

Poly[[diaquatri- μ_4 -succinato-dineodymium(III)] monohydrate]Yong-Ke He,^a Xiao-Fang Wang,^b Li-Tian Zhang,^a Zheng-Bo Han^{a*} and Seik Weng Ng^c^aCollege of Chemistry, Liaoning University, Shenyang 110036, People's Republic of China, ^bDepartment of Pharmaceutical Engineering, Liaoning University, Shenyang 110036, People's Republic of China, and ^cDepartment of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: ceshzb@lnu.edu.cn

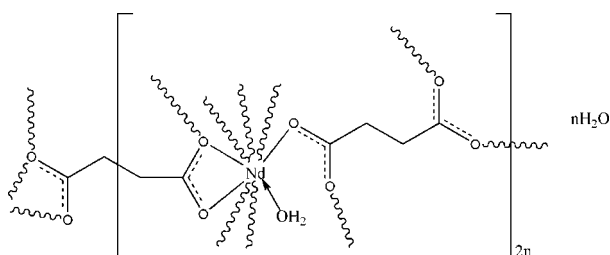
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.024; wR factor = 0.066; data-to-parameter ratio = 14.1.

Carboxylate bridging in the title neodymium(III) coordination polymer, $\{[\text{Nd}_2(\text{C}_4\text{H}_4\text{O}_4)_3(\text{H}_2\text{O})_2]\cdot\text{H}_2\text{O}\}_n$, leads to a three-dimensional network architecture. One of the two independent succinate groups lies on a centre of inversion whereas the other lies on a general position; both engage in μ_4 -bridging. The motif is consolidated by hydrogen bonds that involve the coordinated water molecule. The uncoordinated water molecule, which lies on a twofold rotation axis, is only weakly hydrogen bonded to the network. The Nd^{III} atom shows tricapped trigonal prismatic coordination.

Related literature

For the structure of $[\text{Ho}_2(\text{C}_4\text{H}_4\text{O}_4)_3(\text{H}_2\text{O})_2\cdot\text{H}_2\text{O}]$, see: Bernini *et al.* (2007).



Experimental

Crystal data

 $[\text{Nd}_2(\text{C}_4\text{H}_4\text{O}_4)_3(\text{H}_2\text{O})_2]\cdot\text{H}_2\text{O}$ $M_r = 690.74$ Monoclinic, $C2/c$ $a = 19.966$ (4) Å $b = 7.8761$ (9) Å $c = 13.9861$ (8) Å $\beta = 120.81$ (1)° $V = 1889.0$ (5) Å³ $Z = 4$ Mo $K\alpha$ radiation $\mu = 5.51$ mm⁻¹ $T = 295$ (2) K $0.37 \times 0.35 \times 0.23$ mm

Data collection

Siemens P4 diffractometer

Absorption correction: ψ scan(North *et al.*, 1968) $T_{\text{min}} = 0.194$, $T_{\text{max}} = 0.364$

(expected range = 0.150–0.281)

2342 measured reflections

1859 independent reflections

1759 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.019$

3 standard reflections

every 97 reflections

intensity decay: <1%

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.024$ $wR(F^2) = 0.066$ $S = 1.03$

1859 reflections

132 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.71$ e Å⁻³ $\Delta\rho_{\text{min}} = -1.53$ e Å⁻³

Table 1

Selected bond lengths (Å).

Nd1—O1	2.486 (3)	Nd1—O5	2.519 (3)
Nd1—O2 ⁱ	2.363 (3)	Nd1—O6	2.508 (2)
Nd1—O3 ⁱⁱ	2.572 (3)	Nd1—O6 ⁱ	2.455 (2)
Nd1—O3 ⁱⁱⁱ	2.463 (2)	Nd1—O1W	2.540 (3)
Nd1—O4 ⁱⁱ	2.537 (3)		

Symmetry codes: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $x, -y + 1, z - \frac{1}{2}$; (iii) $-x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H12 \cdots O1 ^{iv}	0.85	2.06	2.899 (4)	168
O1W—H11 \cdots O4 ⁱ	0.85	1.90	2.709 (4)	158

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

Data collection: *XSCANS* (Bruker, 2000); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *pubCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: C12484).

