C14	0.7590 (3)	0.0575 (3)	0.0358 (2)	0.0543 (7)	
H14	0.6733	−0.0005	0.0223	0.065*	
C15	0.7946 (3)	−0.1714 (3)	0.3610 (2)	0.0481 (7)	
H15	0.7494	−0.1990	0.2835	0.058*	
C16	0.8948 (3)	−0.2303 (3)	0.4065 (3)	0.0539 (7)	
H16	0.9314	−0.3047	0.3672	0.065*	
C17	0.8552 (3)	−0.0607 (3)	0.5419 (2)	0.0457 (6)	
H17	0.8617	0.0024	0.6143	0.055*	
N2A	0.4960 (7)	0.2455 (6)	0.4035 (6)	0.0454 (8)	0.50
C18A	0.4180 (9)	0.3048 (8)	0.4730 (7)	0.0555 (9)	0.50
H18A	0.4107	0.2876	0.5419	0.061 (18)*	0.50
N4A	0.3501 (8)	0.3918 (7)	0.4354 (6)	0.0585 (11)	0.50
H4B	0.2948	0.4414	0.4686	0.070*	0.50
C19A	0.3867 (11)	0.3854 (11)	0.3339 (8)	0.0812 (16)	0.50
H19A	0.3531	0.4330	0.2849	0.097*	0.50
C20A	0.4792 (10)	0.2998 (8)	0.3137 (6)	0.0687 (14)	0.50
H20A	0.5236	0.2806	0.2510	0.082*	0.50
N2B	0.4733 (7)	0.2211 (7)	0.3869 (6)	0.0454 (8)	0.50
C18B	0.4021 (9)	0.2941 (9)	0.4556 (7)	0.0555 (9)	0.50
H18B	0.3984	0.2916	0.5298	0.067*	0.50
N4B	0.3359 (9)	0.3724 (8)	0.4044 (6)	0.0585 (11)	0.50
H4C	0.2791	0.4238	0.4328	0.070*	0.50
C19B	0.3710 (12)	0.3589 (11)	0.3024 (8)	0.0812 (16)	0.50
H19B	0.3458	0.4067	0.2514	0.097*	0.50
C20B	0.4506 (10)	0.2612 (9)	0.2896 (7)	0.0687 (14)	0.50
H20B	0.4858	0.2253	0.2237	0.082*	0.50

