Di-$\mu_3$-chlorido-tetra-$\mu_2$-chlorido-dichloridotetrakis(N,N-di-ethylethane-1,2-diamine-$\kappa^2N,N'\prime$)tetracadmium(II)

Abdul-Razak H. Al-Sudani, Myasim Qasim Abdulridha and Benson M. Kariuki

IUCrData (2019). 4, x191618

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Di-μ₃-chlorido-tetra-μ₂-chlorido-dichlorido-tetrakis(N,N-diethylethane-1,2-diamine-κ²N,N')-tetracadmium(II)

Abdul-Razak H. Al-Sudani, Myasim Qasim Abdulridha and Benson M. Kariuki

In the title compound, [Cd₄Cl₈(C₆H₁₆N₂)₄], the Cd²⁺ cations and Cl⁻/Co⁻ anions form Cd₄Cl₈ clusters with six bridging and two pendant Cl⁻/Co⁻ ions. Cd···Cl distances range from 2.5158 (19) to 2.8227 (18) Å in the cluster. A similar M₄Cl₈ core has been reported for an NiII complex (Kermagoret et al., 2007). Each Cd²⁺ cation has a distorted octahedral coordination completed by four Cl⁻/Co⁻ ions and two nitrogen atoms of the bidentate amino ligand. The cluster consists of pairs of face-sharing hexahedra linked by a shared edge.

Structure description

The coordination chemistry of cadmium is of interest to a wide range of disciplines ranging from toxicology to catalysis (Melnik et al., 2009; Andersen et al., 1984).

In the crystal structure, each complex unit has four amino ligands with two nitrogen atoms of each ligand coordinating to one Cd²⁺ ion (Fig. 1). The complex is centrosymmetric with the asymmetric unit consisting of half of the complex unit. One ligand of the asymmetric unit is disordered with two components of 0.553 (13) and 0.447 (13) occupancy.

The Cd²⁺ cations and Cl⁻ ions form Cd₄Cl₈ clusters with six bridging and two pendant Cl⁻ ions. Cd···Cl distances range from 2.5158 (19) to 2.8227 (18) Å in the cluster. A similar M₄Cl₈ core has been reported for an NiII complex (Kermagoret et al., 2007). Each Cd²⁺ cation has a distorted octahedral coordination completed by four Cl⁻ ions and two nitrogen atoms of the bidentate amino ligand. The cluster consists of pairs of face-sharing hexahedra linked by a shared edge. The complex units are linked by intermolecular N···H···Cl contacts with N···Cl distances in the range 3.407 (6) to 3.548 (6) Å and N···H···Cl angles in the range 140.5 to 146.3° (Fig. 2, Table 1). Each complex unit donates four and accepts four N···H···Cl contacts with each pendant Cl⁻ accepting two bonds from different units.

Keywords: crystal structure; metal cluster; N···H···Cl contact; cadmium.
Synthesis and crystallization

The cadmium complex was prepared by direct reaction of equimolar amounts of cadmium dichloride and N-diethylaminoethylamine in ethanol at room temperature. The white solid obtained was separated by filtration after three hours, washed with 5 ml cold ethanol and then three times (5 ml each) with diethyl ether. Based on the cadmium dichloride used, the yield was 85%. Crystallization from warm methanol solution in open air produced colourless crystals.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The geometry and displacement parameters associated with the disordered atoms of the ligand were restrained during refinement.

Acknowledgements

Continued support by Cardiff University is acknowledged.

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Sheldrick, G. M. (2015). Acta Cryst. C71, 3–8.

