

Bis[4-(2-hydroxybenzylideneamino)-benzoato- κO^1]tetrakis(methanol- κO)-cadmium

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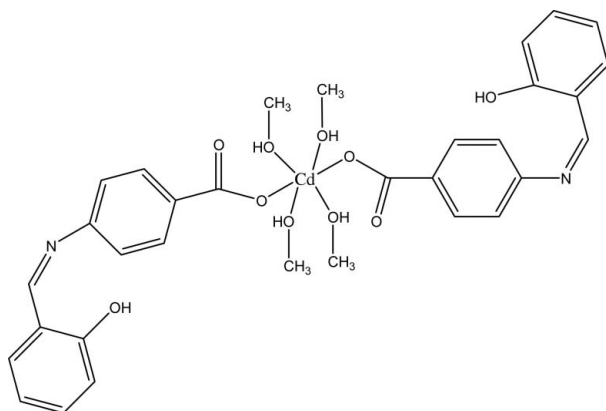
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(C-C) = 0.012$ Å; R factor = 0.072; wR factor = 0.166; data-to-parameter ratio = 13.7.

In the title mononuclear complex, $[Cd(C_{14}H_{10}NO_3)_2(CH_3OH)_4]$, the Cd^{2+} cation is situated on an inversion centre. It exhibits a distorted octahedral coordination, defined by two carboxylate O atoms from two monodentate anions and by four O atoms from four methanol molecules. The crystal structure comprises intramolecular $O-H \cdots O$ and $O-H \cdots N$, and intermolecular $O-H \cdots O$ hydrogen bonds. The latter help to construct a layered structure extending parallel to (100).

Related literature

For background to Schiff base ligands, see: Garnovskii *et al.* (1993); Banerjee *et al.* (2004); Zhong *et al.* (2009). For background to cadmium complexes, see: Meng *et al.* (2004); Wang *et al.* (2010).



Experimental

Crystal data

$[Cd(C_{14}H_{10}NO_3)_2(CH_3OH)_4]$
 $M_r = 721.04$
 Monoclinic, $P2_1/c$
 $a = 15.564$ (3) Å
 $b = 11.937$ (2) Å
 $c = 8.8946$ (18) Å
 $\beta = 99.69$ (3)°

$V = 1629.0$ (6) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.73$ mm⁻¹
 $T = 293$ K
 $0.21 \times 0.19 \times 0.16$ mm

Data collection

Rigaku Saturn diffractometer
 Absorption correction: multi-scan
 (*CrystalClear*; Rigaku/MS, 2006)
 $T_{min} = 0.862$, $T_{max} = 0.892$

7793 measured reflections
 2760 independent reflections
 2137 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.055$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.072$
 $wR(F^2) = 0.166$
 $S = 1.13$
 2760 reflections

202 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 0.97$ e Å⁻³
 $\Delta\rho_{min} = -0.63$ e Å⁻³

Table 1

Selected bond lengths (Å).

Cd1—O1	2.230 (5)	Cd1—O3	2.315 (5)
Cd1—O4	2.295 (5)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O4—H4 \cdots O2	0.87	1.87	2.653 (7)	150
O5—H5 \cdots N1	0.82	1.90	2.632 (9)	148
O3—H3 \cdots O2 ¹	0.85	1.83	2.640 (7)	160

Symmetry code: (i) $-x + 2, y + \frac{1}{2}, -z + \frac{5}{2}$.

Data collection: *CrystalClear* (Rigaku/MS, 2006); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2478).

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supplementary materials

Acta Cryst. (2011). E67, m685-m686 [doi:10.1107/S1600536811015364]

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Y. Wang, X. Wang, Y.-X. Li, H.-X. Yang and Y.-J. Liu

Comment

Schiff base ligands played an important role in the development of coordination chemistry due to their metal binding ability (Garnovskii *et al.*, 1993). Schiff bases and their metal complexes have numerous applications in biological systems and material sciences (Banerjee *et al.*, 2004; Zhong *et al.*, 2009). The Cd^{2+} ion is a good model atom to construct complexes owing to its property to form bonds with different types of donors simultaneously, and to its various coordination modes (Meng *et al.*, 2004; Wang *et al.*, 2010). In this work, we describe the synthesis and structure of the title complex, $[Cd(C_{14}H_{10}NO_3)_2(CH_3OH)_4]$, (I).

In complex (I), the Cd^{2+} ion is situated on an inversion centre and is six-coordinated by two carboxylate O atoms from two monodentate ligands and by four O atoms from four methanol molecules (Fig. 1). The dihedral angle between the phenyl ring and the benzylidenimino moiety is $23.4(4)^\circ$.

