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Bis[4-hydroxy-*N*′-(4-methoxy-2-oxidobenzylidene-κO^2)benzohydrazidato-$\kappa^2 O,N'$]cadmium(II) dimethyl sulfoxide disolvate

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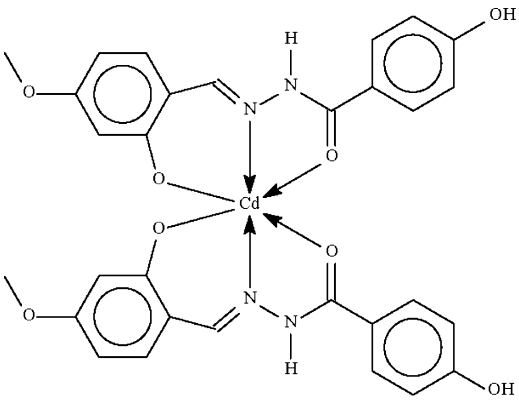
Key indicators: single-crystal X-ray study; T = 118 K; mean σ(C–C) = 0.009 Å; R factor = 0.059; wR factor = 0.153; data-to-parameter ratio = 15.4.

The metal atom in the title compound, $[Cd(C_{15}H_{13}N_2O_4)_2]\cdot 2C_2H_6OS$, is twice O,N,O'-chelated by two symmetry-related Schiff base ligands to define a *trans*-N_2O_4 octahedral geometry. Each anion occupies meridional sites of the octahedron; the metal atom lies on a special position of site symmetry 2. The dimethyl sulfoxide molecule is a hydrogen-bond acceptor to the –NH– unit, and O—H···O hydrogen bonds link molecules into a supramolecular chain.

Related literature

For the monohydrated Schiff base ligand, see: Mohd Lair *et al.* (2009).



Experimental

Crystal data

$[Cd(C_{15}H_{13}N_2O_4)_2]\cdot 2C_2H_6OS$
M_r = 839.20
Monoclinic, $C2/c$
a = 23.891 (2) Å
b = 10.439 (1) Å
c = 19.874 (1) Å
β = 132.137 (4)°
V = 3675.3 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.77 mm^{-1}
T = 118 K
0.12 × 0.06 × 0.03 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.507, T_{max} = 0.745
(expected range = 0.665–0.977)
10208 measured reflections
3243 independent reflections
2147 reflections with $I > 2\sigma(I)$
R_{int} = 0.103

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.153
S = 1.02
3243 reflections
211 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.90 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O1^{i}	0.84	1.79	2.603 (6)	163
N2—H2···O5	0.88	1.93	2.766 (6)	159

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

We thank the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2421).

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supplementary materials

Acta Cryst. (2009). E**65**, m541 [**doi:10.1107/S1600536809013774**]

Bis[4-hydroxy-*N*'-(4-methoxy-2-oxidobenzylidene-κO^2)benzohydrazidato-$\kappa^2 O,N'$]cadmium(II) dimethyl sulfoxide disolvate

N. Mohd Lair, H. Mohd Ali and S. W. Ng

Comment

(type here to add)

Experimental

4-Hydroxy-*N*'-(2-hydroxy-4-methoxybenzylidene)benzohydrazide monohydrate (0.30 g, 1 mmol) and cadmium diacetate (0.14 g, 0.5 mmol) were heated in ethanol (50 ml) for 4 h. The solvent was removed and the product was recrystallized from DMSO to give prismatic crystals.

Refinement

Owing to the small number of observed reflections, the aromatic rings were refined as rigid hexagons with sides of 1.39 Å in order to reduce the number of refined parameters. Hydrogen atoms were placed at calculated positions (C–H 0.95–0.98, N–H 0.88, O–H 0.84 Å) and were treated as riding on their parent carbon atoms, with U(H) set to 1.2–1.5 times U_{eq}(C,N,O). The final difference Fourier map had a large peak/deep hole in the vicinity of the Cd atom.

