Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Lanthanite-(Nd), $Nd_2(CO_3)_3 \cdot 8H_2O$

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Received 16 January 2013; accepted 30 January 2013

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(O–C) = 0.007 Å; H-atom completeness 0%; R factor = 0.020; wR factor = 0.057; data-to-parameter ratio = 15.4.

Lanthanite-(Nd), ideally $Nd_2(CO_3)_3 \cdot 8H_2O$ [dineodymium(III) tricarbonate octahydrate], is a member of the lanthanite mineral group characterized by the general formula $REE_2(CO_3)_3 \cdot 8H_2O$, where REE is a 10-coordinated rare earth element. Based on single-crystal X-ray diffraction of a natural sample from Mitsukoshi, Hizen-cho, Karatsu City, Saga Prefecture, Japan, this study presents the first structure determination of lanthanite-(Nd). Its structure is very similar to that of other members of the lanthanite group. It is composed of infinite sheets made up of corner- and edge-sharing of two NdO_{10}-polyhedra (both with site symmetry ..2) and two carbonate triangles (site symmetries ..2 and 1) parallel to the ab plane, and stacked perpendicular to c. These layers are linked to one another only through hydrogen bonding involving the water molecules.

Related literature

For background to the lanthanite mineral group, see: Berzelius (1825); Blake (1853); Coutinho (1955); Shinn & Eick (1968); Ansell *et al.* (1976); Dal Negro *et al.* (1977); Cesbron *et al.* (1979); Roberts *et al.* (1980); Fujimori (1981); Svisero & Mascarenhas (1981); Nagashima *et al.* (1986); Atencio *et al.* (1989); Coimbra *et al.* (1989); Graham *et al.* (2007). For information on dawsonite, see: Corazza *et al.* (1977). For details of rigid-body motion, see: Downs *et al.* (1992). For resources for bond-valence calculations, see: Brese & O'Keeffe (1991).

Experimental

Crystal data

$Nd_2(CO_3)_3 \cdot 8H_2O$
M_r = 612.64
Orthorhombic, $Pccn$
a = 8.9391 (4) Å
b = 9.4694 (4) Å
c = 16.9374 (8) Å
V = 1433.72 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 7.25 mm^{-1}
T = 296 K
0.20 × 0.18 × 0.02 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2005)
T_{min} = 0.325, T_{max} = 0.869
9235 measured reflections
1570 independent reflections
1373 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.057
S = 1.12
1570 reflections
102 parameters
H-atom parameters not refined
$\Delta\rho_{max}$ = 0.81 e Å^{-3}
$\Delta\rho_{min}$ = −0.59 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å).

D—H···A	D···A	D—H···A	D···A
OW1···O1	2.645 (4)	OW3···OW1^{iv}	2.795 (4)
OW1···OW1^{i}	2.772 (5)	OW3···O5	2.928 (4)
OW1···OW4^{ii}	2.792 (5)	OW3···OW3^{vi}	2.994 (6)
OW1···OW3^{iii}	2.795 (4)	OW4···OW1^{vii}	2.792 (5)
OW2···O1^{iv}	2.645 (3)	OW4···OW2^{i}	2.833 (5)
OW2···OW2^{i}	2.786 (5)	OW4···OW4^{viii}	2.909 (9)
OW2···O5	2.815 (4)	OW4···OW2^{i}	3.231 (6)
OW2···OW4^{i}	2.833 (5)		
OW3···O2^{v}	2.626 (5)		

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XtalDraw* (Downs & Hall-Wallace, 2003); software used to prepare material for publication: *publCIF* (Westrip, 2010).

The authors gratefully acknowledge Marcus Origlieri for providing the lanthanite-(Nd) sample to the RRUFF Project. Funding support of this study was given by the Arizona Science Foundation, the Brazilian government (CNPq 202469/2011–5) and NASA NNX11AP82A, Mars Science Laboratory Investigations. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(*s*) and do not necessarily reflect the views of the National Aeronautics and Space Administration.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2719).

