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# Di-$\mu$-nicotinamide-$\kappa^2N^1$:$O$;$\kappa^2O$:$N^1$-bis[aquabis(3-chlorobenzoato-$\kappa^2O,O'$)-cadmium]

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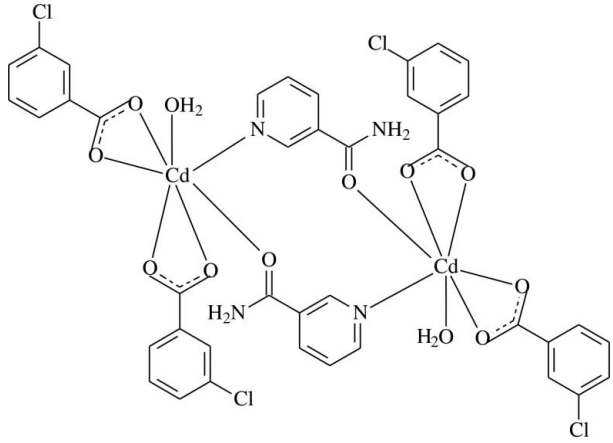
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.020; $wR$ factor = 0.052; data-to-parameter ratio = 14.6.

In the centrosymmetric dinuclear title compound, $[Cd_2(C_7H_4ClO_2)_4(C_6H_6N_2O)_2(H_2O)_2]$, the $Cd^{II}$ atom is coordinated by one N atom from one bridging nicotinamide ligand and one O atom from another symmetry-related bridging nicotinamide ligand, four O atoms from two 3-chlorobenzoate ligands and one water molecule in an irregular geometry. The dihedral angles between the carboxylate groups and the adjacent benzene rings are 6.98 (12) and 2.42 (13)°, while the benzene rings are oriented at a dihedral angle of 4.33 (6)°. Intermolecular O—H···O, N—H···O and weak C—H···O hydrogen bonds link the molecules into a three-dimensional network. $\pi$–$\pi$ interactions, indicated by short centroid–centroid distances [3.892 (1) Å between the pyridine rings and 3.683 (1) Å between the benzene rings] further stabilize the structure.

## Related literature

For niacin, see: Krishnamachari (1974). For the nicotinic acid derivative *N*,*N*-diethylnicotinamide, see: Bigoli *et al.* (1972). For related structures, see: Hökelek *et al.* (2009*a*,*b*, 2010*a*,*b*); Necefoğlu *et al.* (2011*a*,*b*); Greenaway *et al.* (1984).



## Experimental

### Crystal data

$[Cd_2(C_7H_4ClO_2)_4(C_6H_6N_2O)_2(H_2O)_2]$
$M_r$ = 1127.32
Triclinic, $P\overline{1}$
$a$ = 7.5835 (2) Å
$b$ = 12.3652 (3) Å
$c$ = 12.4893 (3) Å
$\alpha$ = 66.878 (2)°
$\beta$ = 78.678 (3)°
$\gamma$ = 83.222 (3)°
$V$ = 1055.02 (5) Å$^3$
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 1.33 mm$^{-1}$
$T$ = 296 K
0.38 × 0.24 × 0.12 mm

### Data collection

Bruker SMART BREEZE CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2012)
$T_{min}$ = 0.689, $T_{max}$ = 0.853
18369 measured reflections
4310 independent reflections
4106 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.052
$S$ = 1.09
4310 reflections
296 parameters
103 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.50 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Cd1—O1 | 2.3234 (14) | Cd1—O5$^{i}$ | 2.3175 (12) |
| Cd1—O2 | 2.4800 (13) | Cd1—O6 | 2.3019 (14) |
| Cd1—O3 | 2.5447 (15) | Cd1—N1 | 2.3384 (14) |
| Cd1—O4 | 2.3110 (16) | | |

Symmetry code: (i) $-x+1, -y+2, -z+1$.

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H21···O3$^{i}$ | 0.83 (3) | 2.26 (2) | 3.026 (2) | 155 (2) |
| N2—H22···O2$^{ii}$ | 0.83 (2) | 2.09 (2) | 2.913 (2) | 170 (2) |
| O6—H61···O1$^{iii}$ | 0.85 (4) | 2.15 (4) | 2.897 (2) | 146 (3) |
| O6—H62···O3$^{iii}$ | 0.81 (3) | 1.94 (3) | 2.710 (2) | 158 (3) |
| C8—H8···O5$^{i}$ | 0.93 | 2.43 | 3.158 (2) | 135 |
| C10—H10···O2$^{ii}$ | 0.93 | 2.54 | 3.403 (3) | 154 |

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

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2387).

