Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{[(5-Bromo-2-oxidophenyl)methyleneamino]methanesulfonato-κ^3O,N,O'}(methanol-κO)(1,10-phenanthroline-κ^2N,N')cadmium(II)

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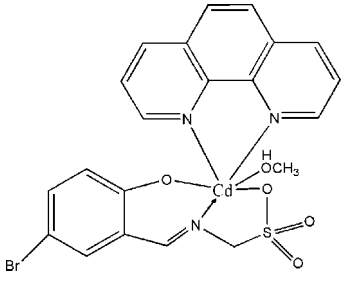
Received 9 July 2007; accepted 27 July 2007

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.006 Å; R factor = 0.040; wR factor = 0.106; data-to-parameter ratio = 15.1.

The title compound, $[Cd(C_8H_6BrNO_4S)(C_{12}H_8N_2)(CH_4O)]$, incorporating a Schiff base formed by aminomethanesulfonic acid and 5-bromosalicylaldehyde, was synthesized in a water–methanol solution. In the structure, the Cd^{II} atom is six-coordinated by one O atom from a methanol molecule, two N atoms from a 1,10-phenanthroline ligand, and one N and two O atoms from the Schiff base in a distorted octahedral coordination geometry. A one-dimensional chain structure is formed *via* C—H···O hydrogen bonds.

Related literature

For related literature, see: Casella & Gullotti (1981); Zhang *et al.* (2005).



Experimental

Crystal data

$[Cd(C_8H_6BrNO_4S)(C_{12}H_8N_2)(CH_4O)]$
M_r = 616.76
Monoclinic, $P2_1/c$
a = 18.712 (3) Å
b = 13.801 (1) Å
c = 8.3681 (12) Å
β = 97.791 (2)°
V = 2141.1 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.02 mm^{-1}
T = 294 (2) K
0.24 × 0.20 × 0.18 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.485, T_{max} = 0.585
11883 measured reflections
4382 independent reflections
2754 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.106
S = 1.03
4382 reflections
290 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O1	1.977 (3)	Cd1—N2	2.135 (3)
Cd1—N1	2.084 (3)	Cd1—O5	2.237 (3)
Cd1—N3	2.115 (3)	Cd1—O2	2.381 (3)
O1—Cd1—N1	90.95 (11)	N3—Cd1—O5	86.72 (11)
O1—Cd1—N3	96.80 (11)	N2—Cd1—O5	157.97 (11)
N1—Cd1—N3	170.89 (11)	O1—Cd1—O2	169.29 (10)
O1—Cd1—N2	100.49 (12)	N1—Cd1—O2	78.36 (10)
N1—Cd1—N2	104.63 (12)	N3—Cd1—O2	93.80 (10)
N3—Cd1—N2	78.72 (12)	N2—Cd1—O2	83.10 (11)
O1—Cd1—O5	97.54 (12)	O5—Cd1—O2	81.46 (10)
N1—Cd1—O5	87.53 (11)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O3	0.93	2.38	2.759 (4)	104
C7—H7···O3^{i}	0.93	2.58	3.113 (5)	117
C8—H8B···O4^{i}	0.97	2.53	3.388 (5)	147
C18—H18···O5	0.93	2.57	3.109 (5)	117

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

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

This work was supported by the Construct Program of the Key Discipline in Hunan Province and Hunan Provincial Natural Science Foundation of China (grant No. 05 J J30015).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2072).

