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Bis[6,6′-dimethoxy-2,2′-(ethane-1,2-diyldiimino-dimethylene)diphenolato-κ^2N,N',O,O']cerium(IV)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.009 Å
Disorder in main residue
R factor = 0.041
wR factor = 0.090
Data-to-parameter ratio = 14.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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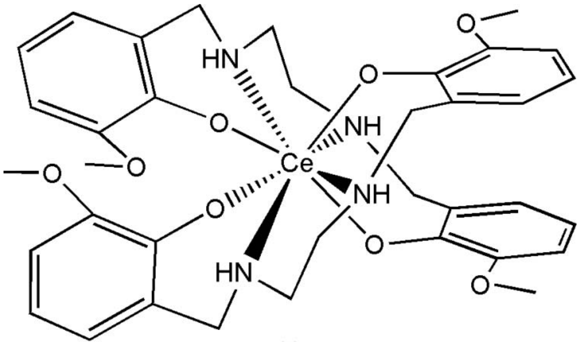
In the title compound, [Ce($C_{18}H_{22}N_2O_4$)$_2$], the Ce atoms are eight-coordinate and there are three independent molecules in the asymmetric unit. Two tetradentate *N*,*N*′-(2-hydroxy-3-methoxybenzyl)ethane-1,2-diamine ligands are coordinated to each Ce^{IV} atom. The molecules are linked into a chain by three C—H···O hydrogen bonds. Neighbouring chains are connected by van der Waals forces, resulting in a three-dimensional network.

Comment

Diamine derivatives are potentially multidentate ligands. We have focused our investigations on *o*-vanillin diamine derivatives and the coordination chemistry of *o*-vanillin diamine derivatives with metals. Having reported the ligand of the title complex (Xia *et al.*, 2006), we report here the crystal structure of the title complex, (I) (Fig. 1).



(I)

In the title complex (I), the cerium(IV) centre is eight-coordinated by four N atoms and four O atoms of two *N*,*N*′-(2-hydroxy-3-methoxybenzyl)ethane-1,2-diamine ligands (Table 1). The asymmetric unit consists of three molecules. The intramolecular dihedral angles between benzene rings range from 9.6 (2) to 38.3 (2)°.

The molecules of (I) are linked by C—H···O hydrogen bonds (Fig. 2 and Table 2) into a chain parallel to the *c* axis. Neighbouring chains are linked into a three-dimensional network by van der Waals forces.

Experimental

A solution of cerium(IV) nitrate (1 mmol) in ethanol (10 ml) was added to a solution of 6,6′-dimethoxy-2,2′-(ethane-1,2-diyldiimino-dimethylene)diphenol (2 mmol) in ethanol (20 ml). The reaction mixture was stirred for 3 h in air and then filtered. X-ray quality crystals of (I) were obtained by evaporation of an ethanol solution

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Crystal data

$[Ce(C_{18}H_{22}N_2O_4)_2]$
$M_r = 800.87$
Monoclinic, $P2_1/c$
$a = 23.166\ (3)$ Å
$b = 17.803\ (2)$ Å
$c = 27.883\ (4)$ Å
$\beta = 110.116\ (3)°$
$V = 10798\ (2)$ Å^3
$Z = 12$
$D_x = 1.478$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.32$ mm^{-1}
$T = 298\ (2)$ K
Block, dark red
0.39 × 0.35 × 0.32 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.627$, $T_{max} = 0.677$
53789 measured reflections
18893 independent reflections
9384 reflections with $I > 2\sigma(I)$
$R_{int} = 0.087$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.090$
$S = 0.94$
18893 reflections
1328 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0235P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.40$ e Å^{-3}
$\Delta\rho_{min} = -1.02$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Ce1—O7	2.184 (4)	Ce2—N7	2.610 (4)
Ce1—O1	2.192 (3)	Ce2—N5	2.617 (4)
Ce1—O3	2.205 (3)	Ce2—N8	2.619 (4)
Ce1—O5	2.207 (4)	Ce2—N6	2.624 (4)
Ce1—N2	2.611 (4)	Ce3—O17	2.177 (4)
Ce1—N3	2.612 (4)	Ce3—O19	2.189 (4)
Ce1—N1	2.649 (4)	Ce3—O21	2.207 (3)
Ce1—N4	2.656 (4)	Ce3—O23	2.215 (3)
Ce2—O9	2.198 (3)	Ce3—N10	2.613 (5)
Ce2—O11	2.200 (4)	Ce3—N11	2.616 (4)
Ce2—O13	2.205 (3)	Ce3—N12	2.626 (4)
Ce2—O15	2.211 (3)	Ce3—N9	2.636 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
C26—H26B···O17^{i}	0.96	2.54	3.358 (7)	143
C16—H16B···O19^{ii}	0.96	2.60	3.411 (7)	143
C55—H55A···O6^{ii}	0.97	2.69	3.634 (6)	166