Table 1

| D—H···A | D—H | D···A | D···A |
|---------|------|-------|-------|
| N2—H2C···Cl4 | 0.89 | 2.82 | 3.548 (6) | 141 |
| N2—H2D···Cl4 | 0.89 | 2.63 | 3.407 (6) | 146 |
| N4—H4D···Cl4 | 0.89 | 2.71 | 3.463 (6) | 143 |

Table 2

| Crystal data | Chemical formula | Chemical formula |
|--------------|------------------|------------------|
|               | [Cd2Cl4(C6H16N2)2] | 599.01           |
| Crystal system, space group | Triclinic, PT |
| Crystal system, space group | Triclinic, PT |
| Temperature (K) | 293 |
| V (Å³) | 9.3622 (10), 9.4023 (10), 12.4248 (9) |
| Z | 87.667 (7), 86.171 (7), 81.993 (9) |
| Radiation type | Mo Kα |
| Crystal size (mm) | 2.60 × 0.17 × 0.06 |

Data collection

| Diffactometer | Rigaku Oxford Diffraction SuperNova, Dual, Cu at home/near, Atlas |
|---------------|---------------------------------------------------------------|
| Absorption correction | Multi-scan (CrysAlis PRO; Rigaku OD, 2018) |
| Tmin, Tmax | 0.498, 1.000 |
| No. of measured, independent and observed [I > 2σ(I)] reflections | 15671, 5120, 3897 |
| Rint | 0.042 |
| R | 0.050, 0.131, 1.07 |
| No. of reflections | 5120 |
| No. of parameters | 247 |
| No. of restraints | 390 |
| H-atom treatment | H-atom parameters constrained |

Refrinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The geometry and displacement parameters associated with the disordered atoms of the ligand were restrained during refinement.

Acknowledgements

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References

Andersen, O. (1984). *EHP, Environ. Health Perspect.* 54, 249–266.
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Figure 1

An ORTEP representation of the complex showing 50% probability ellipsoids (only the major component of the disordered ligand is shown). Symmetry code: (i) 1 − x, 1 − y, − z.

Figure 2

A segment of the crystal packing showing intermolecular N-H···Cl contacts as red dotted lines.
full crystallographic data

*IUCrData* (2019). *4*, x191618  [https://doi.org/10.1107/S2414314619016183]

Di-$\mu_3$-chlorido-tetra-$\mu_2$-chlorido-dichloridotetakis(N,N-diethylethane-1,2-diamine-$\kappa^2$N,N$'$)tetracadmium(II)

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Di-$\mu_3$-chlorido-tetra-$\mu_2$-chlorido-dichloridotetakis(N,N-diethylethane-1,2-diamine-$\kappa^2$N,N$'$)tetracadmium(II)

Crystal data

$[\text{Cd}_2\text{Cl}_4(\text{C}_{6}\text{H}_{16}\text{N}_2)_2]$

$M_r = 599.01$

Triclinic, $P\bar{1}$

$a = 9.3622$ (10) Å

$b = 9.4023$ (10) Å

$c = 12.4248$ (9) Å

$\alpha = 87.667$ (7)°

$\beta = 86.171$ (7)°

$\gamma = 81.993$ (9)°

$V = 1080.08$ (18) Å$^3$

$Z = 2$

$F(000) = 592$

$D_c = 1.842$ Mg m$^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3382 reflections

$\theta = 4.3$–29.0°

$\mu = 2.46$ mm$^{-1}$

$T = 293$ K

Plate, colourless

$0.26 \times 0.17 \times 0.06$ mm

Data collection

Rigaku Oxford Diffraction SuperNova, Dual, Cu at home/near, Atlas diffractometer

$\omega$ scans

Absorption correction: multi-scan

(CrysAlisPro; Rigaku OD, 2018)

$T_{\text{min}} = 0.498$, $T_{\text{max}} = 1.000$

15671 measured reflections

5120 independent reflections

3897 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.042$

$\theta_{\text{max}} = 29.9^\circ$, $\theta_{\text{min}} = 2.2^\circ$

$h = -12\rightarrow 12$

$k = -13\rightarrow 11$

$l = -16\rightarrow 17$

Refinement

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.050$

$wR(F^2) = 0.131$

$S = 1.07$

5120 reflections

247 parameters

390 restraints

Hydrogen site location: inferred from neighbour sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_c^2) + (0.0348P)^2 + 6.2177P]$

where $P = (F_c^2 + 2F_s^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 1.01$ e Å$^{-3}$

$\Delta\rho_{\text{min}} = -1.42$ 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.** Non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed in calculated positions and refined using a riding model. Methyl C—H bonds were fixed at 0.96 Å, with displacement parameters 1.5 times \( U_{eq}(C) \). C—H distances for methylene groups were set to 0.97 Å and their \( U_{eq}(H) \) set to 1.2 times the \( U_{eq}(C) \). N—H distances for methylene groups were set to 0.89 Å and their \( U_{eq}(H) \) set to 1.2 times the \( U_{eq}(N) \).

**Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)**

| Atom | \( x \)   | \( y \)   | \( z \)   | \( U_{eq} \times \) \( U_{eq} \) | Occ. (<1) |
|------|----------|----------|----------|-----------------|----------|
| C1   | 0.3866 (10) | 0.7344 (10) | 0.3329 (9) | 0.082 (3) |          |
| H1A  | 0.465814 | 0.696964 | 0.284423 | 0.123* |          |
| H1B  | 0.407495 | 0.704330 | 0.405591 | 0.123* |          |
| H1C  | 0.372739 | 0.837455 | 0.326914 | 0.123* |          |
| C2   | 0.2507 (8) | 0.6784 (7) | 0.3041 (7) | 0.0558 (19) |          |
| H2A  | 0.173933 | 0.708569 | 0.358127 | 0.067* |          |
| H2B  | 0.221937 | 0.722091 | 0.235435 | 0.067* |          |
| C3   | 0.2355 (13) | 0.4747 (12) | 0.4994 (6) | 0.089 (3) |          |
| H3A  | 0.142236 | 0.444258 | 0.496016 | 0.133* |          |
| H3B  | 0.223962 | 0.575986 | 0.511236 | 0.133* |          |
| H3C  | 0.284821 | 0.423647 | 0.557614 | 0.133* |          |
| C4   | 0.3231 (8) | 0.4433 (8) | 0.3941 (5) | 0.0545 (18) |          |
| H4A  | 0.419740 | 0.466318 | 0.401386 | 0.065* |          |
| H4B  | 0.331569 | 0.340956 | 0.382622 | 0.065* |          |
| C5   | 0.1245 (7) | 0.4757 (8) | 0.2735 (5) | 0.0514 (17) |          |
| H5A  | 0.132528 | 0.371930 | 0.281572 | 0.062* |          |
| H5B  | 0.051170 | 0.516084 | 0.326825 | 0.062* |          |
| C6   | 0.0763 (8) | 0.5190 (9) | 0.1657 (6) | 0.060 (2) |          |
| H6A  | 0.063721 | 0.622981 | 0.158022 | 0.073* |          |
| H6B  | −0.016600 | 0.487290 | 0.157711 | 0.073* |          |
| N1   | 0.2651 (5) | 0.5211 (5) | 0.2966 (4) | 0.0394 (12) |          |
| C7   | 0.714 (4) | −0.077 (3) | 0.4663 (12) | 0.073 (6) | 0.553 (13) |
| H7A  | 0.635299 | −0.063720 | 0.520053 | 0.110* | 0.553 (13) |
| H7B  | 0.730646 | −0.176329 | 0.446588 | 0.110* | 0.553 (13) |
| H7C  | 0.799720 | −0.052313 | 0.494931 | 0.110* | 0.553 (13) |
| C8   | 0.6775 (13) | 0.0172 (16) | 0.3676 (9) | 0.048 (3) | 0.553 (13) |
| H8A  | 0.588856 | −0.007556 | 0.341762 | 0.057* | 0.553 (13) |
| H8B  | 0.657684 | 0.116019 | 0.389934 | 0.057* | 0.553 (13) |
| C9   | 0.926 (2) | 0.1786 (15) | 0.3716 (14) | 0.072 (5) | 0.553 (13) |
| H9A  | 1.021730 | 0.188722 | 0.390221 | 0.108* | 0.553 (13) |
| H9B  | 0.889663 | 0.258784 | 0.326183 | 0.108* | 0.553 (13) |
| H9C  | 0.863855 | 0.175657 | 0.436148 | 0.108* | 0.553 (13) |
| C10  | 0.9295 (11) | 0.0413 (15) | 0.3123 (12) | 0.060 (4) | 0.553 (13) |
| H10A | 0.969293 | −0.038212 | 0.358338 | 0.072* | 0.553 (13) |
| H10B | 0.995039 | 0.044716 | 0.248637 | 0.072* | 0.553 (13) |
| C11  | 0.8223 (14) | −0.1326 (11) | 0.2264 (10) | 0.056 (3) | 0.553 (13) |
| H11A | 0.922980 | −0.142333 | 0.200069 | 0.067* | 0.553 (13) |
| H11B | 0.813489 | −0.206590 | 0.282200 | 0.067* | 0.553 (13) |
| C12  | 0.7378 (10) | −0.1610 (8) | 0.1385 (7) | 0.064 (2) | 0.553 (13) |
### Atomic displacement parameters (Å²)