References

Bruker (2001). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Casella, L. & Gullotti, M. (1981). *J. Am. Chem. Soc.* **103**, 6338–6347.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Zhang, S.-H., Jiang, Y.-M. & Yu, K.-B. (2005). *Acta Cryst.* E**61**, m209–m211.

  doi:10.1107/S1600536807036811

supplementary materials

Acta Cryst. (2007). E**63**, m2250 [**doi:10.1107/S1600536807036811**]

{[(5-Bromo-2-oxidophenyl)methyleneamino]methanesulfonato-κ^3O,N,O'}(methanol-κO)(1,10-phenanthroline-κ^2N,N')cadmium(II)

J.-S. Xu, C.-H. Zhang, D.-Z. Kuang, Y.-L. Feng and Y.-L. Peng

Comment

During the last two decades, the Schiff base complexes containing sulfur and the complexes of amino acid Schiff bases have aroused increasing interest because of their antiviral, anticancer and antibacterial activities (Casella & Gullotti, 1981; Zhang *et al.*, 2005). We have utilized aminomethanesulfonic acid and 5-bromosalicylaldehyde as ligands and investigated their reaction with cadmium acetate. We report here the structure of the title compound.

In the title compound, the Cd^{II} atom is six-coordinated by the imine N atom, the phenolate O atom and a sulfonate O atom from the tridentate Schiff base ligand, two N atoms from a phenanthroline ligand and one O atom from a methanol molecule. Thus the Cd^{II} atom has a distorted octahedral geometry (Fig. 1). The Cd—O distances are in a range of 1.977 (3)–2.381 (3) Å, and the mean Cd—O bond length is 2.198 (3) Å (Table 1). The Cd—N distances range from 2.084 (3) to 2.135 (3) Å. The Schiff base ligand adopts a κ^3O,N,O'-tridentate mode, forming a five-membered ring and a six-membered ring. An O—H···O hydrogen bond between the coordinated O atom of the methanol molecule and an uncoordinated O atom of the sulfonate group and C—H···O hydrogen bonds are observed (Table 2).

Experimental

An aqueous solution (5 ml) of $Cd(ClO_4)_2{\cdot}6H_2O$ (0.422 g, 1.0 mmol) was added dropwise to a methanol solution (15 ml) of NaOH (0.041 g, 1.0 mmol), 5-bromosalicylaldehyde (0.202 g, 1.0 mmol) and aminomethanesulfonic acid (0.112 g, 1.0 mmol). The reaction mixture was refluxed for 4 h and added a methanol solution containing 1,10-phenanthroline (0.201 g, 1.0 mmol). The reaction mixture was refluxed for 6 h and then filtered. The resulting yellow filtrate was allowed to stand at room temperature for one month to afford yellow block-shaped crystals. Analysis, calculated for $C_{21}H_{18}BrCdN_3O_5S$: C 40.86, H 2.92, N 6.81%; found: C 39.96, H 2.84, N 6.87%.

Refinement

All H atoms were positioned geometrically and refined as riding, with C—H = 0.93(CH), 0.97(CH_2), 0.96(CH_3) and 0.93 (OH) Å and U_{iso}(H)=1.5U_{eq}(C) for CH_3 group and U_{iso}(H)=1.2U_{eq}(C, O) for the others.

Figures

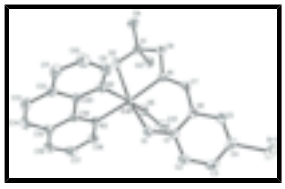


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

{[(5-Bromo-2-oxidophenyl)methyleneamino]methanesulfonato- κ^3O,N,O'}(methanol-κO)(1,10-phenanthroline-κ^2N,N')cadmium(II)

Crystal data

$[Cd(C_8H_6BrNO_4S)(C_{12}H_8N_2)(CH_4O)]$	F_{000} = 1216
M_r = 616.76	D_x = 1.913 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3340 reflections
a = 18.712 (3) Å	θ = 2.2–25.9º
b = 13.801 (1) Å	μ = 3.02 mm^{-1}
c = 8.3681 (12) Å	T = 294 (2) K
β = 97.791 (2)º	Block, yellow
V = 2141.1 (5) Å^3	0.24 × 0.20 × 0.18 mm
Z = 4	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	4382 independent reflections
Radiation source: fine-focus sealed tube	2754 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.061
T = 294(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −21→23
T_{min} = 0.485, T_{max} = 0.585	k = −14→17
11883 measured reflections	l = −10→10

