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# Poly[($\mu_3$-biphenyl-3,3′-dicarboxylato)-(1,10-phenanthroline)cadmium]

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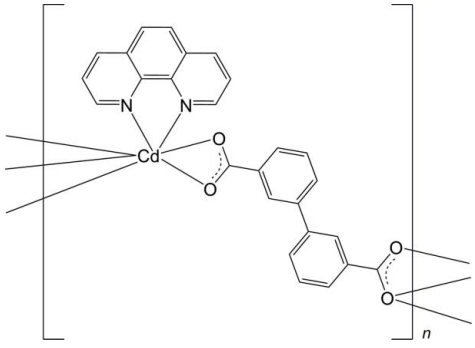
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.033; $wR$ factor = 0.075; data-to-parameter ratio = 16.4.

In the title compound, $[Cd(C_{14}H_8O_4)(C_{12}H_8N_2)]_n$, the $Cd^{II}$ ion is seven-coordinated in a distorted pentagonal–bipyramidal coordination geometry by five O atoms from bridging biphenyl-3,3′-dicarboylate (dpda) ligands and two N atoms from a 1,10-phenanthroline (1,10-phen) ligand. In the crystal, dinuclear units with a Cd···Cd separation of 3.8208 (7) Å are observed. Each of these dinuclear units is bridged *via* 3,3′-bpda in a chelating/chelating and bridging fashion, generating a zigzag chain along the *c* axis. Neighboring chains are further packed *via* weak $\pi$–$\pi$ interactions between interchain parallel 1,10-phen rings [centroid–centroid distance = 3.5197 (9) Å] into a three-dimensional supramolecular architecture.

## Related literature

For the use of biphenyldicarboxylato ligands in supramolecular chemistry, see: Furukawa *et al.* (2008); Qu (2007); Zhu (2010).




## Experimental

### Crystal data

$[Cd(C_{14}H_8O_4)(C_{12}H_8N_2)]$
$M_r$ = 532.81
Monoclinic, $C2/c$
$a$ = 26.1947 (17) Å
$b$ = 9.7258 (5) Å
$c$ = 21.2247 (14) Å
$\beta$ = 127.411 (1)°
$V$ = 4295.0 (5) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 1.05 mm$^{-1}$
$T$ = 296 K
0.22 × 0.16 × 0.12 mm

### Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.804, $T_{max}$ = 0.887
12984 measured reflections
4902 independent reflections
3799 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.075
$S$ = 1.04
4902 reflections
298 parameters
20 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.68 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.39 e Å$^{-3}$

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2322).

## References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Furukawa, H., Kim, J., Ockwig, N. W., O'Keeffe, M. & Yaghi, O. M. (2008). *J. Am. Chem. Soc.* **130**, 11650–11661.
Qu, Z. (2007). *Chin. J. Inorg. Chem.* **23**, 1837–1839.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhu, B.-Y. (2010). *Acta Cryst.* E**66**, m1214.

# supporting information

*Acta Cryst.* (2011). E**67**, m1557 [doi:10.1107/S1600536811042085]

## Poly[($\mu_3$-biphenyl-3,3′-dicarboxylato)(1,10-phenanthroline)cadmium]

**Yu-E Qiu**

### S1. Comment

Polycarboxylate ligands have been widely used to construct coordination polymers due to their versatile coordination modes. The use of biphenyldicarboxylic acid and its derivatives have been reported in literature (Qu, 2007; Furukawa *et al.*, 2008; Zhu, 2010). The title coordination polymer $[Cd(C_{14}H_8O_4)(C_{12}H_8N_2)]_n$, (I), was obtained under hydrothermal conditions and herein its crystal structure is reported.

There is one $Cd^{II}$ cation, one 3,3′-biphenyl-dicarboxylate anion (3,3′-bpda) and one 1,10-phenanthroline (1,10-phen) ligand observed in the asymmetric unit of (I). The $Cd^{II}$ ion is seven coordinated in a distorted pentagonal bipyramidal coordination geometry by five O atoms ($O1^{ii}$, $O2^{i}$, $O2^{ii}$, O3, O4) from bridging 3,3′-bpda with Cd—O bond lengths in the range of 2.258 (2)–2.515 (3) Å, two N atoms (N1, N2) from two 1,10-phen ligands with Cd—N bond lengths of 2.336 (3) and 2.368 (3) Å (Fig. 1). In the crystal structure of (I), dinuclear units with a Cd···Cd separation of 3.8208 (7) Å are observed. Each of these dinuclear units is bridged *via* 3,3′-bpda in a $\mu_1\ \eta^1{:}\eta^1/\mu_2\ \eta^1{:}\eta^2$ coordination mode into one dimensional zigzag chains. Parallel 1, 10-phen ligands are attached to the outside of the zigzag chain with centroid distances of 3.5197 (9) Å indicating weak $\pi$-$\pi$ stacking interactions (Fig. 2). Neighboring chains are further packed *via* weak $\pi$-$\pi$ interactions between interchain parallel 1,10-phen rings into the resulting three dimensional supramolecular architecture.