| Atom | $U^{11}$  | $U^{22}$  | $U^{33}$  | $U^{12}$  | $U^{13}$  | $U^{23}$  |
|------|-----------|-----------|-----------|-----------|-----------|-----------|
| C1   | 0.085 (7) | 0.066 (6) | 0.097 (7) | −0.025 (5)| 0.027 (6) | −0.028 (5)|
| C2   | 0.059 (5) | 0.041 (4) | 0.064 (4) | −0.002 (3)| 0.017 (4) | −0.010 (3)|
| C3   | 0.109 (8) | 0.107 (8) | 0.044 (5) | −0.001 (6)| 0.013 (5) | 0.000 (5) |
| C4   | 0.056 (4) | 0.064 (5) | 0.042 (4) | −0.005 (4)| 0.001 (3) | −0.002 (3)|
| C5   | 0.040 (4) | 0.064 (4) | 0.049 (4) | −0.008 (3)| 0.013 (3) | −0.005 (3)|
| C6   | 0.040 (4) | 0.068 (5) | 0.068 (5) | 0.007 (3) | 0.001 (4) | 0.001 (4) |
| N1   | 0.037 (3) | 0.043 (3) | 0.038 (3) | −0.007 (2)| 0.004 (2) | −0.002 (2)|
| C7   | 0.102 (12)| 0.076 (13)| 0.043 (9) | −0.022 (11)| −0.010 (9)| 0.023 (8)|
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|     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|
| C8  | 0.051 (6) | 0.051 (7) | 0.044 (6) | 0.018 (5) | 0.003 (5) | 0.005 (5) |
| C9  | 0.076 (11) | 0.056 (9) | 0.091 (12) | 0.023 (8) | 0.033 (9) | 0.003 (8) |
| C10 | 0.057 (7) | 0.059 (8) | 0.055 (7) | 0.024 (6) | 0.002 (6) | 0.016 (6) |
| C11 | 0.065 (6) | 0.039 (5) | 0.058 (6) | 0.007 (5) | 0.004 (5) | 0.001 (5) |
| C12 | 0.076 (5) | 0.047 (4) | 0.070 (4) | -0.014 (4) | -0.012 (4) | 0.000 (3) |
| N3  | 0.063 (3) | 0.039 (3) | 0.042 (3) | 0.011 (2) | 0.006 (3) | -0.001 (2) |
| C7A | 0.109 (16) | 0.080 (18) | 0.061 (13) | 0.007 (15) | 0.009 (12) | 0.006 (11) |
| C8A | 0.065 (8) | 0.049 (8) | 0.049 (7) | -0.011 (7) | -0.007 (7) | 0.005 (6) |
| C9A | 0.082 (14) | 0.087 (14) | 0.093 (14) | -0.018 (11) | -0.018 (12) | -0.005 (12) |
| C10A| 0.059 (7) | 0.058 (8) | 0.069 (8) | 0.019 (7) | 0.002 (7) | 0.014 (7) |
| C11A| 0.055 (6) | 0.039 (6) | 0.051 (6) | -0.008 (5) | 0.006 (6) | -0.001 (5) |
| C12A| 0.076 (5) | 0.047 (4) | 0.070 (4) | -0.014 (4) | -0.012 (4) | 0.000 (3) |
| N3A | 0.063 (3) | 0.039 (3) | 0.042 (3) | 0.001 (2) | -0.006 (3) | -0.001 (2) |
| N2  | 0.044 (3) | 0.043 (3) | 0.044 (3) | -0.008 (2) | -0.001 (2) | -0.001 (2) |
| N4  | 0.054 (4) | 0.045 (3) | 0.042 (3) | 0.001 (3) | -0.004 (3) | -0.005 (2) |
| C11 | 0.0453 (9) | 0.0411 (8) | 0.0549 (10) | -0.0014 (7) | 0.0034 (8) | 0.0047 (7) |
| C12 | 0.0476 (9) | 0.0430 (8) | 0.0370 (8) | -0.0030 (7) | 0.0026 (7) | 0.0002 (6) |
| C13 | 0.0386 (9) | 0.0483 (9) | 0.0544 (10) | 0.0014 (7) | -0.0098 (7) | -0.0096 (7) |
| C14 | 0.0472 (10) | 0.0562 (11) | 0.0829 (14) | -0.0023 (8) | 0.0150 (10) | 0.0002 (10) |
| Cd1 | 0.0324 (3) | 0.0429 (3) | 0.0388 (3) | 0.00378 (19) | 0.00272 (19) | -0.00057 (19) |
| Cd2 | 0.0398 (3) | 0.0354 (3) | 0.0466 (3) | 0.00223 (19) | 0.0016 (2) | 0.0013 (2) |

