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 Di- μ -chlorido-bis[(2,2'-bibenzimidazole)-chloridocadmium(II)]

Ge Liu

Chifeng University, Chifeng 024000, People's Republic of China

Correspondence e-mail: liu_ge2008@163.com

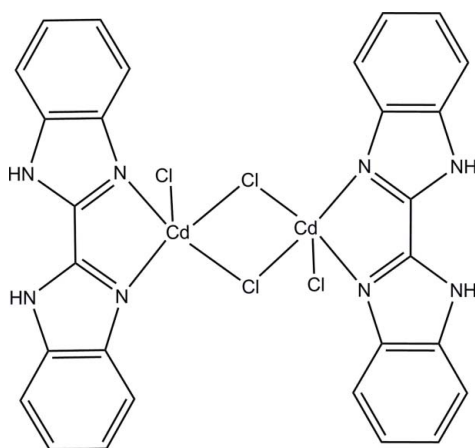
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.033; wR factor = 0.060; data-to-parameter ratio = 17.6.

The title binuclear complex, $[\text{Cd}_2\text{Cl}_4(\text{C}_{14}\text{H}_{10}\text{N}_4)_2]$, was synthesized by the hydrothermal reaction of CdCl_2 and the ligand 2,2'-bibenzimidazole. The molecule lies on an inversion center and the metal center displays a strongly distorted trigonal-bipyramidal geometry. The Cd^{II} ions are coordinated by two N atoms from the organic ligand, and by one terminal and two bridging chloride anions. The crystal structure involves intermolecular $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen bonds, resulting in a one-dimensional supramolecular structure.

Related literature

For the synthesis of 2,2'-bibenzimidazole, see: Fieselmann *et al.* (1978). For general properties of Cd^{II} -based complex polymers, see: Meng *et al.* (2004).



Experimental

Crystal data

 $[\text{Cd}_2\text{Cl}_4(\text{C}_{14}\text{H}_{10}\text{N}_4)_2]$
 $M_r = 835.12$

 Monoclinic, $C2/c$
 $a = 11.824$ (2) Å
 $b = 10.784$ (2) Å
 $c = 22.828$ (5) Å
 $\beta = 91.10$ (3)°
 $V = 2910.1$ (10) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.86$ mm⁻¹
 $T = 293$ (2) K
 $0.17 \times 0.16 \times 0.12$ mm

Data collection

 Rigaku R-AXIS RAPID-S
 diffractometer
 Absorption correction: none
 14677 measured reflections

 3337 independent reflections
 2840 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.035$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.060$
 $S = 1.14$
 3337 reflections

 190 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.29$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.34$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

| | | | |
|------------|------------|-------------------------|-------------|
| Cd1—N4 | 2.305 (2) | Cd1—Cl1 | 2.5725 (10) |
| Cd1—N1 | 2.338 (2) | Cd1—Cl1 ⁱ | 2.5903 (10) |
| Cd1—Cl2 | 2.4602 (8) | | |
| N4—Cd1—Cl2 | 118.63 (6) | Cl2—Cd1—Cl1 | 96.65 (3) |
| N4—Cd1—Cl1 | 144.04 (6) | N1—Cd1—Cl1 ⁱ | 154.49 (6) |

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

Table 2

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|--|--------------|--------------------|-------------|----------------------|
| $\text{N3}-\text{H16}\cdots\text{Cl2}^{\text{ii}}$ | 0.86 | 2.39 | 3.221 (2) | 163 |

 Symmetry code: (ii) $x - \frac{1}{2}, y - \frac{1}{2}, z$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); 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 thanks Chifeng University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2211).