Figures

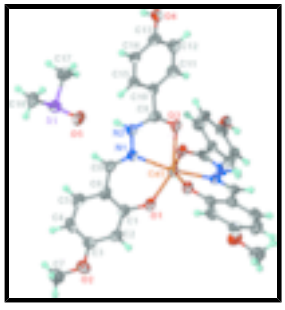


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $Cd(C_{15}H_{13}N_2O_4)_2{\cdot}2DMSO$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

Bis[4-hydroxy-*N*'-(4-methoxy-2-oxidobenzylidene- κO^2)benzohydrazidato-$\kappa^2 O,N'$]cadmium(II) dimethyl sulfoxide disolvate

Crystal data

$[Cd(C_{15}H_{13}N_2O_4)_2]{\cdot}2C_2H_6OS$	F_{000} = 1720
M_r = 839.20	D_x = 1.517 Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation λ = 0.71073 Å

Hall symbol: -C 2yc	Cell parameters from 638 reflections
a = 23.891 (2) Å	θ = 2.2–18.8º
b = 10.439 (1) Å	μ = 0.77 mm^{-1}
c = 19.874 (1) Å	T = 118 K
β = 132.137 (4)º	Prism, yellow
V = 3675.3 (4) Å^3	0.12 × 0.06 × 0.03 mm
Z = 4	

Data collection

Bruker SMART APEX diffractometer	3243 independent reflections
Radiation source: fine-focus sealed tube	2147 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.103
T = 118 K	θ_{max} = 25.0º
ω scans	θ_{min} = 2.1º
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	h = −28→28
T_{min} = 0.507, T_{max} = 0.745	k = −12→12
10208 measured reflections	l = −23→23

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.059	H-atom parameters constrained
$wR(F^2)$ = 0.153	$w = 1/[\sigma^2(F_o^2) + (0.0692P)^2 + 0.0136P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.001
3243 reflections	$\Delta\rho_{max}$ = 1.31 e Å^{-3}
211 parameters	$\Delta\rho_{min}$ = −0.90 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	0.5000	0.32500 (7)	0.7500	0.0253 (2)
S1	0.18289 (10)	0.48574 (18)	0.67220 (12)	0.0335 (5)
O1	0.4272 (2)	0.1893 (4)	0.6323 (3)	0.0276 (10)
O2	0.2426 (3)	−0.1133 (5)	0.4273 (3)	0.0373 (12)
O3	0.5137 (2)	0.4972 (4)	0.8391 (3)	0.0264 (10)
O4	0.4911 (2)	0.8669 (4)	1.0697 (3)	0.0304 (11)
H4	0.4624	0.8507	1.0791	0.046*
N1	0.3944 (3)	0.3437 (5)	0.7273 (3)	0.0227 (12)
N2	0.3971 (3)	0.4373 (5)	0.7788 (4)	0.0262 (13)
H2	0.3589	0.4493	0.7755	0.031*

