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Bis{μ-4,4′,6,6′-tetrabromo-2,2′-[*o*-phenylenebis(nitrilomethylidyne)]diphenolato}-bis[(dimethylformamide)cadmium(II)]

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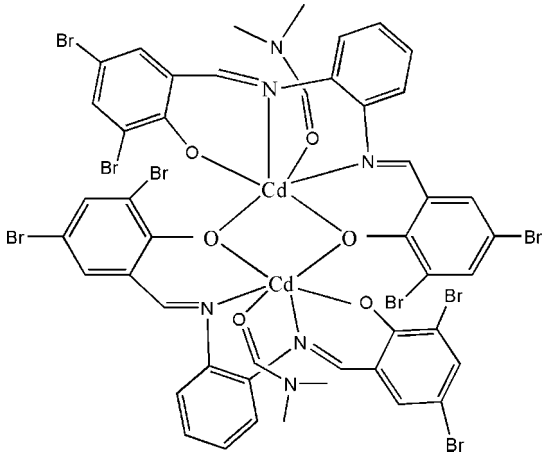
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.016 Å; R factor = 0.059; wR factor = 0.209; data-to-parameter ratio = 15.3.

The Schiff base ligand derived from the condensation of 3,5-dibromosalicylaldehyde and 1,2-phenylenediamine, in the presence of dimethylformamide, forms the centrosymmetric title neutral binuclear distorted complex, $[Cd_2(C_{20}H_{10}Br_4N_2O_2)_2(C_3H_7NO)_2]$, with the two octahedral Cd atoms linked by two O atoms. All bond lengths and angles show normal values.

Related literature

For related literature, see: Elzbieta *et al.* (1964); Wang *et al.* (2003); Wu *et al.* (2005).



Experimental

Crystal data

$[Cd_2(C_{20}H_{10}Br_4N_2O_2)_2(C_3H_7NO)_2]$
M_r = 1630.87
Triclinic, $P\overline{1}$
a = 9.6831 (8) Å
b = 12.0433 (10) Å
c = 12.4877 (10) Å
α = 95.942 (1)°
β = 108.822 (1)°
γ = 90.313 (1)°
V = 1369.82 (19) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 6.66 mm^{-1}
T = 296 (2) K
0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
11120 measured reflections
4716 independent reflections
2815 reflections with $I > 2\sigma(I)$
R_{int} = 0.062

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.210
S = 1.04
4716 reflections
309 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.63 e Å^{-3}
$\Delta\rho_{min}$ = −2.23 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O2	2.265 (6)	Cd1—N2	2.352 (8)
Cd1—O1	2.279 (6)	Cd1—O3	2.371 (9)
Cd1—O1^{i}	2.341 (7)	Cd1—N1	2.391 (8)
O2—Cd1—O1	129.1 (3)	O2—Cd1—N2	80.5 (3)
O2—Cd1—O1^{i}	84.5 (2)	O1—Cd1—N2	150.0 (3)
O1—Cd1—O1^{i}	73.6 (3)	N2—Cd1—N1	71.6 (3)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Bruker, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2060).

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supporting information

Acta Cryst. (2008). E**64**, m36 [https://doi.org/10.1107/S1600536807059612]

Bis{μ-4,4′,6,6′-tetrabromo-2,2′-[*o*-phenylenebis(nitrilomethylidyne)]diphenolato}bis[(dimethylformamide)cadmium(II)]

Shaomin Shi, Xuegang Song, Zongqiu Hu and Xieqing Yu

S1. Comment

The crystal structure and some properties of 4,4′,6,6′-tetrabromo- 2,2′-[1,2-phenylenebis(nitrilomethylidyne)]diphenolato Ni(II) and Zn(II) complex were previously reported by Wang *et al.* (2003) and Wu *et al.* (2005), respectively. We report here the synthesis and crystal structure of a novel binuclear complex {bis[*N*,*N*′-1,2-phenylenediaminebis(3,5-dibromo-salicylideneiminato)]- bisdimethylformamide-diCadmium(II)}. In the title compound,every molecule forms a centro-symmetric dimer and each Cd atom is six-coordinated by one oxygen atom of dimethylformamide, two O and two amino N atom of the ligand 4,4′,6,6′-tetrabromo-2,2′-[1,2-phenylenebis-(nitrilomethylidyne)]diphenol and the μ-O atom from another ligand,forming a distorted octahedron (Fig. 1).