### S2. Experimental

To a 16 ml Teflon-lined stainless steel vessel was loaded 3,3′-biphenyl-dicarboxylic acid (0.0242 g, 0.1 mmol), 1,10-phenanthroline (0.0198 g, 0.1 mmol), NaOH (0.0080 g, 0.2 mmol) and $Cd(NO_3)_2 \times 4H_2O$ (0.0308 g, 0.1 mmol), then it was sealed and heated to 160 °C for 72 h. After being cooled down to room temperature at a rate of -5 °C/h, colorless block shaped crystals are obtained after filtration. Yield: 0.025 g (47% based on Cd).

### S3. Refinement

All H atoms bonded to C atoms were added according to theoretical models, assigned isotropic displacement parameters and allowed to ride on their respective parent atoms [C—H = 0.93–0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$].

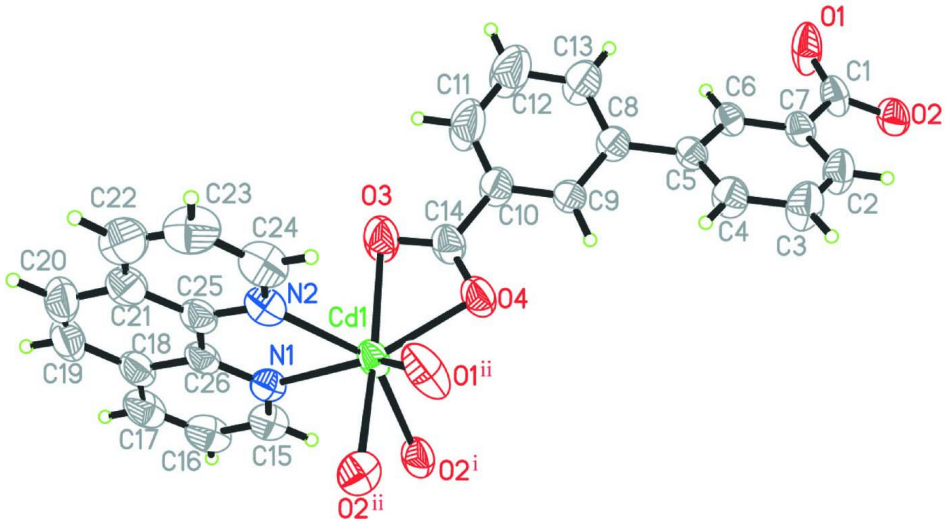


**Figure 1**

Anisotropic displacement ellipsoid plot of (I) at the 50% probability level. H atoms are represented by circles of arbitrary size. Symmetry code: (i)-*x* + 1, -*y* + 2, -*z* + 1; (ii)*x*, -*y* + 2, *z* - 1/2.

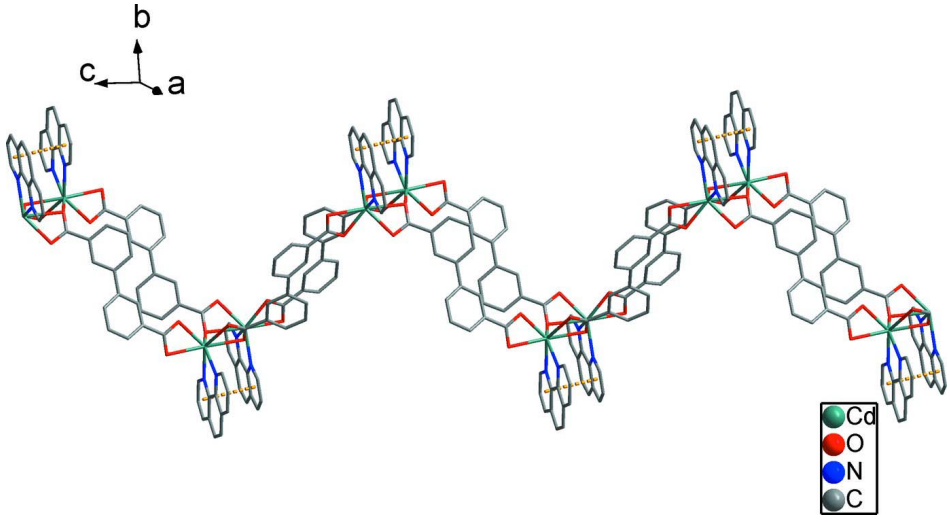


**Figure 2**

The one–dimensional zigzag chain structure of (I).

