Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# *catena*-Poly[[diiodidocadmium(II)]-$\mu$-4,4′-di-4-pyridyl-2,2′-disulfanediyldipyrimidine]

**Hai-Bin Zhu**

School of Chemistry and Chemical Engineering, Southeast University, Nanjing 211189, People's Republic of China, and School of Material Science and Engineering, Southeast University, Nanjing 211189, People's Republic of China
Correspondence e-mail: zhuhaibin@seu.edu.cn

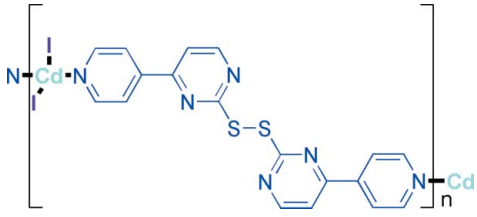
Received 20 November 2009; accepted 27 November 2009

Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.027; $wR$ factor = 0.057; data-to-parameter ratio = 15.4.

In the title compound, $[CdI_2(C_{18}H_{12}N_6S_2)]_n$, the 4,4′-di-4-pyridyl-2,2′-disulfanediyldipyrimidine ($L$) ligand bridges two $Cd^{II}$ centers, forming polymeric zigzag chains extending along the $b$ axis. The $Cd^{II}$ ions are coordinated by two N atoms from two $L$ ligands and two iodide anions in a distorted tetrahedral geometry.

## Related literature

For coordination polymers with 4,4′-dipyridinedisulfide, see: Horikoshi & Mochida (2006). For coordination complexes with the title ligand $L$, see: Zhu *et al.* (2009).




## Experimental

### Crystal data

$[CdI_2(C_{18}H_{12}N_6S_2)]$
$M_r$ = 742.69
Triclinic, $P\overline{1}$
$a$ = 10.0145 (7) Å
$b$ = 10.7294 (8) Å
$c$ = 11.7217 (9) Å
$\alpha$ = 93.133 (1)°
$\beta$ = 109.886 (1)°
$\gamma$ = 97.726 (1)°
$V$ = 1166.81 (15) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 3.78 mm$^{-1}$
$T$ = 298 K
0.20 × 0.15 × 0.12 mm

### Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 1.9, $T_{max}$ = 28.9
5935 measured reflections
4037 independent reflections
3073 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.015

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.057
$S$ = 0.99
4037 reflections
262 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.35 e Å$^{-3}$

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT-Plus* (Bruker, 2007); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The author acknowledges the finanical support from the China Postdoctoral Reseach Fund (grant No. 20070411010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2663).

## References

Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *APEX2* and *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
Horikoshi, R. & Mochida, T. (2006). *Coord. Chem. Rev.* **250**, 2595–2609.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhu, H. B., Wang, H., Kong, F., Gou, S. H. & Sun, Y. M. (2009). *J. Mol. Struct.* **936**, 99–103.

# supporting information

*Acta Cryst.* (2010). E**66**, m1 [doi:10.1107/S1600536809051162]

## *catena*-Poly[[diiodidocadmium(II)]-$\mu$-4,4′-di-4-pyridyl-2,2′-disulfanediyldipyrimidine]

**Hai-Bin Zhu**

### S1. Comment

Over past few years, organic aromatic disulfide has received considerable attention due to both its conformational flexibility and axial chirality (Horikoshi *et al.*, 2006). In our previous study, we have reported two one-dimensional $Zn^{II}$ and $Fe^{II}$ coordination polymers with the ligand *L* ( = 2, 2′-dithiobis(4-pyridin-4-ylpyrimidine) (Zhu *et al.*, 2009). Herein, we report new one-dimensional $Cd^{II}$ coordination chain generated by althernative linking of Cd center and ligand *L*.

The $Cd^{II}$ ion in the title complex adopts a tetrahedral coordination geometry completed by two N atoms from two ligands *L* [Cd1—N1 2.287 (3) Å; Cd1—N6 2.289 (4) Å] and two I anions [I1—Cd1 2.6938 (4) Å; I2—Cd1 2.6962 (4) Å]. In *L*, the C—S—S—C torsion angle is 84.1 (2)°.