S2. Experimental

The title complex was synthesized in two stages. In the first stage, 3,5-dibromosalicylaldehyde was prepared according to Elzbieta *et al.* (1964). (1964). To ethanol (100 ml) containing 1,2-phenylenediamine (6 g), two mole equivalents of 3,5-dibromosalicylaldehyde in ethanol (50 ml) were slowly added with continuous stirring; the Schiff base molecule, *viz*. 4,4′,6,6′-tetrabromo-2,2′-[1,2-phenylenebis(nitrilomethylidyne)]diphenol, precipitated immediately. In the second stage, the ligand (0.3 mmol), $Cd(OAc)_2$ (0.6 mmol), DMF (30 ml) were refluxed for 2 h. The hot solution was filtered and allowed to stand at room temperature undisturbed for about one month, resulting in yellow crystals.

S3. Refinement

After their location in the difference map, all H-atoms were fixed geometrically at ideal positions and allowed to ride on the parent C or N atoms with $C_{aromatic}$—H = 0.93 Å, $C_{methine}$—H = 0.96 Å and N—H = 0.83 (3) Å and $U_{iso}(H) = 1.2U_{eq}$ (C of aromatic and N) or $U_{iso}(H) = 1.5U_{eq}$(C of methine). Because the crystal approximated a sphere and the maximum transmission factor was 0.3943 an absorption correction was not considered necessary.

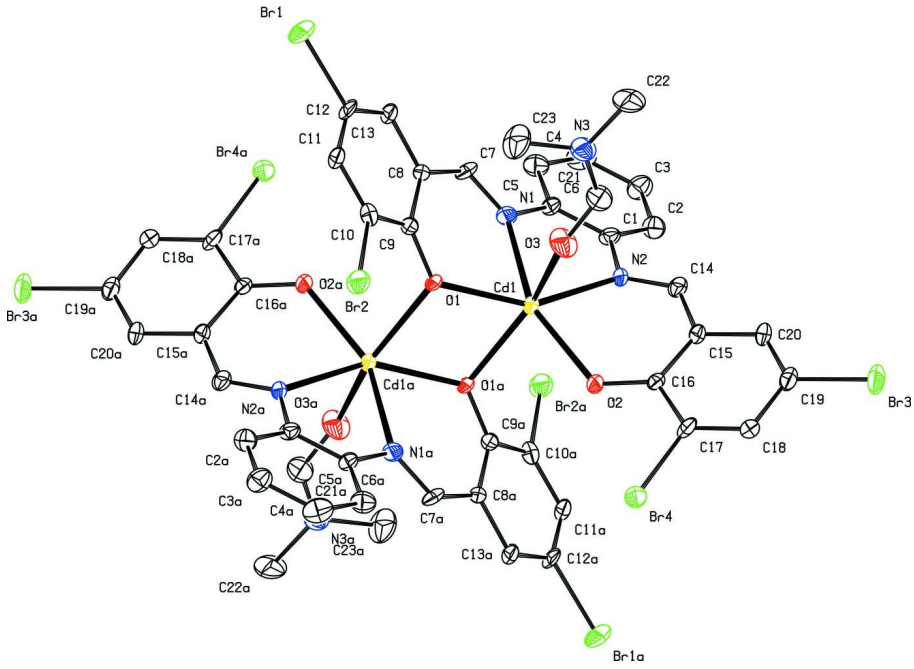

Figure 1

Molecular structure of (I) showing 30% probability displacement ellipsoids.

