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Diammonium diaquapentanitratocerate(III) dihydrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(O–N) = 0.007 Å
H-atom completeness 63%
R factor = 0.027
wR factor = 0.075
Data-to-parameter ratio = 15.3

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

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The structure of the title compound, $(NH_4)_2[Ce(NO_3)_5(H_2O)_2]\cdot 2H_2O$, consists of complex diaquapentanitratocerate(III) anions with 12-coordinate Ce atoms, ammonium cations and uncoordinated water molecules. The complex anion lies on a crystallographic twofold axis.

Comment

The title compound was obtained as a by-product while attempting to synthesize a Ce complex with furan-2-carboxylic acid. The crystals are isomorphous with previously reported analogous compounds of La (Eriksson *et al.*, 1982) and Pr (Meyer *et al.*, 1990). The crystals are composed of complex diaquapentanitratocerate(III) anions, ammonium cations and water of crystallization. The cerium atom is located on a crystallographic twofold axis, which runs also through atoms N1 and O2 (Fig. 1).

The complex may be viewed as a distorted pentagonal prism formed by the five nitrate groups with coordinated water molecules capping the two pentagonal faces. The crystal structure also contains uncoordinated water molecules and ammonium cations which are hardly distinguishable by X-ray diffraction. The present interpretation of the peaks in the Fourier map was based on analysis of the hydrogen bonds

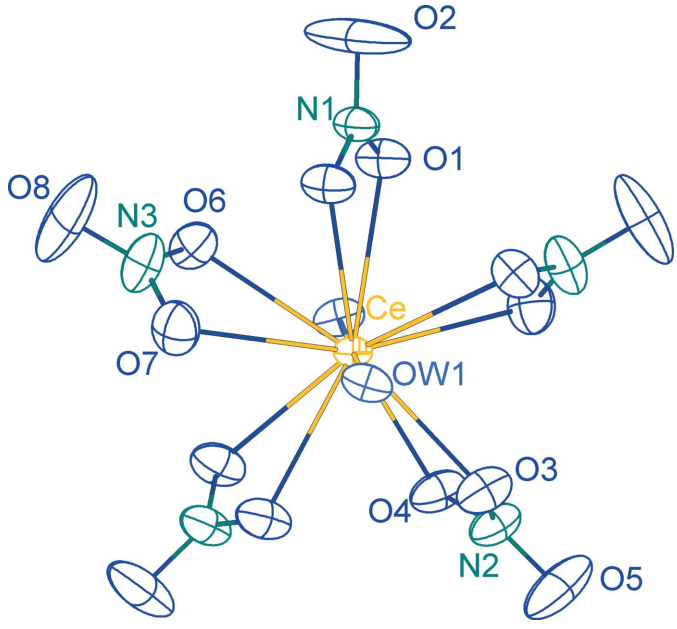

Figure 1
View of the complex anion showing the atom-labelling scheme. Only symmetry-independent atoms have been labelled and displacement ellipsoids are drawn at the 50% probability level. Unlabelled atoms are generated by the symmetry code $-x, y, \frac{1}{2} - z$.

formed; the site occupied by the atom which forms the greatest number of relevant contacts with acceptor (*i.e.* nitrate) O atoms was labelled N4, the other O*W*2; however, as atoms N4 and O*W*2 form hydrogen-bonded chains in the following manner, ···N4···N4···O*W*2···O*W*2···N4···N4···, it seems most probable that ammonium cations and water molecules actually alternate in their occupation of the N4 and O*W*2 sites..

Experimental

Ammonium cerium(IV) nitrate (1 mmol, 0.546 g) dissolved in water (3 ml) was added to an aqueous solution (12 ml) of furan-2-carboxylic acid (3 mmol, 0.336 g). This solution yielded crystals after 10 d. Analysis: calculated: Ce 25.19, N 17.63, H 2.54%, found: Ce 23.65, N 17.39, H 2.72%.

Crystal data

$(NH_4)_2[Ce(NO_3)_5(H_2O)_2]\cdot 2H_2O$
$M_r = 558.32$
Monoclinic, $C2/c$
$a = 11.089\ (7)$ Å
$b = 8.936\ (5)$ Å
$c = 17.963\ (13)$ Å
$\beta = 101.77\ (6)^\circ$
$V = 1742.6\ (19)$ Å^3
$Z = 4$
$D_x = 2.128$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7829 reflections
$\theta = 3$–28.5°
$\mu = 2.72$ mm^{-1}
$T = 293\ (2)$ K
Irregular fragment, colourless
0.4 × 0.35 × 0.3 mm

Data collection

Kuma KM-4 with a CCD counter diffractometer
ω scans
Absorption correction: analytical (Clark & Reid, 1995)
$T_{min} = 0.392$, $T_{max} = 0.467$
5214 measured reflections
2014 independent reflections
1990 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 28.4^\circ$
$h = -14 \rightarrow 14$
$k = -11 \rightarrow 11$
$l = -16 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.075$
$S = 1.16$
2014 reflections
132 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.03P)^2 + 9.6P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.76$ e Å^{-3}
$\Delta\rho_{min} = -0.74$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Ce—O*W*1	2.545 (3)	Ce—O7	2.678 (4)
Ce—O3	2.636 (3)	Ce—O4	2.681 (3)
Ce—O6	2.678 (4)	Ce—O1	2.707 (3)

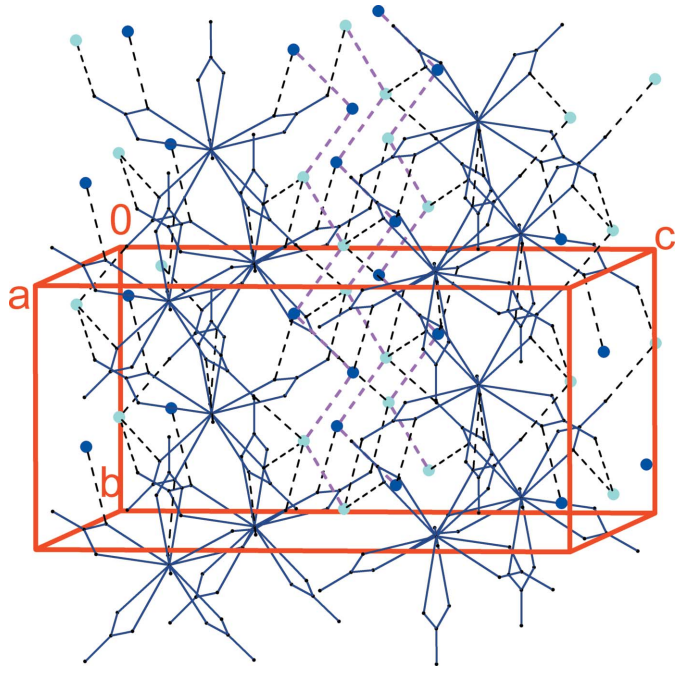

Figure 2
View of the packing and the hydrogen bonds (dashed lines). Atom N4 and its symmetry-equivalent are turquoise, all O*W*2 atoms are blue and the N4···N4′, N4···O*W*2, and O*W*2···O*W*2′ hydrogen bonds are drawn in purple.

The H atoms bonded to O*W*1 were located in a difference Fourier map and were freely refined. The other H atoms could not be located.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Crystal Impact, 2005); software used to prepare material for publication: *SHELXL97*.

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