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.040	H-atom parameters constrained
$wR(F^2)$ = 0.106	$w = 1/[\sigma^2(F_o^2) + (0.0445P)^2 + 0.319P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
4382 reflections	$\Delta\rho_{max} = 0.59$ e Å^{-3}
290 parameters	$\Delta\rho_{min} = -0.56$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	y	z	U_{iso}*/U_{eq}
Cd1	0.26012 (2)	−0.00001 (3)	1.04615 (6)	0.03781 (15)
Br1	−0.04473 (3)	0.29929 (4)	0.64972 (7)	0.0725 (2)
S1	0.33001 (5)	0.11933 (7)	1.35725 (12)	0.0389 (3)
O1	0.18426 (15)	0.00142 (18)	0.8572 (3)	0.0473 (7)
O2	0.34653 (14)	0.02965 (19)	1.2771 (3)	0.0441 (7)
O3	0.26898 (15)	0.1068 (2)	1.4462 (3)	0.0499 (7)
O4	0.39171 (15)	0.1656 (2)	1.4478 (4)	0.0572 (8)
N1	0.25062 (15)	0.1493 (2)	1.0740 (4)	0.0331 (7)
N2	0.35398 (17)	−0.0178 (2)	0.9297 (4)	0.0373 (8)
N3	0.27402 (16)	−0.1520 (2)	1.0582 (4)	0.0344 (7)
C1	0.1391 (2)	0.0703 (3)	0.8111 (5)	0.0371 (9)
C2	0.0840 (2)	0.0536 (3)	0.6811 (5)	0.0465 (11)
H2	0.0835	−0.0050	0.6263	0.056*
C3	0.0315 (2)	0.1199 (3)	0.6328 (5)	0.0511 (12)
H3	−0.0044	0.1054	0.5482	0.061*
C4	0.0316 (2)	0.2091 (3)	0.7097 (5)	0.0451 (11)
C5	0.0855 (2)	0.2317 (3)	0.8304 (5)	0.0387 (9)
H5	0.0863	0.2924	0.8789	0.046*
C6	0.14027 (19)	0.1634 (3)	0.8828 (4)	0.0315 (8)
C7	0.19513 (19)	0.1974 (3)	1.0094 (4)	0.0314 (8)
H7	0.1898	0.2599	1.0476	0.038*
C8	0.3014 (2)	0.1992 (3)	1.1928 (5)	0.0398 (10)
H8A	0.2786	0.2560	1.2319	0.048*
H8B	0.3428	0.2204	1.1437	0.048*
C9	0.3917 (2)	0.0482 (3)	0.8632 (5)	0.0504 (11)
H9	0.3771	0.1126	0.8647	0.060*
C10	0.4520 (2)	0.0258 (3)	0.7915 (6)	0.0591 (13)
H10	0.4764	0.0744	0.7441	0.071*
C11	0.4754 (2)	−0.0664 (3)	0.7904 (5)	0.0532 (12)
H11	0.5165	−0.0816	0.7440	0.064*
C12	0.4372 (2)	−0.1397 (3)	0.8599 (5)	0.0401 (10)
C13	0.4551 (2)	−0.2402 (3)	0.8598 (5)	0.0541 (12)
H13	0.4968	−0.2593	0.8194	0.065*
C14	0.4137 (2)	−0.3080 (3)	0.9160 (6)	0.0533 (12)
H14	0.4266	−0.3729	0.9116	0.064*
C15	0.3498 (2)	−0.2816 (3)	0.9831 (5)	0.0393 (10)
C16	0.3033 (3)	−0.3490 (3)	1.0419 (5)	0.0493 (11)
H16	0.3126	−0.4150	1.0363	0.059*
C17	0.2447 (2)	−0.3174 (3)	1.1070 (5)	0.0502 (11)