### Poly[($\mu_3$-biphenyl-3,3′-dicarboxylato)(1,10-phenanthroline)cadmium]

*Crystal data*

$[Cd(C_{14}H_8O_4)(C_{12}H_8N_2)]$
$M_r$ = 532.81
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
*a* = 26.1947 (17) Å
*b* = 9.7258 (5) Å
*c* = 21.2247 (14) Å
$\beta$ = 127.411 (1)°
*V* = 4295.0 (5) Å$^3$
*Z* = 8
*F*(000) = 2128
$D_x$ = 1.648 Mg m$^{-3}$
Mo *Kα* radiation, $\lambda$ = 0.71073 Å
Cell parameters from 4252 reflections
$\theta$ = 2.3–26.6°
$\mu$ = 1.05 mm$^{-1}$
*T* = 296 K
Block, colorless
0.22 × 0.16 × 0.12 mm

*Data collection*

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.804, $T_{max}$ = 0.887
12984 measured reflections
4902 independent reflections
3799 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029
$\theta_{max}$ = 27.5°, $\theta_{min}$ = 2.0°
$h$ = −33→34
$k$ = −12→12
$l$ = −22→27

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.075
$S$ = 1.04
4902 reflections
298 parameters
20 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0264P)^2 + 5.2631P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.68 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.39 e Å$^{-3}$

*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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cd1 | 0.576743 (12) | 0.54986 (2) | 0.356955 (13) | 0.03981 (9) |
| O4 | 0.58387 (13) | 0.7247 (2) | 0.43196 (14) | 0.0562 (6) |
| O2 | 0.53633 (12) | 1.4416 (2) | 0.71597 (14) | 0.0510 (6) |
| N1 | 0.55605 (13) | 0.3153 (3) | 0.35361 (14) | 0.0391 (6) |
| N2 | 0.66457 (14) | 0.4227 (3) | 0.38232 (16) | 0.0462 (7) |
| O1 | 0.60664 (16) | 1.2882 (2) | 0.80000 (16) | 0.0743 (9) |
| O3 | 0.63552 (15) | 0.5452 (3) | 0.50456 (15) | 0.0715 (8) |
| C8 | 0.63079 (16) | 0.9542 (3) | 0.62890 (18) | 0.0419 (7) |
| C22 | 0.7643 (2) | 0.2526 (5) | 0.4166 (2) | 0.0690 (11) |
| H22 | 0.7980 | 0.1969 | 0.4287 | 0.083* |
| C15 | 0.50313 (17) | 0.2623 (4) | 0.33813 (19) | 0.0493 (8) |
| H15 | 0.4707 | 0.3218 | 0.3267 | 0.059* |
| C9 | 0.61051 (15) | 0.8739 (3) | 0.56284 (18) | 0.0384 (7) |
| H9 | 0.5779 | 0.9068 | 0.5125 | 0.046* |
| C6 | 0.60253 (15) | 1.1531 (3) | 0.67908 (18) | 0.0378 (7) |
| H6 | 0.6193 | 1.1044 | 0.7256 | 0.045* |