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# supporting information

*Acta Cryst.* (2013). E**69**, m389–m390 [https://doi.org/10.1107/S1600536813015948]

## Di-$\mu$-nicotinamide-$\kappa^2N^1$:$O$;$\kappa^2O$:$N^1$-bis[aquabis(3-chlorobenzoato-$\kappa^2O,O'$)cadmium]

**Nihat Bozkurt, Nefise Dilek, Nagihan Çaylak Delibaş, Hacali Necefoğlu and Tuncer Hökelek**

### S1. Comment

As a part of our ongoing investigations of transition metal complexes of nicotinamide (NA), one form of niacin (Krishnamachari, 1974), and/or the nicotinic acid derivative *N*,*N*-diethylnicotinamide (DENA), an important respiratory stimulant (Bigoli *et al.*, 1972), the title compound was synthesized and its crystal structure is reported herein.

The title compound, (I), consists of dimeric units located around a crystallographic symmetry center and made up of two Cd cations, four 3-chlorobenzoate (CB) anions, which act in bidentate modes, two nicotinamide (NA) ligands and two water molecules (Fig. 1). Both of the $Cd^{II}$ centres are seven-coordinated, and the two monomeric units are bridged through the two nicotinamide (NA) ligands about an inversion center. The Cd1···Cd1a [symmetry code: (a) 1 - *x*, - *y*, 1 - *z*] distance is 7.1647 (3)Å. In the molecule, two Cd—O bond distances [2.4800 (13)Å and 2.5447 (15)Å] are significantly longer than the other four, and the average Cd—O bond length is 2.3798 (14)Å (Table 1). The Cd atom is displaced out of the least-squares planes of the carboxylate groups (O1/C1/O2) and (O3/C14/O4) by -0.2003 (1)Å and -0.3909 (1)Å, respectively.

The dihedral angles between the planar carboxylate groups and the adjacent benzene rings *A* (C2—C7) and *C* (C15—C20) are 6.98 (12)° and 2.42 (13)°, respectively, while those between rings *A*, *B* (N1/C8—C12) and *C* are A/B = 80.48 (7)°, A/C = 4.33 (6)°, B/C = 81.80 (7)°.

In (I), the O1-Cd1-O2 and O3-Cd1-O4 angles are 54.22 (4)° and 53.32 (5) °, respectively. The corresponding O—M—O (where M is a metal) angles are 57.75 (2)° in $[Cu(C_7H_5O_2F)(C_7H_4O_2F)_2(C_6H_6N_2O)_2]$, (II) (Necefoğlu *et al.*, 2011*a*), 60.32 (4)° in $[Co(C_8H_7O_3)_2(C_6H_6N_2O)(H_2O)_2]$, (III) (Hökelek *et al.*, 2010*a*), 59.02 (8)° in $[Zn(C_8H_8NO_2)_2(C_6H_6N_2O)_2].H_2O$, (IV) (Hökelek *et al.*, 2009*a*), 60.03 (6)° in $[Zn(C_9H_{10}NO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$, (V) (Hökelek *et al.*, 2009*b*), 57.53 (5)°, 56.19 (5)° and 59.04 (4)° in $[Zn(C_8H_7O_3)_2(C_6H_6N_2O)_2]$, (VI) (Hökelek *et al.*, 2010*b*), 57.61 (8)° in $[Mn_2(C_7H_4O_2Br)_4(C_6H_6N_2O)_2(H_2O)_2]$, (VII) (Necefoğlu *et al.*, 2011*b*) and 55.2 (1)° in $[Cu(Asp)_2(py)_2]$ (where Asp is acetylsalicylate and py is pyridine) [(VIII); Greenaway *et al.*, 1984].

In the crystal structure, intermolecular O—H···O, N—H···O and C—H···O hydrogen bonds link the molecules into a three dimensional network (Table 2), in which they may be effective in the stabilization of the structure. The $\pi$···$\pi$ contacts between the pyridine rings and between the benzene rings, Cg2—$Cg2^{i}$ and Cg1—$Cg3^{ii}$ [symmetry codes: (i) 2 - *x*, - *y*, - *z*; (ii) 1 - *x*, 1 - *y*, 1 - *z*, where Cg1, Cg2 and Cg3 are the centroids of the rings *A* (C2—C7), *B* (N1/C8—C12) and *C* (C15—C20), respectively] may further stabilize the structure, with centroid-centroid distances of 3.892 (1)Å and 3.683 (1)Å, respectively.

## S2. Experimental

The title compound was prepared by the reaction of $3CdSO_4.8H_2O$ (1.283 g, 5 mmol) in $H_2O$ (50 ml) and nicotinamide (1.220 g, 10 mmol) in $H_2O$ (50 ml) with sodium 3-chlorobenzoate (1.790 g, 10 mmol) in $H_2O$ (100 ml) at room temperature. The mixture was filtered and set aside to crystallize at ambient temperature for two weeks, giving colorless single crystals.