References

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supplementary materials

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Di- μ -chlorido-bis[(2,2'-bibenzimidazole)chloridocadmium(II)]

G. Liu

Comment

Bibenzimidazole has the potential to function as a bis-bidentate nitrogen ligand by coordinating to metal ions as a chelate. On the other hand, Cd^{II}-containing coordination polymers have attracted much attention as they are able to bond to different donors ligands simultaneously, because of the Cd^{II} large radius. Various coordination modes and potential applications in catalysis, fluorescent materials, NLO materials and so on (Meng *et al.* 2004) have been described. Here we report the crystal structure of the title complex prepared from CdCl₂ and bibenzimidazole ligand (see experimental).

As show in Fig. 1, the complex lies on an inversion center, and Cd atoms have strongly distorted trigonal-bipyramidal geometry, being coordinated by two N atoms from the organic ligand, and by one terminal and two bridging Cl⁻ anions. The two Cd centers are bridged by two chloride ions to give a dinuclear cadmium complex. Intermolecular N—H \cdots Cl hydrogen bonds extend the dinuclear complex to a one dimensional chain in the crystal structure (Fig. 2).

Experimental

A mixture of CdCl₂ (0.073 g, 0.40 mmol), bibenzimidazole (0.070 g, 0.30 mmol) and H₂O (10 ml) was placed in a Teflon reactor, then heated to 433 K at 10.8 K/h; after maintaining the reaction at 433 K for three days, it was cooled to 303 K at 10.8 K/h. Crystals suitable for X-ray analysis were obtained.

Refinement

Raw diffraction data were used for refinement, since semi-empirical correction failed to properly correct absorption effects. All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with N—H = 0.86 Å, C—H = 0.93 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier atom})$.

Figures

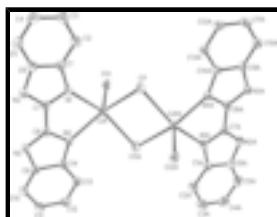


Fig. 1. The structure of the title compound with displacement ellipsoids at the 30% probability level.

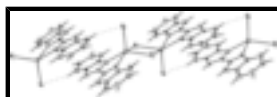


Fig. 2. One dimensional chain formed by hydrogen bonds (dashed lines) in the crystal structure of the title compound.

Di- μ -chlorido-bis[(2,2'-bibenzimidazole)chloridocadmium(II)]

Crystal data

| | |
|---|---|
| [Cd ₂ Cl ₄ (C ₁₄ H ₁₀ N ₄) ₂] | $F_{000} = 1632$ |
| $M_r = 835.12$ | $D_x = 1.906 \text{ Mg m}^{-3}$ |
| Monoclinic, $C2/c$ | Mo $K\alpha$ radiation |
| Hall symbol: $-C 2yc$ | $\lambda = 0.71073 \text{ \AA}$ |
| $a = 11.824 (2) \text{ \AA}$ | Cell parameters from 13595 reflections |
| $b = 10.784 (2) \text{ \AA}$ | $\theta = 3.1\text{--}27.5^\circ$ |
| $c = 22.828 (5) \text{ \AA}$ | $\mu = 1.86 \text{ mm}^{-1}$ |
| $\beta = 91.10 (3)^\circ$ | $T = 293 (2) \text{ K}$ |
| $V = 2910.1 (10) \text{ \AA}^3$ | Prism, yellow |
| $Z = 4$ | $0.17 \times 0.16 \times 0.12 \text{ mm}$ |

Data collection

| | |
|--|--|
| Rigaku R-Axis RAPID-S diffractometer | 2840 reflections with $I > 2\sigma(I)$ |
| Radiation source: fine-focus sealed tube | $R_{\text{int}} = 0.035$ |
| Monochromator: graphite | $\theta_{\text{max}} = 27.5^\circ$ |
| $T = 293(2) \text{ K}$ | $\theta_{\text{min}} = 3.1^\circ$ |
| ω scans | $h = -15 \rightarrow 15$ |
| Absorption correction: none | $k = -14 \rightarrow 14$ |
| 14677 measured reflections | $l = -29 \rightarrow 29$ |
| 3337 independent reflections | |