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supplementary materials

Acta Cryst. (2013). E**69**, i15–i16 [doi:10.1107/S1600536813003164]

Lanthanite-(Nd), $Nd_2(CO_3)_3\cdot 8H_2O$

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Comment

Crystals of the lanthanite group minerals exhibit a thin, platy habit and are characterized by the general formula $REE_2(CO_3)_3\cdot 8H_2O$, where *REE* is a 10-coordinated rare earth element. The group consists of lanthanite-(La), lanthanite-(Ce) and lanthanite-(Nd). The first of these minerals was found by Berzelius (1825) during one of his excursions to Bastnäs, Västmanland, Sweden, where he studied the local minerals and formulated the fundamentals of modern chemistry. Over 150 years later, Dal Negro *et al.* (1977) refined the crystal structure of the Bastnäs lanthanite and reported it in the non-standard setting *Pbnb* of space group No. 56. The chemistry of a different sample from this locality was later determined to be dominated by Ce (Atencio *et al.*, 1989). Of the lanthanite group minerals, the structure of lanthanite-(Ce) is the only one previously determined from a natural sample. However, Shinn & Eick (1968) synthesized lanthanite-(La) and performed a refinement in the standard setting *Pccn* of space group No. 56.

Lanthanite-(Nd) from Bethlehem, Pennsylvania, US, was first described by Blake (1853), although it was not possible to discriminate the Nd-dominance at that time. It was not until Atencio *et al.* (1989) analyzed a Bethlehem sample that it was found to be Nd-rich. Lanthanite-(Nd) has since been reported from other localities, including Curitiba, Brazil (Coutinho, 1955; Ansell *et al.*, 1976; Cesbron *et al.*, 1979; Roberts *et al.*, 1980; Fujimori, 1981; Svisero & Mascarenhas, 1981); Saga Prefecture, Japan (Nagashima *et al.*, 1986); Santa Isabel, São Paulo, Brazil (Coimbra *et al.*, 1989); and Whitianga, Coromandel Peninsula, New Zealand (Graham *et al.*, 2007). With the exception of those found in Whitianga, all lanthanite-(Nd) samples from these localities, including the one used in this study, exhibit a predominance of Nd with sub-equal La and a notable depletion of Ce. In reference to this phenomenon, Atencio *et al.* (1989) stated that lanthanite minerals comprise two distinct groups: one in which the proportions of La, Ce and Nd are similar and another in which La and Nd are similar in abundance while Ce is severely depleted or entirely absent. This trend presumably stems from differences in formational conditions, but the exact mechanism(*s*) remain(*s*) unclear.

Many of the studies referenced above reported lanthanite-(Nd) unit-cell parameters, but none reported the crystal structure. This study presents the first crystal structure refinement of lanthanite-(Nd). In the course of identifying minerals for the RRUFF project (http://rruff.info), we found an un-twinned lanthanite-(Nd) sample from Mitsukoshi, Hizen-cho, Karatsu City, Saga Prefecture, Japan and performed single-crystal X-ray diffraction.