O5	0.2603 (2)	0.4283 (5)	0.7353 (4)	0.0432 (13)
C1	0.35890 (17)	0.1366 (4)	0.5922 (3)	0.0261 (16)
C2	0.3336 (2)	0.0367 (4)	0.5313 (3)	0.0291 (16)
H2A	0.3643	0.0060	0.5204	0.035*
C3	0.2633 (2)	−0.0181 (4)	0.4865 (3)	0.0295 (16)
C4	0.21840 (18)	0.0268 (4)	0.5025 (3)	0.0339 (17)
H4A	0.1704	−0.0107	0.4719	0.041*
C5	0.2437 (2)	0.1267 (4)	0.5634 (3)	0.0326 (17)
H5	0.2130	0.1574	0.5743	0.039*
C6	0.3140 (2)	0.1815 (4)	0.6082 (3)	0.0286 (15)
C7	0.1732 (4)	−0.1797 (8)	0.3856 (5)	0.0438 (19)
H7A	0.1662	−0.2488	0.3471	0.066*
H7B	0.1309	−0.1196	0.3484	0.066*
H7C	0.1754	−0.2159	0.4328	0.066*
C8	0.3314 (4)	0.2851 (6)	0.6694 (5)	0.0269 (16)
H8	0.2915	0.3119	0.6658	0.032*
C9	0.4604 (4)	0.5100 (6)	0.8344 (4)	0.0269 (15)
C10	0.4616 (2)	0.6071 (4)	0.8911 (2)	0.0236 (15)
C11	0.5075 (2)	0.7141 (4)	0.9198 (3)	0.0289 (16)
H11	0.5330	0.7276	0.8990	0.035*
C12	0.5159 (2)	0.8012 (3)	0.9790 (3)	0.0314 (17)
H12	0.5472	0.8743	0.9986	0.038*
C13	0.4785 (2)	0.7813 (4)	1.0094 (3)	0.0282 (16)
C14	0.4326 (2)	0.6744 (4)	0.9807 (3)	0.0241 (14)
H14	0.4071	0.6609	1.0015	0.029*
C15	0.4242 (2)	0.5873 (3)	0.9215 (3)	0.0244 (15)
H15	0.3929	0.5142	0.9019	0.029*
C16	0.1442 (4)	0.4487 (8)	0.7214 (5)	0.0372 (18)
H16A	0.1335	0.3567	0.7154	0.056*
H16B	0.0974	0.4970	0.6902	0.056*
H16C	0.1805	0.4720	0.7858	0.056*
C17	0.1980 (4)	0.6515 (7)	0.6951 (5)	0.0424 (19)
H17A	0.2175	0.6882	0.6690	0.064*
H17B	0.2346	0.6653	0.7609	0.064*
H17C	0.1502	0.6932	0.6682	0.064*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0238 (4)	0.0338 (4)	0.0243 (4)	0.000	0.0186 (3)	0.000
S1	0.0368 (10)	0.0355 (11)	0.0337 (11)	−0.0019 (8)	0.0259 (9)	−0.0040 (9)
O1	0.025 (2)	0.037 (3)	0.027 (3)	0.000 (2)	0.019 (2)	0.000 (2)
O2	0.041 (3)	0.041 (3)	0.032 (3)	−0.010 (2)	0.026 (3)	−0.012 (2)
O3	0.025 (2)	0.035 (3)	0.029 (3)	−0.001 (2)	0.022 (2)	−0.003 (2)
O4	0.034 (3)	0.038 (3)	0.032 (3)	−0.007 (2)	0.028 (2)	−0.010 (2)
N1	0.024 (3)	0.026 (3)	0.020 (3)	−0.001 (2)	0.016 (2)	0.000 (2)
N2	0.030 (3)	0.033 (3)	0.025 (3)	0.000 (3)	0.022 (3)	−0.005 (3)
O5	0.035 (3)	0.042 (3)	0.061 (4)	0.004 (2)	0.036 (3)	0.002 (3)

C1	0.025 (3)	0.031 (4)	0.020 (4)	0.006 (3)	0.014 (3)	0.007 (3)
C2	0.034 (4)	0.033 (4)	0.027 (4)	0.007 (3)	0.024 (3)	0.002 (3)
C3	0.037 (4)	0.025 (4)	0.032 (4)	−0.003 (3)	0.025 (4)	0.000 (3)
C4	0.024 (3)	0.045 (5)	0.021 (4)	−0.012 (3)	0.010 (3)	−0.006 (3)
C5	0.030 (4)	0.044 (5)	0.026 (4)	0.005 (3)	0.019 (3)	0.003 (3)
C6	0.027 (3)	0.035 (4)	0.026 (4)	0.007 (3)	0.018 (3)	0.010 (4)
C7	0.047 (4)	0.044 (5)	0.035 (4)	−0.004 (4)	0.025 (4)	−0.002 (4)
C8	0.027 (4)	0.024 (4)	0.035 (4)	0.003 (3)	0.024 (3)	0.005 (3)
C9	0.027 (4)	0.027 (4)	0.022 (4)	0.007 (3)	0.015 (3)	0.006 (3)
C10	0.021 (3)	0.029 (4)	0.020 (4)	−0.002 (3)	0.014 (3)	0.000 (3)
C11	0.035 (4)	0.034 (4)	0.029 (4)	−0.001 (3)	0.026 (3)	−0.002 (3)
C12	0.033 (4)	0.036 (5)	0.035 (4)	−0.006 (3)	0.027 (3)	0.001 (3)
C13	0.035 (4)	0.033 (4)	0.022 (4)	0.005 (3)	0.021 (3)	0.002 (3)
C14	0.025 (3)	0.029 (4)	0.021 (3)	0.004 (3)	0.017 (3)	0.003 (3)
C15	0.026 (3)	0.026 (4)	0.020 (4)	−0.002 (3)	0.015 (3)	0.001 (3)
C16	0.031 (4)	0.051 (5)	0.037 (5)	−0.004 (3)	0.025 (4)	−0.006 (4)
C17	0.050 (4)	0.039 (5)	0.047 (5)	0.004 (4)	0.035 (4)	−0.001 (4)