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supplementary materials

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Poly[[diaquatri- μ_4 -succinato-dineodymium(III)] monohydrate]

Y.-K. He, X.-F. Wang, L.-T. Zhang, Z.-B. Han and S. W. Ng

Comment

The holonium ion reacts with succinic acid under hydrothermal conditions to form polymeric $[\text{Ho}_2(\text{C}_4\text{H}_4\text{O}_4)_3(\text{H}_2\text{O})_4 \cdot 6\text{H}_2\text{O}]$ and $[\text{Ho}_2(\text{C}_4\text{H}_4\text{O}_4)_3(\text{H}_2\text{O})_2 \cdot \text{H}_2\text{O}]$ (Bernini *et al.*, 2007). The latter compound is a dihydrate. With the neodymium cation in place of the holonium cation, the reaction yields the title compound, which has the corresponding formulation.

The title compound is polymeric owing to carboxylate bridging; the geometry of the metal atom is a tricapped trigonal prism (Fig. 2).

Experimental

Neodymium nitrate hexahydrate (0.4 mmol, 0.175 g), succinic acid (1 mmol, 0.118 g), sodium hydroxide (1 mmol, 0.04 g) and water (10 ml) were placed in a 23-ml Teflon-lined Parr bomb. The bomb was heated at 453 K for 3 d and then cooled to room temperature at a rate of 5 K h⁻¹ (yield 70%). CH&N elemental analysis for C₁₂H₁₈Nd₂O₁₅ (found%/calc%): C 20.79/20.87, H 2.57/2.63.

Refinement

The methylene H atoms were placed at calculated positions (C—H = 0.97 Å) in the riding model approximation, with their U_{iso} values set to 1.2 times U_{eq} of the parent atoms. The H atoms of O1w were placed in chemically sensible positions on the basis of hydrogen bonds but were not refined (O—H = 0.85 Å). The H atom on O2w, which lies on a twofold axis, was similarly placed; however, O2w is only a weak hydrogen bond donor to O1w. The final difference Fourier map had a deep hole in the vicinity of Nd1 but was otherwise featureless.

Figures

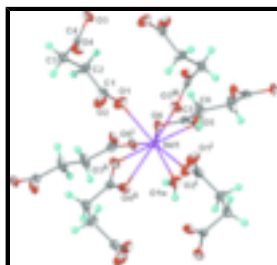


Fig. 1. Part of the polymeric structure of the title compound. Displacement ellipsoids are drawn at the 70% probability level, and H atoms as spheres of arbitrary radii. Symmetry codes are given in Table 1.

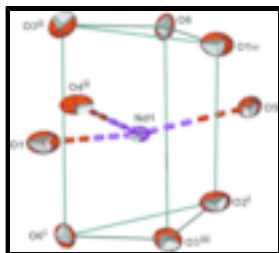


Fig. 2. Geometry of the neodymium atom in the title compound.

Poly[[diaquatri- μ_4 -succinato-dineodymium(III)] monohydrate]

Crystal data

$[\text{Nd}_2(\text{C}_4\text{H}_4\text{O}_4)_3(\text{H}_2\text{O})_2] \cdot \text{H}_2\text{O}$

$M_r = 690.74$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 19.966\ (4)\ \text{\AA}$

$b = 7.8761\ (9)\ \text{\AA}$

$c = 13.9861\ (8)\ \text{\AA}$

$\beta = 120.81\ (1)^\circ$

$V = 1889.0\ (5)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 1320$

$D_x = 2.429\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 28 reflections