### S2. Experimental

Slowly added is the $CH_2Cl_2$ (5 ml) solution of ligand *L* (0.1 mmol) into the $CdI_2$ (0.1 mmol) solution in methanol (10 ml). The mixture was kept on standing for three days to give single crystals suitable for X-ray diffraction analysis.

### S3. Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 Å and *U*iso(H) = 1.2*U*eq(C).

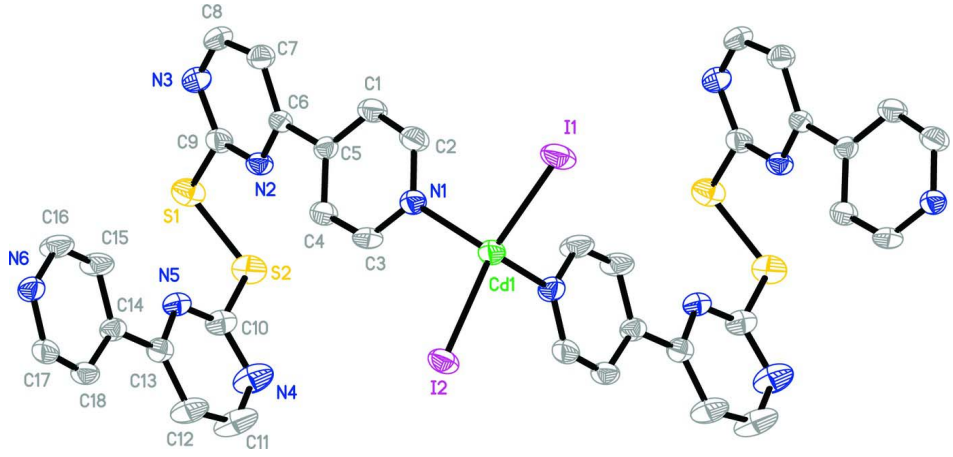



**Figure 1**

The coordination environment of the $Cd^{II}$ center in the title compound with 30% probability displacement ellipsoids. Unlabelled atoms are related with the labelled ones by symmetry operation (*x, y + 1, z*). H atoms omitted for clarity.

**_catena_-Poly[[diiodidocadmium(II)]-$\mu$-4,4′-di-4-pyridyl-2,2′- disulfanediyldipyrimidine]**

*Crystal data*

$[CdI_2(C_{18}H_{12}N_6S_2)]$
$M_r = 742.69$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 10.0145\ (7)$ Å
$b = 10.7294\ (8)$ Å
$c = 11.7217\ (9)$ Å
$\alpha = 93.133\ (1)°$
$\beta = 109.886\ (1)°$
$\gamma = 97.726\ (1)°$
$V = 1166.81\ (15)$ Å$^3$
$Z = 2$
$F(000) = 696$
$D_x = 2.114$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4037 reflections
$\theta = 2.3–25.5°$
$\mu = 3.78$ mm$^{-1}$
$T = 298$ K
Block, colourless
0.20 × 0.15 × 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)
$T_{min} = 1.9$, $T_{max} = 28.9$
5935 measured reflections
4037 independent reflections
3073 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$
$h = -7\rightarrow11$
$k = -12\rightarrow12$
$l = -13\rightarrow13$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.057$
$S = 0.99$
4037 reflections
262 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0238P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å$^{-3}$
$\Delta\rho_{min} = -0.35$ 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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| I2 | 1.04050 (3) | 0.30244 (3) | −0.04759 (3) | 0.06234 (11) |
| I1 | 0.58853 (3) | 0.01728 (3) | −0.20478 (3) | 0.07768 (13) |
| Cd1 | 0.80005 (3) | 0.17348 (3) | −0.02843 (3) | 0.05367 (11) |