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

All H atoms were treated as riding atoms, with C—H = 0.93–0.97 Å, and N—H = 0.91 Å, and with $U_{iso}(H) = 1.2U_{eq}$(aryl and methylene C, and N) [C—H = 0.96 Å and with $U_{iso}(H) = 1.5U_{eq}$(C) for methyl groups]. The methyl groups bonded to O24 are disordered over two sites. The coordinates of these two sites were refined with the occupancies tied to sum to unity. The site occupancies for C06A and attached H atoms and C06B and attached H atoms refined to 0.62 (1) and 0.38 (1), respectively.The highest peak in the final difference map is located 0.89 Å from atom Ce3 and the deepest hole is located 0.82 Å from atom Ce3.

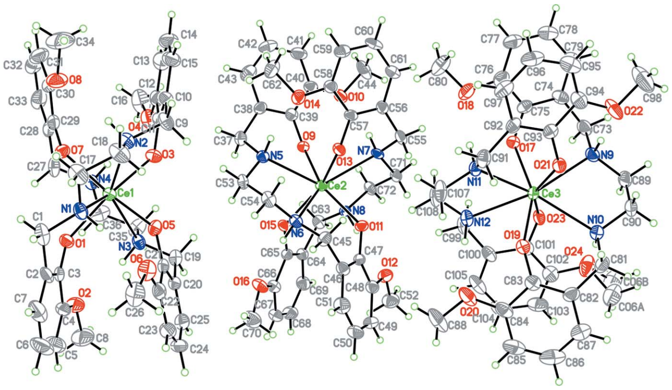

Figure 1
The asymmetric unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. Only one disorder component is shown.

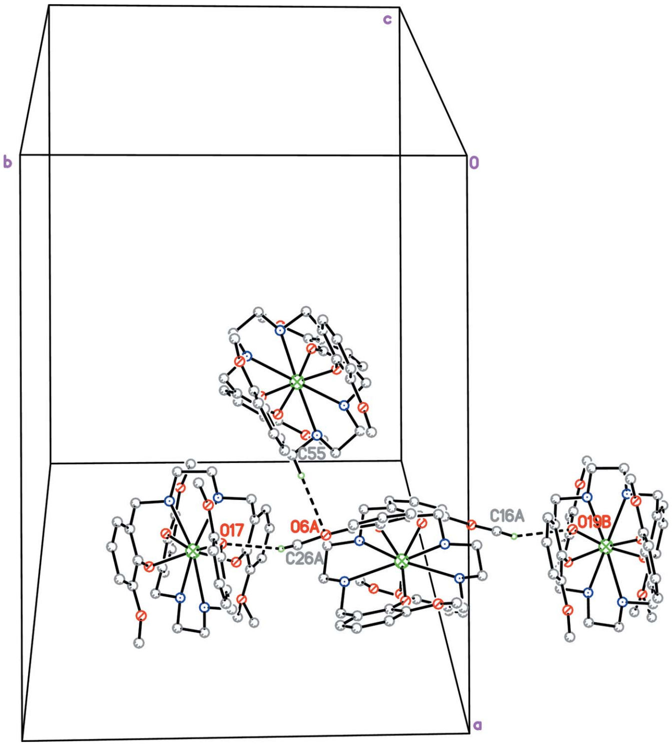

Figure 2
A portion of the crystal structure of (I), showing the formation of a hydrogen-bonded chain built from C—H···O interactions (dashed lines). For clarity, H atoms not involved in hydrogen bonds have been omitted and only one disorder component is shown. [Symmetry codes: (A) $1-x, -\frac{1}{2}+y, \frac{1}{2}-z$; (B) $x, -1+y, z$.]

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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