| | | | | |
|---|---|---|---|---|
| C25 | 0.66020 (16) | 0.2840 (3) | 0.38477 (18) | 0.0429 (8) |
| C7 | 0.57685 (16) | 1.2827 (3) | 0.66989 (18) | 0.0398 (7) |
| C5 | 0.60382 (15) | 1.0940 (3) | 0.62004 (18) | 0.0372 (7) |
| C21 | 0.70931 (19) | 0.1938 (4) | 0.4015 (2) | 0.0540 (9) |
| C26 | 0.60325 (16) | 0.2285 (3) | 0.37016 (17) | 0.0410 (7) |
| C24 | 0.71735 (19) | 0.4739 (4) | 0.3960 (2) | 0.0607 (10) |
| H24 | 0.7207 | 0.5686 | 0.3937 | 0.073* |
| C14 | 0.61750 (17) | 0.6662 (3) | 0.4976 (2) | 0.0462 (8) |
| C10 | 0.63737 (18) | 0.7474 (4) | 0.5699 (2) | 0.0510 (9) |
| C23 | 0.7685 (2) | 0.3906 (5) | 0.4137 (2) | 0.0713 (12) |
| H23 | 0.8049 | 0.4303 | 0.4234 | 0.086* |
| C2 | 0.5534 (2) | 1.3575 (4) | 0.6021 (2) | 0.0577 (10) |
| H2 | 0.5363 | 1.4447 | 0.5957 | 0.069* |
| C1 | 0.57283 (18) | 1.3394 (3) | 0.7327 (2) | 0.0475 (8) |
| C3 | 0.5556 (2) | 1.3028 (4) | 0.5438 (2) | 0.0668 (12) |
| H3 | 0.5407 | 1.3539 | 0.4986 | 0.080* |
| C17 | 0.5397 (2) | 0.0336 (4) | 0.3544 (2) | 0.0605 (11) |
| H17 | 0.5336 | −0.0606 | 0.3544 | 0.073* |
| C4 | 0.57985 (18) | 1.1717 (4) | 0.5526 (2) | 0.0513 (9) |
| H4 | 0.5801 | 1.1351 | 0.5123 | 0.062* |
| C16 | 0.4936 (2) | 0.1214 (4) | 0.3381 (2) | 0.0600 (10) |
| H16 | 0.4555 | 0.0885 | 0.3270 | 0.072* |
| C19 | 0.6478 (2) | −0.0034 (4) | 0.3886 (2) | 0.0646 (11) |
| H19 | 0.6439 | −0.0982 | 0.3901 | 0.078* |
| C11 | 0.6841 (3) | 0.6979 (5) | 0.6435 (3) | 0.0999 (17) |
| H11 | 0.7014 | 0.6111 | 0.6491 | 0.120* |
| C18 | 0.59693 (19) | 0.0839 (3) | 0.37142 (19) | 0.0505 (9) |
| C13 | 0.6786 (2) | 0.9026 (5) | 0.7021 (2) | 0.0867 (16) |
| H13 | 0.6926 | 0.9536 | 0.7470 | 0.104* |
| C12 | 0.7065 (3) | 0.7767 (6) | 0.7108 (3) | 0.118 (2) |
| H12 | 0.7399 | 0.7446 | 0.7610 | 0.142* |
| C20 | 0.7008 (2) | 0.0496 (4) | 0.4026 (2) | 0.0659 (11) |
| H20 | 0.7332 | −0.0095 | 0.4135 | 0.079* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cd1 | 0.05906 (17) | 0.02976 (12) | 0.03860 (14) | −0.00476 (11) | 0.03382 (12) | −0.00224 (10) |
| O4 | 0.0822 (18) | 0.0413 (13) | 0.0422 (14) | 0.0027 (13) | 0.0362 (14) | −0.0058 (11) |
| O2 | 0.0564 (15) | 0.0473 (13) | 0.0569 (15) | 0.0043 (12) | 0.0383 (13) | −0.0115 (11) |
| N1 | 0.0439 (15) | 0.0375 (14) | 0.0341 (14) | −0.0049 (12) | 0.0227 (12) | 0.0023 (11) |
| N2 | 0.0523 (17) | 0.0492 (17) | 0.0444 (16) | −0.0107 (14) | 0.0332 (14) | −0.0059 (13) |
| O1 | 0.145 (3) | 0.0429 (14) | 0.0609 (17) | 0.0272 (16) | 0.0757 (19) | 0.0103 (12) |
| O3 | 0.107 (2) | 0.0565 (13) | 0.0489 (9) | 0.0251 (13) | 0.0461 (13) | 0.0007 (11) |
| C8 | 0.0485 (19) | 0.0465 (18) | 0.0372 (17) | 0.0058 (16) | 0.0295 (15) | −0.0008 (15) |
| C22 | 0.066 (3) | 0.094 (3) | 0.058 (2) | 0.010 (3) | 0.043 (2) | −0.002 (2) |
| C15 | 0.055 (2) | 0.049 (2) | 0.046 (2) | −0.0103 (17) | 0.0320 (18) | 0.0016 (16) |
| C9 | 0.0429 (18) | 0.0410 (17) | 0.0334 (16) | 0.0023 (14) | 0.0243 (14) | −0.0009 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C6 | 0.0468 (18) | 0.0352 (15) | 0.0384 (17) | −0.0041 (14) | 0.0295 (15) | −0.0034 (13) |