## S3. Refinement

Atoms H61, H62 (for $H_2O$) and H21, H22 (for $NH_2$) were located in a difference Fourier map and were freely refined. The C-bound H-atoms were positioned geometrically with C—H = 0.93Å for aromatic H-atoms, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

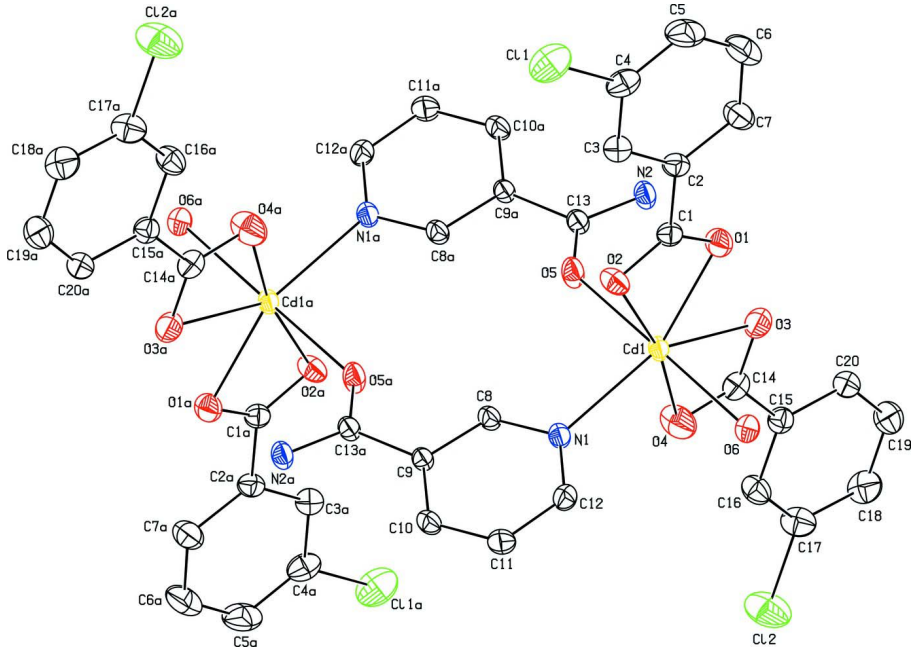


**Figure 1**

The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level [symmetry code: (a) 1 - *x*, - *y*, 1 - *z*].

**Di-$\mu$-nicotinamide-$\kappa^2N^1$:$O$;$\kappa^2O$:$N^1$-bis[aquabis(3-chlorobenzoato-$\kappa^2O,O'$)cadmium]**

*Crystal data*

$[Cd_2(C_7H_4ClO_2)_4(C_6H_6N_2O)_2(H_2O)_2]$
$M_r = 1127.32$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.5835$ (2) Å
$b = 12.3652$ (3) Å
$c = 12.4893$ (3) Å
$\alpha = 66.878$ (2)°
$\beta = 78.678$ (3)°
$\gamma = 83.222$ (3)°
$V = 1055.02$ (5) Å$^3$
$Z = 1$
$F(000) = 560$
$D_x = 1.774$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9868 reflections
$\theta = 2.7$–$28.4$°
$\mu = 1.33$ mm$^{-1}$
$T = 296$ K
Block, colorless
0.38 × 0.24 × 0.12 mm

*Data collection*

Bruker SMART BREEZE CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2012)
$T_{min}$ = 0.689, $T_{max}$ = 0.853
18369 measured reflections
4310 independent reflections
4106 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020
$\theta_{max}$ = 26.4°, $\theta_{min}$ = 1.8°
$h$ = −9→9
$k$ = −15→15
$l$ = −15→13

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.052
$S$ = 1.09
4310 reflections
296 parameters
103 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0281P)^2 + 0.3773P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.50 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cd1 | 0.460563 (15) | 0.713174 (9) | 0.502386 (11) | 0.02850 (5) |
| Cl1 | 0.20058 (11) | 1.03333 (7) | −0.11806 (6) | 0.0761 (2) |
| Cl2 | 0.76396 (11) | 0.40476 (8) | 1.09335 (6) | 0.0821 (2) |
| O1 | 0.53731 (18) | 0.68689 (12) | 0.32444 (12) | 0.0428 (3) |
| O2 | 0.31326 (17) | 0.81613 (13) | 0.32598 (12) | 0.0409 (3) |
| O3 | 0.7424 (2) | 0.58157 (12) | 0.54856 (12) | 0.0454 (3) |
| O4 | 0.5701 (2) | 0.64166 (16) | 0.67878 (14) | 0.0635 (5) |
| O5 | 0.35989 (16) | 1.12711 (11) | 0.55996 (14) | 0.0421 (3) |
| O6 | 0.2965 (2) | 0.54660 (13) | 0.57771 (15) | 0.0428 (3) |
| H61 | 0.340 (4) | 0.488 (3) | 0.631 (3) | 0.086 (11)* |
| H62 | 0.266 (4) | 0.523 (2) | 0.532 (2) | 0.059 (8)* |
| N1 | 0.22851 (19) | 0.80844 (12) | 0.59063 (13) | 0.0305 (3) |
| N2 | 0.0768 (2) | 1.19067 (14) | 0.60728 (15) | 0.0359 (3) |
| H21 | 0.110 (3) | 1.259 (2) | 0.5826 (19) | 0.040 (6)* |
| H22 | −0.033 (3) | 1.1805 (19) | 0.6266 (19) | 0.040 (6)* |