**Geometric parameters (Å, °)**

| C1—C2 | 1.512 (10) | C12—H12A | 0.9700 |
| C1—H1A | 0.9600 | C12—H12B | 0.9700 |
| C1—H1B | 0.9600 | C7A—Cd2 | 2.427 (5) |
| C1—H1C | 0.9600 | C1—N1 | 1.473 (7) |
| C2—N1 | 1.473 (7) | C7A—H7D | 0.9600 |
| C2—H2A | 0.9700 | C7A—H7E | 0.9600 |
| C2—H2B | 0.9700 | C7A—H7F | 0.9600 |
| C3—C4 | 1.514 (9) | C8A—N3A | 1.479 (9) |
| C3—H3A | 0.9600 | C8A—H8C | 0.9700 |
| C3—H3B | 0.9600 | C8A—H8D | 0.9700 |
| C3—H3C | 0.9600 | C9A—C10A | 1.514 (12) |
| C4—N1 | 1.484 (8) | C9A—H9D | 0.9600 |
| C4—H4A | 0.9700 | C9A—H9E | 0.9600 |
| C4—H4B | 0.9700 | C9A—H9F | 0.9600 |
| C5—C6 | 1.465 (9) | C10A—N3A | 1.467 (10) |
| C5—N1 | 1.488 (7) | C10A—H10C | 0.9700 |
| C5—H5A | 0.9700 | C10A—H10D | 0.9700 |
| C5—H5B | 0.9700 | C11A—C12A | 1.436 (10) |
| C6—N2 | 1.473 (9) | C11A—N3A | 1.508 (9) |
| C6—H6A | 0.9700 | C11A—H11C | 0.9700 |
| C6—H6B | 0.9700 | C11A—H11D | 0.9700 |
| N1—Cd1 | 2.419 (5) | C12A—N4 | 1.437 (9) |
| C7—C8 | 1.516 (11) | C12A—H12C | 0.9700 |
| C7—H7A | 0.9600 | C12A—H12D | 0.9700 |
| Bond      | Distance (Å) | Bond      | Distance (Å) |
|-----------|--------------|-----------|--------------|
| C7—H7B   | 0.9600       | N3A—Cd2  | 2.427 (5)    |
| C7—H7C   | 0.9600       | N2—Cd1   | 2.282 (6)    |
| C8—N3    | 1.455 (9)    | N2—H2C   | 0.8900       |
| C8—H8A   | 0.9700       | N2—H2D   | 0.8900       |
| C8—H8B   | 0.9700       | N4—Cd2   | 2.285 (6)    |
| C9—C10   | 1.507 (12)   | N4—H4C   | 0.8900       |
| C9—H9A   | 0.9600       | N4—H4D   | 0.8900       |
| C9—H9B   | 0.9600       | Cl1—Cd1  | 2.6302 (17)  |
| C9—H9C   | 0.9600       | Cl1—Cd2  | 2.8227 (18)  |
| C10—N3   | 1.514 (10)   | Cl2—Cd1  | 2.6625 (17)  |
| C10—H10A | 0.9700       | Cl2—Cd1i | 2.7509 (16)  |
| C10—H10B | 0.9700       | Cl2—Cd2i | 2.8027 (17)  |
| C11—C12  | 1.445 (10)   | Cl3—Cd2  | 2.5952 (18)  |
| C11—N3   | 1.495 (9)    | Cl3—Cd1  | 2.5983 (18)  |
| C11—H11A | 0.9700       | Cl4—Cd2  | 2.5158 (19)  |
| C11—H11B | 0.9700       | Cd1—Cd2  | 3.4713 (8)   |
| C12—N4   | 1.437 (9)    |          |              |