| C25 | 0.052 (2) | 0.0461 (19) | 0.0315 (17) | −0.0015 (16) | 0.0260 (16) | −0.0051 (14) |
| C7 | 0.0506 (19) | 0.0361 (16) | 0.0413 (17) | −0.0006 (14) | 0.0324 (16) | −0.0045 (14) |
| C5 | 0.0402 (17) | 0.0390 (16) | 0.0388 (17) | −0.0025 (13) | 0.0273 (15) | −0.0064 (13) |
| C21 | 0.061 (2) | 0.067 (2) | 0.0387 (19) | 0.0051 (19) | 0.0325 (18) | −0.0048 (17) |
| C26 | 0.054 (2) | 0.0372 (17) | 0.0282 (16) | −0.0054 (15) | 0.0231 (15) | −0.0034 (13) |
| C24 | 0.065 (3) | 0.066 (3) | 0.061 (2) | −0.016 (2) | 0.044 (2) | −0.0065 (19) |
| C14 | 0.061 (2) | 0.0433 (14) | 0.0453 (19) | 0.0021 (16) | 0.0380 (18) | −0.0038 (15) |
| C10 | 0.068 (2) | 0.0494 (19) | 0.0386 (18) | 0.0156 (18) | 0.0343 (18) | 0.0033 (15) |
| C23 | 0.056 (3) | 0.103 (4) | 0.070 (3) | −0.008 (2) | 0.046 (2) | −0.003 (3) |
| C2 | 0.086 (3) | 0.0426 (19) | 0.056 (2) | 0.0179 (19) | 0.049 (2) | 0.0063 (17) |
| C1 | 0.074 (2) | 0.0332 (17) | 0.053 (2) | −0.0027 (17) | 0.048 (2) | −0.0059 (16) |
| C3 | 0.107 (3) | 0.057 (2) | 0.053 (2) | 0.024 (2) | 0.057 (2) | 0.0156 (18) |
| C17 | 0.083 (3) | 0.039 (2) | 0.048 (2) | −0.019 (2) | 0.034 (2) | −0.0024 (16) |
| C4 | 0.071 (2) | 0.053 (2) | 0.0431 (19) | 0.0113 (18) | 0.0417 (19) | −0.0005 (16) |
| C16 | 0.071 (3) | 0.055 (2) | 0.050 (2) | −0.024 (2) | 0.035 (2) | −0.0018 (18) |
| C19 | 0.093 (3) | 0.0386 (19) | 0.055 (2) | 0.006 (2) | 0.041 (2) | −0.0048 (17) |
| C11 | 0.136 (4) | 0.084 (3) | 0.060 (3) | 0.060 (3) | 0.050 (3) | 0.004 (2) |
| C18 | 0.072 (3) | 0.0370 (17) | 0.0343 (18) | −0.0015 (17) | 0.0277 (18) | −0.0024 (14) |
| C13 | 0.112 (4) | 0.089 (3) | 0.037 (2) | 0.051 (3) | 0.034 (2) | −0.002 (2) |
| C12 | 0.150 (4) | 0.109 (3) | 0.056 (3) | 0.073 (3) | 0.042 (3) | 0.006 (2) |
| C20 | 0.088 (3) | 0.056 (2) | 0.054 (2) | 0.023 (2) | 0.043 (2) | −0.0011 (19) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cd1—O4 | 2.258 (2) | C6—H6 | 0.9300 |
| Cd1—N1 | 2.336 (3) | C25—C21 | 1.413 (5) |
| Cd1—N2 | 2.368 (3) | C25—C26 | 1.432 (4) |
| Cd1—O2$^{i}$ | 2.368 (2) | C7—C2 | 1.380 (4) |
| Cd1—O1$^{ii}$ | 2.388 (2) | C7—C1 | 1.505 (4) |
| Cd1—O2$^{ii}$ | 2.497 (2) | C5—C4 | 1.387 (4) |
| Cd1—O3 | 2.515 (3) | C21—C20 | 1.423 (5) |
| Cd1—C14 | 2.731 (3) | C26—C18 | 1.419 (4) |
| O4—C14 | 1.245 (4) | C24—C23 | 1.406 (6) |
| O2—C1 | 1.271 (4) | C24—H24 | 0.9300 |
| O2—Cd1$^{i}$ | 2.368 (2) | C14—C10 | 1.509 (4) |
| O2—Cd1$^{iii}$ | 2.497 (2) | C10—C11 | 1.360 (5) |
| N1—C15 | 1.320 (4) | C23—H23 | 0.9300 |
| N1—C26 | 1.355 (4) | C2—C3 | 1.378 (5) |
| N2—C24 | 1.325 (4) | C2—H2 | 0.9300 |
| N2—C25 | 1.358 (4) | C3—C4 | 1.386 (5) |
| O1—C1 | 1.238 (4) | C3—H3 | 0.9300 |
| O1—Cd1$^{iii}$ | 2.388 (2) | C17—C16 | 1.341 (6) |
| O3—C14 | 1.243 (4) | C17—C18 | 1.401 (6) |
| C8—C13 | 1.367 (5) | C17—H17 | 0.9300 |
| C8—C9 | 1.397 (4) | C4—H4 | 0.9300 |
| C8—C5 | 1.491 (4) | C16—H16 | 0.9300 |
| C22—C23 | 1.352 (6) | C19—C20 | 1.336 (6) |