The crystal structure of (I) comprises intramolecular O—H \cdots O and O—H \cdots N hydrogen bonds that help to stabilize the molecular conformation. Intermolecular O—H \cdots O hydrogen bonds between methanol molecules and the free carboxylate O atoms of neighbouring molecules construct a layered structure extending parallel to (100), as shown in Fig. 2.

Experimental

N-(4-carboxyphenyl)salicylideneimine (0.04 mmol, 0.0097 g) in methanol (6 ml) was added dropwise to a methanol solution (5 ml) of $CdCl_2$ (0.02 mmol, 0.0037 g) in methanol. The resulting solution was allowed to stand at room temperature. After two weeks good quality crystals with pale yellow colour were obtained and were dried in air.

Refinement

H atoms bound to C atoms were generated geometrically and refined as riding atoms with C—H = 0.93 Å and $U_{iso}(H) = 1.2 \times U_{eq}(C)$. H atoms bound to O atoms were found from difference maps and refined with distance restraints between 0.82—0.87 Å and $U_{iso}(H) = 1.5 \times U_{eq}(O)$.

Figures

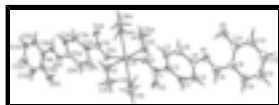


Fig. 1. View of the molecular structure of (I), showing the labelling of the non-H atoms and atomic displacement parameters at the 30% probability level. [Symmetry code: A) $-x+2, -y+1, -z+3$.]

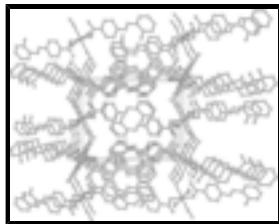


Fig. 2. View of the packing of the structure of (I), showing intermolecular hydrogen bonding (dotted lines). H atoms have been omitted for clarity.

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Crystal data

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$M_r = 721.04$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 15.564\ (3)\ \text{\AA}$

$b = 11.937\ (2)\ \text{\AA}$

$c = 8.8946\ (18)\ \text{\AA}$

$\beta = 99.69\ (3)^\circ$

$V = 1629.0\ (6)\ \text{\AA}^3$

$Z = 2$

$F(000) = 740$

$D_x = 1.470\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3109 reflections

$\theta = 2.2\text{--}28.0^\circ$

$\mu = 0.73\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Prism, pale yellow

$0.21 \times 0.19 \times 0.16\ \text{mm}$

Data collection

Rigaku Saturn
diffractometer

Radiation source: fine-focus sealed tube
graphite

Detector resolution: $28.5714\ \text{pixels mm}^{-1}$
 ω scans

Absorption correction: multi-scan
(*CrystalClear*; Rigaku/MSC, 2006)

$T_{\min} = 0.862$, $T_{\max} = 0.892$

7793 measured reflections

2760 independent reflections

2137 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.055$

$\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 2.2^\circ$

$h = -18 \rightarrow 18$

$k = -14 \rightarrow 10$

$l = -10 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.072$

$wR(F^2) = 0.166$

$S = 1.13$

2760 reflections

202 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0483P)^2 + 5.4285P]$

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

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

$\Delta\rho_{\max} = 0.97\ \text{e \AA}^{-3}$

0 restraints

$$\Delta\rho_{\min} = -0.63 \text{ e } \text{\AA}^{-3}$$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	1.0000	0.5000	1.5000	0.0478 (3)
N1	0.5587 (4)	0.4273 (6)	0.7851 (7)	0.0592 (17)
O1	0.8888 (4)	0.4749 (4)	1.3094 (6)	0.0591 (15)
O2	0.9173 (4)	0.3047 (4)	1.2333 (7)	0.0740 (18)
O3	1.0768 (4)	0.5897 (4)	1.3338 (6)	0.0684 (16)
H3	1.0698	0.6603	1.3269	0.103*
O4	1.0614 (3)	0.3361 (4)	1.4350 (6)	0.0605 (14)
H4	1.0252	0.3053	1.3620	0.091*
O5	0.4108 (4)	0.5348 (5)	0.7011 (8)	0.0810 (19)
H5	0.4577	0.5198	0.7542	0.122*
C1	0.8710 (5)	0.3913 (6)	1.2257 (8)	0.0513 (18)
C2	0.7912 (5)	0.3969 (6)	1.1089 (7)	0.0467 (17)
C3	0.7585 (5)	0.3037 (6)	1.0221 (9)	0.062 (2)
H3A	0.7881	0.2358	1.0373	0.075*
C4	0.6827 (5)	0.3101 (6)	0.9135 (9)	0.066 (2)
H4A	0.6622	0.2472	0.8570	0.079*
C5	0.6378 (5)	0.4124 (6)	0.8902 (8)	0.0519 (19)
C6	0.6693 (5)	0.5042 (7)	0.9765 (9)	0.061 (2)
H6	0.6398	0.5722	0.9619	0.073*
C7	0.7443 (6)	0.4964 (6)	1.0843 (8)	0.062 (2)
H7	0.7638	0.5592	1.1419	0.074*
C8	0.5382 (5)	0.3639 (7)	0.6702 (9)	0.063 (2)
H8	0.5776	0.3100	0.6491	0.076*
C9	0.4532 (5)	0.3738 (7)	0.5696 (9)	0.059 (2)
C10	0.4316 (6)	0.2979 (8)	0.4527 (10)	0.076 (3)
H10	0.4725	0.2449	0.4347	0.092*
C11	0.3504 (7)	0.2990 (8)	0.3616 (11)	0.084 (3)
H11	0.3353	0.2445	0.2870	0.101*
C12	0.2932 (6)	0.3808 (9)	0.3826 (11)	0.082 (3)
H12	0.2400	0.3841	0.3170	0.099*
C13	0.3112 (6)	0.4603 (8)	0.4994 (11)	0.076 (3)