| | | | | |
|---|---|---|---|---|
| C1 | 0.4252 (2) | 0.76332 (15) | 0.27256 (16) | 0.0322 (4) |
| C2 | 0.4302 (2) | 0.79357 (16) | 0.14374 (16) | 0.0342 (4) |
| C3 | 0.3235 (3) | 0.88734 (17) | 0.08028 (17) | 0.0386 (4) |
| H3 | 0.2453 | 0.9300 | 0.1181 | 0.046* |
| C4 | 0.3347 (3) | 0.91633 (19) | −0.03919 (18) | 0.0476 (5) |
| C5 | 0.4493 (4) | 0.8553 (3) | −0.0977 (2) | 0.0640 (7) |
| H5 | 0.4561 | 0.8766 | −0.1785 | 0.077* |
| C6 | 0.5542 (4) | 0.7616 (3) | −0.0341 (2) | 0.0681 (7) |
| H6 | 0.6318 | 0.7192 | −0.0725 | 0.082* |
| C7 | 0.5445 (3) | 0.7307 (2) | 0.0856 (2) | 0.0497 (5) |
| H7 | 0.6152 | 0.6672 | 0.1275 | 0.060* |
| C8 | 0.2617 (2) | 0.91606 (15) | 0.57989 (16) | 0.0312 (4) |
| H8 | 0.3762 | 0.9434 | 0.5445 | 0.037* |
| C9 | 0.1366 (2) | 0.98948 (14) | 0.61809 (15) | 0.0271 (3) |
| C10 | −0.0336 (2) | 0.94833 (16) | 0.67092 (17) | 0.0354 (4) |
| H10 | −0.1225 | 0.9951 | 0.6971 | 0.042* |
| C11 | −0.0685 (3) | 0.83632 (17) | 0.68393 (18) | 0.0415 (4) |
| H11 | −0.1813 | 0.8063 | 0.7200 | 0.050* |
| C12 | 0.0650 (2) | 0.76927 (15) | 0.64305 (17) | 0.0351 (4) |
| H12 | 0.0398 | 0.6939 | 0.6524 | 0.042* |
| C13 | 0.1971 (2) | 1.10895 (15) | 0.59403 (15) | 0.0297 (3) |
| C14 | 0.6964 (3) | 0.57773 (16) | 0.65218 (17) | 0.0386 (4) |
| C15 | 0.7945 (2) | 0.49355 (16) | 0.74759 (17) | 0.0346 (4) |
| C16 | 0.7431 (3) | 0.48946 (19) | 0.86197 (18) | 0.0429 (4) |
| H16 | 0.6506 | 0.5397 | 0.8790 | 0.051* |
| C17 | 0.8306 (3) | 0.4102 (2) | 0.94991 (19) | 0.0494 (5) |
| C18 | 0.9655 (3) | 0.3336 (2) | 0.9270 (2) | 0.0538 (5) |
| H18 | 1.0216 | 0.2793 | 0.9876 | 0.065* |
| C19 | 1.0164 (3) | 0.3383 (2) | 0.8131 (2) | 0.0527 (5) |
| H19 | 1.1086 | 0.2877 | 0.7965 | 0.063* |
| C20 | 0.9308 (3) | 0.41792 (17) | 0.72359 (18) | 0.0404 (4) |
| H20 | 0.9652 | 0.4205 | 0.6470 | 0.049* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cd1 | 0.02751 (7) | 0.02414 (7) | 0.03423 (8) | 0.00202 (5) | −0.00289 (5) | −0.01339 (5) |
| Cl1 | 0.0897 (5) | 0.0728 (4) | 0.0522 (4) | 0.0005 (4) | −0.0339 (3) | −0.0001 (3) |
| Cl2 | 0.0835 (5) | 0.1212 (6) | 0.0423 (3) | 0.0194 (4) | −0.0211 (3) | −0.0333 (4) |
| O1 | 0.0440 (7) | 0.0409 (7) | 0.0385 (7) | 0.0112 (6) | −0.0088 (6) | −0.0123 (6) |
| O2 | 0.0344 (7) | 0.0516 (8) | 0.0382 (7) | 0.0078 (6) | −0.0040 (5) | −0.0224 (6) |
| O3 | 0.0644 (9) | 0.0350 (7) | 0.0377 (8) | −0.0055 (6) | −0.0119 (6) | −0.0122 (6) |
| O4 | 0.0594 (10) | 0.0753 (11) | 0.0474 (9) | 0.0313 (9) | −0.0172 (8) | −0.0197 (8) |
| O5 | 0.0267 (6) | 0.0326 (7) | 0.0697 (10) | −0.0027 (5) | 0.0032 (6) | −0.0273 (7) |
| O6 | 0.0511 (8) | 0.0310 (7) | 0.0461 (9) | −0.0080 (6) | 0.0020 (7) | −0.0172 (7) |
| N1 | 0.0301 (7) | 0.0272 (7) | 0.0351 (8) | 0.0009 (5) | −0.0029 (6) | −0.0146 (6) |
| N2 | 0.0293 (8) | 0.0296 (8) | 0.0502 (10) | 0.0022 (6) | −0.0013 (7) | −0.0201 (7) |