| | | | |
|---|---|---|---|
| C22—C21 | 1.393 (5) | C19—C18 | 1.428 (6) |
| C22—H22 | 0.9300 | C19—H19 | 0.9300 |
| C15—C16 | 1.393 (5) | C11—C12 | 1.398 (6) |
| C15—H15 | 0.9300 | C11—H11 | 0.9300 |
| C9—C10 | 1.380 (4) | C13—C12 | 1.380 (6) |
| C9—H9 | 0.9300 | C13—H13 | 0.9300 |
| C6—C7 | 1.385 (4) | C12—H12 | 0.9300 |
| C6—C5 | 1.398 (4) | C20—H20 | 0.9300 |

| | | | |
|---|---|---|---|
| O4—Cd1—N1 | 132.46 (9) | C4—C5—C6 | 117.3 (3) |
| O4—Cd1—N2 | 125.46 (10) | C4—C5—C8 | 120.7 (3) |
| N1—Cd1—N2 | 70.87 (9) | C6—C5—C8 | 122.0 (3) |
| O4—Cd1—O2$^{i}$ | 88.24 (9) | C22—C21—C25 | 117.3 (4) |
| N1—Cd1—O2$^{i}$ | 80.75 (9) | C22—C21—C20 | 123.4 (4) |
| N2—Cd1—O2$^{i}$ | 145.46 (8) | C25—C21—C20 | 119.3 (4) |
| O4—Cd1—O1$^{ii}$ | 87.04 (9) | N1—C26—C18 | 121.6 (3) |
| N1—Cd1—O1$^{ii}$ | 140.34 (9) | N1—C26—C25 | 119.2 (3) |
| N2—Cd1—O1$^{ii}$ | 83.53 (10) | C18—C26—C25 | 119.2 (3) |
| O2$^{i}$—Cd1—O1$^{ii}$ | 108.10 (10) | N2—C24—C23 | 122.6 (4) |
| O4—Cd1—O2$^{ii}$ | 127.82 (8) | N2—C24—H24 | 118.7 |
| N1—Cd1—O2$^{ii}$ | 94.27 (8) | C23—C24—H24 | 118.7 |
| N2—Cd1—O2$^{ii}$ | 86.32 (8) | O3—C14—O4 | 121.7 (3) |
| O2$^{i}$—Cd1—O2$^{ii}$ | 76.36 (8) | O3—C14—C10 | 120.2 (3) |
| O1$^{ii}$—Cd1—O2$^{ii}$ | 53.28 (8) | O4—C14—C10 | 118.1 (3) |
| O4—Cd1—O3 | 53.83 (8) | O3—C14—Cd1 | 66.77 (18) |
| N1—Cd1—O3 | 88.58 (8) | O4—C14—Cd1 | 54.92 (16) |
| N2—Cd1—O3 | 86.12 (9) | C10—C14—Cd1 | 172.8 (2) |
| O2$^{i}$—Cd1—O3 | 113.01 (9) | C11—C10—C9 | 118.9 (3) |
| O1$^{ii}$—Cd1—O3 | 120.11 (10) | C11—C10—C14 | 119.8 (3) |
| O2$^{ii}$—Cd1—O3 | 170.56 (9) | C9—C10—C14 | 121.2 (3) |
| O4—Cd1—C14 | 26.82 (9) | C22—C23—C24 | 119.6 (4) |
| N1—Cd1—C14 | 111.54 (9) | C22—C23—H23 | 120.2 |
| N2—Cd1—C14 | 106.69 (10) | C24—C23—H23 | 120.2 |
| O2$^{i}$—Cd1—C14 | 101.72 (9) | C3—C2—C7 | 119.8 (3) |
| O1$^{ii}$—Cd1—C14 | 104.46 (9) | C3—C2—H2 | 120.1 |
| O2$^{ii}$—Cd1—C14 | 153.63 (9) | C7—C2—H2 | 120.1 |
| O3—Cd1—C14 | 27.01 (9) | O1—C1—O2 | 121.8 (3) |
| C14—O4—Cd1 | 98.26 (19) | O1—C1—C7 | 119.2 (3) |
| C1—O2—Cd1$^{i}$ | 129.8 (2) | O2—C1—C7 | 119.0 (3) |
| C1—O2—Cd1$^{iii}$ | 89.51 (19) | C2—C3—C4 | 120.0 (3) |
| Cd1$^{i}$—O2—Cd1$^{iii}$ | 103.50 (8) | C2—C3—H3 | 120.0 |
| C15—N1—C26 | 118.5 (3) | C4—C3—H3 | 120.0 |
| C15—N1—Cd1 | 125.3 (2) | C16—C17—C18 | 120.0 (3) |
| C26—N1—Cd1 | 116.2 (2) | C16—C17—H17 | 120.0 |
| C24—N2—C25 | 117.8 (3) | C18—C17—H17 | 120.0 |
| C24—N2—Cd1 | 126.5 (3) | C3—C4—C5 | 121.5 (3) |
| C25—N2—Cd1 | 115.8 (2) | C3—C4—H4 | 119.2 |
| C1—O1—Cd1$^{iii}$ | 95.4 (2) | C5—C4—H4 | 119.2 |