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H13	0.2700	0.5136	0.5149	0.091*
C14	0.3917 (6)	0.4568 (7)	0.5904 (9)	0.062 (2)
C15	1.0839 (5)	0.5457 (5)	1.1902 (7)	0.091 (3)
H15A	1.1181	0.5955	1.1392	0.137*
H15B	1.0269	0.5378	1.1305	0.137*
H15C	1.1118	0.4738	1.2027	0.137*
C16	1.1049 (5)	0.2536 (5)	1.5305 (7)	0.079 (3)
H16A	1.1236	0.1942	1.4708	0.118*
H16B	1.0663	0.2241	1.5943	0.118*
H16C	1.1547	0.2867	1.5931	0.118*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0584 (5)	0.0351 (4)	0.0469 (4)	0.0027 (4)	0.0006 (3)	-0.0028 (3)
N1	0.055 (4)	0.069 (4)	0.053 (4)	0.000 (3)	0.004 (3)	0.003 (3)
O1	0.064 (4)	0.047 (3)	0.061 (3)	0.006 (2)	-0.005 (3)	-0.015 (2)
O2	0.073 (4)	0.047 (3)	0.090 (4)	0.010 (3)	-0.022 (3)	-0.015 (3)
O3	0.098 (5)	0.048 (3)	0.063 (3)	-0.011 (3)	0.023 (3)	0.006 (2)
O4	0.063 (4)	0.043 (3)	0.069 (3)	0.011 (2)	-0.006 (3)	-0.008 (2)
O5	0.064 (4)	0.086 (4)	0.094 (5)	0.018 (3)	0.015 (4)	-0.003 (3)
C1	0.060 (5)	0.047 (4)	0.046 (4)	-0.004 (4)	0.005 (4)	0.000 (3)
C2	0.045 (4)	0.054 (4)	0.041 (4)	-0.008 (3)	0.006 (3)	-0.001 (3)
C3	0.066 (6)	0.046 (4)	0.069 (5)	0.001 (4)	-0.004 (4)	-0.003 (4)
C4	0.066 (6)	0.053 (4)	0.068 (5)	-0.007 (4)	-0.018 (4)	-0.006 (4)
C5	0.051 (5)	0.060 (5)	0.045 (4)	-0.001 (4)	0.006 (4)	0.008 (3)
C6	0.064 (5)	0.059 (4)	0.056 (5)	0.006 (4)	-0.001 (4)	0.000 (4)
C7	0.085 (6)	0.050 (4)	0.045 (4)	0.000 (4)	-0.007 (4)	0.001 (3)
C8	0.057 (5)	0.067 (5)	0.065 (5)	0.004 (4)	0.008 (4)	0.003 (4)
C9	0.043 (5)	0.070 (5)	0.060 (5)	-0.007 (4)	0.001 (4)	0.013 (4)
C10	0.078 (7)	0.072 (6)	0.074 (6)	-0.002 (5)	-0.002 (5)	-0.003 (5)
C11	0.078 (7)	0.082 (7)	0.085 (7)	-0.013 (6)	-0.007 (6)	-0.007 (5)
C12	0.061 (6)	0.097 (7)	0.082 (7)	-0.010 (5)	-0.010 (5)	0.022 (6)
C13	0.056 (6)	0.085 (6)	0.085 (7)	0.011 (5)	0.005 (5)	0.013 (5)
C14	0.057 (6)	0.076 (5)	0.055 (5)	-0.009 (4)	0.012 (4)	0.000 (4)
C15	0.137 (10)	0.059 (5)	0.084 (7)	0.012 (6)	0.036 (7)	0.005 (5)
C16	0.085 (7)	0.055 (5)	0.096 (7)	0.023 (5)	0.016 (6)	0.020 (5)