C2—C1—H1A 109.5 C10A—C9A—H9D 109.5
C2—C1—H1B 109.5 C10A—C9A—H9E 109.5
H1A—C1—H1B 109.5 H9D—C9A—H9E 109.5
C2—C1—H1C 109.5 H9D—C9A—H9F 109.5
H1A—C1—H1C 109.5 H9D—C9A—H9F 109.5
H1B—C1—H1C 109.5 H9E—C9A—H9F 109.5
N1—C2—C1 114.4 (6) N3A—C10A—C9A 112.3 (11)
N1—C2—H2A 108.7 N3A—C10A—H10C 109.1
C1—C2—H2A 108.7 C9A—C10A—H10C 109.1
N1—C2—H2B 108.7 N3A—C10A—H10D 109.1
C1—C2—H2B 108.7 C9A—C10A—H10D 109.1
H2A—C2—H2B 107.6 H10C—C10A—H10D 107.9
C4—C3—H3A 109.5 C12A—C11A—N3A 116.9 (8)
C4—C3—H3B 109.5 C12A—C11A—H11C 108.1
H3A—C3—H3B 109.5 N3A—C11A—H11C 108.1
C4—C3—H3C 109.5 C12A—C11A—H11D 108.1
H3A—C3—H3C 109.5 N3A—C11A—H11D 108.1
N1—C4—C3 116.0 (6) C11A—C12A—N4 118.4 (8)
N1—C4—H4A 108.3 C11A—C12A—H12C 107.7
C3—C4—H4A 108.3 N4—C12A—H12C 107.7
N1—C4—H4B 108.3 C11A—C12A—H12D 107.7
C3—C4—H4B 108.3 N4—C12A—H12D 107.7
H4A—C4—H4B 107.4 H12C—C12A—H12D 107.1
C6—C5—N1 114.4 (6) C10A—N3A—C8A 114.8 (10)
C6—C5—H5A 108.7 C10A—N3A—C11A 112.0 (9)
N1—C5—H5A 108.7 C8A—N3A—C11A 106.0 (8)
C6—C5—H5B 108.7 C10A—N3A—Cd2 114.9 (9)
N1—C5—H5B 108.7 C8A—N3A—Cd2 107.9 (8)
H5A—C5—H5B 107.6 C11A—N3A—Cd2 99.9 (6)
| Bond                  | Length (Å) | Bond                  | Length (Å) | Bond                  | Length (Å) |
|----------------------|------------|----------------------|------------|----------------------|------------|
| C5—C6—N2            | 1.118 (6)  | C6—N2—Cd1           | 1.098 (4)  | C6—N2—H2C           | 1.097      |
| C5—C6—H6A           | 1.093      | C6—N2—H2D           | 1.097      | Cd1—N2—H2C           | 1.097      |
| N2—C6—H6A           | 1.093      | C6—N2—H2D           | 1.097      | Cd1—N2—H2D           | 1.097      |
| C5—C6—H6B           | 1.093      | H2C—N2—H2D          | 1.082      | H2C—N2—H2D          | 1.082      |
| H6A—C6—H6B          | 1.079      | C2—N1—C4            | 1.130 (5)  | C12A—N4—Cd2         | 1.102 (4)  |
| C2—N1—C5            | 1.110 (5)  | C12—N4—Cd2         | 1.102 (4)  | C12—N4—Cd2         | 1.102 (4)  |
| C4—N1—C5            | 1.110 (5)  | Cd2—N4—H4C         | 1.096      | Cd2—N4—H4C         | 1.096      |
| C2—N1—Cd1           | 1.129 (4)  | Cd2—N4—H4D         | 1.096      | Cd2—N4—H4D         | 1.096      |
| C4—N1—Cd1           | 1.109 (4)  | Cd2—N4—H4D         | 1.096      | Cd2—N4—H4D         | 1.096      |