Geometric parameters (Å, °)

Cd1—O1	2.246 (4)	C4—H4A	0.9500
Cd1—O1^{i}	2.246 (4)	C5—C6	1.3900
Cd1—N1^{i}	2.254 (5)	C5—H5	0.9500
Cd1—N1	2.254 (5)	C6—C8	1.464 (7)
Cd1—O3	2.386 (4)	C7—H7A	0.9800
Cd1—O3^{i}	2.386 (4)	C7—H7B	0.9800
S1—O5	1.497 (5)	C7—H7C	0.9800
S1—C17	1.764 (7)	C8—H8	0.9500
S1—C16	1.782 (6)	C9—C10	1.500 (7)
O1—C1	1.362 (5)	C10—C11	1.3900
O2—C3	1.355 (5)	C10—C15	1.3900
O2—C7	1.439 (8)	C11—C12	1.3900
O3—C9	1.221 (7)	C11—H11	0.9500
O4—C13	1.356 (5)	C12—C13	1.3900
O4—H4	0.8400	C12—H12	0.9500
N1—C8	1.280 (8)	C13—C14	1.3900
N1—N2	1.385 (7)	C14—C15	1.3900
N2—C9	1.356 (8)	C14—H14	0.9500
N2—H2	0.8800	C15—H15	0.9500
C1—C2	1.3900	C16—H16A	0.9800
C1—C6	1.3900	C16—H16B	0.9800
C2—C3	1.3900	C16—H16C	0.9800
C2—H2A	0.9500	C17—H17A	0.9800
C3—C4	1.3900	C17—H17B	0.9800
C4—C5	1.3900	C17—H17C	0.9800
O1—Cd1—O1^{i}	101.8 (2)	C5—C6—C8	112.7 (3)
O1—Cd1—N1^{i}	104.12 (16)	C1—C6—C8	127.3 (3)
O1^{i}—Cd1—N1^{i}	82.26 (16)	O2—C7—H7A	109.5