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| C14—O3—Cd1 | 86.2 (2) | C17—C16—C15 | 119.5 (4) |
| C13—C8—C9 | 117.5 (3) | C17—C16—H16 | 120.2 |
| C13—C8—C5 | 121.0 (3) | C15—C16—H16 | 120.2 |
| C9—C8—C5 | 121.4 (3) | C20—C19—C18 | 120.7 (4) |
| C23—C22—C21 | 119.9 (4) | C20—C19—H19 | 119.7 |
| C23—C22—H22 | 120.1 | C18—C19—H19 | 119.7 |
| C21—C22—H22 | 120.1 | C10—C11—C12 | 120.4 (4) |
| N1—C15—C16 | 123.1 (4) | C10—C11—H11 | 119.8 |
| N1—C15—H15 | 118.5 | C12—C11—H11 | 119.8 |
| C16—C15—H15 | 118.5 | C17—C18—C26 | 117.4 (4) |
| C10—C9—C8 | 122.1 (3) | C17—C18—C19 | 123.1 (4) |
| C10—C9—H9 | 118.9 | C26—C18—C19 | 119.5 (4) |
| C8—C9—H9 | 118.9 | C8—C13—C12 | 121.6 (4) |
| C7—C6—C5 | 121.5 (3) | C8—C13—H13 | 119.2 |
| C7—C6—H6 | 119.3 | C12—C13—H13 | 119.2 |
| C5—C6—H6 | 119.3 | C13—C12—C11 | 119.3 (4) |
| N2—C25—C21 | 122.8 (3) | C13—C12—H12 | 120.3 |
| N2—C25—C26 | 117.9 (3) | C11—C12—H12 | 120.3 |
| C21—C25—C26 | 119.4 (3) | C19—C20—C21 | 121.9 (4) |
| C2—C7—C6 | 119.8 (3) | C19—C20—H20 | 119.0 |
| C2—C7—C1 | 120.3 (3) | C21—C20—H20 | 119.0 |
| C6—C7—C1 | 119.9 (3) | | |

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| N1—Cd1—O4—C14 | 45.0 (3) | Cd1—N2—C24—C23 | 177.4 (3) |
| N2—Cd1—O4—C14 | −51.1 (2) | Cd1—O3—C14—O4 | 0.5 (4) |
| O2$^{i}$—Cd1—O4—C14 | 120.7 (2) | Cd1—O3—C14—C10 | −178.2 (3) |
| O1$^{ii}$—Cd1—O4—C14 | −131.0 (2) | Cd1—O4—C14—O3 | −0.5 (4) |
| O2$^{ii}$—Cd1—O4—C14 | −168.08 (19) | Cd1—O4—C14—C10 | 178.2 (3) |
| O3—Cd1—O4—C14 | 0.3 (2) | O4—Cd1—C14—O3 | 179.5 (4) |
| O4—Cd1—N1—C15 | 60.5 (3) | N1—Cd1—C14—O3 | 33.6 (3) |
| N2—Cd1—N1—C15 | −178.5 (3) | N2—Cd1—C14—O3 | −41.9 (2) |
| O2$^{i}$—Cd1—N1—C15 | −18.5 (2) | O2$^{i}$—Cd1—C14—O3 | 118.2 (2) |
| O1$^{ii}$—Cd1—N1—C15 | −125.7 (3) | O1$^{ii}$—Cd1—C14—O3 | −129.4 (2) |
| O2$^{ii}$—Cd1—N1—C15 | −93.9 (2) | O2$^{ii}$—Cd1—C14—O3 | −158.9 (2) |
| O3—Cd1—N1—C15 | 95.1 (2) | N1—Cd1—C14—O4 | −145.9 (2) |
| O4—Cd1—N1—C26 | −118.5 (2) | N2—Cd1—C14—O4 | 138.5 (2) |
| N2—Cd1—N1—C26 | 2.46 (19) | O2$^{i}$—Cd1—C14—O4 | −61.3 (2) |
| O2$^{i}$—Cd1—N1—C26 | 162.5 (2) | O1$^{ii}$—Cd1—C14—O4 | 51.1 (2) |
| O1$^{ii}$—Cd1—N1—C26 | 55.2 (3) | O2$^{ii}$—Cd1—C14—O4 | 21.6 (3) |
| O2$^{ii}$—Cd1—N1—C26 | 87.1 (2) | O3—Cd1—C14—O4 | −179.5 (4) |
| O3—Cd1—N1—C26 | −83.9 (2) | O4—Cd1—C14—C10 | −12.9 (19) |
| O4—Cd1—N2—C24 | −51.3 (3) | N1—Cd1—C14—C10 | −158.8 (19) |
| N1—Cd1—N2—C24 | 179.7 (3) | N2—Cd1—C14—C10 | 126 (2) |
| O2$^{i}$—Cd1—N2—C24 | 143.2 (3) | O2$^{i}$—Cd1—C14—C10 | −74 (2) |
| O1$^{ii}$—Cd1—N2—C24 | 30.4 (3) | O1$^{ii}$—Cd1—C14—C10 | 38 (2) |
| O2$^{ii}$—Cd1—N2—C24 | 83.9 (3) | O2$^{ii}$—Cd1—C14—C10 | 9 (2) |
| O3—Cd1—N2—C24 | −90.5 (3) | O3—Cd1—C14—C10 | 168 (2) |
| O4—Cd1—N2—C25 | 127.0 (2) | C8—C9—C10—C11 | 1.4 (6) |