H17	0.2138	−0.3612	1.1470	0.060*
C18	0.2319 (2)	−0.2181 (3)	1.1125 (5)	0.0431 (10)
H18	0.1917	−0.1970	1.1566	0.052*
C19	0.33226 (19)	−0.1828 (3)	0.9920 (4)	0.0323 (9)
C20	0.37606 (18)	−0.1110 (3)	0.9276 (4)	0.0317 (9)
O5	0.18771 (15)	−0.0173 (2)	1.2362 (4)	0.0511 (8)
H5A	0.2086	−0.0352	1.3391	0.061*
C21	0.1118 (3)	−0.0026 (4)	1.2097 (7)	0.0739 (16)
H21A	0.1014	0.0585	1.1569	0.111*
H21B	0.0933	−0.0027	1.3112	0.111*
H21C	0.0895	−0.0538	1.1429	0.111*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0392 (3)	0.0302 (3)	0.0458 (3)	0.0055 (2)	0.0122 (2)	−0.0006 (2)
Br1	0.0512 (3)	0.0899 (4)	0.0723 (4)	0.0222 (3)	−0.0059 (2)	0.0143 (3)
S1	0.0378 (5)	0.0417 (6)	0.0371 (6)	0.0036 (5)	0.0047 (4)	−0.0008 (5)
O1	0.0520 (17)	0.0361 (16)	0.0517 (18)	0.0076 (14)	−0.0011 (14)	−0.0076 (14)
O2	0.0494 (16)	0.0403 (16)	0.0433 (16)	0.0087 (13)	0.0092 (13)	0.0024 (13)
O3	0.0525 (17)	0.0535 (18)	0.0477 (17)	0.0026 (14)	0.0211 (14)	−0.0016 (15)
O4	0.0467 (17)	0.069 (2)	0.0511 (18)	−0.0030 (15)	−0.0094 (14)	−0.0088 (16)
N1	0.0333 (17)	0.0318 (17)	0.0342 (18)	−0.0026 (14)	0.0045 (14)	−0.0027 (14)
N2	0.0396 (18)	0.033 (2)	0.0407 (19)	0.0013 (15)	0.0113 (15)	0.0006 (15)
N3	0.0377 (18)	0.0308 (18)	0.0347 (18)	0.0003 (14)	0.0052 (14)	0.0009 (15)
C1	0.042 (2)	0.036 (2)	0.034 (2)	−0.0053 (19)	0.0087 (18)	0.0001 (18)
C2	0.060 (3)	0.039 (3)	0.039 (2)	−0.012 (2)	0.001 (2)	−0.005 (2)
C3	0.045 (3)	0.062 (3)	0.042 (3)	−0.018 (2)	−0.010 (2)	0.008 (2)
C4	0.035 (2)	0.060 (3)	0.040 (2)	0.002 (2)	0.0036 (18)	0.010 (2)
C5	0.040 (2)	0.039 (2)	0.039 (2)	0.0059 (19)	0.0098 (18)	−0.0005 (19)
C6	0.0295 (19)	0.035 (2)	0.031 (2)	−0.0006 (17)	0.0071 (16)	0.0006 (17)
C7	0.034 (2)	0.028 (2)	0.034 (2)	−0.0003 (17)	0.0099 (16)	0.0005 (17)
C8	0.036 (2)	0.037 (2)	0.045 (2)	−0.0044 (18)	0.0017 (18)	−0.0007 (19)
C9	0.056 (3)	0.037 (2)	0.062 (3)	0.000 (2)	0.021 (2)	0.003 (2)
C10	0.058 (3)	0.052 (3)	0.073 (3)	−0.007 (2)	0.030 (3)	0.011 (3)
C11	0.040 (2)	0.064 (3)	0.060 (3)	0.002 (2)	0.021 (2)	−0.007 (2)
C12	0.035 (2)	0.042 (2)	0.043 (2)	0.0046 (19)	0.0033 (18)	−0.007 (2)
C13	0.045 (3)	0.059 (3)	0.061 (3)	0.016 (2)	0.013 (2)	−0.006 (3)
C14	0.059 (3)	0.038 (3)	0.062 (3)	0.019 (2)	0.006 (2)	−0.009 (2)
C15	0.048 (2)	0.031 (2)	0.036 (2)	0.0024 (19)	−0.0040 (19)	−0.0019 (18)
C16	0.067 (3)	0.032 (2)	0.046 (3)	0.001 (2)	−0.006 (2)	−0.002 (2)
C17	0.061 (3)	0.039 (3)	0.049 (3)	−0.013 (2)	0.003 (2)	0.003 (2)
C18	0.042 (2)	0.044 (3)	0.044 (2)	−0.0046 (19)	0.0075 (19)	−0.001 (2)
C19	0.031 (2)	0.032 (2)	0.033 (2)	0.0038 (17)	−0.0017 (16)	−0.0037 (18)
C20	0.033 (2)	0.032 (2)	0.030 (2)	0.0031 (17)	0.0009 (16)	−0.0044 (17)
O5	0.0486 (17)	0.0553 (19)	0.0529 (18)	0.0001 (14)	0.0192 (14)	0.0029 (15)
C21	0.054 (3)	0.098 (4)	0.077 (4)	−0.009 (3)	0.034 (3)	−0.012 (3)