| C1 | 0.0283 (8) | 0.0334 (9) | 0.0335 (9) | −0.0042 (7) | −0.0019 (7) | −0.0117 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C2 | 0.0309 (8) | 0.0385 (9) | 0.0321 (9) | −0.0056 (7) | −0.0004 (7) | −0.0133 (7) |
| C3 | 0.0379 (9) | 0.0408 (10) | 0.0366 (10) | −0.0029 (8) | −0.0055 (8) | −0.0140 (8) |
| C4 | 0.0524 (12) | 0.0499 (11) | 0.0354 (11) | −0.0120 (9) | −0.0107 (9) | −0.0065 (9) |
| C5 | 0.0791 (17) | 0.0805 (17) | 0.0312 (11) | −0.0132 (14) | −0.0016 (11) | −0.0206 (11) |
| C6 | 0.0763 (18) | 0.0812 (18) | 0.0502 (14) | 0.0032 (14) | 0.0068 (12) | −0.0384 (14) |
| C7 | 0.0484 (12) | 0.0561 (13) | 0.0443 (12) | 0.0056 (10) | −0.0013 (9) | −0.0240 (10) |
| C8 | 0.0249 (8) | 0.0310 (8) | 0.0389 (10) | −0.0014 (6) | 0.0020 (7) | −0.0176 (7) |
| C9 | 0.0259 (8) | 0.0270 (8) | 0.0295 (8) | 0.0012 (6) | −0.0030 (6) | −0.0134 (7) |
| C10 | 0.0284 (8) | 0.0366 (9) | 0.0406 (10) | −0.0002 (7) | 0.0045 (7) | −0.0191 (8) |
| C11 | 0.0306 (9) | 0.0411 (10) | 0.0489 (12) | −0.0095 (7) | 0.0088 (8) | −0.0178 (9) |
| C12 | 0.0357 (9) | 0.0282 (8) | 0.0403 (10) | −0.0048 (7) | −0.0020 (7) | −0.0127 (7) |
| C13 | 0.0273 (8) | 0.0300 (8) | 0.0342 (9) | 0.0005 (6) | −0.0021 (7) | −0.0167 (7) |
| C14 | 0.0415 (10) | 0.0341 (9) | 0.0385 (10) | −0.0038 (8) | −0.0101 (8) | −0.0098 (8) |
| C15 | 0.0317 (9) | 0.0337 (9) | 0.0380 (10) | −0.0029 (7) | −0.0055 (7) | −0.0127 (8) |
| C16 | 0.0375 (10) | 0.0509 (11) | 0.0425 (11) | 0.0084 (8) | −0.0089 (8) | −0.0220 (9) |
| C17 | 0.0425 (11) | 0.0649 (14) | 0.0395 (11) | 0.0019 (10) | −0.0117 (9) | −0.0173 (10) |
| C18 | 0.0424 (11) | 0.0559 (13) | 0.0525 (13) | 0.0086 (9) | −0.0170 (10) | −0.0078 (10) |
| C19 | 0.0398 (11) | 0.0489 (12) | 0.0624 (14) | 0.0113 (9) | −0.0064 (10) | −0.0184 (11) |
| C20 | 0.0382 (10) | 0.0390 (10) | 0.0414 (11) | −0.0016 (8) | 0.0000 (8) | −0.0155 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cd1—O1 | 2.3234 (14) | C3—H3 | 0.9300 |
| Cd1—O2 | 2.4800 (13) | C4—C5 | 1.373 (4) |
| Cd1—O3 | 2.5447 (15) | C5—C6 | 1.383 (4) |
| Cd1—O4 | 2.3110 (16) | C5—H5 | 0.9300 |
| Cd1—O5$^{i}$ | 2.3175 (12) | C6—H6 | 0.9300 |
| Cd1—O6 | 2.3019 (14) | C7—C6 | 1.379 (3) |
| Cd1—N1 | 2.3384 (14) | C7—H7 | 0.9300 |
| Cd1—C1 | 2.7496 (18) | C8—H8 | 0.9300 |
| Cl1—C4 | 1.739 (2) | C9—C8 | 1.383 (2) |
| Cl2—C17 | 1.740 (2) | C9—C10 | 1.385 (2) |
| O1—C1 | 1.257 (2) | C9—C13 | 1.497 (2) |
| O2—C1 | 1.257 (2) | C10—C11 | 1.381 (3) |
| O3—C14 | 1.256 (2) | C10—H10 | 0.9300 |
| O4—C14 | 1.247 (3) | C11—H11 | 0.9300 |
| O5—Cd1$^{i}$ | 2.3175 (12) | C12—C11 | 1.380 (3) |
| O5—C13 | 1.241 (2) | C12—H12 | 0.9300 |
| O6—H61 | 0.85 (3) | C15—C14 | 1.499 (3) |
| O6—H62 | 0.82 (3) | C15—C16 | 1.387 (3) |
| N1—C8 | 1.333 (2) | C15—C20 | 1.380 (3) |
| N1—C12 | 1.332 (2) | C16—C17 | 1.377 (3) |
| N2—C13 | 1.317 (2) | C16—H16 | 0.9300 |
| N2—H21 | 0.83 (2) | C17—C18 | 1.376 (3) |
| N2—H22 | 0.83 (2) | C18—H18 | 0.9300 |
| C1—C2 | 1.496 (3) | C19—C18 | 1.378 (3) |
| C2—C7 | 1.386 (3) | C19—H19 | 0.9300 |
| C3—C2 | 1.392 (3) | C20—C19 | 1.382 (3) |