Refinement

| | |
|--|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.033$ | H-atom parameters constrained |
| $wR(F^2) = 0.060$ | $w = 1/[\sigma^2(F_o^2) + (0.0213P)^2 + 2.9529P]$ |
| $S = 1.14$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 3337 reflections | $(\Delta/\sigma)_{\text{max}} = 0.002$ |
| 190 parameters | $\Delta\rho_{\text{max}} = 0.29 \text{ e \AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{\text{min}} = -0.34 \text{ e \AA}^{-3}$ |
| | Extinction correction: none |

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

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|----|------------|------------|--------------|----------------------------------|
| C1 | 0.7642 (2) | 0.8420 (3) | 0.65287 (12) | 0.0352 (6) |

| | | | | |
|-----|---------------|---------------|--------------|--------------|
| C2 | 0.8455 (3) | 0.8628 (3) | 0.69666 (14) | 0.0488 (8) |
| H2 | 0.9096 | 0.9102 | 0.6896 | 0.059* |
| C3 | 0.8279 (3) | 0.8110 (3) | 0.75062 (15) | 0.0567 (9) |
| H3 | 0.8804 | 0.8252 | 0.7807 | 0.068* |
| C4 | 0.7338 (3) | 0.7380 (3) | 0.76151 (14) | 0.0569 (9) |
| H4 | 0.7252 | 0.7037 | 0.7985 | 0.068* |
| C5 | 0.6533 (3) | 0.7156 (3) | 0.71877 (13) | 0.0523 (9) |
| H5 | 0.5909 | 0.6658 | 0.7259 | 0.063* |
| C6 | 0.6688 (2) | 0.7699 (3) | 0.66449 (12) | 0.0370 (6) |
| C7 | 0.6614 (2) | 0.8380 (2) | 0.57409 (11) | 0.0314 (6) |
| C8 | 0.6263 (2) | 0.8657 (2) | 0.51432 (11) | 0.0314 (6) |
| C9 | 0.5301 (2) | 0.8803 (2) | 0.43105 (11) | 0.0319 (6) |
| C10 | 0.4514 (2) | 0.8770 (3) | 0.38526 (13) | 0.0409 (7) |
| H10 | 0.3817 | 0.8381 | 0.3889 | 0.049* |
| C11 | 0.4822 (3) | 0.9342 (3) | 0.33429 (13) | 0.0450 (7) |
| H11 | 0.4318 | 0.9343 | 0.3025 | 0.054* |
| C12 | 0.5875 (3) | 0.9926 (3) | 0.32871 (13) | 0.0441 (7) |
| H12 | 0.6050 | 1.0302 | 0.2934 | 0.053* |
| C13 | 0.6652 (2) | 0.9957 (2) | 0.37397 (12) | 0.0378 (6) |
| H13 | 0.7349 | 1.0343 | 0.3700 | 0.045* |