Geometric parameters (\AA , $^\circ$)

Cd1—O1	2.230 (5)	C5—C6	1.380 (10)
Cd1—O1 ⁱ	2.230 (5)	C6—C7	1.384 (11)
Cd1—O4 ⁱ	2.295 (5)	C6—H6	0.9300
Cd1—O4	2.295 (5)	C7—H7	0.9300
Cd1—O3 ⁱ	2.315 (5)	C8—C9	1.472 (10)
Cd1—O3	2.315 (5)	C8—H8	0.9300
N1—C8	1.270 (9)	C9—C10	1.377 (11)
N1—C5	1.425 (9)	C9—C14	1.412 (11)

O1—C1	1.248 (8)	C10—C11	1.382 (12)
O2—C1	1.255 (8)	C10—H10	0.9300
O3—C15	1.403 (8)	C11—C12	1.356 (13)
O3—H3	0.8507	C11—H11	0.9300
O4—C16	1.398 (7)	C12—C13	1.401 (13)
O4—H4	0.8668	C12—H12	0.9300
O5—C14	1.352 (10)	C13—C14	1.373 (12)
O5—H5	0.8200	C13—H13	0.9300
C1—C2	1.481 (9)	C15—H15A	0.9600
C2—C7	1.391 (10)	C15—H15B	0.9600
C2—C3	1.400 (9)	C15—H15C	0.9600
C3—C4	1.395 (10)	C16—H16A	0.9600
C3—H3A	0.9300	C16—H16B	0.9599
C4—C5	1.405 (10)	C16—H16C	0.9601
C4—H4A	0.9300		
O1—Cd1—O1 ⁱ	180.000 (1)	C5—C6—C7	120.7 (7)
O1—Cd1—O4 ⁱ	90.19 (17)	C5—C6—H6	119.6
O1 ⁱ —Cd1—O4 ⁱ	89.81 (17)	C7—C6—H6	119.6
O1—Cd1—O4	89.81 (17)	C6—C7—C2	121.7 (7)
O1 ⁱ —Cd1—O4	90.19 (17)	C6—C7—H7	119.1
O4 ⁱ —Cd1—O4	180.000 (1)	C2—C7—H7	119.1
O1—Cd1—O3 ⁱ	90.3 (2)	N1—C8—C9	121.4 (8)
O1 ⁱ —Cd1—O3 ⁱ	89.7 (2)	N1—C8—H8	119.3
O4 ⁱ —Cd1—O3 ⁱ	87.23 (19)	C9—C8—H8	119.3
O4—Cd1—O3 ⁱ	92.77 (19)	C10—C9—C14	118.4 (8)
O1—Cd1—O3	89.7 (2)	C10—C9—C8	119.1 (8)
O1 ⁱ —Cd1—O3	90.3 (2)	C14—C9—C8	122.5 (8)
O4 ⁱ —Cd1—O3	92.77 (19)	C9—C10—C11	121.3 (9)
O4—Cd1—O3	87.23 (19)	C9—C10—H10	119.4
O3 ⁱ —Cd1—O3	180.000 (1)	C11—C10—H10	119.4
C8—N1—C5	121.8 (7)	C12—C11—C10	118.9 (9)
C1—O1—Cd1	128.8 (5)	C12—C11—H11	120.5
C15—O3—Cd1	122.5 (4)	C10—C11—H11	120.5
C15—O3—H3	109.5	C11—C12—C13	122.4 (9)
Cd1—O3—H3	115.5	C11—C12—H12	118.8
C16—O4—Cd1	128.8 (4)	C13—C12—H12	118.8
C16—O4—H4	110.1	C14—C13—C12	117.7 (9)
Cd1—O4—H4	107.7	C14—C13—H13	121.1
C14—O5—H5	109.5	C12—C13—H13	121.1
O1—C1—O2	124.0 (7)	O5—C14—C13	118.4 (9)
O1—C1—C2	117.3 (7)	O5—C14—C9	120.5 (7)
O2—C1—C2	118.7 (6)	C13—C14—C9	121.0 (8)
C7—C2—C3	117.3 (7)	O3—C15—H15A	109.5
C7—C2—C1	120.3 (6)	O3—C15—H15B	109.5
C3—C2—C1	122.3 (7)	H15A—C15—H15B	109.5
C4—C3—C2	121.6 (7)	O3—C15—H15C	109.5

