

catena-Poly[[[diaquaneodymium(III)]bis(μ -difluoroacetato- κ^2 O:O')][diaquaneodymium(III)]tetrakis-(μ -difluoroacetato- κ^2 O:O')] monohydrate]

Alexander Rohde and Werner Urland*

Institut für Anorganische Chemie, Universität Hannover, Callinstrasse 9, D-30167 Hannover, Germany

Correspondence e-mail: urland@acc.uni-hannover.de

Key indicators

Single-crystal X-ray study
 T = 293 K
 Mean σ (C–C) = 0.007 Å
 R factor = 0.026
 wR factor = 0.064
 Data-to-parameter ratio = 12.6

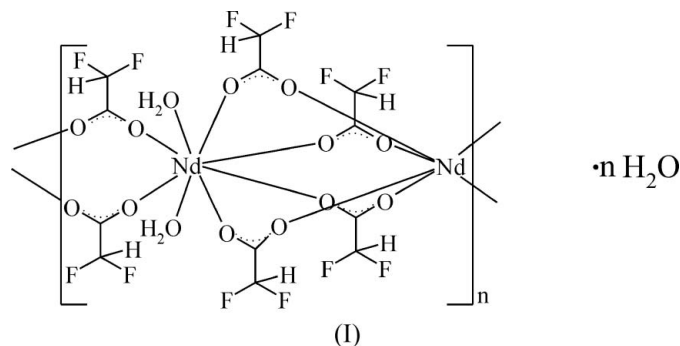
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound, $\{[\text{Nd}(\text{C}_2\text{HF}_2\text{O}_2)_3(\text{H}_2\text{O})_2] \cdot \text{H}_2\text{O}\}_n$, was synthesized by the reaction of Nd_2O_3 with difluoroacetic acid in water. The compound consists of chains, running along the *b* axis. The Nd^{3+} ion is coordinated by eight O atoms, giving a distorted square antiprism.

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Comment

In connection with our investigations of the structural chemistry of lanthanide (Ln) halogenoacetates, we directed our attention to the neodymium compound with difluoroacetic acid.



The title compound, (I), crystallizes isotypically with the praseodymium, erbium (Oczko & Starynowicz, 2000) and gadolinium (Rohde *et al.*, 2004) compounds. The asymmetric unit is shown in Fig. 1. The Nd^{3+} ion is coordinated by eight O atoms from six carboxylate groups and two water molecules (Table 1), giving a distorted square antiprism. The characteristic structural units are polymeric $[\text{Nd}(\text{C}_2\text{HF}_2\text{O}_2)_3(\text{H}_2\text{O})_2]_n$ chains, running along [010] with bidentate bridging carboxylate groups (Fig. 2). The chains are made up of dimers, which are connected by two carboxylate groups. In the dimers the Nd^{3+} ions are bridged by four carboxylate groups. As a consequence of this structural behaviour, there are two different $\text{Nd} \cdots \text{Nd}$ distances [4.443 (1) and 5.183 (1) Å].

Besides the coordinated water molecules (O1W and O2W), there is a non-coordinated water molecule (O3W). These water molecules and some of the O and F atoms of the carboxylate groups are connected through a complicated pattern of hydrogen-bonding interactions involving numerous $\text{O} \cdots \text{H} \cdots \text{O}$ and $\text{O} \cdots \text{H} \cdots \text{F}$ links, giving a three-dimensional network (Table 2).

Experimental

The title compound was prepared by the reaction of Nd_2O_3 (0.35 g, 2 mmol Nd^{3+} ; Strem Chemicals, 99.9%) with difluoroacetic acid

(0.96 g, 10 mmol; Aldrich, 98%) in H₂O (5 ml) at about 333 K. After the oxide was dissolved, the solution was cooled to room temperature. Violet crystals of (I) were formed after a few weeks.

Crystal data

[Nd(C₂HF₂O₂)₃(H₂O)₂]₃·H₂O
M_r = 483.37
 Triclinic, *P* $\bar{1}$
a = 8.405 (2) Å
b = 9.508 (3) Å
c = 9.639 (3) Å
 α = 66.67 (3)°
 β = 79.34 (3)°
 γ = 77.74 (3)°

V = 686.8 (4) Å³
Z = 2
D_x = 2.337 Mg m⁻³
 Mo *K*α radiation
 μ = 3.90 mm⁻¹
T = 293 (2) K
 Block, violet
 0.22 × 0.13 × 0.13 mm

Data collection

Stoe IPDS area-detector
 diffractometer
 φ scans
 Absorption correction: none
 9819 measured reflections

2512 independent reflections
 2246 reflections with *I* > 2σ(*I*)
*R*_{int} = 0.042
 θ_{\max} = 26.1°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.026
wR (*F*²) = 0.064
 S = 1.03
 2512 reflections
 199 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0443P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.69 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -1.20 \text{ e \AA}^{-3}$

Table 1

Selected bond lengths (Å).