Geometric parameters (Å, °)

Cd1—O1	1.977 (3)	C7—H7	0.9300
Cd1—N1	2.084 (3)	C8—H8A	0.9700
Cd1—N3	2.115 (3)	C8—H8B	0.9700
Cd1—N2	2.135 (3)	C9—C10	1.383 (6)
Cd1—O5	2.237 (3)	C9—H9	0.9300
Cd1—O2	2.381 (3)	C10—C11	1.347 (6)
Br1—C4	1.910 (4)	C10—H10	0.9300
S1—O4	1.441 (3)	C11—C12	1.409 (6)
S1—O3	1.455 (3)	C11—H11	0.9300
S1—O2	1.461 (3)	C12—C20	1.402 (5)
S1—C8	1.788 (4)	C12—C13	1.427 (6)
O1—C1	1.296 (4)	C13—C14	1.339 (6)
N1—C7	1.288 (4)	C13—H13	0.9300
N1—C8	1.453 (4)	C14—C15	1.436 (6)
N2—C9	1.321 (5)	C14—H14	0.9300
N2—C20	1.352 (4)	C15—C19	1.406 (5)
N3—C18	1.324 (5)	C15—C16	1.407 (6)
N3—C19	1.356 (5)	C16—C17	1.361 (6)
C1—C2	1.412 (5)	C16—H16	0.9300
C1—C6	1.418 (5)	C17—C18	1.393 (5)
C2—C3	1.362 (6)	C17—H17	0.9300
C2—H2	0.9300	C18—H18	0.9300
C3—C4	1.388 (6)	C19—C20	1.437 (5)
C3—H3	0.9300	O5—C21	1.422 (5)
C4—C5	1.363 (5)	O5—H5A	0.9300
C5—C6	1.417 (5)	C21—H21A	0.9600
C5—H5	0.9300	C21—H21B	0.9600
C6—C7	1.449 (5)	C21—H21C	0.9600
O1—Cd1—N1	90.95 (11)	C6—C7—H7	116.9
O1—Cd1—N3	96.80 (11)	N1—C8—S1	109.5 (2)
N1—Cd1—N3	170.89 (11)	N1—C8—H8A	109.8
O1—Cd1—N2	100.49 (12)	S1—C8—H8A	109.8
N1—Cd1—N2	104.63 (12)	N1—C8—H8B	109.8
N3—Cd1—N2	78.72 (12)	S1—C8—H8B	109.8
O1—Cd1—O5	97.54 (12)	H8A—C8—H8B	108.2
N1—Cd1—O5	87.53 (11)	N2—C9—C10	122.9 (4)
N3—Cd1—O5	86.72 (11)	N2—C9—H9	118.6
N2—Cd1—O5	157.97 (11)	C10—C9—H9	118.6
O1—Cd1—O2	169.29 (10)	C11—C10—C9	120.0 (4)
N1—Cd1—O2	78.36 (10)	C11—C10—H10	120.0
N3—Cd1—O2	93.80 (10)	C9—C10—H10	120.0
N2—Cd1—O2	83.10 (11)	C10—C11—C12	119.5 (4)
O5—Cd1—O2	81.46 (10)	C10—C11—H11	120.3
O4—S1—O3	114.30 (18)	C12—C11—H11	120.3
O4—S1—O2	114.37 (17)	C20—C12—C11	116.8 (4)
O3—S1—O2	111.35 (16)	C20—C12—C13	118.7 (4)