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Crystal data

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Hall symbol: -P 1
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$b = 12.0433\ (10)$ Å
$c = 12.4877\ (10)$ Å
$\alpha = 95.942\ (1)°$
$\beta = 108.822\ (1)°$
$\gamma = 90.313\ (1)°$
$V = 1369.82\ (19)$ Å^3
$Z = 1$
$F(000) = 776$
$D_x = 1.977$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3027 reflections
$\theta = 2.3–26.4°$
$\mu = 6.66$ mm^{-1}
$T = 296$ K
Block, yellow
0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
11120 measured reflections
4716 independent reflections
2815 reflections with $I > 2\sigma(I)$
$R_{int} = 0.062$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$
$h = -11\rightarrow11$
$k = -14\rightarrow14$
$l = -14\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.210$
$S = 1.04$
4716 reflections
309 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
$w = 1/[\sigma^2(F_o^2) + (0.1219P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.63$ e Å^{-3}
$\Delta\rho_{min} = -2.23$ 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	0.11948 (8)	0.12544 (6)	0.51678 (6)	0.0395 (3)
Br1	0.4487 (2)	−0.23438 (14)	1.02145 (13)	0.0916 (6)
Br2	0.23171 (17)	−0.28244 (10)	0.53098 (11)	0.0675 (4)
Br3	0.44885 (19)	0.53322 (12)	0.20894 (13)	0.0840 (5)
Br4	0.07472 (16)	0.13462 (11)	0.09195 (10)	0.0688 (5)
C1	0.1356 (12)	0.3654 (9)	0.6670 (8)	0.043 (3)
C2	0.1149 (13)	0.4809 (10)	0.6945 (10)	0.055 (3)
H2	0.1184	0.5315	0.6438	0.066*
C3	0.0895 (15)	0.5198 (11)	0.7953 (11)	0.067 (4)
H3	0.0813	0.5958	0.8132	0.080*
C4	0.0764 (17)	0.4440 (12)	0.8695 (11)	0.078 (4)
H4	0.0541	0.4685	0.9349	0.093*
C5	0.0982 (14)	0.3268 (11)	0.8430 (10)	0.060 (3)
H5	0.0948	0.2766	0.8939	0.072*
C6	0.1244 (11)	0.2880 (8)	0.7418 (8)	0.038 (2)
C7	0.1996 (12)	0.1034 (10)	0.7944 (8)	0.048 (3)
H7	0.2190	0.1357	0.8690	0.057*
C8	0.2330 (12)	−0.0143 (9)	0.7800 (8)	0.046 (3)
C9	0.1989 (11)	−0.0823 (9)	0.6713 (9)	0.043 (3)
C10	0.2592 (12)	−0.1937 (9)	0.6746 (10)	0.047 (3)
C11	0.3300 (13)	−0.2379 (10)	0.7774 (10)	0.056 (3)
H11	0.3616	−0.3106	0.7773	0.068*
C12	0.3519 (14)	−0.1694 (11)	0.8801 (11)	0.061 (3)
C13	0.3081 (12)	−0.0600 (10)	0.8842 (10)	0.053 (3)
H13	0.3272	−0.0165	0.9538	0.063*