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|---|---|---|---|
| C3—C4 | 1.378 (3) | C20—H20 | 0.9300 |
| | | | |
| O1—Cd1—O2 | 54.22 (4) | C4—C3—H3 | 120.3 |
| O1—Cd1—O3 | 82.45 (4) | C3—C4—Cl1 | 119.17 (18) |
| O1—Cd1—N1 | 137.15 (5) | C5—C4—Cl1 | 119.11 (18) |
| O1—Cd1—C1 | 27.07 (5) | C5—C4—C3 | 121.7 (2) |
| O2—Cd1—O3 | 136.12 (4) | C4—C5—C6 | 118.8 (2) |
| O2—Cd1—C1 | 27.20 (5) | C4—C5—H5 | 120.6 |
| O3—Cd1—C1 | 109.10 (5) | C6—C5—H5 | 120.6 |
| O4—Cd1—O1 | 135.63 (5) | C5—C6—H6 | 119.7 |
| O4—Cd1—O2 | 169.88 (5) | C7—C6—C5 | 120.5 (2) |
| O4—Cd1—O3 | 53.32 (5) | C7—C6—H6 | 119.7 |
| O4—Cd1—O5$^{i}$ | 88.27 (6) | C2—C7—H7 | 119.8 |
| O4—Cd1—N1 | 87.04 (5) | C6—C7—C2 | 120.4 (2) |
| O4—Cd1—C1 | 162.39 (6) | C6—C7—H7 | 119.8 |
| O5$^{i}$—Cd1—O1 | 93.65 (5) | N1—C8—C9 | 124.08 (15) |
| O5$^{i}$—Cd1—O2 | 88.64 (5) | N1—C8—H8 | 118.0 |
| O5$^{i}$—Cd1—O3 | 87.51 (4) | C9—C8—H8 | 118.0 |
| O5$^{i}$—Cd1—N1 | 90.96 (5) | C8—C9—C10 | 117.80 (15) |
| O5$^{i}$—Cd1—C1 | 90.09 (5) | C8—C9—C13 | 116.21 (15) |
| O6—Cd1—O1 | 89.05 (5) | C10—C9—C13 | 125.95 (15) |
| O6—Cd1—O2 | 96.40 (6) | C9—C10—H10 | 120.7 |
| O6—Cd1—O3 | 88.63 (5) | C11—C10—C9 | 118.53 (16) |
| O6—Cd1—O4 | 86.82 (7) | C11—C10—H10 | 120.7 |
| O6—Cd1—O5$^{i}$ | 174.96 (6) | C10—C11—H11 | 120.2 |
| O6—Cd1—N1 | 89.95 (5) | C12—C11—C10 | 119.61 (16) |
| O6—Cd1—C1 | 94.24 (6) | C12—C11—H11 | 120.2 |
| N1—Cd1—O2 | 83.38 (5) | N1—C12—C11 | 122.44 (16) |
| N1—Cd1—O3 | 140.36 (5) | N1—C12—H12 | 118.8 |
| N1—Cd1—C1 | 110.52 (5) | C11—C12—H12 | 118.8 |
| C1—O1—Cd1 | 95.71 (11) | O5—C13—N2 | 122.76 (16) |
| C1—O2—Cd1 | 88.42 (11) | O5—C13—C9 | 117.92 (15) |
| C14—O3—Cd1 | 86.39 (12) | N2—C13—C9 | 119.30 (15) |
| C14—O4—Cd1 | 97.51 (13) | O3—C14—C15 | 119.50 (18) |
| C13—O5—Cd1$^{i}$ | 136.29 (11) | O4—C14—O3 | 121.95 (18) |
| Cd1—O6—H62 | 118.6 (19) | O4—C14—C15 | 118.55 (18) |
| Cd1—O6—H61 | 115 (2) | C16—C15—C14 | 119.32 (17) |
| H62—O6—H61 | 108 (3) | C20—C15—C14 | 120.79 (18) |
| C8—N1—Cd1 | 115.65 (11) | C20—C15—C16 | 119.86 (18) |
| C12—N1—Cd1 | 126.66 (11) | C15—C16—H16 | 120.4 |
| C12—N1—C8 | 117.53 (15) | C17—C16—C15 | 119.19 (19) |
| C13—N2—H21 | 117.5 (16) | C17—C16—H16 | 120.4 |
| C13—N2—H22 | 123.5 (15) | C16—C17—Cl2 | 118.88 (17) |
| H21—N2—H22 | 118 (2) | C18—C17—C16 | 121.3 (2) |
| O1—C1—O2 | 121.43 (17) | C18—C17—Cl2 | 119.75 (17) |
| O1—C1—C2 | 118.66 (16) | C17—C18—C19 | 119.2 (2) |
| O1—C1—Cd1 | 57.23 (10) | C17—C18—H18 | 120.4 |
| O2—C1—Cd1 | 64.37 (10) | C19—C18—H18 | 120.4 |