| | | | | |
|---|---|---|---|---|
| S1 | 0.66738 (13) | 0.72678 (11) | 0.58132 (11) | 0.0647 (3) |
| S2 | 0.83801 (13) | 0.63432 (12) | 0.62502 (11) | 0.0666 (3) |
| N1 | 0.6891 (4) | 0.3069 (3) | 0.0542 (3) | 0.0487 (9) |
| N2 | 0.6043 (3) | 0.5841 (3) | 0.3679 (3) | 0.0466 (8) |
| N3 | 0.4190 (4) | 0.6770 (3) | 0.4080 (4) | 0.0593 (10) |
| C6 | 0.5105 (4) | 0.5314 (3) | 0.2591 (4) | 0.0426 (10) |
| C4 | 0.7136 (4) | 0.4798 (4) | 0.2009 (4) | 0.0526 (11) |
| H4A | 0.7736 | 0.5465 | 0.2565 | 0.063* |
| C9 | 0.5529 (4) | 0.6526 (4) | 0.4357 (4) | 0.0508 (11) |
| C8 | 0.3282 (5) | 0.6238 (4) | 0.2986 (5) | 0.0618 (13) |
| H8A | 0.2334 | 0.6379 | 0.2739 | 0.074* |
| C3 | 0.7684 (4) | 0.4046 (4) | 0.1332 (4) | 0.0523 (11) |
| H3B | 0.8655 | 0.4238 | 0.1437 | 0.063* |
| C5 | 0.5695 (4) | 0.4544 (3) | 0.1849 (4) | 0.0423 (10) |
| C2 | 0.5492 (5) | 0.2843 (4) | 0.0378 (4) | 0.0632 (13) |
| H2B | 0.4911 | 0.2178 | −0.0191 | 0.076* |
| C1 | 0.4868 (5) | 0.3542 (4) | 0.1005 (4) | 0.0606 (13) |
| H1A | 0.3889 | 0.3343 | 0.0864 | 0.073* |
| C7 | 0.3683 (4) | 0.5492 (4) | 0.2207 (4) | 0.0530 (11) |
| H7A | 0.3026 | 0.5122 | 0.1454 | 0.064* |
| N5 | 0.9147 (3) | 0.7871 (3) | 0.4735 (3) | 0.0474 (8) |
| C13 | 1.0157 (4) | 0.8354 (4) | 0.4271 (4) | 0.0493 (11) |
| C14 | 0.9704 (4) | 0.9207 (4) | 0.3321 (4) | 0.0459 (10) |
| C10 | 0.9551 (5) | 0.7070 (4) | 0.5546 (4) | 0.0571 (12) |
| N4 | 1.0789 (5) | 0.6629 (4) | 0.5948 (4) | 0.0815 (13) |
| C18 | 1.0671 (4) | 0.9895 (4) | 0.2893 (4) | 0.0548 (12) |
| H18A | 1.1651 | 0.9878 | 0.3252 | 0.066* |
| C15 | 0.8267 (5) | 0.9313 (4) | 0.2767 (5) | 0.0637 (13) |
| H15A | 0.7576 | 0.8889 | 0.3036 | 0.076* |
| C12 | 1.1494 (5) | 0.7979 (5) | 0.4649 (5) | 0.0737 (14) |
| H12A | 1.2198 | 0.8306 | 0.4345 | 0.088* |
| C11 | 1.1754 (6) | 0.7115 (6) | 0.5484 (5) | 0.0934 (18) |
| H11A | 1.2650 | 0.6856 | 0.5736 | 0.112* |
| C17 | 1.0191 (5) | 1.0597 (4) | 0.1950 (5) | 0.0566 (12) |
| H17A | 1.0864 | 1.1044 | 0.1676 | 0.068* |
| N6 | 0.8813 (4) | 1.0678 (3) | 0.1399 (3) | 0.0537 (9) |
| C16 | 0.7870 (5) | 1.0040 (4) | 0.1829 (5) | 0.0697 (14) |
| H16A | 0.6900 | 1.0097 | 0.1470 | 0.084* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| I2 | 0.04535 (17) | 0.0650 (2) | 0.0747 (2) | −0.00692 (14) | 0.02573 (16) | −0.00033 (16) |
| I1 | 0.04633 (19) | 0.0866 (2) | 0.0967 (3) | −0.00948 (16) | 0.03348 (19) | −0.0232 (2) |
| Cd1 | 0.04412 (19) | 0.05401 (19) | 0.0674 (3) | 0.00516 (14) | 0.02683 (18) | 0.00403 (16) |
| S1 | 0.0556 (7) | 0.0817 (8) | 0.0595 (9) | 0.0022 (6) | 0.0296 (7) | −0.0090 (7) |
| S2 | 0.0583 (8) | 0.0876 (9) | 0.0536 (9) | 0.0064 (6) | 0.0201 (6) | 0.0158 (7) |
| N1 | 0.043 (2) | 0.051 (2) | 0.053 (2) | 0.0078 (17) | 0.0185 (18) | 0.0044 (18) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N2 | 0.0358 (19) | 0.053 (2) | 0.053 (2) | 0.0038 (16) | 0.0198 (18) | 0.0010 (17) |