C14	0.2264 (12)	0.3819 (9)	0.5122 (9)	0.047 (3)
H14	0.2668	0.4505	0.5515	0.057*
C15	0.2428 (12)	0.3542 (8)	0.3983 (9)	0.043 (3)
C16	0.1701 (11)	0.2569 (8)	0.3189 (8)	0.040 (2)
C17	0.1859 (14)	0.2533 (10)	0.2058 (9)	0.052 (3)
C18	0.2647 (13)	0.3316 (10)	0.1731 (9)	0.054 (3)
H18	0.2704	0.3248	0.0998	0.065*
C19	0.3385 (13)	0.4247 (9)	0.2558 (10)	0.051 (3)
C20	0.3231 (13)	0.4366 (9)	0.3635 (10)	0.055 (3)
H20	0.3657	0.4991	0.4141	0.066*
C21	0.4950 (16)	0.1462 (13)	0.6135 (13)	0.076 (4)
H21	0.5067	0.2211	0.6046	0.091*
C22	0.7544 (17)	0.1575 (18)	0.7356 (15)	0.132 (8)
H22A	0.7803	0.1603	0.8169	0.198*
H22B	0.7512	0.2321	0.7146	0.198*
H22C	0.8259	0.1173	0.7107	0.198*
C23	0.591 (2)	−0.0177 (14)	0.7041 (16)	0.111 (6)
H23A	0.6012	−0.0188	0.7830	0.167*
H23B	0.6651	−0.0617	0.6865	0.167*
H23C	0.4965	−0.0480	0.6577	0.167*
N1	0.1447 (10)	0.1698 (8)	0.7134 (7)	0.047 (2)
N2	0.1608 (10)	0.3198 (7)	0.5632 (7)	0.045 (2)
N3	0.6088 (12)	0.0998 (10)	0.6810 (9)	0.069 (3)
O1	0.1178 (8)	−0.0490 (5)	0.5721 (6)	0.0445 (18)
O2	0.0985 (8)	0.1756 (6)	0.3426 (6)	0.0477 (19)
O3	0.3735 (9)	0.0995 (9)	0.5606 (9)	0.087 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0502 (5)	0.0319 (4)	0.0337 (5)	−0.0075 (3)	0.0083 (4)	0.0092 (3)
Br1	0.1109 (13)	0.0818 (11)	0.0657 (10)	0.0087 (9)	−0.0052 (9)	0.0452 (9)
Br2	0.0899 (10)	0.0448 (7)	0.0618 (8)	0.0056 (7)	0.0157 (7)	0.0085 (6)
Br3	0.1124 (12)	0.0685 (9)	0.0833 (10)	−0.0282 (9)	0.0447 (10)	0.0229 (8)
Br4	0.0918 (11)	0.0691 (9)	0.0404 (7)	−0.0234 (7)	0.0162 (7)	0.0018 (6)
C1	0.055 (7)	0.040 (6)	0.031 (5)	0.007 (5)	0.009 (5)	0.003 (5)
C2	0.064 (8)	0.045 (7)	0.057 (8)	0.004 (6)	0.021 (6)	0.007 (6)
C3	0.086 (10)	0.058 (8)	0.062 (8)	0.010 (7)	0.032 (8)	0.005 (7)
C4	0.101 (11)	0.087 (11)	0.054 (8)	0.028 (9)	0.039 (8)	0.000 (8)
C5	0.068 (8)	0.057 (8)	0.054 (8)	0.006 (6)	0.018 (7)	0.009 (6)
C6	0.040 (6)	0.039 (6)	0.034 (6)	0.008 (5)	0.007 (5)	0.008 (5)
C7	0.053 (7)	0.063 (8)	0.025 (5)	0.015 (6)	0.007 (5)	0.016 (5)
C8	0.060 (7)	0.041 (6)	0.030 (6)	−0.017 (5)	0.002 (5)	0.007 (5)
C9	0.033 (6)	0.050 (7)	0.044 (6)	−0.007 (5)	0.003 (5)	0.017 (5)
C10	0.048 (7)	0.036 (6)	0.055 (7)	−0.007 (5)	0.014 (6)	0.008 (5)
C11	0.062 (8)	0.040 (6)	0.066 (8)	−0.002 (6)	0.013 (7)	0.029 (6)
C12	0.060 (8)	0.062 (8)	0.054 (8)	0.000 (6)	−0.002 (6)	0.044 (7)
C13	0.052 (7)	0.051 (7)	0.049 (7)	−0.008 (6)	0.002 (6)	0.023 (6)

C14	0.059 (7)	0.029 (5)	0.049 (7)	0.004 (5)	0.009 (6)	0.010 (5)
C15	0.049 (6)	0.034 (6)	0.045 (6)	−0.001 (5)	0.010 (5)	0.017 (5)
C16	0.048 (6)	0.035 (6)	0.032 (5)	0.002 (5)	0.004 (5)	0.011 (5)
C17	0.071 (8)	0.053 (7)	0.037 (6)	0.009 (6)	0.017 (6)	0.023 (5)
C18	0.062 (8)	0.062 (8)	0.037 (6)	−0.011 (6)	0.012 (6)	0.012 (6)
C19	0.052 (7)	0.048 (7)	0.059 (8)	0.005 (5)	0.020 (6)	0.025 (6)
C20	0.073 (8)	0.031 (6)	0.056 (7)	−0.012 (6)	0.012 (7)	0.012 (5)
C21	0.066 (10)	0.071 (10)	0.090 (11)	0.003 (8)	0.020 (9)	0.022 (8)
C22	0.060 (11)	0.20 (2)	0.109 (15)	−0.039 (13)	−0.017 (10)	0.049 (15)
C23	0.108 (14)	0.094 (13)	0.135 (16)	0.037 (11)	0.034 (12)	0.045 (12)
N1	0.056 (6)	0.054 (6)	0.031 (5)	−0.006 (5)	0.013 (4)	0.002 (4)
N2	0.063 (6)	0.031 (5)	0.035 (5)	−0.015 (4)	0.007 (4)	0.006 (4)
N3	0.051 (7)	0.083 (8)	0.072 (8)	−0.002 (6)	0.016 (6)	0.015 (7)
O1	0.052 (5)	0.032 (4)	0.038 (4)	0.000 (3)	−0.006 (3)	0.020 (3)
O2	0.066 (5)	0.046 (4)	0.031 (4)	−0.015 (4)	0.016 (4)	0.006 (3)
O3	0.040 (5)	0.098 (8)	0.121 (9)	−0.001 (5)	0.021 (6)	0.013 (6)