Cd1	0.626073 (19)	0.085390 (18)	0.425047 (14)	0.03928 (6)
Cl1	0.69914 (15)	0.49427 (11)	1.16945 (7)	0.1012 (4)
Cl2	1.02250 (10)	0.16260 (9)	−0.15082 (7)	0.0746 (2)
N1	0.7692 (2)	−0.0639 (2)	0.44682 (17)	0.0401 (5)
N3	0.9319 (2)	−0.1599 (2)	0.52090 (19)	0.0489 (5)
H3B	0.9938	−0.1761	0.5711	0.059*
O1	0.7451 (2)	0.25174 (19)	0.61312 (15)	0.0546 (5)
O2	0.56444 (19)	0.10523 (19)	0.61424 (14)	0.0494 (5)
O3	0.82065 (19)	0.19455 (19)	0.34830 (14)	0.0477 (4)
O4	0.6460 (2)	0.0404 (2)	0.22683 (16)	0.0581 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O5A	0.0736 (17)	0.0680 (16)	0.124 (5)	0.0230 (14)	0.027 (3)	0.009 (3)
O5B	0.0736 (17)	0.0680 (16)	0.124 (5)	0.0230 (14)	0.027 (3)	0.009 (3)
C1	0.0445 (13)	0.0372 (12)	0.0332 (11)	0.0116 (10)	0.0065 (10)	0.0082 (9)
C2	0.0452 (13)	0.0386 (12)	0.0336 (12)	0.0088 (10)	0.0033 (10)	0.0094 (10)
C3	0.0622 (17)	0.0435 (14)	0.0447 (14)	0.0001 (13)	0.0082 (12)	0.0092 (11)
C4	0.083 (2)	0.0455 (15)	0.0433 (15)	−0.0057 (15)	−0.0006 (15)	0.0029 (12)
C5	0.098 (2)	0.0496 (16)	0.0310 (13)	0.0163 (16)	0.0124 (14)	0.0027 (12)
C6	0.078 (2)	0.0646 (18)	0.0427 (15)	0.0091 (16)	0.0230 (14)	0.0079 (13)
C7	0.0552 (16)	0.0560 (16)	0.0398 (13)	0.0010 (13)	0.0097 (12)	0.0056 (12)
C8	0.0498 (14)	0.0519 (14)	0.0403 (13)	0.0192 (12)	0.0166 (11)	0.0232 (11)
C9	0.0536 (15)	0.0448 (13)	0.0400 (12)	0.0168 (11)	0.0166 (11)	0.0203 (10)
C10	0.0657 (18)	0.0606 (17)	0.0377 (13)	−0.0004 (14)	0.0130 (12)	0.0165 (12)
C11	0.073 (2)	0.0671 (18)	0.0534 (16)	0.0005 (16)	0.0249 (14)	0.0238 (14)
C12	0.0739 (18)	0.0608 (16)	0.0480 (14)	0.0265 (14)	0.0305 (13)	0.0289 (12)
C13	0.076 (2)	0.0637 (18)	0.0352 (13)	0.0161 (15)	0.0140 (13)	0.0159 (12)
C14	0.0573 (17)	0.0638 (17)	0.0425 (14)	0.0066 (14)	0.0102 (12)	0.0195 (13)
C15	0.0490 (15)	0.0540 (15)	0.0373 (13)	0.0112 (12)	0.0089 (11)	0.0076 (11)
C16	0.0543 (16)	0.0526 (15)	0.0546 (16)	0.0185 (13)	0.0161 (13)	0.0104 (13)
C17	0.0487 (14)	0.0458 (14)	0.0404 (13)	0.0046 (11)	0.0084 (11)	0.0121 (11)
N2A	0.0395 (17)	0.0445 (18)	0.0528 (16)	0.0057 (14)	0.0054 (13)	0.0191 (13)
C18A	0.0504 (19)	0.0526 (17)	0.071 (2)	0.0097 (15)	0.0181 (17)	0.0279 (16)
N4A	0.0477 (16)	0.0519 (18)	0.077 (3)	0.0151 (14)	0.0111 (19)	0.0204 (19)
C19A	0.092 (3)	0.089 (3)	0.069 (4)	0.034 (3)	−0.001 (3)	0.037 (3)
C20A	0.082 (3)	0.074 (4)	0.055 (3)	0.025 (3)	0.005 (2)	0.028 (2)
N2B	0.0395 (17)	0.0445 (18)	0.0528 (16)	0.0057 (14)	0.0054 (13)	0.0191 (13)
C18B	0.0504 (19)	0.0526 (17)	0.071 (2)	0.0097 (15)	0.0181 (17)	0.0279 (16)
N4B	0.0477 (16)	0.0519 (18)	0.077 (3)	0.0151 (14)	0.0111 (19)	0.0204 (19)
C19B	0.092 (3)	0.089 (3)	0.069 (4)	0.034 (3)	−0.001 (3)	0.037 (3)
C20B	0.082 (3)	0.074 (4)	0.055 (3)	0.025 (3)	0.005 (2)	0.028 (2)
Cd1	0.04308 (10)	0.04348 (10)	0.03381 (9)	0.00937 (7)	0.01179 (7)	0.01330 (7)
Cl1	0.1674 (11)	0.0783 (6)	0.0397 (4)	0.0108 (6)	0.0227 (5)	−0.0056 (4)
Cl2	0.1043 (6)	0.0850 (5)	0.0566 (4)	0.0302 (5)	0.0472 (4)	0.0339 (4)
N1	0.0424 (11)	0.0413 (10)	0.0387 (10)	0.0089 (9)	0.0114 (9)	0.0137 (8)
N3	0.0444 (12)	0.0562 (13)	0.0484 (12)	0.0108 (10)	0.0048 (10)	0.0221 (10)

O1	0.0646 (12)	0.0542 (11)	0.0405 (9)	−0.0011 (9)	0.0170 (9)	0.0092 (8)
O2	0.0541 (11)	0.0495 (10)	0.0345 (9)	−0.0020 (9)	0.0080 (8)	0.0029 (8)
O3	0.0560 (11)	0.0568 (11)	0.0340 (9)	0.0156 (9)	0.0121 (8)	0.0162 (8)
O4	0.0567 (11)	0.0715 (13)	0.0480 (10)	0.0004 (10)	0.0182 (9)	0.0223 (9)