O1—Cd1—N1	82.26 (16)	O2—C7—H7B	109.5
O1^{i}—Cd1—N1	104.12 (16)	H7A—C7—H7B	109.5
N1^{i}—Cd1—N1	170.1 (3)	O2—C7—H7C	109.5
O1—Cd1—O3	150.75 (14)	H7A—C7—H7C	109.5
O1^{i}—Cd1—O3	94.45 (15)	H7B—C7—H7C	109.5
N1^{i}—Cd1—O3	102.05 (16)	N1—C8—C6	127.4 (5)
N1—Cd1—O3	70.17 (16)	N1—C8—H8	116.3
O1—Cd1—O3^{i}	94.45 (15)	C6—C8—H8	116.3
O1^{i}—Cd1—O3^{i}	150.75 (14)	O3—C9—N2	122.3 (6)
N1^{i}—Cd1—O3^{i}	70.17 (16)	O3—C9—C10	121.5 (6)
N1—Cd1—O3^{i}	102.05 (16)	N2—C9—C10	116.1 (5)
O3—Cd1—O3^{i}	82.3 (2)	C11—C10—C15	120.0
O5—S1—C17	104.7 (3)	C11—C10—C9	117.7 (3)
O5—S1—C16	104.9 (3)	C15—C10—C9	122.0 (4)
C17—S1—C16	99.3 (4)	C12—C11—C10	120.0
C1—O1—Cd1	130.6 (3)	C12—C11—H11	120.0
C3—O2—C7	117.6 (5)	C10—C11—H11	120.0
C9—O3—Cd1	114.2 (4)	C11—C12—C13	120.0
C13—O4—H4	109.5	C11—C12—H12	120.0
C8—N1—N2	116.5 (5)	C13—C12—H12	120.0
C8—N1—Cd1	128.4 (4)	O4—C13—C14	122.6 (3)
N2—N1—Cd1	114.9 (3)	O4—C13—C12	117.3 (3)
C9—N2—N1	118.2 (5)	C14—C13—C12	120.0
C9—N2—H2	120.9	C13—C14—C15	120.0
N1—N2—H2	120.9	C13—C14—H14	120.0
O1—C1—C2	117.6 (3)	C15—C14—H14	120.0
O1—C1—C6	122.4 (3)	C14—C15—C10	120.0
C2—C1—C6	120.0	C14—C15—H15	120.0
C1—C2—C3	120.0	C10—C15—H15	120.0
C1—C2—H2A	120.0	S1—C16—H16A	109.5
C3—C2—H2A	120.0	S1—C16—H16B	109.5
O2—C3—C2	116.1 (3)	H16A—C16—H16B	109.5
O2—C3—C4	123.9 (3)	S1—C16—H16C	109.5
C2—C3—C4	120.0	H16A—C16—H16C	109.5
C5—C4—C3	120.0	H16B—C16—H16C	109.5
C5—C4—H4A	120.0	S1—C17—H17A	109.5
C3—C4—H4A	120.0	S1—C17—H17B	109.5
C4—C5—C6	120.0	H17A—C17—H17B	109.5
C4—C5—H5	120.0	S1—C17—H17C	109.5
C6—C5—H5	120.0	H17A—C17—H17C	109.5
C5—C6—C1	120.0	H17B—C17—H17C	109.5
O1^{i}—Cd1—O1—C1	90.7 (4)	C3—C4—C5—C6	0.0
N1^{i}—Cd1—O1—C1	175.5 (4)	C4—C5—C6—C1	0.0
N1—Cd1—O1—C1	−12.2 (4)	C4—C5—C6—C8	180.0 (4)
O3—Cd1—O1—C1	−31.7 (6)	O1—C1—C6—C5	178.1 (4)
O3^{i}—Cd1—O1—C1	−113.8 (4)	C2—C1—C6—C5	0.0

O1—Cd1—O3—C9	24.1 (6)	O1—C1—C6—C8	−1.8 (6)
O1^{i}—Cd1—O3—C9	−99.9 (4)	C2—C1—C6—C8	−179.9 (5)
N1^{i}—Cd1—O3—C9	177.1 (4)	N2—N1—C8—C6	−178.8 (5)
N1—Cd1—O3—C9	3.5 (4)	Cd1—N1—C8—C6	6.1 (9)
O3^{i}—Cd1—O3—C9	109.4 (5)	C5—C6—C8—N1	171.3 (6)
O1—Cd1—N1—C8	2.3 (5)	C1—C6—C8—N1	−8.8 (9)
O1^{i}—Cd1—N1—C8	−97.9 (5)	Cd1—O3—C9—N2	−3.9 (8)
O3—Cd1—N1—C8	172.4 (6)	Cd1—O3—C9—C10	175.5 (4)
O3^{i}—Cd1—N1—C8	95.3 (5)	N1—N2—C9—O3	1.4 (9)
O1—Cd1—N1—N2	−172.8 (4)	N1—N2—C9—C10	−178.1 (5)
O1^{i}—Cd1—N1—N2	86.9 (4)	O3—C9—C10—C11	25.7 (7)
O3—Cd1—N1—N2	−2.8 (4)	N2—C9—C10—C11	−154.8 (4)
O3^{i}—Cd1—N1—N2	−79.9 (4)	O3—C9—C10—C15	−148.5 (5)
C8—N1—N2—C9	−173.7 (6)	N2—C9—C10—C15	31.0 (7)
Cd1—N1—N2—C9	2.1 (7)	C15—C10—C11—C12	0.0
Cd1—O1—C1—C2	−168.0 (3)	C9—C10—C11—C12	−174.3 (4)
Cd1—O1—C1—C6	13.8 (6)	C10—C11—C12—C13	0.0
O1—C1—C2—C3	−178.2 (4)	C11—C12—C13—O4	177.6 (4)
C6—C1—C2—C3	0.0	C11—C12—C13—C14	0.0
C7—O2—C3—C2	174.7 (5)	O4—C13—C14—C15	−177.4 (4)
C7—O2—C3—C4	−6.5 (7)	C12—C13—C14—C15	0.0
C1—C2—C3—O2	178.9 (5)	C13—C14—C15—C10	0.0
C1—C2—C3—C4	0.0	C11—C10—C15—C14	0.0
O2—C3—C4—C5	−178.8 (5)	C9—C10—C15—C14	174.1 (4)
C2—C3—C4—C5	0.0		