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| O2—C1—C2 | 119.89 (16) | C18—C19—C20 | 120.2 (2) |
| C2—C1—Cd1 | 172.93 (12) | C18—C19—H19 | 119.9 |
| C3—C2—C1 | 120.25 (17) | C20—C19—H19 | 119.9 |
| C7—C2—C1 | 120.45 (17) | C15—C20—C19 | 120.2 (2) |
| C7—C2—C3 | 119.28 (18) | C15—C20—H20 | 119.9 |
| C2—C3—H3 | 120.3 | C19—C20—H20 | 119.9 |
| C4—C3—C2 | 119.33 (19) | | |

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|---|---|---|---|
| O2—Cd1—O1—C1 | 2.65 (10) | Cd1—O1—C1—O2 | −4.98 (18) |
| O3—Cd1—O1—C1 | −170.02 (11) | Cd1—O1—C1—C2 | 173.31 (13) |
| O4—Cd1—O1—C1 | −174.29 (11) | Cd1—O2—C1—O1 | 4.64 (17) |
| O5$^{i}$—Cd1—O1—C1 | −83.03 (11) | Cd1—O2—C1—C2 | −173.62 (14) |
| O6—Cd1—O1—C1 | 101.24 (11) | Cd1—O3—C14—O4 | −8.9 (2) |
| N1—Cd1—O1—C1 | 12.33 (14) | Cd1—O3—C14—C15 | 170.72 (15) |
| O1—Cd1—O2—C1 | −2.64 (10) | Cd1—O4—C14—O3 | 9.8 (2) |
| O3—Cd1—O2—C1 | 7.87 (13) | Cd1—O4—C14—C15 | −169.75 (14) |
| O4—Cd1—O2—C1 | 165.1 (3) | Cd1$^{i}$—O5—C13—N2 | −3.1 (3) |
| O5$^{i}$—Cd1—O2—C1 | 92.85 (11) | Cd1$^{i}$—O5—C13—C9 | 175.50 (12) |
| O6—Cd1—O2—C1 | −86.82 (11) | C12—N1—C8—C9 | −1.0 (3) |
| N1—Cd1—O2—C1 | −176.03 (11) | Cd1—N1—C12—C11 | −174.35 (15) |
| O1—Cd1—O3—C14 | −171.24 (11) | C8—N1—C12—C11 | 1.0 (3) |
| O2—Cd1—O3—C14 | −179.82 (10) | O1—C1—C2—C3 | −172.19 (17) |
| O4—Cd1—O3—C14 | 5.05 (11) | O1—C1—C2—C7 | 6.0 (3) |
| O5$^{i}$—Cd1—O3—C14 | 94.75 (11) | O2—C1—C2—C3 | 6.1 (3) |
| O6—Cd1—O3—C14 | −82.01 (11) | O2—C1—C2—C7 | −175.64 (18) |
| N1—Cd1—O3—C14 | 6.26 (14) | C1—C2—C7—C6 | −177.4 (2) |
| C1—Cd1—O3—C14 | −176.02 (10) | C3—C2—C7—C6 | 0.8 (3) |
| O1—Cd1—O4—C14 | 0.16 (19) | C4—C3—C2—C1 | 177.72 (17) |
| O2—Cd1—O4—C14 | −165.6 (3) | C4—C3—C2—C7 | −0.5 (3) |
| O3—Cd1—O4—C14 | −5.11 (12) | C2—C3—C4—Cl1 | 179.81 (15) |
| O5$^{i}$—Cd1—O4—C14 | −93.29 (14) | C2—C3—C4—C5 | −0.2 (3) |
| O6—Cd1—O4—C14 | 85.54 (14) | Cl1—C4—C5—C6 | −179.3 (2) |
| N1—Cd1—O4—C14 | 175.66 (14) | C3—C4—C5—C6 | 0.7 (4) |
| C1—Cd1—O4—C14 | −8.5 (3) | C2—C7—C6—C5 | −0.4 (4) |
| O1—Cd1—N1—C8 | −95.81 (14) | C4—C5—C6—C7 | −0.4 (4) |
| O1—Cd1—N1—C12 | 79.59 (17) | C10—C9—C8—N1 | 0.1 (3) |
| O2—Cd1—N1—C8 | −87.92 (13) | C13—C9—C8—N1 | −177.73 (16) |
| O2—Cd1—N1—C12 | 87.48 (15) | C8—C9—C10—C11 | 0.8 (3) |
| O3—Cd1—N1—C8 | 87.85 (14) | C13—C9—C10—C11 | 178.40 (18) |
| O3—Cd1—N1—C12 | −96.76 (16) | C8—C9—C13—O5 | −11.4 (2) |
| O4—Cd1—N1—C8 | 88.82 (13) | C8—C9—C13—N2 | 167.21 (17) |
| O4—Cd1—N1—C12 | −95.78 (16) | C10—C9—C13—O5 | 170.94 (18) |
| O5$^{i}$—Cd1—N1—C8 | 0.60 (13) | C10—C9—C13—N2 | −10.4 (3) |
| O5$^{i}$—Cd1—N1—C12 | 176.00 (15) | C9—C10—C11—C12 | −0.8 (3) |
| O6—Cd1—N1—C8 | 175.64 (13) | N1—C12—C11—C10 | −0.1 (3) |
| O6—Cd1—N1—C12 | −8.96 (15) | C16—C15—C14—O3 | −179.91 (18) |
| C1—Cd1—N1—C8 | −89.86 (13) | C16—C15—C14—O4 | −0.3 (3) |
| C1—Cd1—N1—C12 | 85.54 (15) | C20—C15—C14—O3 | −2.0 (3) |