Nd1—O32 ⁱ	2.374 (4)	Nd1—O21	2.464 (3)
Nd1—O12 ⁱⁱ	2.378 (3)	Nd1—O2W	2.497 (4)
Nd1—O22 ⁱⁱ	2.411 (3)	Nd1—O11	2.502 (3)
Nd1—O31	2.448 (3)	Nd1—O1W	2.577 (3)

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

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O1W—H11W···O3W ⁱⁱⁱ	0.85	2.12	2.793 (5)	136
O1W—H11W···O31	0.85	2.28	2.836 (5)	124
O1W—H11W···O11	0.85	2.49	2.951 (5)	115
O1W—H12W···O3W	0.85	2.26	2.768 (5)	118
O1W—H12W···O21	0.85	2.27	2.945 (5)	136
O2W—H21W···F11 ^{iv}	0.85	2.54	3.393 (8)	178
O2W—H22W···O1W ⁱ	0.85	2.17	2.823 (5)	133
O2W—H22W···O32	0.85	2.51	3.145 (6)	132
O3W—H31W···F32 ^v	0.85	2.51	3.157 (6)	134
O3W—H31W···F21	0.85	2.51	2.959 (5)	114
O3W—H32W···O11 ⁱⁱⁱ	0.85	2.28	2.880 (6)	128

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

All H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.98 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C). The H atoms of the water O atoms were located in a Fourier map and refined as riding [O—H = 0.85 Å and *U*_{iso}(H) = 1.2 *U*_{eq}(O)]. The

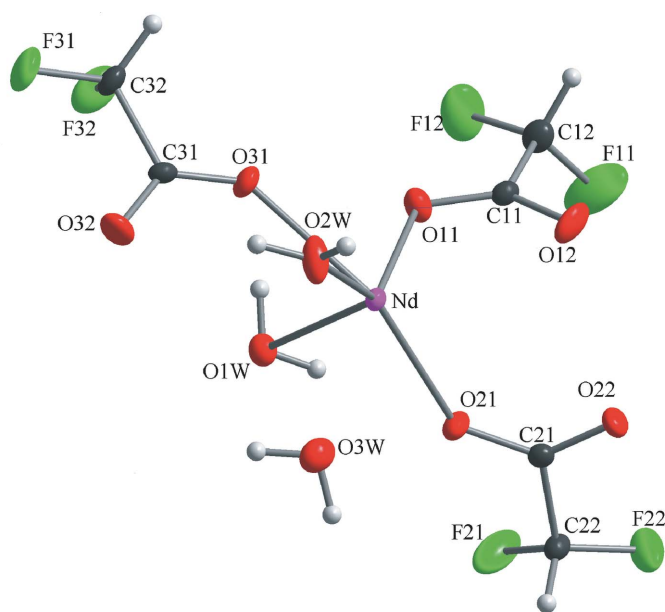


Figure 1

View of the asymmetric unit of (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

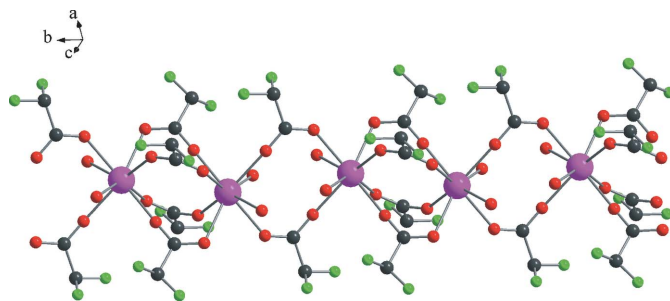


Figure 2

Polymeric chain of (I). H atoms have been omitted for clarity.

deepest electron density hole in the final difference Fourier synthesis is located 0.85 Å from atom Nd1.

Data collection: *IPDS Software* (Stoe & Cie, 1998); cell refinement: *IPDS Software*; data reduction: *IPDS Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

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