The general structure feature of lanthanite-(Nd) is that of infinite sheets of corner- and edge-sharing NdO_{10}- and carbonate-polyhedra (Fig. 1) parallel to the *ab* plane, and stacked perpendicular to *c*. The layers are linked to one another only by hydrogen bonding between water molecules (Fig. 2). This accounts for the micaceous cleavage of the lanthanite minerals (Fig. 3) (Dal Negro *et al.*, 1977). There are two distinct Nd-sites (Nd1 and Nd2 at Wyckoff positions 4 *c* and 4 *d*), as well as two C-sites (C1 and C2 at Wyckoff positions 4 *d* and 8 *e*). Nd1 and Nd2 share an edge (O3 and O4) in the *a*-direction, forming a chain. The chains are linked in the *b*-direction by NdO_{10} polyhedra sharing a corner (O5) and sharing edges with the C2 carbonate group. Nd1 is bonded to two water molecules (OW1 and OW2) while Nd2 is bonded to one (OW3) that protrude from the primary sheet in the *c*-direction. The C1 carbonate group also projects from the sheet along *c*. According to bond valence calculations (Brese & O′Keeffe, 1991), without accounting for hydrogen bonding, each O-atom of the C1 carbonate group is under-bonded, with bond valence sums of 1.64 and 1.47 bond valence units for O1 and O2, respectively. The two O1 atoms are bonded only to Nd2 and C1, resulting in an underbonding that is satisfied by hydrogen bonding as an acceptor of OW1 and OW2 (Table 1). The apex O-atom, O2, is not bonded to any cation other than C1 and therefore has much larger thermal displacement parameters and a shorter bond length (1.243 (8) Å) than usually found in carbonate groups. The C1—O2 bond is close to satisfying the rigid-body criteria of equal displacement amplitudes of C1 and O2 along the C1—O2 bond direction. The bond length, corrected for rigid-body motion is 1.268 Å (Downs *et al.*, 1992). O2 is also the acceptor of an hydrogen bond from the OW3 atom of the adjacent sheet, thus connecting the two sheets. There are not many minerals with dangling O atoms in CO_3 groups, but these features are also observed in the crystal structures of isotypic lanthanite-(La) (Shinn & Eick, 1968), lanthanite-(Ce) (Dal Negro *et al.*, 1977) and in dawsonite, $NaAlCO_3(OH)_2$ (Corazza *et al.*, 1977). The last water molecule, OW4, is not bonded to any cation, but instead is situated between the OW1 of a given polyhedral layer and OW2 of the adjacent layer, linking the two layers together through hydrogen bonds.

Experimental

The lanthanite-(Nd) specimen used in this study was from Mitsukoshi, Hizen-cho, Karatsu City, Saga Prefecture, Japan, and is in the collection of the RRUFF project (deposition No. R060993; http://rruff.info). The experimental empirical formula, $(Nd_{0.95}La_{0.61}Pr_{0.17}Sm_{0.12}Gd_{0.08}Y_{0.04}Eu_{0.03})_{\Sigma=2}(CO_3)_3{\cdot}7.97H_2O$, was based on 17 O atoms and was determined from data of a CAMECA SX100 electron microprobe at the conditions of 15 keV, 10 nA, and a beam size of 20 μm. An average of 23 analysis points yielded (wt. %): H_2O 23.50 (by difference), CO_2 21.60, Y_2O_3 0.70, La_2O_3 16.32, Pr_2O_3 4.56, Nd_2O_3 26.06, Sm_2O_3 3.49, Eu_2O_3 0.87, Gd_2O_3 2.40, Tb_2O_3 0.12, Dy_2O_3 0.45.

Refinement

Due to similar X-ray scattering lengths, all rare earth elements were treated as Nd. The highest residual peak in the difference Fourier maps was located at (1/4, 3/4, 0.3413), 1.03 Å from Nd2, and the deepest hole at (0.2515, 0.8358, 0.2813), 0.81 Å from Nd2. H-atoms from water molecules could not be assigned reliably and were excluded from refinement.

Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XtalDraw* (Downs & Hall-Wallace, 2003); software used to prepare material for publication: *publCIF* (Westrip, 2010).