| N3 | 0.048 (2) | 0.063 (2) | 0.073 (3) | 0.0126 (19) | 0.028 (2) | 0.005 (2) |
| C6 | 0.036 (2) | 0.040 (2) | 0.053 (3) | 0.0036 (18) | 0.017 (2) | 0.009 (2) |
| C4 | 0.043 (2) | 0.056 (3) | 0.056 (3) | 0.003 (2) | 0.016 (2) | −0.002 (2) |
| C9 | 0.043 (3) | 0.053 (2) | 0.059 (3) | 0.003 (2) | 0.024 (2) | 0.007 (2) |
| C8 | 0.042 (3) | 0.066 (3) | 0.085 (4) | 0.019 (2) | 0.028 (3) | 0.014 (3) |
| C3 | 0.032 (2) | 0.066 (3) | 0.059 (3) | 0.002 (2) | 0.020 (2) | 0.005 (2) |
| C5 | 0.037 (2) | 0.044 (2) | 0.049 (3) | 0.0089 (18) | 0.019 (2) | 0.010 (2) |
| C2 | 0.043 (3) | 0.063 (3) | 0.076 (4) | −0.003 (2) | 0.020 (3) | −0.019 (3) |
| C1 | 0.041 (2) | 0.064 (3) | 0.074 (4) | 0.002 (2) | 0.021 (2) | −0.008 (3) |
| C7 | 0.043 (3) | 0.059 (3) | 0.053 (3) | 0.009 (2) | 0.011 (2) | 0.004 (2) |
| N5 | 0.0379 (19) | 0.061 (2) | 0.042 (2) | 0.0099 (16) | 0.0132 (17) | 0.0014 (18) |
| C13 | 0.045 (2) | 0.055 (2) | 0.050 (3) | 0.007 (2) | 0.021 (2) | −0.009 (2) |
| C14 | 0.038 (2) | 0.054 (2) | 0.047 (3) | 0.0098 (19) | 0.018 (2) | −0.004 (2) |
| C10 | 0.045 (3) | 0.077 (3) | 0.050 (3) | 0.014 (2) | 0.016 (2) | 0.002 (3) |
| N4 | 0.066 (3) | 0.125 (4) | 0.070 (3) | 0.038 (3) | 0.033 (3) | 0.037 (3) |
| C18 | 0.036 (2) | 0.061 (3) | 0.068 (4) | 0.004 (2) | 0.022 (2) | 0.000 (2) |
| C15 | 0.040 (3) | 0.087 (3) | 0.075 (4) | 0.008 (2) | 0.031 (3) | 0.024 (3) |
| C12 | 0.047 (3) | 0.113 (4) | 0.076 (4) | 0.027 (3) | 0.033 (3) | 0.024 (3) |
| C11 | 0.059 (3) | 0.154 (6) | 0.087 (5) | 0.052 (4) | 0.034 (3) | 0.046 (4) |
| C17 | 0.043 (3) | 0.054 (3) | 0.077 (4) | 0.001 (2) | 0.029 (3) | 0.003 (3) |
| N6 | 0.046 (2) | 0.054 (2) | 0.069 (3) | 0.0120 (17) | 0.028 (2) | 0.0135 (18) |
| C16 | 0.038 (3) | 0.091 (4) | 0.092 (4) | 0.017 (2) | 0.033 (3) | 0.034 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| I2—Cd1 | 2.6962 (4) | C2—H2B | 0.9300 |
| I1—Cd1 | 2.6938 (5) | C1—H1A | 0.9300 |
| Cd1—N1 | 2.287 (3) | C7—H7A | 0.9300 |
| Cd1—N6$^{i}$ | 2.290 (4) | N5—C10 | 1.314 (5) |
| S1—C9 | 1.771 (4) | N5—C13 | 1.360 (5) |
| S1—S2 | 2.0205 (19) | C13—C12 | 1.383 (6) |
| S2—C10 | 1.774 (4) | C13—C14 | 1.470 (6) |
| N1—C3 | 1.326 (5) | C14—C18 | 1.383 (5) |
| N1—C2 | 1.334 (5) | C14—C15 | 1.386 (6) |
| N2—C9 | 1.325 (4) | C10—N4 | 1.330 (6) |
| N2—C6 | 1.338 (5) | N4—C11 | 1.325 (6) |
| N3—C9 | 1.334 (5) | C18—C17 | 1.359 (6) |
| N3—C8 | 1.336 (5) | C18—H18A | 0.9300 |
| C6—C7 | 1.383 (5) | C15—C16 | 1.362 (6) |
| C6—C5 | 1.480 (5) | C15—H15A | 0.9300 |
| C4—C5 | 1.378 (5) | C12—C11 | 1.370 (7) |
| C4—C3 | 1.388 (5) | C12—H12A | 0.9300 |
| C4—H4A | 0.9300 | C11—H11A | 0.9300 |
| C8—C7 | 1.376 (5) | C17—N6 | 1.326 (5) |
| C8—H8A | 0.9300 | C17—H17A | 0.9300 |
| C3—H3B | 0.9300 | N6—C16 | 1.343 (5) |
| C5—C1 | 1.381 (5) | N6—Cd1$^{ii}$ | 2.290 (4) |