O4—S1—C8	105.46 (18)	C11—C12—C13	124.4 (4)
O3—S1—C8	107.03 (18)	C14—C13—C12	122.1 (4)
O2—S1—C8	103.24 (17)	C14—C13—H13	118.9
C1—O1—Cd1	127.9 (2)	C12—C13—H13	118.9
S1—O2—Cd1	110.84 (14)	C13—C14—C15	120.8 (4)
C7—N1—C8	117.2 (3)	C13—C14—H14	119.6
C7—N1—Cd1	122.6 (2)	C15—C14—H14	119.6
C8—N1—Cd1	119.2 (2)	C19—C15—C16	117.6 (4)
C9—N2—C20	118.0 (3)	C19—C15—C14	118.6 (4)
C9—N2—Cd1	129.3 (3)	C16—C15—C14	123.8 (4)
C20—N2—Cd1	112.8 (2)	C17—C16—C15	119.9 (4)
C18—N3—C19	118.2 (3)	C17—C16—H16	120.1
C18—N3—Cd1	128.6 (3)	C15—C16—H16	120.1
C19—N3—Cd1	113.1 (2)	C16—C17—C18	118.6 (4)
O1—C1—C2	119.3 (4)	C16—C17—H17	120.7
O1—C1—C6	124.5 (3)	C18—C17—H17	120.7
C2—C1—C6	116.2 (4)	N3—C18—C17	123.6 (4)
C3—C2—C1	122.7 (4)	N3—C18—H18	118.2
C3—C2—H2	118.6	C17—C18—H18	118.2
C1—C2—H2	118.6	N3—C19—C15	122.1 (4)
C2—C3—C4	120.2 (4)	N3—C19—C20	117.9 (3)
C2—C3—H3	119.9	C15—C19—C20	120.0 (3)
C4—C3—H3	119.9	N2—C20—C12	122.9 (4)
C5—C4—C3	120.0 (4)	N2—C20—C19	117.4 (3)
C5—C4—Br1	119.8 (3)	C12—C20—C19	119.7 (3)
C3—C4—Br1	120.1 (3)	C21—O5—Cd1	124.2 (3)
C4—C5—C6	120.6 (4)	C21—O5—H5A	117.9
C4—C5—H5	119.7	Cd1—O5—H5A	117.9
C6—C5—H5	119.7	O5—C21—H21A	109.5
C1—C6—C5	120.1 (3)	O5—C21—H21B	109.5
C1—C6—C7	124.9 (3)	H21A—C21—H21B	109.5
C5—C6—C7	115.0 (3)	O5—C21—H21C	109.5
N1—C7—C6	126.2 (3)	H21A—C21—H21C	109.5
N1—C7—H7	116.9	H21B—C21—H21C	109.5
N1—Cd1—O1—C1	−14.3 (3)	C4—C5—C6—C7	178.6 (3)
N3—Cd1—O1—C1	160.9 (3)	C8—N1—C7—C6	176.4 (3)
N2—Cd1—O1—C1	−119.4 (3)	Cd1—N1—C7—C6	−14.8 (5)
O5—Cd1—O1—C1	73.3 (3)	C1—C6—C7—N1	0.7 (6)
O2—Cd1—O1—C1	−10.6 (8)	C5—C6—C7—N1	−178.7 (4)
O4—S1—O2—Cd1	−153.75 (17)	C7—N1—C8—S1	138.6 (3)
O3—S1—O2—Cd1	74.79 (18)	Cd1—N1—C8—S1	−30.6 (3)
C8—S1—O2—Cd1	−39.73 (19)	O4—S1—C8—N1	166.6 (3)
O1—Cd1—O2—S1	19.0 (7)	O3—S1—C8—N1	−71.3 (3)
N1—Cd1—O2—S1	22.80 (16)	O2—S1—C8—N1	46.3 (3)
N3—Cd1—O2—S1	−152.52 (16)	C20—N2—C9—C10	0.4 (6)
N2—Cd1—O2—S1	129.34 (17)	Cd1—N2—C9—C10	179.9 (3)
O5—Cd1—O2—S1	−66.42 (16)	N2—C9—C10—C11	−1.3 (7)
O1—Cd1—N1—C7	18.1 (3)	C9—C10—C11—C12	1.2 (7)
N2—Cd1—N1—C7	119.2 (3)	C10—C11—C12—C20	−0.1 (6)