Geometric parameters (Å, º)

Cd1—O2	2.265 (6)	C10—C11	1.406 (15)
Cd1—O1	2.279 (6)	C11—C12	1.405 (17)
Cd1—O1^{i}	2.341 (7)	C11—H11	0.9300
Cd1—N2	2.352 (8)	C12—C13	1.387 (17)
Cd1—O3	2.371 (9)	C13—H13	0.9300
Cd1—N1	2.391 (8)	C14—N2	1.313 (12)
Br1—C12	1.958 (11)	C14—C15	1.486 (15)
Br2—C10	1.929 (11)	C14—H14	0.9300
Br3—C19	1.933 (10)	C15—C20	1.441 (13)
Br4—C17	1.949 (12)	C15—C16	1.468 (14)
C1—C6	1.414 (13)	C16—O2	1.307 (11)
C1—C2	1.429 (15)	C16—C17	1.465 (14)
C1—N2	1.449 (13)	C17—C18	1.383 (15)
C2—C3	1.394 (16)	C18—C19	1.453 (16)
C2—H2	0.9300	C18—H18	0.9300
C3—C4	1.399 (18)	C19—C20	1.394 (15)
C3—H3	0.9300	C20—H20	0.9300
C4—C5	1.448 (18)	C21—O3	1.245 (16)
C4—H4	0.9300	C21—N3	1.320 (16)
C5—C6	1.401 (15)	C21—H21	0.9300
C5—H5	0.9300	C22—N3	1.486 (18)
C6—N1	1.460 (13)	C22—H22A	0.9600
C7—N1	1.331 (13)	C22—H22B	0.9600
C7—C8	1.463 (15)	C22—H22C	0.9600
C7—H7	0.9300	C23—N3	1.492 (19)
C8—C13	1.438 (14)	C23—H23A	0.9600
C8—C9	1.448 (15)	C23—H23B	0.9600
C9—O1	1.339 (12)	C23—H23C	0.9600
C9—C10	1.466 (15)	O1—Cd1^{i}	2.341 (7)