Geometric parameters (Å, °)

O5A—H5A	0.858 (10)	C15—H15	0.9300
O5A—H5B	0.851 (10)	C16—N3	1.354 (4)
O5B—H5C	0.846 (10)	C16—H16	0.9300
O5B—H5D	0.845 (10)	C17—N1	1.316 (3)
C1—O1	1.250 (3)	C17—N3	1.334 (4)
C1—O2	1.264 (3)	C17—H17	0.9300
C1—C2	1.500 (3)	N2A—C18A	1.308 (8)
C2—C7	1.381 (4)	N2A—C20A	1.378 (9)
C2—C3	1.384 (3)	N2A—Cd1	2.259 (7)
C3—C4	1.386 (4)	C18A—N4A	1.326 (9)
C3—H3A	0.9300	C18A—H18A	0.9300
C4—C5	1.371 (5)	N4A—C19A	1.343 (10)
C4—H4A	0.9300	N4A—H4B	0.8600
C5—C6	1.369 (4)	C19A—C20A	1.343 (10)
C5—Cl1	1.737 (3)	C19A—H19A	0.9300
C6—C7	1.381 (4)	C20A—H20A	0.9300
C6—H6	0.9300	N2B—C18B	1.311 (9)
C7—H7	0.9300	N2B—C20B	1.375 (9)
C8—O4	1.248 (3)	N2B—Cd1	2.256 (7)
C8—O3	1.262 (3)	C18B—N4B	1.330 (9)
C8—C9	1.501 (3)	C18B—H18B	0.9300
C9—C10	1.380 (4)	N4B—C19B	1.330 (10)
C9—C14	1.381 (4)	N4B—H4C	0.8600
C10—C11	1.385 (4)	C19B—C20B	1.340 (11)
C10—H10	0.9300	C19B—H19B	0.9300
C11—C12	1.381 (4)	C20B—H20B	0.9300
C11—H11	0.9300	Cd1—N1	2.251 (2)
C12—C13	1.360 (4)	Cd1—O4	2.3989 (19)
C12—Cl2	1.743 (3)	Cd1—O2^{i}	2.4261 (18)
C13—C14	1.387 (4)	Cd1—O1	2.4584 (17)
C13—H13	0.9300	Cd1—O2	2.4622 (17)
C14—H14	0.9300	Cd1—O3	2.5453 (19)
C15—C16	1.345 (4)	N3—H3B	0.8600
C15—N1	1.377 (3)	O2—Cd1^{i}	2.4260 (18)
H5A—O5A—H5B	104.1 (16)	N4A—C19A—C20A	109.7 (9)
H5C—O5B—H5D	106.3 (16)	N4A—C19A—H19A	125.2
O1—C1—O2	121.4 (2)	C20A—C19A—H19A	125.2
O1—C1—C2	119.8 (2)	C19A—C20A—N2A	107.0 (8)
O2—C1—C2	118.8 (2)	C19A—C20A—H20A	126.5
C7—C2—C3	119.0 (2)	N2A—C20A—H20A	126.5
C7—C2—C1	120.7 (2)	C18B—N2B—C20B	104.0 (7)