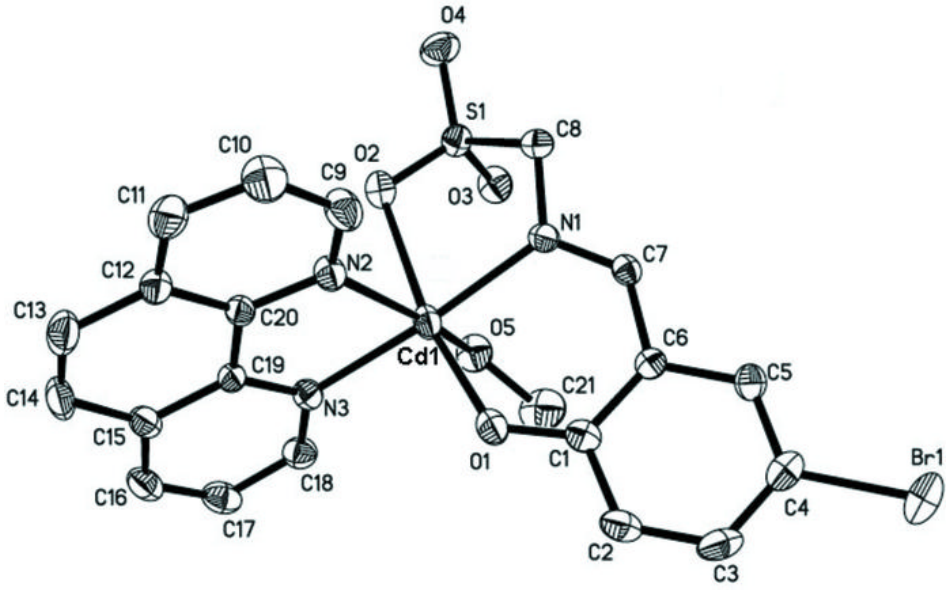
O5—Cd1—N1—C7	−79.4 (3)	C10—C11—C12—C13	177.2 (4)
O2—Cd1—N1—C7	−161.2 (3)	C20—C12—C13—C14	2.8 (6)
O1—Cd1—N1—C8	−173.3 (3)	C11—C12—C13—C14	−174.5 (4)
N2—Cd1—N1—C8	−72.2 (3)	C12—C13—C14—C15	−1.5 (7)
O5—Cd1—N1—C8	89.2 (3)	C13—C14—C15—C19	−1.5 (6)
O2—Cd1—N1—C8	7.4 (3)	C13—C14—C15—C16	179.0 (4)
O1—Cd1—N2—C9	83.0 (4)	C19—C15—C16—C17	−1.1 (6)
N1—Cd1—N2—C9	−10.7 (4)	C14—C15—C16—C17	178.5 (4)
N3—Cd1—N2—C9	178.0 (4)	C15—C16—C17—C18	0.5 (6)
O5—Cd1—N2—C9	−132.5 (4)	C19—N3—C18—C17	0.8 (6)
O2—Cd1—N2—C9	−86.8 (4)	Cd1—N3—C18—C17	176.6 (3)
O1—Cd1—N2—C20	−97.4 (3)	C16—C17—C18—N3	−0.3 (6)
N1—Cd1—N2—C20	168.9 (2)	C18—N3—C19—C15	−1.5 (5)
N3—Cd1—N2—C20	−2.4 (2)	Cd1—N3—C19—C15	−177.9 (3)
O5—Cd1—N2—C20	47.1 (4)	C18—N3—C19—C20	177.6 (3)
O2—Cd1—N2—C20	92.9 (2)	Cd1—N3—C19—C20	1.1 (4)
O1—Cd1—N3—C18	−75.9 (3)	C16—C15—C19—N3	1.6 (5)
N2—Cd1—N3—C18	−175.3 (3)	C14—C15—C19—N3	−178.0 (3)
O5—Cd1—N3—C18	21.3 (3)	C16—C15—C19—C20	−177.4 (3)
O2—Cd1—N3—C18	102.5 (3)	C14—C15—C19—C20	3.0 (5)
O1—Cd1—N3—C19	100.1 (2)	C9—N2—C20—C12	0.7 (5)
N2—Cd1—N3—C19	0.7 (2)	Cd1—N2—C20—C12	−178.9 (3)