O2—Cd1—O1	129.1 (3)	C12—C13—H13	120.3
O2—Cd1—O1^{i}	84.5 (2)	C8—C13—H13	120.3
O1—Cd1—O1^{i}	73.6 (3)	N2—C14—C15	126.8 (9)
O2—Cd1—N2	80.5 (3)	N2—C14—H14	116.6
O1—Cd1—N2	150.0 (3)	C15—C14—H14	116.6
O1^{i}—Cd1—N2	120.4 (3)	C20—C15—C16	120.5 (10)
O2—Cd1—O3	92.4 (3)	C20—C15—C14	115.5 (9)
O1—Cd1—O3	83.4 (3)	C16—C15—C14	123.7 (9)
O1^{i}—Cd1—O3	147.1 (3)	O2—C16—C17	119.8 (9)
N2—Cd1—O3	91.1 (3)	O2—C16—C15	125.5 (9)
O2—Cd1—N1	151.8 (3)	C17—C16—C15	114.6 (9)
O1—Cd1—N1	79.2 (3)	C18—C17—C16	124.8 (11)
O1^{i}—Cd1—N1	106.3 (3)	C18—C17—Br4	118.6 (8)
N2—Cd1—N1	71.6 (3)	C16—C17—Br4	116.4 (8)
O3—Cd1—N1	91.7 (3)	C17—C18—C19	118.5 (10)
C6—C1—C2	119.1 (10)	C17—C18—H18	120.7
C6—C1—N2	116.5 (9)	C19—C18—H18	120.7
C2—C1—N2	124.3 (9)	C20—C19—C18	120.0 (9)
C3—C2—C1	121.7 (11)	C20—C19—Br3	121.9 (9)
C3—C2—H2	119.2	C18—C19—Br3	118.1 (8)
C1—C2—H2	119.2	C19—C20—C15	121.5 (10)
C2—C3—C4	119.8 (12)	C19—C20—H20	119.3
C2—C3—H3	120.1	C15—C20—H20	119.3
C4—C3—H3	120.1	O3—C21—N3	126.3 (14)
C3—C4—C5	119.0 (11)	O3—C21—H21	116.8
C3—C4—H4	120.5	N3—C21—H21	116.8
C5—C4—H4	120.5	N3—C22—H22A	109.5
C6—C5—C4	121.1 (11)	N3—C22—H22B	109.5
C6—C5—H5	119.5	H22A—C22—H22B	109.5
C4—C5—H5	119.5	N3—C22—H22C	109.5
C5—C6—C1	119.2 (10)	H22A—C22—H22C	109.5
C5—C6—N1	121.6 (9)	H22B—C22—H22C	109.5
C1—C6—N1	119.1 (9)	N3—C23—H23A	109.5
N1—C7—C8	127.6 (10)	N3—C23—H23B	109.5
N1—C7—H7	116.2	H23A—C23—H23B	109.5
C8—C7—H7	116.2	N3—C23—H23C	109.5
C13—C8—C9	120.7 (10)	H23A—C23—H23C	109.5
C13—C8—C7	114.5 (10)	H23B—C23—H23C	109.5
C9—C8—C7	124.7 (9)	C7—N1—C6	121.1 (9)
O1—C9—C8	124.0 (10)	C7—N1—Cd1	125.2 (7)
O1—C9—C10	120.1 (10)	C6—N1—Cd1	112.4 (6)
C8—C9—C10	115.8 (9)	C14—N2—C1	119.9 (9)
C11—C10—C9	122.3 (11)	C14—N2—Cd1	123.4 (7)
C11—C10—Br2	120.2 (9)	C1—N2—Cd1	115.6 (6)
C9—C10—Br2	117.5 (8)	C21—N3—C22	123.9 (13)
C12—C11—C10	118.4 (11)	C21—N3—C23	118.5 (12)
C12—C11—H11	120.8	C22—N3—C23	117.6 (14)