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| N1—Cd1—N2—C25 | −2.0 (2) | C8—C9—C10—C14 | −176.3 (3) |
| O2$^{i}$—Cd1—N2—C25 | −38.5 (3) | O3—C14—C10—C11 | 12.1 (6) |
| O1$^{ii}$—Cd1—N2—C25 | −151.3 (2) | O4—C14—C10—C11 | −166.7 (4) |
| O2$^{ii}$—Cd1—N2—C25 | −97.8 (2) | O3—C14—C10—C9 | −170.2 (4) |
| O3—Cd1—N2—C25 | 87.8 (2) | O4—C14—C10—C9 | 11.0 (5) |
| O4—Cd1—O3—C14 | −0.3 (2) | C21—C22—C23—C24 | 0.5 (6) |
| N1—Cd1—O3—C14 | −149.0 (2) | N2—C24—C23—C22 | 0.5 (6) |
| N2—Cd1—O3—C14 | 140.1 (2) | C6—C7—C2—C3 | 0.2 (6) |
| O2$^{i}$—Cd1—O3—C14 | −69.7 (2) | C1—C7—C2—C3 | −178.0 (4) |
| O1$^{ii}$—Cd1—O3—C14 | 59.9 (3) | Cd1$^{iii}$—O1—C1—O2 | −2.7 (4) |
| O2$^{ii}$—Cd1—O3—C14 | 103.3 (5) | Cd1$^{iii}$—O1—C1—C7 | 174.9 (3) |
| C26—N1—C15—C16 | 0.1 (5) | Cd1$^{i}$—O2—C1—O1 | −104.7 (4) |
| Cd1—N1—C15—C16 | −178.9 (2) | Cd1$^{iii}$—O2—C1—O1 | 2.6 (4) |
| C13—C8—C9—C10 | −0.4 (5) | Cd1$^{i}$—O2—C1—C7 | 77.7 (4) |
| C5—C8—C9—C10 | 176.5 (3) | Cd1$^{iii}$—O2—C1—C7 | −175.0 (3) |
| C24—N2—C25—C21 | 0.3 (5) | C2—C7—C1—O1 | −163.1 (4) |
| Cd1—N2—C25—C21 | −178.1 (2) | C6—C7—C1—O1 | 18.7 (5) |
| C24—N2—C25—C26 | 179.9 (3) | C2—C7—C1—O2 | 14.6 (5) |
| Cd1—N2—C25—C26 | 1.5 (3) | C6—C7—C1—O2 | −163.6 (3) |
| C5—C6—C7—C2 | −1.8 (5) | C7—C2—C3—C4 | 1.4 (6) |
| C5—C6—C7—C1 | 176.4 (3) | C2—C3—C4—C5 | −1.5 (6) |
| C7—C6—C5—C4 | 1.6 (5) | C6—C5—C4—C3 | 0.0 (5) |
| C7—C6—C5—C8 | −179.4 (3) | C8—C5—C4—C3 | −178.9 (4) |
| C13—C8—C5—C4 | 149.9 (4) | C18—C17—C16—C15 | 0.2 (5) |
| C9—C8—C5—C4 | −26.9 (5) | N1—C15—C16—C17 | −0.1 (5) |
| C13—C8—C5—C6 | −29.0 (5) | C9—C10—C11—C12 | −2.7 (8) |
| C9—C8—C5—C6 | 154.2 (3) | C14—C10—C11—C12 | 175.1 (5) |
| C23—C22—C21—C25 | −1.0 (5) | C16—C17—C18—C26 | −0.3 (5) |
| C23—C22—C21—C20 | 179.4 (4) | C16—C17—C18—C19 | −179.5 (3) |
| N2—C25—C21—C22 | 0.6 (5) | N1—C26—C18—C17 | 0.4 (5) |
| C26—C25—C21—C22 | −179.0 (3) | C25—C26—C18—C17 | −178.1 (3) |
| N2—C25—C21—C20 | −179.8 (3) | N1—C26—C18—C19 | 179.6 (3) |
| C26—C25—C21—C20 | 0.6 (5) | C25—C26—C18—C19 | 1.1 (5) |
| C15—N1—C26—C18 | −0.3 (4) | C20—C19—C18—C17 | 178.4 (4) |
| Cd1—N1—C26—C18 | 178.9 (2) | C20—C19—C18—C26 | −0.7 (5) |
| C15—N1—C26—C25 | 178.2 (3) | C9—C8—C13—C12 | 0.7 (7) |
| Cd1—N1—C26—C25 | −2.7 (3) | C5—C8—C13—C12 | −176.2 (5) |
| N2—C25—C26—N1 | 0.8 (4) | C8—C13—C12—C11 | −2.0 (10) |
| C21—C25—C26—N1 | −179.6 (3) | C10—C11—C12—C13 | 3.0 (10) |
| N2—C25—C26—C18 | 179.3 (3) | C18—C19—C20—C21 | 0.3 (6) |
| C21—C25—C26—C18 | −1.1 (4) | C22—C21—C20—C19 | 179.3 (4) |
| C25—N2—C24—C23 | −0.9 (5) | C25—C21—C20—C19 | −0.2 (6) |

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