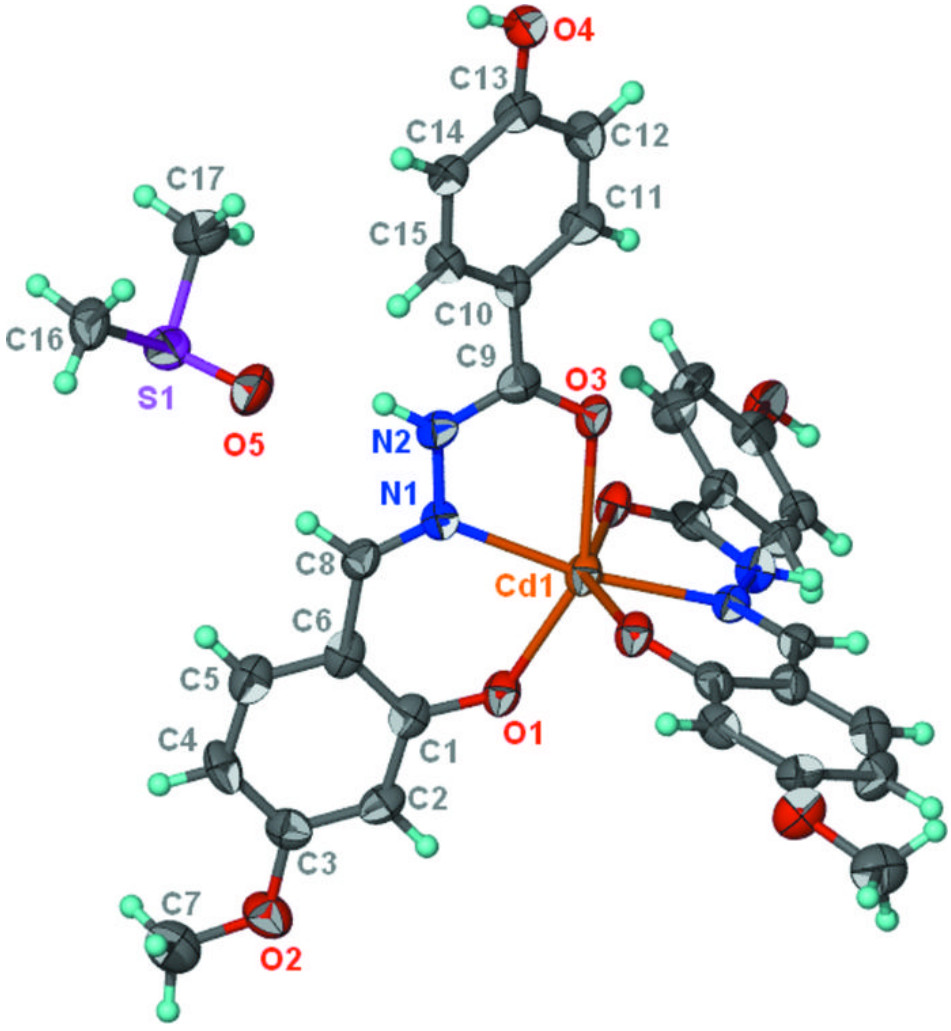
Symmetry codes: (i) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···O1^{ii}	0.84	1.79	2.603 (6)	163
N2—H2···O5	0.88	1.93	2.766 (6)	159

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

Fig. 1


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