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Crystal structure of *N,N'*-(2-hydroxypropane-1,3-diyl)bis(pyridine-2-alimine)- $\kappa^5 N,N',N'',N''',O$]-tris(nitrato- $\kappa^2 O,O'$) cerium(III), $C_{15}H_{16}CeN_7O_{10}$

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.50 × 0.36 × 0.35 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	2.15 mm ⁻¹
Diffractometer, scan mode:	AFC10/Saturn724+, φ and ω
$\theta_{\max}$, completeness:	30.0°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	23,110, 6365, 0.032
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 5978
$N(\text{param})_{\text{refined}}$:	302
Programs:	CrystalClear [1], Olex2 [2], SHELX [3]

Source of material

1,3-Bis(2-pyridylmethyleneamino)-2-propanol (HL) ligand was synthesized according to a literature procedure [4]. An acetonitrile solution (20 mL) of $CeCl_3 \cdot 6H_2O$ (0.043 g, 0.2 mmol) was added $NaNO_3$ (0.051 g, 0.6 mmol) and then an acetonitrile solution (20 mL) of HL (0.051 g, 0.2 mmol) was added dropwise. The resulting solution was stirred for 3 h and then filtered. Light-yellow crystals were obtained by slow evaporation of the filtrate after four weeks. **Yield:** 92 mg (64 %). **Anal.** $C_{15}H_{16}CeN_7O_{10}$, 594.47 g/mol): C, 30.31; H, 2.71; N, 16.49. Found: C, 30.44; H, 2.84; N, 16.62%. **FT-IR** (KBr pellet, cm^{-1}): 3385(s/br), 1657(s), 1464(br), 1306(s), 1038(s), 820(w).

Experimental details

Hydrogen atoms were idealized and refined using rigid groups (with the SHELX program [3]).

Comment

Schiff bases have been extensively used for the synthesis of transition metal complexes. Mononuclear, binuclear and polynuclear transition metal complexes have been prepared and characterized [5–7]. Till now, only several mononuclear lanthanide complexes of Schiff ligands

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Abstract

$C_{15}H_{16}CeN_7O_{10}$, monoclinic, $P2_1/n$ (no. 14), $a = 7.8762(12)$ Å, $b = 21.330(3)$ Å, $c = 13.181(2)$ Å, $\beta = 99.536(2)^\circ$, $V = 2183.8(6)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0285$, $wR_{\text{ref}}(F^2) = 0.0523$, $T = 103$ K.