$\theta = 5.2\text{--}12.4^\circ$

$\mu = 5.51\ \text{mm}^{-1}$

$T = 295\ (2)\ \text{K}$

Block, purple

$0.37 \times 0.35 \times 0.23\ \text{mm}$

Data collection

Siemens P4
diffractometer

Radiation source: medium-focus sealed tube

Monochromator: graphite

$T = 295\ (2)\ \text{K}$

ω - 2θ scans

Absorption correction: ψ scan
(North *et al.*, 1968)

$T_{\min} = 0.194$, $T_{\max} = 0.364$

2342 measured reflections

1859 independent reflections

1759 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.019$

$\theta_{\max} = 26.0^\circ$

$\theta_{\min} = 2.4^\circ$

$h = -1 \rightarrow 24$

$k = -1 \rightarrow 9$

$l = -17 \rightarrow 15$

3 standard reflections

every 97 reflections

intensity decay: $<1\%$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.024$

$wR(F^2) = 0.066$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0385P)^2 + 5.3046P]$

where $P = (F_o^2 + 2F_c^2)/3$

$S = 1.03$ $(\Delta/\sigma)_{\max} = 0.001$
 1859 reflections $\Delta\rho_{\max} = 0.71 \text{ e } \text{\AA}^{-3}$
 132 parameters $\Delta\rho_{\min} = -1.53 \text{ e } \text{\AA}^{-3}$
 Primary atom site location: structure-invariant direct methods
 Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Nd1	0.269282 (10)	0.78357 (2)	0.230560 (14)	0.01147 (10)
O1	0.1961 (2)	0.7564 (4)	0.3297 (3)	0.0262 (7)
O2	0.17965 (17)	0.4808 (3)	0.3430 (2)	0.0255 (6)
O3	0.18625 (14)	0.4811 (3)	0.6347 (2)	0.0201 (5)
O4	0.17029 (17)	0.2677 (3)	0.5265 (2)	0.0201 (6)
O5	0.40816 (16)	0.7251 (3)	0.3807 (2)	0.0217 (6)
O6	0.32606 (13)	0.5160 (3)	0.3399 (2)	0.0181 (5)
O1w	0.33554 (16)	0.6094 (3)	0.1495 (2)	0.0234 (6)
H11	0.3218	0.6460	0.0848	0.035*
H12	0.3223	0.5059	0.1454	0.035*
O2w	0.5000	0.5101 (10)	0.2500	0.079 (2)
H21	0.5203	0.5710	0.2206	0.118*
C1	0.1697 (2)	0.6327 (4)	0.3572 (3)	0.0167 (7)
C2	0.1225 (2)	0.6721 (5)	0.4117 (3)	0.0200 (7)
H2A	0.0792	0.7448	0.3624	0.024*
H2B	0.1551	0.7350	0.4798	0.024*
C3	0.0903 (2)	0.5144 (5)	0.4397 (3)	0.0184 (7)
H3A	0.0508	0.5498	0.4563	0.022*
H3B	0.0655	0.4409	0.3750	0.022*
C4	0.15256 (18)	0.4147 (5)	0.5375 (3)	0.0142 (6)
C5	0.39642 (19)	0.5743 (5)	0.3931 (3)	0.0158 (7)
C6	0.4604 (2)	0.4567 (5)	0.4686 (3)	0.0259 (8)
H6A	0.4630	0.3639	0.4250	0.031*
H6B	0.4483	0.4088	0.5219	0.031*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.01244 (14)	0.00748 (15)	0.01412 (14)	0.00056 (6)	0.00653 (10)	0.00027 (6)
O1	0.0398 (18)	0.0149 (11)	0.0377 (18)	-0.0004 (13)	0.0298 (16)	0.0011 (13)
O2	0.0356 (15)	0.0124 (12)	0.0414 (16)	0.0014 (12)	0.0290 (14)	-0.0003 (12)
O3	0.0197 (12)	0.0181 (13)	0.0159 (12)	0.0023 (11)	0.0043 (10)	-0.0034 (10)
O4	0.0293 (15)	0.0117 (12)	0.0159 (13)	-0.0006 (11)	0.0091 (12)	0.0003 (10)
O5	0.0138 (13)	0.0126 (13)	0.0298 (15)	-0.0002 (10)	0.0046 (12)	0.0014 (10)
O6	0.0103 (11)	0.0192 (13)	0.0193 (11)	-0.0015 (10)	0.0035 (10)	0.0041 (10)
O1w	0.0341 (15)	0.0168 (13)	0.0270 (13)	0.0020 (12)	0.0213 (12)	0.0018 (11)
O2w	0.053 (3)	0.094 (5)	0.087 (5)	0.000	0.033 (3)	0.000
C1	0.0182 (17)	0.0142 (16)	0.0167 (16)	0.0018 (13)	0.0082 (14)	0.0006 (13)
C2	0.0279 (19)	0.0160 (16)	0.0225 (18)	0.0049 (16)	0.0174 (16)	0.0037 (15)