| C14 | 0.6356 (2) | 0.9386 (2) | 0.42626 (11) | 0.0306 (6) |
| Cd1 | 0.851704 (16) | 1.006362 (18) | 0.527622 (9) | 0.03487 (7) |
| Cl1 | 1.04814 (6) | 0.95042 (8) | 0.57022 (3) | 0.04315 (18) |
| Cl2 | 0.84050 (6) | 1.21444 (7) | 0.57132 (3) | 0.04270 (18) |
| N1 | 0.75762 (18) | 0.8824 (2) | 0.59515 (10) | 0.0343 (5) |
| N2 | 0.60522 (19) | 0.7697 (2) | 0.61309 (9) | 0.0386 (6) |
| H15 | 0.5416 | 0.7327 | 0.6072 | 0.046* |
| N3 | 0.52742 (18) | 0.8349 (2) | 0.48775 (9) | 0.0347 (5) |
| H16 | 0.4728 | 0.7946 | 0.5032 | 0.042* |
| N4 | 0.69432 (18) | 0.9280 (2) | 0.47931 (9) | 0.0324 (5) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C1 | 0.0327 (15) | 0.0355 (15) | 0.0373 (15) | 0.0013 (11) | 0.0013 (12) | 0.0007 (12) |
| C2 | 0.0377 (17) | 0.058 (2) | 0.0510 (19) | -0.0033 (15) | -0.0065 (15) | 0.0030 (16) |
| C3 | 0.051 (2) | 0.071 (2) | 0.047 (2) | 0.0076 (18) | -0.0105 (16) | -0.0022 (18) |
| C4 | 0.058 (2) | 0.077 (3) | 0.0352 (18) | 0.0122 (19) | 0.0038 (16) | 0.0087 (17) |
| C5 | 0.0448 (19) | 0.067 (2) | 0.0455 (19) | -0.0043 (16) | 0.0112 (15) | 0.0063 (16) |
| C6 | 0.0329 (15) | 0.0432 (17) | 0.0353 (15) | 0.0006 (12) | 0.0052 (12) | -0.0024 (13) |
| C7 | 0.0283 (14) | 0.0314 (14) | 0.0348 (14) | -0.0073 (11) | 0.0049 (11) | -0.0026 (11) |
| C8 | 0.0276 (14) | 0.0320 (14) | 0.0348 (14) | -0.0081 (11) | 0.0037 (11) | -0.0045 (11) |
| C9 | 0.0307 (14) | 0.0312 (14) | 0.0338 (14) | -0.0053 (11) | 0.0019 (11) | -0.0052 (11) |
| C10 | 0.0329 (15) | 0.0450 (17) | 0.0446 (17) | -0.0079 (13) | -0.0029 (13) | -0.0052 (14) |
| C11 | 0.0461 (18) | 0.0484 (18) | 0.0400 (17) | -0.0064 (14) | -0.0103 (14) | -0.0030 (14) |
| C12 | 0.0552 (19) | 0.0410 (17) | 0.0363 (15) | -0.0103 (14) | 0.0022 (14) | 0.0006 (13) |
| C13 | 0.0383 (15) | 0.0364 (15) | 0.0389 (15) | -0.0119 (12) | 0.0071 (12) | -0.0028 (13) |
| C14 | 0.0302 (14) | 0.0282 (13) | 0.0337 (14) | -0.0057 (11) | 0.0044 (11) | -0.0067 (11) |