| C5—N1—Cd1           | 0.995 (4)  | C2—N1—Cd1          | 1.112 (4)  | C2—N1—Cd1          | 1.112 (4)  |
| C8—C7—H7A           | 1.095      | C2—N1—Cd1          | 1.112 (4)  | C2—N1—Cd1          | 1.112 (4)  |
| C8—C7—H7B           | 1.095      | C2—N1—Cd1          | 1.112 (4)  | C2—N1—Cd1          | 1.112 (4)  |
| H7A—C7—H7B          | 1.095      | C2—N1—Cd1          | 1.112 (4)  | C2—N1—Cd1          | 1.112 (4)  |
| C8—C7—H7C           | 1.095      | C2—N1—Cd1          | 1.112 (4)  | C2—N1—Cd1          | 1.112 (4)  |
| H7A—C7—H7C          | 1.095      | C2—N1—Cd1          | 1.112 (4)  | C2—N1—Cd1          | 1.112 (4)  |
| H7B—C7—H7C          | 1.095      | N3—C8—C7           | 1.171 (11) | N3—C8—C7           | 1.171 (11) |
| N3—C8—H8A           | 1.080      | N2—Cd1—N1           | 0.780 (18) | N2—Cd1—N1           | 0.780 (18) |
| C7—C8—H8A           | 1.080      | C10—C9—H9A         | 1.095      | C10—C9—H9A         | 1.095      |
| N3—C8—H8B           | 1.080      | N2—Cd1—C13         | 1.751 (15) | N2—Cd1—C13         | 1.751 (15) |
| C7—C8—H8B           | 1.080      | N1—Cd1—C13         | 0.973 (13) | N1—Cd1—C13         | 0.973 (13) |
| H8A—C8—H8B          | 1.073      | N2—Cd1—C13         | 1.751 (15) | N2—Cd1—C13         | 1.751 (15) |
| C10—C9—H9A          | 1.095      | N1—Cd1—C13         | 0.973 (13) | N1—Cd1—C13         | 0.973 (13) |
| H9A—C9—H9B          | 1.095      | C12—C11—N3         | 1.156 (9)  | C12—C11—N3         | 1.156 (9)  |
| C10—C9—H9C          | 1.095      | C13—Cd1—C12        | 0.854 (5)  | C13—Cd1—C12        | 0.854 (5)  |
| H9B—C9—H9C          | 1.095      | C13—Cd1—C12        | 0.854 (5)  | C13—Cd1—C12        | 0.854 (5)  |
| C9—C10—N3           | 1.156 (9)  | C1—Cd1—C12         | 0.801 (5)  | C1—Cd1—C12         | 0.801 (5)  |
| C9—C10—H10A         | 1.084      | C12—Cd1—C12        | 0.861 (5)  | C12—Cd1—C12        | 0.861 (5)  |
| N3—C10—H10A         | 1.084      | N2—Cd1—C12         | 1.361 (14) | N2—Cd1—C12         | 1.361 (14) |
| C9—C10—H10B         | 1.084      | N1—Cd1—C12         | 1.274 (12) | N1—Cd1—C12         | 1.274 (12) |
| N3—C10—H10B         | 1.084      | C13—Cd1—C12        | 0.482 (4)  | C13—Cd1—C12        | 0.482 (4)  |
| H10A—C10—H10B       | 1.074      | C1—Cd1—C12         | 0.529 (4)  | C1—Cd1—C12         | 0.529 (4)  |