supplementary materials

C3	0.0148 (15)	0.0210 (17)	0.0168 (16)	-0.0009 (14)	0.0062 (13)	0.0010 (14)
C4	0.0118 (15)	0.0158 (16)	0.0163 (16)	-0.0045 (14)	0.0081 (13)	0.0010 (14)
C5	0.0156 (16)	0.0173 (16)	0.0132 (15)	-0.0016 (14)	0.0064 (13)	-0.0024 (14)
C6	0.0139 (18)	0.0179 (18)	0.034 (2)	-0.0009 (16)	0.0033 (16)	0.0052 (16)

Geometric parameters (Å, °)

Nd1—O1	2.486 (3)	O6—C5	1.291 (4)
Nd1—O2 ⁱ	2.363 (3)	O6—Nd1 ^{iv}	2.455 (2)
Nd1—O3 ⁱⁱ	2.572 (3)	O1w—H11	0.85
Nd1—O3 ⁱⁱⁱ	2.463 (2)	O1w—H12	0.85
Nd1—O4 ⁱⁱ	2.537 (3)	O2w—H21	0.86
Nd1—O5	2.519 (3)	C1—C2	1.518 (5)
Nd1—O6	2.508 (2)	C2—C3	1.538 (5)
Nd1—O6 ⁱ	2.455 (2)	C2—H2A	0.97
Nd1—O1w	2.540 (3)	C2—H2B	0.97
O1—C1	1.258 (5)	C3—C4	1.513 (5)
O2—C1	1.245 (4)	C3—H3A	0.97
O2—Nd1 ^{iv}	2.363 (3)	C3—H3B	0.97
O3—C4	1.278 (4)	C4—Nd1 ^v	2.952 (3)
O3—Nd1 ⁱⁱⁱ	2.463 (2)	C5—C6	1.491 (5)
O3—Nd1 ^v	2.572 (3)	C6—C6 ^{vi}	1.522 (7)
O4—C4	1.243 (4)	C6—H6A	0.97
O4—Nd1 ^v	2.537 (3)	C6—H6B	0.97
O5—C5	1.240 (4)		
O2 ⁱ —Nd1—O6 ⁱ	75.74 (9)	C4—O4—Nd1 ^v	96.7 (2)
O2 ⁱ —Nd1—O3 ⁱⁱⁱ	76.80 (9)	C5—O5—Nd1	94.9 (2)
O6 ⁱ —Nd1—O3 ⁱⁱⁱ	69.35 (9)	C5—O6—Nd1 ^{iv}	152.6 (2)
O2 ⁱ —Nd1—O1	143.84 (10)	C5—O6—Nd1	94.1 (2)
O6 ⁱ —Nd1—O1	74.43 (10)	Nd1 ^{iv} —O6—Nd1	111.50 (9)
O3 ⁱⁱⁱ —Nd1—O1	73.88 (10)	Nd1—O1w—H11	109.5
O2 ⁱ —Nd1—O6	131.05 (9)	Nd1—O1w—H12	109.5
O6 ⁱ —Nd1—O6	152.50 (3)	H11—O1w—H12	109.5
O3 ⁱⁱⁱ —Nd1—O6	107.01 (8)	O2—C1—O1	124.7 (3)
O1—Nd1—O6	78.39 (9)	O2—C1—C2	117.9 (3)
O2 ⁱ —Nd1—O5	86.97 (10)	O1—C1—C2	117.4 (3)
O6 ⁱ —Nd1—O5	140.11 (8)	C1—C2—C3	114.2 (3)
O3 ⁱⁱⁱ —Nd1—O5	71.83 (8)	C1—C2—H2A	108.7
O1—Nd1—O5	103.28 (11)	C3—C2—H2A	108.7
O6—Nd1—O5	51.47 (8)	C1—C2—H2B	108.7
O2 ⁱ —Nd1—O4 ⁱⁱ	82.89 (10)	C3—C2—H2B	108.7
O6 ⁱ —Nd1—O4 ⁱⁱ	70.72 (8)	H2A—C2—H2B	107.6
O3 ⁱⁱⁱ —Nd1—O4 ⁱⁱ	138.47 (8)	C4—C3—C2	113.1 (3)
O1—Nd1—O4 ⁱⁱ	105.77 (11)	C4—C3—H3A	109.0