supplementary materials

| | | | | | | |
|-----|--------------|--------------|--------------|--------------|-------------|---------------|
| Cd1 | 0.02621 (11) | 0.03603 (12) | 0.04251 (12) | -0.01089 (8) | 0.00477 (8) | -0.00660 (10) |
| C11 | 0.0287 (3) | 0.0578 (4) | 0.0431 (4) | -0.0050 (3) | 0.0039 (3) | 0.0038 (3) |
| C12 | 0.0364 (4) | 0.0389 (4) | 0.0533 (4) | -0.0110 (3) | 0.0141 (3) | -0.0121 (3) |
| N1 | 0.0256 (11) | 0.0377 (13) | 0.0396 (13) | -0.0070 (9) | 0.0014 (10) | 0.0005 (10) |
| N2 | 0.0336 (13) | 0.0449 (14) | 0.0375 (13) | -0.0157 (11) | 0.0039 (10) | 0.0001 (11) |
| N3 | 0.0265 (12) | 0.0396 (13) | 0.0380 (13) | -0.0141 (10) | 0.0039 (10) | -0.0025 (10) |
| N4 | 0.0288 (12) | 0.0355 (13) | 0.0330 (12) | -0.0111 (10) | 0.0039 (9) | -0.0015 (10) |

Geometric parameters (Å, °)

| | | | |
|----------|-----------|--------------------------|-------------|
| C1—N1 | 1.389 (3) | C9—C14 | 1.403 (3) |
| C1—C2 | 1.393 (4) | C10—C11 | 1.373 (4) |
| C1—C6 | 1.399 (4) | C10—H10 | 0.9300 |
| C2—C3 | 1.372 (4) | C11—C12 | 1.403 (4) |
| C2—H2 | 0.9300 | C11—H11 | 0.9300 |
| C3—C4 | 1.389 (5) | C12—C13 | 1.370 (4) |
| C3—H3 | 0.9300 | C12—H12 | 0.9300 |
| C4—C5 | 1.371 (4) | C13—C14 | 1.393 (4) |
| C4—H4 | 0.9300 | C13—H13 | 0.9300 |
| C5—C6 | 1.386 (4) | C14—N4 | 1.389 (3) |
| C5—H5 | 0.9300 | Cd1—N4 | 2.305 (2) |
| C6—N2 | 1.381 (3) | Cd1—N1 | 2.338 (2) |
| C7—N1 | 1.317 (3) | Cd1—Cl2 | 2.4602 (8) |
| C7—N2 | 1.341 (3) | Cd1—Cl1 | 2.5725 (10) |
| C7—C8 | 1.450 (4) | Cd1—Cl1 ⁱ | 2.5903 (10) |
| C8—N4 | 1.327 (3) | Cl1—Cd1 ⁱ | 2.5903 (10) |
| C8—N3 | 1.348 (3) | N2—H15 | 0.8600 |
| C9—N3 | 1.385 (3) | N3—H16 | 0.8600 |
| C9—C10 | 1.387 (4) | | |
| N1—C1—C2 | 131.0 (3) | C13—C12—C11 | 121.7 (3) |
| N1—C1—C6 | 108.9 (2) | C13—C12—H12 | 119.1 |
| C2—C1—C6 | 120.1 (3) | C11—C12—H12 | 119.1 |
| C3—C2—C1 | 117.6 (3) | C12—C13—C14 | 117.4 (3) |
| C3—C2—H2 | 121.2 | C12—C13—H13 | 121.3 |
| C1—C2—H2 | 121.2 | C14—C13—H13 | 121.3 |
| C2—C3—C4 | 121.8 (3) | N4—C14—C13 | 130.9 (2) |
| C2—C3—H3 | 119.1 | N4—C14—C9 | 109.0 (2) |
| C4—C3—H3 | 119.1 | C13—C14—C9 | 120.2 (3) |
| C5—C4—C3 | 121.3 (3) | N4—Cd1—N1 | 73.49 (8) |
| C5—C4—H4 | 119.3 | N4—Cd1—Cl2 | 118.63 (6) |
| C3—C4—H4 | 119.3 | N1—Cd1—Cl2 | 102.95 (6) |
| C4—C5—C6 | 117.4 (3) | N4—Cd1—Cl1 | 144.04 (6) |
| C4—C5—H5 | 121.3 | N1—Cd1—Cl1 | 93.11 (6) |
| C6—C5—H5 | 121.3 | Cl2—Cd1—Cl1 | 96.65 (3) |
| N2—C6—C5 | 132.8 (3) | N4—Cd1—Cl1 ⁱ | 91.81 (6) |
| N2—C6—C1 | 105.5 (2) | N1—Cd1—Cl1 ⁱ | 154.49 (6) |
| C5—C6—C1 | 121.7 (3) | Cl2—Cd1—Cl1 ⁱ | 102.39 (3) |
| N1—C7—N2 | 113.1 (2) | Cl1—Cd1—Cl1 ⁱ | 86.78 (3) |