C10—C11—H11	120.8	C9—O1—Cd1	126.7 (6)
C13—C12—C11	122.8 (10)	C9—O1—Cd1^{i}	119.4 (5)
C13—C12—Br1	120.0 (10)	Cd1—O1—Cd1^{i}	106.4 (3)
C11—C12—Br1	117.2 (9)	C16—O2—Cd1	127.4 (6)
C12—C13—C8	119.4 (11)	C21—O3—Cd1	142.1 (10)
C6—C1—C2—C3	2.5 (18)	O1—Cd1—N1—C7	24.8 (9)
N2—C1—C2—C3	179.3 (11)	O1^{i}—Cd1—N1—C7	93.9 (9)
C1—C2—C3—C4	−3 (2)	N2—Cd1—N1—C7	−148.7 (9)
C2—C3—C4—C5	4 (2)	O3—Cd1—N1—C7	−58.2 (9)
C3—C4—C5—C6	−3 (2)	O2—Cd1—N1—C6	10.3 (11)
C4—C5—C6—C1	2.6 (18)	O1—Cd1—N1—C6	−168.3 (7)
C4—C5—C6—N1	−179.2 (11)	O1^{i}—Cd1—N1—C6	−99.1 (7)
C2—C1—C6—C5	−2.2 (16)	N2—Cd1—N1—C6	18.2 (6)
N2—C1—C6—C5	−179.2 (10)	O3—Cd1—N1—C6	108.8 (7)
C2—C1—C6—N1	179.6 (10)	C15—C14—N2—C1	−171.1 (10)
N2—C1—C6—N1	2.6 (14)	C15—C14—N2—Cd1	21.1 (15)
N1—C7—C8—C13	172.7 (10)	C6—C1—N2—C14	−153.9 (10)
N1—C7—C8—C9	−5.8 (18)	C2—C1—N2—C14	29.3 (16)
C13—C8—C9—O1	173.6 (9)	C6—C1—N2—Cd1	14.8 (12)
C7—C8—C9—O1	−7.9 (16)	C2—C1—N2—Cd1	−162.0 (9)
C13—C8—C9—C10	−6.4 (14)	O2—Cd1—N2—C14	−33.2 (8)
C7—C8—C9—C10	172.0 (10)	O1—Cd1—N2—C14	137.8 (8)
O1—C9—C10—C11	−172.2 (9)	O1^{i}—Cd1—N2—C14	−111.0 (8)
C8—C9—C10—C11	7.8 (15)	O3—Cd1—N2—C14	59.1 (9)
O1—C9—C10—Br2	5.4 (12)	N1—Cd1—N2—C14	150.6 (9)
C8—C9—C10—Br2	−174.6 (7)	O2—Cd1—N2—C1	158.5 (8)
C9—C10—C11—C12	−4.4 (16)	O1—Cd1—N2—C1	−30.5 (11)
Br2—C10—C11—C12	178.1 (9)	O1^{i}—Cd1—N2—C1	80.7 (8)
C10—C11—C12—C13	−0.7 (18)	O3—Cd1—N2—C1	−109.2 (8)
C10—C11—C12—Br1	179.3 (8)	N1—Cd1—N2—C1	−17.7 (7)
C11—C12—C13—C8	2.0 (18)	O3—C21—N3—C22	175.5 (15)
Br1—C12—C13—C8	−178.0 (8)	O3—C21—N3—C23	−4 (2)
C9—C8—C13—C12	1.9 (16)	C8—C9—O1—Cd1	38.3 (13)
C7—C8—C13—C12	−176.7 (10)	C10—C9—O1—Cd1	−141.6 (7)
N2—C14—C15—C20	−178.6 (11)	C8—C9—O1—Cd1^{i}	−107.3 (9)
N2—C14—C15—C16	8.2 (18)	C10—C9—O1—Cd1^{i}	72.7 (11)
C20—C15—C16—O2	177.7 (11)	O2—Cd1—O1—C9	142.4 (8)
C14—C15—C16—O2	−9.3 (17)	O1^{i}—Cd1—O1—C9	−149.2 (10)
C20—C15—C16—C17	−0.6 (15)	N2—Cd1—O1—C9	−26.1 (11)
C14—C15—C16—C17	172.4 (10)	O3—Cd1—O1—C9	54.6 (8)
O2—C16—C17—C18	−176.9 (11)	N1—Cd1—O1—C9	−38.4 (8)
C15—C16—C17—C18	1.6 (17)	O2—Cd1—O1—Cd1^{i}	−68.4 (4)
O2—C16—C17—Br4	7.9 (14)	O1^{i}—Cd1—O1—Cd1^{i}	0.0
C15—C16—C17—Br4	−173.7 (7)	N2—Cd1—O1—Cd1^{i}	123.1 (5)
C16—C17—C18—C19	0.2 (19)	O3—Cd1—O1—Cd1^{i}	−156.2 (4)
Br4—C17—C18—C19	175.4 (9)	N1—Cd1—O1—Cd1^{i}	110.7 (3)
C17—C18—C19—C20	−3.1 (18)	C17—C16—O2—Cd1	157.1 (8)

C17—C18—C19—Br3	179.8 (9)	C15—C16—O2—Cd1	−21.2 (15)
C18—C19—C20—C15	4.1 (18)	O1—Cd1—O2—C16	−140.1 (8)
Br3—C19—C20—C15	−178.9 (9)	O1^{i}—Cd1—O2—C16	156.2 (9)
C16—C15—C20—C19	−2.2 (17)	N2—Cd1—O2—C16	34.1 (9)
C14—C15—C20—C19	−175.7 (11)	O3—Cd1—O2—C16	−56.6 (9)
C8—C7—N1—C6	−176.7 (10)	N1—Cd1—O2—C16	41.7 (12)
C8—C7—N1—Cd1	−10.9 (16)	N3—C21—O3—Cd1	134.6 (14)
C5—C6—N1—C7	−28.6 (15)	O2—Cd1—O3—C21	99.7 (17)
C1—C6—N1—C7	149.5 (10)	O1—Cd1—O3—C21	−131.3 (17)
C5—C6—N1—Cd1	163.8 (9)	O1^{i}—Cd1—O3—C21	−176.7 (14)
C1—C6—N1—Cd1	−18.1 (11)	N2—Cd1—O3—C21	19.2 (17)
O2—Cd1—N1—C7	−156.6 (8)	N1—Cd1—O3—C21	−52.4 (17)

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