| C12—C11—N3          | 1.172 (7)  | C12—Cd1—C12        | 1.168 (4)  | C12—Cd1—C12        | 1.168 (4)  |
| C12—C11—H11A        | 1.080      | C12—Cd1—C12        | 1.168 (4)  | C12—Cd1—C12        | 1.168 (4)  |
| N3—C11—H11A         | 1.080      | C12—Cd1—C12        | 1.168 (4)  | C12—Cd1—C12        | 1.168 (4)  |
| C12—C11—H11B        | 1.080      | N4—Cd2—N3          | 0.780 (19) | N4—Cd2—N3          | 0.780 (19) |
| N3—C11—H11B         | 1.080      | N4—Cd2—N3A         | 0.780 (19) | N4—Cd2—N3A         | 0.780 (19) |
| H11A—C11—H11B       | 1.072      | N4—Cd2—C14         | 0.955 (17) | N4—Cd2—C14         | 0.955 (17) |
| N4—C12—C11          | 1.174 (8)  | N3—Cd2—C14         | 0.985 (15) | N3—Cd2—C14         | 0.985 (15) |
| N4—C12—H12A         | 1.080      | N3A—Cd2—C14        | 0.985 (15) | N3A—Cd2—C14        | 0.985 (15) |
| C11—C12—H12A        | 1.080      | N4—Cd2—C13         | 1.704 (17) | N4—Cd2—C13         | 1.704 (17) |
| N4—C12—H12B         | 1.080      | N3—Cd2—C13         | 1.029 (13) | N3—Cd2—C13         | 1.029 (13) |
| C11—C12—H12B        | 1.080      | N3A—Cd2—C13        | 1.029 (13) | N3A—Cd2—C13        | 1.029 (13) |
| H12A—C12—H12B       | 1.072      | Cl4—Cd2—C13        | 0.939 (6)  | Cl4—Cd2—C13        | 0.939 (6)  |
C8—N3—C11  115.9 (8)  N4—Cd2—Cl2^i  93.02 (15)
C8—N3—C10  111.3 (8)  N3—Cd2—Cl2^i  164.69 (14)
C11—N3—C10  103.2 (7)  Cl4—Cd2—Cl2^i  94.66 (6)
C8—N3—Cd2  112.4 (7)  Cl3—Cd2—Cl2^i  84.45 (5)
C11—N3—Cd2  103.4 (5)  N4—Cd2—Cl1  87.06 (16)
C10—N3—Cd2  110.0 (6)  N3—Cd2—Cl1  90.86 (14)
C8A—C7A—H7D  109.5  N3A—Cd2—Cl1  90.86 (14)
C8A—C7A—H7E  109.5  Cl4—Cd2—Cl1  170.58 (6)
H7D—C7A—H7E  109.5  Cl3—Cd2—Cl1  83.36 (5)
C8A—C7A—H7F  109.5  Cl2^i—Cd2—Cl1  76.14 (5)
H7E—C7A—H7F  109.5  N4—Cd2—Cd1  123.88 (16)
C8A—C7A—H8C  108.5  Cl4—Cd2—Cd1  124.18 (5)
C8A—C7A—H8D  108.5  Cl3—Cd2—Cd1  48.10 (4)
C7A—C8A—H8C  108.5  Cl2^i—Cd2—Cd1  50.65 (3)
C7A—C8A—H8D  108.5  Cl1—Cd2—Cd1  48.05 (4)
H8C—C8A—H8D  107.5

Symmetry code: (i) −x+1, −y+1, −z.

Hydrogen-bond geometry (Å, °)

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|------|-------|-------|---------|
| N2—H2C···Cl4^i | 0.89 | 2.82 | 3.548 (6) | 141 |
| N2—H2D···Cl4^ii | 0.89 | 2.63 | 3.407 (6) | 146 |
| N4—H4D···Cl4^iii | 0.89 | 2.71 | 3.463 (6) | 143 |

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