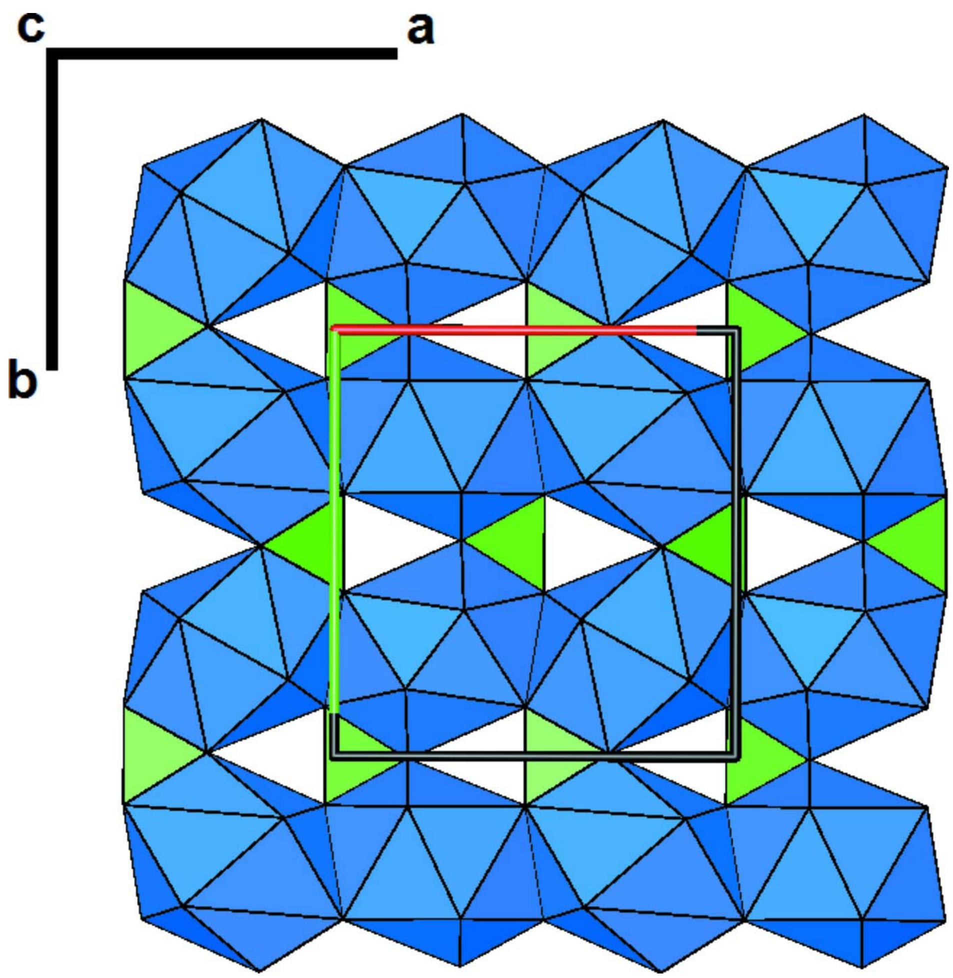

Figure 1

Looking down on a sheet of the lanthanite-(Nd) structure. NdO_{10} polyhedra are represented in blue and carbonate triangles are represented in green.