O6—Nd1—O4 ⁱⁱ	113.63 (8)	C2—C3—H3A	109.0
O5—Nd1—O4 ⁱⁱ	143.08 (10)	C4—C3—H3B	109.0
O2 ⁱ —Nd1—O1w	73.82 (9)	C2—C3—H3B	109.0
O6 ⁱ —Nd1—O1w	134.24 (8)	H3A—C3—H3B	107.8
O3 ⁱⁱⁱ —Nd1—O1w	133.01 (9)	O4—C4—O3	119.0 (3)
O1—Nd1—O1w	142.34 (9)	O4—C4—C3	121.7 (3)
O6—Nd1—O1w	69.04 (8)	O3—C4—C3	119.3 (3)
O5—Nd1—O1w	70.79 (9)	O4—C4—Nd1 ^v	58.60 (18)
O4 ⁱⁱ —Nd1—O1w	72.30 (9)	O3—C4—Nd1 ^v	60.36 (18)
O2 ⁱ —Nd1—O3 ⁱⁱ	127.75 (9)	C3—C4—Nd1 ^v	177.8 (2)
O6 ⁱ —Nd1—O3 ⁱⁱ	103.59 (8)	O5—C5—O6	119.2 (3)
O3 ⁱⁱⁱ —Nd1—O3 ⁱⁱ	153.22 (2)	O5—C5—C6	122.6 (3)
O1—Nd1—O3 ⁱⁱ	79.34 (9)	O6—C5—C6	118.1 (3)
O6—Nd1—O3 ⁱⁱ	66.82 (8)	O5—C5—Nd1	59.91 (19)
O5—Nd1—O3 ⁱⁱ	115.27 (8)	O6—C5—Nd1	59.57 (17)
O4 ⁱⁱ —Nd1—O3 ⁱⁱ	50.33 (8)	C6—C5—Nd1	175.1 (3)
O1w—Nd1—O3 ⁱⁱ	70.94 (9)	C5—C6—C6 ^{vi}	113.0 (4)
C1—O1—Nd1	134.0 (3)	C5—C6—H6A	109.0
C1—O2—Nd1 ^{iv}	147.2 (2)	C6 ^{vi} —C6—H6A	109.0
C4—O3—Nd1 ⁱⁱⁱ	155.3 (2)	C5—C6—H6B	109.0
C4—O3—Nd1 ^v	94.0 (2)	C6 ^{vi} —C6—H6B	109.0
Nd1 ⁱⁱⁱ —O3—Nd1 ^v	109.12 (9)	H6A—C6—H6B	107.8
O2 ⁱ —Nd1—O1—C1	175.0 (3)	O6 ⁱ —Nd1—O6—Nd1 ^{iv}	60.36 (18)
O6 ⁱ —Nd1—O1—C1	139.6 (4)	O3 ⁱⁱⁱ —Nd1—O6—Nd1 ^{iv}	138.18 (10)
O3 ⁱⁱⁱ —Nd1—O1—C1	-147.9 (4)	O1—Nd1—O6—Nd1 ^{iv}	69.23 (11)
O6—Nd1—O1—C1	-36.2 (4)	O5—Nd1—O6—Nd1 ^{iv}	-173.16 (16)
O5—Nd1—O1—C1	-81.6 (4)	O4 ⁱⁱ —Nd1—O6—Nd1 ^{iv}	-33.06 (13)
O4 ⁱⁱ —Nd1—O1—C1	75.3 (4)	O1w—Nd1—O6—Nd1 ^{iv}	-91.53 (11)
O1w—Nd1—O1—C1	-6.0 (5)	O3 ⁱⁱ —Nd1—O6—Nd1 ^{iv}	-14.02 (9)
O3 ⁱⁱ —Nd1—O1—C1	32.1 (4)	C5—Nd1—O6—Nd1 ^{iv}	-169.9 (2)
C5—Nd1—O1—C1	-58.6 (4)	C4 ⁱⁱ —Nd1—O6—Nd1 ^{iv}	-23.57 (11)
C4 ⁱⁱ —Nd1—O1—C1	53.9 (4)	Nd1 ^{iv} —O2—C1—O1	-4.1 (8)
Nd1 ^{iv} —Nd1—O1—C1	-2.3 (3)	Nd1 ^{iv} —O2—C1—C2	176.0 (3)
O2 ⁱ —Nd1—O5—C5	-148.6 (2)	Nd1—O1—C1—O2	4.1 (6)
O6 ⁱ —Nd1—O5—C5	147.99 (19)	Nd1—O1—C1—C2	-176.0 (3)
O3 ⁱⁱⁱ —Nd1—O5—C5	134.3 (2)	O2—C1—C2—C3	-1.8 (5)
O1—Nd1—O5—C5	66.5 (2)	O1—C1—C2—C3	178.3 (3)
O6—Nd1—O5—C5	3.36 (19)	C1—C2—C3—C4	72.9 (4)
O4 ⁱⁱ —Nd1—O5—C5	-74.7 (3)	Nd1 ^v —O4—C4—O3	0.5 (3)
O1w—Nd1—O5—C5	-74.7 (2)	Nd1 ^v —O4—C4—C3	-177.4 (3)
O3 ⁱⁱ —Nd1—O5—C5	-17.9 (3)	Nd1 ⁱⁱⁱ —O3—C4—O4	159.2 (4)