C3—C2—C1	120.3 (2)	C18B—N2B—Cd1	129.1 (6)
C2—C3—C4	120.3 (3)	C20B—N2B—Cd1	126.3 (6)
C2—C3—H3A	119.9	N2B—C18B—N4B	110.6 (8)
C4—C3—H3A	119.9	N2B—C18B—H18B	124.7
C5—C4—C3	119.4 (3)	N4B—C18B—H18B	124.7
C5—C4—H4A	120.3	C19B—N4B—C18B	109.5 (9)
C3—C4—H4A	120.3	C19B—N4B—H4C	125.2
C6—C5—C4	121.3 (2)	C18B—N4B—H4C	125.2
C6—C5—Cl1	119.2 (3)	N4B—C19B—C20B	104.7 (9)
C4—C5—Cl1	119.4 (2)	N4B—C19B—H19B	127.7
C5—C6—C7	119.0 (3)	C20B—C19B—H19B	127.7
C5—C6—H6	120.5	C19B—C20B—N2B	111.0 (8)
C7—C6—H6	120.5	C19B—C20B—H20B	124.5
C6—C7—C2	121.1 (3)	N2B—C20B—H20B	124.5
C6—C7—H7	119.5	N1—Cd1—N2B	174.70 (16)
C2—C7—H7	119.5	N1—Cd1—N2A	175.97 (17)
O4—C8—O3	122.4 (2)	N2B—Cd1—N2A	7.9 (3)
O4—C8—C9	119.0 (2)	N1—Cd1—O4	90.69 (7)
O3—C8—C9	118.6 (2)	N2B—Cd1—O4	85.28 (19)
C10—C9—C14	119.1 (2)	N2A—Cd1—O4	88.26 (18)
C10—C9—C8	120.7 (2)	N1—Cd1—O2^{i}	85.06 (7)
C14—C9—C8	120.1 (2)	N2B—Cd1—O2^{i}	91.85 (18)
C9—C10—C11	120.6 (3)	N2A—Cd1—O2^{i}	98.91 (16)
C9—C10—H10	119.7	O4—Cd1—O2^{i}	94.95 (6)
C11—C10—H10	119.7	N1—Cd1—O1	91.90 (7)
C12—C11—C10	118.8 (3)	N2B—Cd1—O1	93.40 (16)
C12—C11—H11	120.6	N2A—Cd1—O1	86.23 (15)
C10—C11—H11	120.6	O4—Cd1—O1	136.91 (6)
C13—C12—C11	121.8 (3)	O2^{i}—Cd1—O1	128.13 (6)
C13—C12—Cl2	119.7 (2)	N1—Cd1—O2	91.49 (7)
C11—C12—Cl2	118.6 (2)	N2B—Cd1—O2	91.89 (19)
C12—C13—C14	118.8 (3)	N2A—Cd1—O2	90.22 (18)
C12—C13—H13	120.6	O4—Cd1—O2	169.85 (6)
C14—C13—H13	120.6	O2^{i}—Cd1—O2	75.38 (6)
C9—C14—C13	120.9 (3)	O1—Cd1—O2	52.91 (6)
C9—C14—H14	119.6	N1—Cd1—O3	85.92 (7)
C13—C14—H14	119.6	N2B—Cd1—O3	94.3 (2)
C16—C15—N1	109.6 (2)	N2A—Cd1—O3	90.35 (18)
C16—C15—H15	125.2	O4—Cd1—O3	52.74 (6)
N1—C15—H15	125.2	O2^{i}—Cd1—O3	146.27 (5)
C15—C16—N3	106.3 (2)	O1—Cd1—O3	84.57 (6)
C15—C16—H16	126.8	O2—Cd1—O3	137.33 (5)
N3—C16—H16	126.8	C17—N1—C15	105.2 (2)
N1—C17—N3	111.2 (2)	C17—N1—Cd1	127.54 (17)
N1—C17—H17	124.4	C15—N1—Cd1	127.05 (17)
N3—C17—H17	124.4	C17—N3—C16	107.8 (2)
C18A—N2A—C20A	105.2 (7)	C17—N3—H3B	126.1

C18A—N2A—Cd1	127.2 (6)	C16—N3—H3B	126.1
C20A—N2A—Cd1	127.7 (5)	C1—O1—Cd1	92.99 (14)
N2A—C18A—N4A	113.3 (8)	C1—O2—Cd1^{i}	162.86 (16)
N2A—C18A—H18A	123.3	C1—O2—Cd1	92.46 (15)
N4A—C18A—H18A	123.3	Cd1^{i}—O2—Cd1	104.62 (6)
C18A—N4A—C19A	104.8 (8)	C8—O3—Cd1	88.82 (15)
C18A—N4A—H4B	127.6	C8—O4—Cd1	95.99 (15)
C19A—N4A—H4B	127.6		