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The molecular structure is shown in the Figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	U _{iso} [*] /U _{eq}
Ce1	0.30692 (2)	0.65738 (2)	0.20102 (2)	0.00992 (3)
O1	0.17118 (19)	0.75521 (7)	0.09297 (13)	0.0145 (3)
O2	0.4799 (2)	0.76431 (8)	0.24201 (12)	0.0208 (3)
O3	0.4734 (2)	0.70351 (8)	0.37223 (12)	0.0182 (3)
O4	0.6511 (2)	0.78244 (8)	0.38658 (12)	0.0183 (3)
O5	0.4501 (2)	0.69399 (8)	0.04382 (12)	0.0175 (3)
O6	0.3797 (3)	0.59627 (8)	0.04383 (14)	0.0279 (4)
O7	0.5169 (2)	0.63187 (9)	−0.07466 (13)	0.0282 (4)
O8	0.6455 (2)	0.64563 (8)	0.22591 (13)	0.0195 (3)
O9	0.5106 (2)	0.57112 (8)	0.28982 (14)	0.0220 (4)
O10	0.7908 (2)	0.57080 (9)	0.31350 (15)	0.0283 (4)
N1	0.1506 (2)	0.54200 (9)	0.16693 (14)	0.0156 (4)
N2	−0.0181 (2)	0.65209 (9)	0.10659 (14)	0.0135 (3)
N3	0.0851 (2)	0.72711 (9)	0.28013 (14)	0.0159 (4)
N4	0.1955 (3)	0.61797 (9)	0.37868 (15)	0.0179 (4)
N5	0.5368 (2)	0.75083 (8)	0.33349 (14)	0.0138 (3)
N6	0.4503 (2)	0.64061 (10)	0.00202 (15)	0.0179 (4)
N7	0.6500 (3)	0.59462 (9)	0.27747 (14)	0.0156 (4)
C1	0.2269 (3)	0.48667 (11)	0.1885 (2)	0.0261 (5)
H1A	0.3470	0.4861	0.2139	0.031*
C2	0.1397 (4)	0.42971 (12)	0.1757 (2)	0.0300 (6)
H2	0.1997	0.3915	0.1924	0.036*
C3	−0.0343 (4)	0.42937 (11)	0.1387 (2)	0.0261 (5)
H3	−0.0972	0.3912	0.1313	0.031*
C4	−0.1151 (3)	0.48598 (11)	0.11260 (19)	0.0212 (5)
H4	−0.2344	0.4874	0.0851	0.025*
C5	−0.0189 (3)	0.54075 (10)	0.12722 (17)	0.0150 (4)
C6	−0.1019 (3)	0.60088 (11)	0.09589 (17)	0.0159 (4)
H6	−0.2207	0.6016	0.0670	0.019*
C7	−0.1129 (3)	0.70985 (10)	0.07100 (17)	0.0158 (4)
H7A	−0.2221	0.7116	0.0989	0.019*
H7B	−0.1411	0.7098	−0.0050	0.019*
C8	−0.0034 (3)	0.76679 (10)	0.10696 (17)	0.0149 (4)
H8	−0.0492	0.8043	0.0657	0.018*
C9	0.0077 (3)	0.78097 (11)	0.22065 (18)	0.0208 (5)
H9A	0.0789	0.8188	0.2389	0.025*
H9B	−0.1088	0.7890	0.2366	0.025*
C10	0.0271 (3)	0.71220 (11)	0.36152 (17)	0.0176 (4)
H10	−0.0598	0.7372	0.3835	0.021*
C11	0.0928 (3)	0.65723 (11)	0.42135 (17)	0.0163 (4)
C12	0.0474 (4)	0.64682 (13)	0.5178 (2)	0.0272 (6)
H12	−0.0243	0.6757	0.5457	0.033*
C13	0.1085 (4)	0.59372 (15)	0.5723 (2)	0.0379 (7)
H13	0.0801	0.5856	0.6383	0.046*
C14	0.2112 (4)	0.55284 (14)	0.5288 (2)	0.0369 (7)
H14	0.2534	0.5157	0.5640	0.044*
C15	0.2522 (4)	0.56669 (12)	0.4328 (2)	0.0280 (6)
H15	0.3241	0.5384	0.4039	0.034*
H1	0.175 (4)	0.7499 (15)	0.031 (3)	0.037 (9)*

based on 2-pyridinecarbaldehyde have been synthesized [8]. Schiff bases like HL are able to coordinate in a pentadentate mode.

The thermal ellipsoid plot of the title complex is shown in the figure. The structure of [Ce(HL)(NO₃)₃] is composed of a cerium(III), one HL and three nitrate ligands. The central cerium(III) is 11-coordinated with five atoms (N1, N2, N3, N4, O1) of HL and six oxygen atoms (O2, O3, O5, O6, O8, O9) from three bidentate coordinating nitrates. In this complex HL is not deprotonated as expected and exhibits a bent coordination with the angle between the two pyridine rings to be 80.5°. The Ce–O (hydroxyl) distance is 2.6498(16) Å. The two imine nitrogen atoms of HL form shorter bonds at 2.6572(18) Å for Ce1–N2 and 2.6375(19) Å for Ce1–N3, while the pyridine nitrogen atoms of HL form longer bonds at 2.7551(18) Å for Ce1–N1 and 2.7643(19) Å for Ce1–N4. The bond angles of the pentadentate ligand HL around the cerium(III) are 61.05(6)° for N1–Ce–N2, 60.66(5)° for O1–Ce–N2, 62.20(5)° for O1–Ce–N3 and 60.82(6)° for N3–Ce–N4 [8]. The six Ce–O distances from the nitrates are in the range of 2.5897(17) Å to 2.6657(17) Å [9]. 1-D chains are formed by intermolecular hydrogen bonds involving the OH group and the coordinated nitrate anions [O1–H...O4, d(D...A) = 2.816 Å].

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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