supplementary materials

C4 ⁱⁱ —Nd1—O5—C5	-40.4 (3)	Nd1 ^v —O3—C4—O4	-0.5 (3)
Nd1 ^{iv} —Nd1—O5—C5	-0.4 (2)	Nd1 ⁱⁱⁱ —O3—C4—C3	-22.8 (7)
O2 ⁱ —Nd1—O6—C5	35.2 (2)	Nd1 ^v —O3—C4—C3	177.4 (3)
O6 ⁱ —Nd1—O6—C5	-129.7 (2)	Nd1 ⁱⁱⁱ —O3—C4—Nd1 ^v	159.8 (6)
O3 ⁱⁱⁱ —Nd1—O6—C5	-51.89 (19)	C2—C3—C4—O4	-115.1 (4)
O1—Nd1—O6—C5	-120.8 (2)	C2—C3—C4—O3	67.0 (4)
O5—Nd1—O6—C5	-3.23 (19)	Nd1—O5—C5—O6	-5.9 (3)
O4 ⁱⁱ —Nd1—O6—C5	136.87 (19)	Nd1—O5—C5—C6	175.1 (3)
O1w—Nd1—O6—C5	78.41 (19)	Nd1 ^{iv} —O6—C5—O5	165.2 (3)
O3 ⁱⁱ —Nd1—O6—C5	155.9 (2)	Nd1—O6—C5—O5	5.9 (3)
C4 ⁱⁱ —Nd1—O6—C5	146.4 (2)	Nd1 ^{iv} —O6—C5—C6	-15.7 (6)
Nd1 ^{iv} —Nd1—O6—C5	169.9 (2)	Nd1—O6—C5—C6	-175.0 (3)
O2 ⁱ —Nd1—O6—Nd1 ^{iv}	-134.70 (11)		