| | | | |
|---|---|---|---|
| C2—C1 | 1.367 (5) | C16—H16A | 0.9300 |
| | | | |
| N1—Cd1—N6$^{i}$ | 96.12 (11) | C5—C1—H1A | 120.0 |
| N1—Cd1—I1 | 106.24 (9) | C8—C7—C6 | 117.1 (4) |
| N6$^{i}$—Cd1—I1 | 108.88 (8) | C8—C7—H7A | 121.4 |
| N1—Cd1—I2 | 109.95 (8) | C6—C7—H7A | 121.4 |
| N6$^{i}$—Cd1—I2 | 104.57 (8) | C10—N5—C13 | 115.5 (4) |
| I1—Cd1—I2 | 126.810 (15) | N5—C13—C12 | 119.8 (4) |
| C9—S1—S2 | 104.45 (14) | N5—C13—C14 | 116.3 (4) |
| C10—S2—S1 | 106.08 (18) | C12—C13—C14 | 123.7 (4) |
| C3—N1—C2 | 117.0 (3) | C18—C14—C15 | 116.6 (4) |
| C3—N1—Cd1 | 119.2 (2) | C18—C14—C13 | 122.1 (4) |
| C2—N1—Cd1 | 123.3 (3) | C15—C14—C13 | 121.3 (4) |
| C9—N2—C6 | 116.3 (3) | N5—C10—N4 | 129.3 (4) |
| C9—N3—C8 | 114.5 (3) | N5—C10—S2 | 121.9 (3) |
| N2—C6—C7 | 121.2 (3) | N4—C10—S2 | 108.7 (4) |
| N2—C6—C5 | 115.6 (3) | C11—N4—C10 | 114.0 (5) |
| C7—C6—C5 | 123.3 (4) | C17—C18—C14 | 120.1 (4) |
| C5—C4—C3 | 119.2 (4) | C17—C18—H18A | 120.0 |
| C5—C4—H4A | 120.4 | C14—C18—H18A | 120.0 |
| C3—C4—H4A | 120.4 | C16—C15—C14 | 119.9 (4) |
| N2—C9—N3 | 127.8 (4) | C16—C15—H15A | 120.1 |
| N2—C9—S1 | 120.2 (3) | C14—C15—H15A | 120.1 |
| N3—C9—S1 | 112.0 (3) | C11—C12—C13 | 118.2 (4) |
| N3—C8—C7 | 123.1 (4) | C11—C12—H12A | 120.9 |
| N3—C8—H8A | 118.4 | C13—C12—H12A | 120.9 |
| C7—C8—H8A | 118.4 | N4—C11—C12 | 123.1 (5) |
| N1—C3—C4 | 123.3 (4) | N4—C11—H11A | 118.5 |
| N1—C3—H3B | 118.4 | C12—C11—H11A | 118.5 |
| C4—C3—H3B | 118.4 | N6—C17—C18 | 123.5 (4) |
| C4—C5—C1 | 117.2 (3) | N6—C17—H17A | 118.2 |
| C4—C5—C6 | 119.8 (4) | C18—C17—H17A | 118.2 |
| C1—C5—C6 | 122.9 (3) | C17—N6—C16 | 116.9 (4) |
| N1—C2—C1 | 123.2 (4) | C17—N6—Cd1$^{ii}$ | 123.1 (3) |
| N1—C2—H2B | 118.4 | C16—N6—Cd1$^{ii}$ | 119.9 (3) |
| C1—C2—H2B | 118.4 | N6—C16—C15 | 123.0 (4) |
| C2—C1—C5 | 120.0 (4) | N6—C16—H16A | 118.5 |
| C2—C1—H1A | 120.0 | C15—C16—H16A | 118.5 |
| | | | |
| C9—S1—S2—C10 | 84.1 (2) | N3—C8—C7—C6 | −1.0 (6) |
| N6$^{i}$—Cd1—N1—C3 | 76.8 (3) | N2—C6—C7—C8 | 0.5 (6) |
| I1—Cd1—N1—C3 | −171.5 (3) | C5—C6—C7—C8 | −179.6 (4) |
| I2—Cd1—N1—C3 | −31.2 (3) | C10—N5—C13—C12 | 0.9 (6) |
| N6$^{i}$—Cd1—N1—C2 | −95.6 (4) | C10—N5—C13—C14 | 177.3 (3) |
| I1—Cd1—N1—C2 | 16.2 (4) | N5—C13—C14—C18 | 171.0 (3) |
| I2—Cd1—N1—C2 | 156.5 (3) | C12—C13—C14—C18 | −12.8 (6) |
| C9—N2—C6—C7 | 0.4 (5) | N5—C13—C14—C15 | −12.1 (5) |
| C9—N2—C6—C5 | −179.5 (3) | C12—C13—C14—C15 | 164.2 (4) |