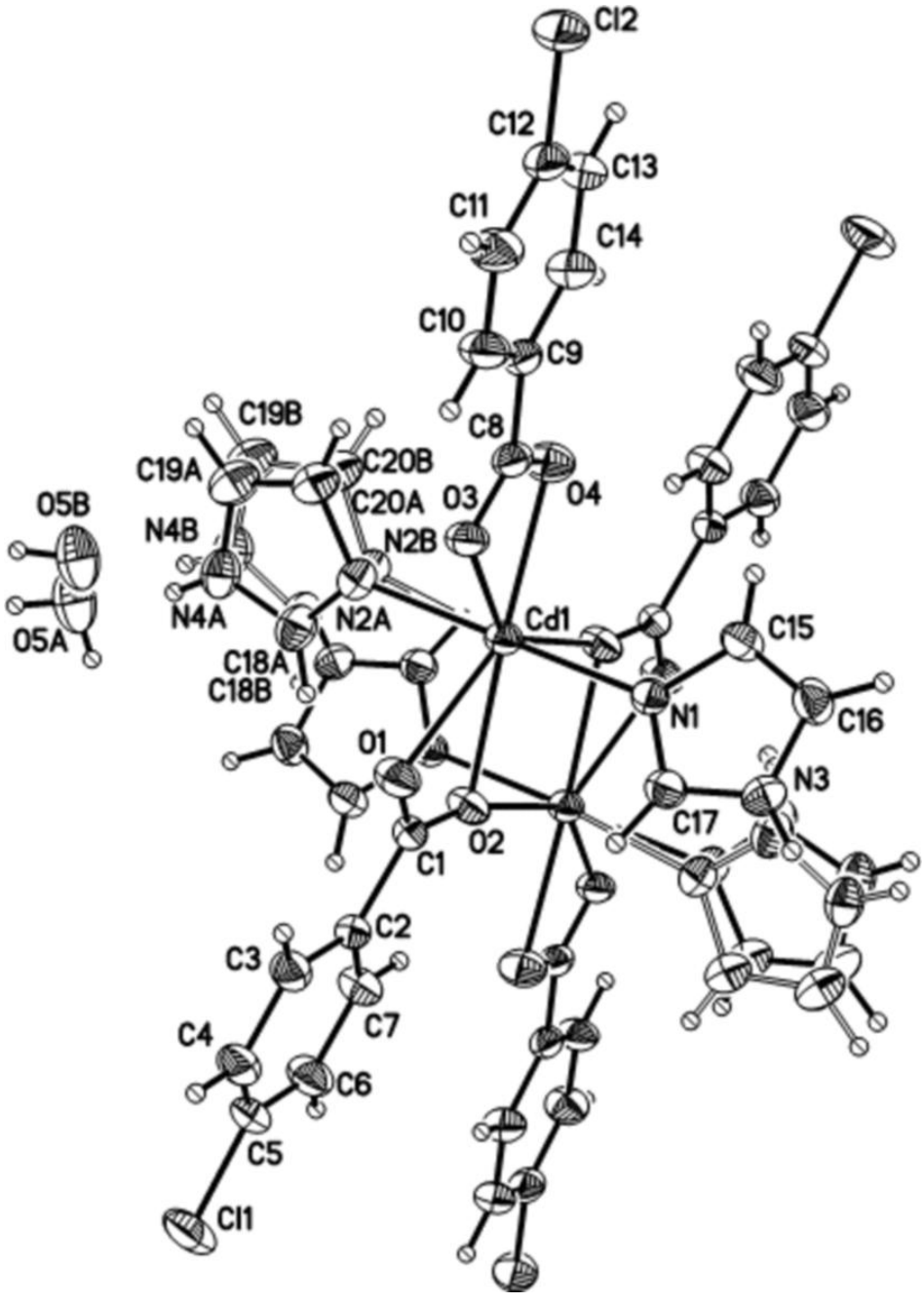
Symmetry codes: (i) −*x*+1, −*y*, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4B—H4C···O5B	0.86	1.94	2.781 (12)	165
N4A—H4B···O5A	0.86	1.95	2.789 (11)	167
N3—H3B···O3^{ii}	0.86	1.98	2.799 (3)	160
O5B—H5D···O5A^{iii}	0.845 (10)	2.25 (5)	3.000 (7)	148 (8)
O5B—H5C···O1^{iv}	0.846 (10)	2.11 (6)	2.716 (9)	128 (6)
O5A—H5B···O3^{iv}	0.851 (10)	1.93 (3)	2.707 (7)	151 (5)

Symmetry codes: (ii) −*x*+2, −*y*, −*z*+1; (iii) −*x*, −*y*+1, −*z*+1; (iv) −*x*+1, −*y*+1, −*z*+1.

Fig. 1


Cl2
C12
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C11
C14
C10
C9
C8
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N4B
N2B
N4A
N2A
Cd1
C15
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C18A
C18B
N1
C16
O1
N3
C17
O2
C1
C2
C3
C7
C4
C6
C5
Cl1

Fig. 2