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C4—C3—H3A	119.2	H15A—C15—H15C	109.5
C2—C3—H3A	119.2	H15B—C15—H15C	109.5
C3—C4—C5	119.4 (7)	O4—C16—H16A	110.1
C3—C4—H4A	120.3	O4—C16—H16B	109.4
C5—C4—H4A	120.3	H16A—C16—H16B	109.5
C6—C5—C4	119.1 (7)	O4—C16—H16C	108.9
C6—C5—N1	116.9 (7)	H16A—C16—H16C	109.5
C4—C5—N1	124.0 (7)	H16B—C16—H16C	109.5
O4 ⁱ —Cd1—O1—C1	-171.4 (7)	C3—C4—C5—N1	-178.4 (7)
O4—Cd1—O1—C1	8.6 (7)	C8—N1—C5—C6	157.7 (8)
O3 ⁱ —Cd1—O1—C1	-84.2 (7)	C8—N1—C5—C4	-24.4 (12)
O3—Cd1—O1—C1	95.8 (7)	C4—C5—C6—C7	0.2 (12)
O1—Cd1—O3—C15	-47.5 (5)	N1—C5—C6—C7	178.2 (7)
O1 ⁱ —Cd1—O3—C15	132.5 (5)	C5—C6—C7—C2	0.8 (13)
O4 ⁱ —Cd1—O3—C15	-137.7 (5)	C3—C2—C7—C6	-1.3 (12)
O4—Cd1—O3—C15	42.3 (5)	C1—C2—C7—C6	-179.8 (7)
O1—Cd1—O4—C16	-140.8 (6)	C5—N1—C8—C9	174.8 (7)
O1 ⁱ —Cd1—O4—C16	39.2 (6)	N1—C8—C9—C10	-175.5 (8)
O3 ⁱ —Cd1—O4—C16	-50.5 (6)	N1—C8—C9—C14	3.0 (13)
O3—Cd1—O4—C16	129.5 (6)	C14—C9—C10—C11	-2.9 (13)
Cd1—O1—C1—O2	-2.5 (12)	C8—C9—C10—C11	175.6 (8)
Cd1—O1—C1—C2	178.8 (5)	C9—C10—C11—C12	4.0 (15)
O1—C1—C2—C7	6.8 (11)	C10—C11—C12—C13	-4.0 (16)
O2—C1—C2—C7	-171.9 (8)	C11—C12—C13—C14	3.0 (15)
O1—C1—C2—C3	-171.6 (7)	C12—C13—C14—O5	178.3 (8)
O2—C1—C2—C3	9.7 (11)	C12—C13—C14—C9	-1.9 (14)
C7—C2—C3—C4	1.0 (12)	C10—C9—C14—O5	-178.3 (8)
C1—C2—C3—C4	179.4 (7)	C8—C9—C14—O5	3.2 (13)
C2—C3—C4—C5	-0.1 (13)	C10—C9—C14—C13	1.9 (13)
C3—C4—C5—C6	-0.5 (12)	C8—C9—C14—C13	-176.6 (8)

Symmetry codes: (i) $-x+2, -y+1, -z+3$.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O4—H4 \cdots O2	0.87	1.87	2.653 (7)	150
O5—H5 \cdots N1	0.82	1.90	2.632 (9)	148
O3—H3 \cdots O2 ⁱⁱ	0.85	1.83	2.640 (7)	160

Symmetry codes: (ii) $-x+2, y+1/2, -z+5/2$.

Fig. 1

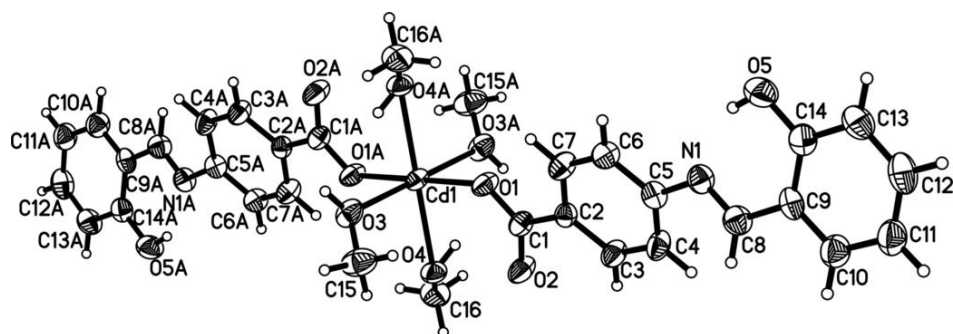


Fig. 2