Symmetry codes: (i) $-x+1/2, y+1/2, -z+1/2$; (ii) $x, -y+1, z-1/2$; (iii) $-x+1/2, -y+3/2, -z+1$; (iv) $-x+1/2, y-1/2, -z+1/2$; (v) $x, -y+1, z+1/2$; (vi) $-x+1, -y+1, -z+1$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H12 \cdots O1 ^{iv}	0.85	2.06	2.899 (4)	168
O1W—H11 \cdots O4 ⁱ	0.85	1.90	2.709 (4)	158

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

Fig. 1

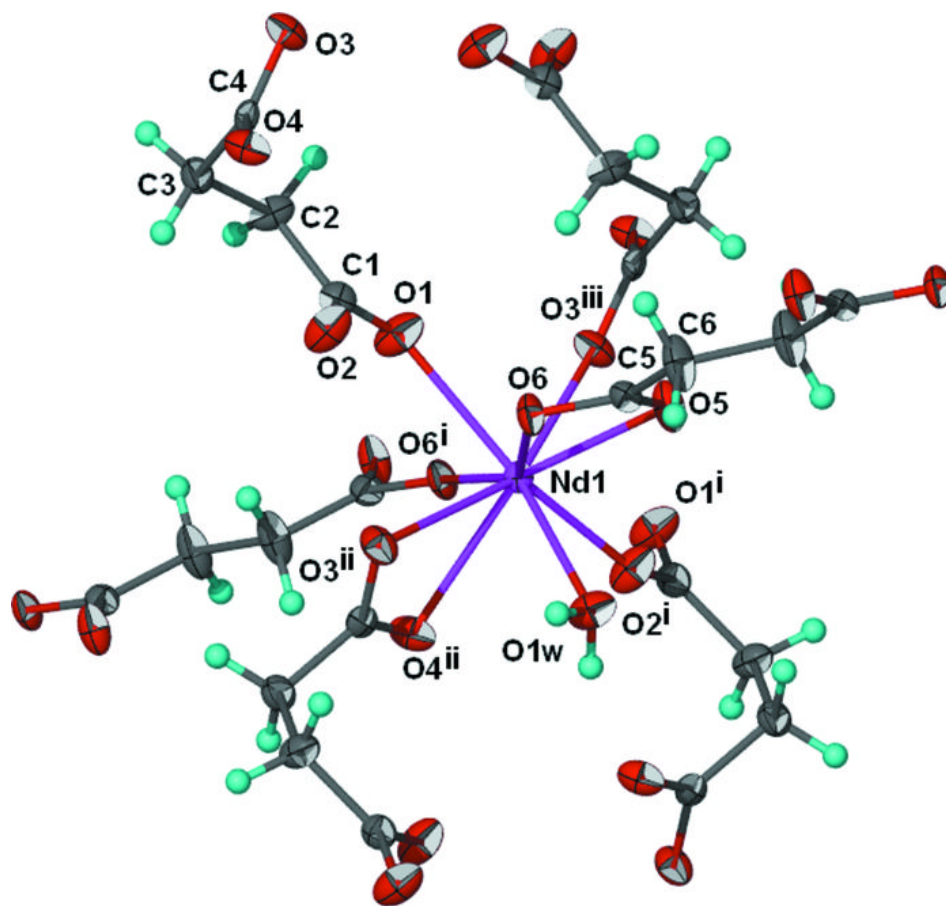


Fig. 2