| | | | |
|---|---|---|---|
| C6—N2—C9—N3 | −1.0 (6) | C13—N5—C10—N4 | −2.6 (7) |
| C6—N2—C9—S1 | −180.0 (3) | C13—N5—C10—S2 | −180.0 (3) |
| C8—N3—C9—N2 | 0.6 (6) | S1—S2—C10—N5 | −11.3 (4) |
| C8—N3—C9—S1 | 179.6 (3) | S1—S2—C10—N4 | 170.8 (3) |
| S2—S1—C9—N2 | −18.5 (3) | N5—C10—N4—C11 | 2.6 (8) |
| S2—S1—C9—N3 | 162.4 (3) | S2—C10—N4—C11 | −179.7 (4) |
| C9—N3—C8—C7 | 0.4 (6) | C15—C14—C18—C17 | −2.1 (6) |
| C2—N1—C3—C4 | 2.3 (6) | C13—C14—C18—C17 | 175.0 (4) |
| Cd1—N1—C3—C4 | −170.5 (3) | C18—C14—C15—C16 | 1.9 (6) |
| C5—C4—C3—N1 | −1.2 (6) | C13—C14—C15—C16 | −175.2 (4) |
| C3—C4—C5—C1 | −0.3 (6) | N5—C13—C12—C11 | 0.5 (7) |
| C3—C4—C5—C6 | 178.2 (4) | C14—C13—C12—C11 | −175.7 (4) |
| N2—C6—C5—C4 | −26.6 (5) | C10—N4—C11—C12 | −0.9 (8) |
| C7—C6—C5—C4 | 153.5 (4) | C13—C12—C11—N4 | −0.4 (9) |
| N2—C6—C5—C1 | 151.8 (4) | C14—C18—C17—N6 | 0.6 (6) |
| C7—C6—C5—C1 | −28.1 (6) | C18—C17—N6—C16 | 1.2 (6) |
| C3—N1—C2—C1 | −2.0 (7) | C18—C17—N6—Cd1$^{ii}$ | −175.0 (3) |
| Cd1—N1—C2—C1 | 170.5 (4) | C17—N6—C16—C15 | −1.4 (7) |
| N1—C2—C1—C5 | 0.6 (7) | Cd1$^{ii}$—N6—C16—C15 | 174.9 (4) |
| C4—C5—C1—C2 | 0.6 (6) | C14—C15—C16—N6 | −0.1 (7) |
| C6—C5—C1—C2 | −177.9 (4) | | |

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