| | | | |
|--|--------------|-----------------------------|--------------|
| N1—C7—C8 | 119.9 (2) | Cd1—C11—Cd1 ⁱ | 93.22 (3) |
| N2—C7—C8 | 127.0 (2) | C7—N1—C1 | 105.3 (2) |
| N4—C8—N3 | 112.6 (2) | C7—N1—Cd1 | 112.71 (17) |
| N4—C8—C7 | 120.4 (2) | C1—N1—Cd1 | 141.87 (18) |
| N3—C8—C7 | 127.1 (2) | C7—N2—C6 | 107.1 (2) |
| N3—C9—C10 | 131.9 (2) | C7—N2—H15 | 126.4 |
| N3—C9—C14 | 105.5 (2) | C6—N2—H15 | 126.4 |
| C10—C9—C14 | 122.5 (3) | C8—N3—C9 | 107.4 (2) |
| C11—C10—C9 | 116.2 (3) | C8—N3—H16 | 126.3 |
| C11—C10—H10 | 121.9 | C9—N3—H16 | 126.3 |
| C9—C10—H10 | 121.9 | C8—N4—C14 | 105.6 (2) |
| C10—C11—C12 | 122.0 (3) | C8—N4—Cd1 | 112.97 (16) |
| C10—C11—H11 | 119.0 | C14—N4—Cd1 | 140.52 (16) |
| C12—C11—H11 | 119.0 | | |
| N1—C1—C2—C3 | 179.2 (3) | C6—C1—N1—C7 | 1.1 (3) |
| C6—C1—C2—C3 | -0.3 (5) | C2—C1—N1—Cd1 | -2.8 (5) |
| C1—C2—C3—C4 | 1.3 (5) | C6—C1—N1—Cd1 | 176.7 (2) |
| C2—C3—C4—C5 | -0.8 (5) | N4—Cd1—N1—C7 | -4.14 (18) |
| C3—C4—C5—C6 | -0.8 (5) | C12—Cd1—N1—C7 | 112.26 (18) |
| C4—C5—C6—N2 | -178.4 (3) | C11—Cd1—N1—C7 | -150.18 (18) |
| C4—C5—C6—C1 | 1.9 (5) | C11 ⁱ —Cd1—N1—C7 | -61.1 (2) |
| N1—C1—C6—N2 | -0.7 (3) | N4—Cd1—N1—C1 | -179.5 (3) |
| C2—C1—C6—N2 | 178.8 (3) | C12—Cd1—N1—C1 | -63.1 (3) |
| N1—C1—C6—C5 | 179.1 (3) | C11—Cd1—N1—C1 | 34.5 (3) |
| C2—C1—C6—C5 | -1.3 (4) | C11 ⁱ —Cd1—N1—C1 | 123.5 (3) |
| N1—C7—C8—N4 | 5.0 (4) | N1—C7—N2—C6 | 0.7 (3) |
| N2—C7—C8—N4 | -175.5 (3) | C8—C7—N2—C6 | -178.9 (3) |
| N1—C7—C8—N3 | -175.0 (3) | C5—C6—N2—C7 | -179.7 (3) |
| N2—C7—C8—N3 | 4.6 (5) | C1—C6—N2—C7 | 0.0 (3) |
| N3—C9—C10—C11 | 178.9 (3) | N4—C8—N3—C9 | -0.1 (3) |
| C14—C9—C10—C11 | 0.0 (4) | C7—C8—N3—C9 | 179.8 (3) |
| C9—C10—C11—C12 | 0.1 (5) | C10—C9—N3—C8 | -178.9 (3) |
| C10—C11—C12—C13 | -0.1 (5) | C14—C9—N3—C8 | 0.1 (3) |
| C11—C12—C13—C14 | -0.2 (4) | N3—C8—N4—C14 | 0.1 (3) |
| C12—C13—C14—N4 | -178.9 (3) | C7—C8—N4—C14 | -179.9 (2) |
| C12—C13—C14—C9 | 0.4 (4) | N3—C8—N4—Cd1 | 171.44 (17) |
| N3—C9—C14—N4 | 0.0 (3) | C7—C8—N4—Cd1 | -8.5 (3) |
| C10—C9—C14—N4 | 179.1 (2) | C13—C14—N4—C8 | 179.3 (3) |
| N3—C9—C14—C13 | -179.5 (2) | C9—C14—N4—C8 | 0.0 (3) |
| C10—C9—C14—C13 | -0.3 (4) | C13—C14—N4—Cd1 | 11.9 (5) |
| N4—Cd1—C11—Cd1 ⁱ | 88.65 (9) | C9—C14—N4—Cd1 | -167.4 (2) |
| N1—Cd1—C11—Cd1 ⁱ | 154.46 (6) | N1—Cd1—N4—C8 | 6.56 (18) |
| C12—Cd1—C11—Cd1 ⁱ | -102.11 (3) | C12—Cd1—N4—C8 | -89.44 (19) |
| C11 ⁱ —Cd1—C11—Cd1 ⁱ | 0.0 | C11—Cd1—N4—C8 | 78.4 (2) |
| N2—C7—N1—C1 | -1.1 (3) | C11 ⁱ —Cd1—N4—C8 | 165.38 (18) |
| C8—C7—N1—C1 | 178.5 (2) | N1—Cd1—N4—C14 | 173.4 (3) |
| N2—C7—N1—Cd1 | -178.16 (18) | C12—Cd1—N4—C14 | 77.4 (3) |