O5—Cd1—N3—C19	−162.7 (2)	C9—N2—C20—C19	−176.5 (3)
O2—Cd1—N3—C19	−81.5 (2)	Cd1—N2—C20—C19	3.8 (4)
Cd1—O1—C1—C2	−173.8 (3)	C11—C12—C20—N2	−0.8 (5)
Cd1—O1—C1—C6	6.0 (6)	C13—C12—C20—N2	−178.4 (3)
O1—C1—C2—C3	175.4 (4)	C11—C12—C20—C19	176.4 (3)
C6—C1—C2—C3	−4.4 (6)	C13—C12—C20—C19	−1.2 (5)
C1—C2—C3—C4	1.5 (7)	N3—C19—C20—N2	−3.4 (5)
C2—C3—C4—C5	2.0 (6)	C15—C19—C20—N2	175.7 (3)
C2—C3—C4—Br1	−176.6 (3)	N3—C19—C20—C12	179.2 (3)
C3—C4—C5—C6	−2.3 (6)	C15—C19—C20—C12	−1.7 (5)
Br1—C4—C5—C6	176.3 (3)	O1—Cd1—O5—C21	−14.5 (3)
O1—C1—C6—C5	−175.8 (4)	N1—Cd1—O5—C21	76.2 (3)
C2—C1—C6—C5	4.0 (5)	N3—Cd1—O5—C21	−110.9 (3)
O1—C1—C6—C7	4.8 (6)	N2—Cd1—O5—C21	−159.3 (3)
C2—C1—C6—C7	−175.3 (3)	O2—Cd1—O5—C21	154.8 (3)
C4—C5—C6—C1	−0.8 (6)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5A···O3	0.93	2.38	2.759 (4)	104
C7—H7···O3^{i}	0.93	2.58	3.113 (5)	117
C8—H8B···O4^{i}	0.97	2.53	3.388 (5)	147
C18—H18···O5	0.93	2.57	3.109 (5)	117

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

Fig. 1


O4
S1
C8
C10
O2
C9
O3
C11
N1
C7
C12
N2
C13
C20
O5
C6
Cd1
C19
C21
C5
C14
N3
C15
O1
C1
Br1
C18
C16
C4
C17
C2
C3