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Diaquatris(nicotinato-*κO*)bis(1,10-phenanthroline-κ^2N,N')cerium(III) trihydrate

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean *σ*(C–C) = 0.006 Å
R factor = 0.034
wR factor = 0.077
Data-to-parameter ratio = 14.4

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

In the title compound, $[Ce(C_6H_4NO_2)_3(C_{12}H_8N_2)_2(H_2O)_2]\cdot 3H_2O$, the Ce^{III} atom shows a capped trigonal prismatic N_4O_5 coordination. The Ce—O and Ce—N bond distances are 2.390 (2)–2.517 (2) and 2.730 (3)–2.752 (3) Å, respectively.

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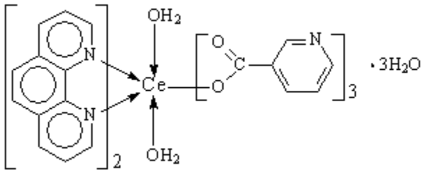
Comment

Diaquatris(nicotinato-*κO*)bis(1,10-phenanthroline-κ^2N,N')-cerium(III) trihydrate, (I) (Fig. 1), is isostructural with the neodymium(III) analog (Liu & Wang, 2004), the two structures featuring extensive hydrogen bonds (Table 2) that give rise to a layer motif. In (I), the Ce atom shows a capped trigonal prismatic coordination (Fig. 2). Selected bond lengths and angles are listed in Table 1.



(I)

Experimental

An aqueous solution (5 ml) of nicotinic acid (0.037 g, 0.3 mmol) was mixed with an aqueous solution (3 ml) of cerium chloride hexahy-

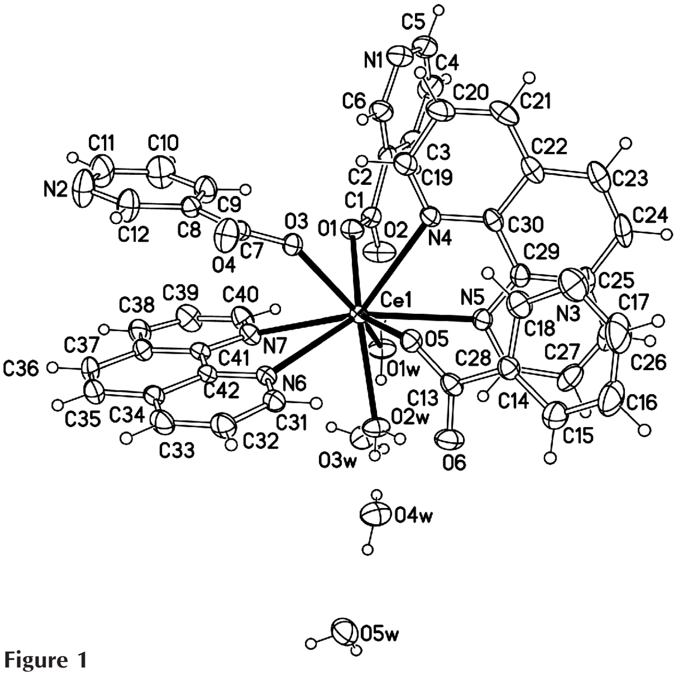


Figure 1
*ORTEP*II (Johnson, 1976) plot of (I), with displacement ellipsoids at the 30% probability level.

drate (0.035 g, 0.1 mmol) and an ethanol solution (5 ml) of 1,10-phenanthroline (0.054 g, 0.3 mmol). The mixture was filtered. Colorless crystals separated from the solution after several days (yield 31%).

Crystal data

$[Ce(C_6H_4NO_2)_3(C_{12}H_8N_2)_2(H_2O)_2]\cdot 3H_2O$
$M_r = 956.91$
Triclinic, $P\overline{1}$
$a = 9.058$ (1) Å
$b = 12.931$ (1) Å
$c = 17.879$ (1) Å
$\alpha = 85.011$ (1)°
$\beta = 80.643$ (1)°
$\gamma = 84.314$ (1)°
$V = 2050.8$ (3) Å^3
$Z = 2$
$D_x = 1.550$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 976 reflections
$\theta = 1.9$–24.3°
$\mu = 1.18$ mm^{-1}
$T = 295$ (2) K
Prism, colorless
0.22 × 0.20 × 0.18 mm