| | | | |
|---|---|---|---|
| O1—Cd1—C1—O2 | 175.29 (18) | C20—C15—C14—O4 | 177.61 (19) |
| O2—Cd1—C1—O1 | −175.29 (18) | C14—C15—C16—C17 | 178.51 (19) |
| O3—Cd1—C1—O1 | 10.47 (12) | C20—C15—C16—C17 | 0.6 (3) |
| O3—Cd1—C1—O2 | −174.24 (10) | C14—C15—C20—C19 | −178.02 (18) |
| O4—Cd1—C1—O1 | 13.3 (3) | C16—C15—C20—C19 | −0.1 (3) |
| O4—Cd1—C1—O2 | −171.40 (18) | C15—C16—C17—Cl2 | −179.44 (16) |
| O5$^{i}$—Cd1—C1—O1 | 97.86 (11) | C15—C16—C17—C18 | −1.2 (3) |
| O5$^{i}$—Cd1—C1—O2 | −86.85 (11) | Cl2—C17—C18—C19 | 179.63 (18) |
| O6—Cd1—C1—O1 | −79.54 (11) | C16—C17—C18—C19 | 1.4 (4) |
| O6—Cd1—C1—O2 | 95.75 (11) | C20—C19—C18—C17 | −1.0 (4) |
| N1—Cd1—C1—O1 | −171.08 (10) | C15—C20—C19—C18 | 0.3 (3) |
| N1—Cd1—C1—O2 | 4.21 (12) | | |

Symmetry code: (i) −*x*+1, −*y*+2, −*z*+1.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H21···O3$^{i}$ | 0.83 (3) | 2.26 (2) | 3.026 (2) | 155 (2) |
| N2—H22···O2$^{ii}$ | 0.83 (2) | 2.09 (2) | 2.913 (2) | 170 (2) |
| O6—H61···O1$^{iii}$ | 0.85 (4) | 2.15 (4) | 2.897 (2) | 146 (3) |
| O6—H62···O3$^{iii}$ | 0.81 (3) | 1.94 (3) | 2.710 (2) | 158 (3) |
| C8—H8···O5$^{i}$ | 0.93 | 2.43 | 3.158 (2) | 135 |
| C10—H10···O2$^{ii}$ | 0.93 | 2.54 | 3.403 (3) | 154 |

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