supplementary materials

| | | | |
|--------------|------------|------------------------------|------------|
| C8—C7—N1—Cd1 | 1.4 (3) | Cl1—Cd1—N4—C14 | -114.8 (3) |
| C2—C1—N1—C7 | -178.4 (3) | Cl1 ⁱ —Cd1—N4—C14 | -27.8 (3) |

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|-----------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| N3—H16 \cdots Cl2 ⁱⁱ | 0.86 | 2.39 | 3.221 (2) | 163 |

Symmetry codes: (ii) $x-1/2, y-1/2, z$.

Fig. 1

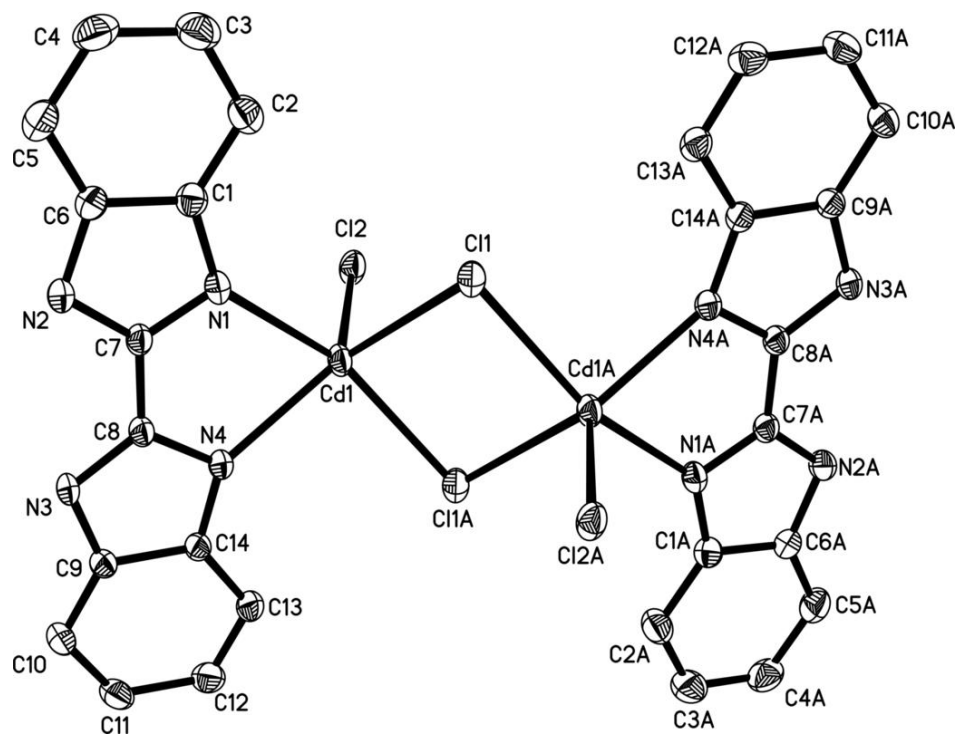


Fig. 2