Data collection

Bruker SMART area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.781$, $T_{max} = 0.816$
11983 measured reflections
8380 independent reflections
6984 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 26.5°$
$h = -11 \rightarrow 8$
$k = -16 \rightarrow 16$
$l = -22 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.077$
$S = 1.03$
8380 reflections
580 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0282P)^2 + 1.2625P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.56$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ce1—O1	2.497 (2)	Ce1—N4	2.750 (3)
Ce1—O3	2.390 (2)	Ce1—N5	2.733 (3)
Ce1—O5	2.517 (2)	Ce1—N6	2.752 (3)
Ce1—O1*w*	2.517 (2)	Ce1—N7	2.730 (3)
Ce1—O2*w*	2.508 (2)		
O1—Ce1—O3	78.5 (1)	O5—Ce1—N5	68.3 (1)
O1—Ce1—O5	138.7 (1)	O5—Ce1—N6	76.3 (1)
O1—Ce1—O1*w*	70.5 (1)	O5—Ce1—N7	135.9 (1)
O1—Ce1—O2*w*	139.8 (1)	O1*w*—Ce1—O2*w*	69.5 (1)
O1—Ce1—N4	68.8 (1)	O1*w*—Ce1—N4	114.1 (1)
O1—Ce1—N5	92.3 (1)	O1*w*—Ce1—N5	72.6 (1)
O1—Ce1—N6	130.3 (1)	O1*w*—Ce1—N6	118.2 (1)
O1—Ce1—N7	78.8 (1)	O1*w*—Ce1—N7	75.5 (1)
O3—Ce1—O5	87.6 (1)	O2*w*—Ce1—N4	132.8 (1)
O3—Ce1—O1*w*	141.9 (1)	O2*w*—Ce1—N5	79.1 (1)
O3—Ce1—O2*w*	135.5 (1)	O2*w*—Ce1—N6	69.0 (1)
O3—Ce1—N4	72.4 (1)	O2*w*—Ce1—N7	88.2 (1)
O3—Ce1—N5	131.3 (1)	N4—Ce1—N5	59.9 (1)
O3—Ce1—N6	67.4 (1)	N4—Ce1—N6	127.7 (1)
O3—Ce1—N7	77.3 (1)	N4—Ce1—N7	139.0 (1)
O5—Ce1—O1*w*	130.4 (1)	N5—Ce1—N6	137.4 (1)
O5—Ce1—O2*w*	74.1 (1)	N5—Ce1—N7	148.1 (1)
O5—Ce1—N4	69.9 (1)	N6—Ce1—N7	59.6 (1)

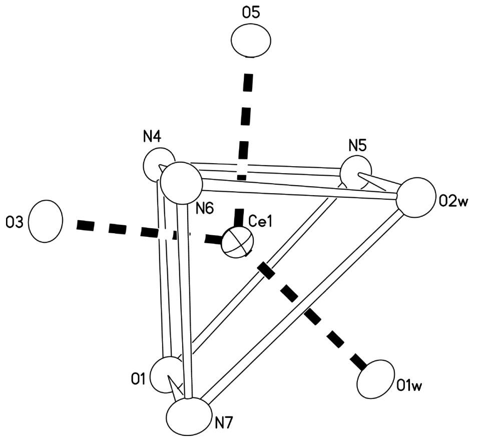


Figure 2
The capped trigonal prismatic geometry around the Ce atom in (I).

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

D—H···A	D—H	H···A	D···A	D—H···A
O1*w*—H1*w*1···O2	0.85 (1)	1.79 (2)	2.628 (4)	167 (4)
O1*w*—H1*w*2···O3*w*	0.85 (1)	1.92 (2)	2.748 (4)	165 (4)
O2*w*—H2*w*1···O6	0.86 (1)	1.78 (1)	2.614 (4)	163 (3)
O2*w*—H2*w*2···O4*w*	0.85 (1)	1.85 (1)	2.706 (4)	177 (4)
O3*w*—H3*w*1···O4^{i}	0.84 (1)	1.90 (1)	2.735 (4)	171 (4)
O3*w*—H3*w*2···O5^{i}	0.84 (1)	2.05 (1)	2.883 (4)	171 (4)
O4*w*—H4*w*1···O3*w*	0.84 (1)	1.97 (2)	2.781 (4)	163 (4)
O4*w*—H4*w*2···O5*w*	0.84 (1)	1.93 (1)	2.766 (4)	171 (4)
O5*w*—H5*w*1···N1^{ii}	0.85 (1)	2.06 (2)	2.873 (5)	160 (4)
O5*w*—H5*w*2···N2^{iii}	0.84 (1)	2.07 (2)	2.890 (5)	165 (4)

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

The aromatic H atoms were positioned geometrically [C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$] and were included in the refinement in the riding-model approximation. The water H atoms were located and refined with distance restraints [O—H = 0.85 (1) Å and H···H = 1.39 (1) Å] and with $U_{iso}(H) = 1.2U_{eq}(O)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; method used to solve structure: atomic coordinates taken from published Nd structure; program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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