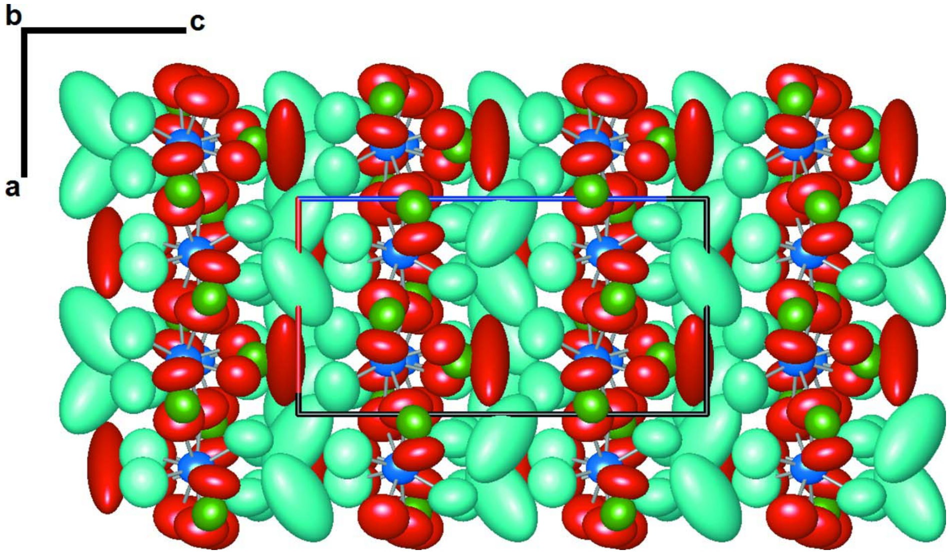

Figure 2

The crystal structure of lanthanite-(Nd) represented with displacement ellipsoids at the 99% probability level. Blue, green, red and cyan represent Nd, C, O atoms and H_2O molecules, respectively.

Figure 3

Photograph of the lanthanite-(Nd) specimen analyzed in this study, illustrating its platy habit.

Dineodymium(III) tricarbonate octahydrate

Crystal data

$Nd_2(CO_3)_3·8H_2O$
$M_r = 612.64$
Orthorhombic, *Pccn*
Hall symbol: -P 2ab 2ac
$a = 8.9391\ (4)$ Å
$b = 9.4694\ (4)$ Å
$c = 16.9374\ (8)$ Å
$V = 1433.72\ (11)$ Å^3
$Z = 4$

$F(000) = 1160$
$D_x = 2.838$ Mg m^{-3}
Mo *Kα* radiation, $\lambda = 0.71073$ Å
Cell parameters from 6318 reflections
$\theta = 2.3–27.5°$
$\mu = 7.25$ mm^{-1}
$T = 296$ K
Platy, pink
0.20 × 0.18 × 0.02 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2005)
$T_{min} = 0.325$, $T_{max} = 0.869$

9235 measured reflections
1570 independent reflections
1373 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
$h = -11 \rightarrow 11$
$k = -10 \rightarrow 11$
$l = -21 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.020$
$wR(F^2) = 0.057$
$S = 1.12$
1570 reflections
102 parameters
0 restraints

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.0225P)^2 + 5.4801P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.81$ e Å^{-3}
$\Delta\rho_{min} = -0.59$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Nd1	0.2500	0.2500	0.250082 (15)	0.01450 (9)
Nd2	0.2500	0.7500	0.280450 (15)	0.01381 (9)
C1	0.2500	0.7500	0.1061 (3)	0.0211 (11)
C2	0.4597 (4)	0.4972 (3)	0.28322 (19)	0.0142 (6)
O1	0.3229 (3)	0.6575 (3)	0.14676 (14)	0.0181 (5)

O2	0.2500	0.7500	0.0327 (3)	0.069 (2)
O3	0.0234 (3)	0.3837 (3)	0.20815 (16)	0.0210 (5)
O4	0.0234 (3)	0.6160 (3)	0.23732 (16)	0.0216 (5)
O5	0.3158 (3)	0.4931 (3)	0.29412 (15)	0.0192 (5)
OW1	0.3170 (3)	0.3820 (3)	0.12154 (16)	0.0232 (5)
OW2	0.1140 (3)	0.3219 (3)	0.37844 (16)	0.0261 (6)
OW3	0.1241 (3)	0.6457 (3)	0.40530 (17)	0.0343 (7)
OW4	0.3878 (6)	0.3889 (5)	0.4972 (3)	0.0749 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.01417 (13)	0.01111 (16)	0.01822 (16)	0.00172 (9)	0.000	0.000
Nd2	0.01354 (13)	0.01037 (16)	0.01752 (16)	−0.00126 (9)	0.000	0.000
C1	0.018 (2)	0.022 (3)	0.023 (3)	0.003 (2)	0.000	0.000
C2	0.0165 (15)	0.0119 (17)	0.0143 (14)	0.0004 (12)	−0.0013 (12)	0.0014 (12)
O1	0.0181 (11)	0.0150 (12)	0.0212 (12)	0.0022 (9)	−0.0017 (9)	−0.0018 (10)
O2	0.095 (5)	0.094 (5)	0.017 (2)	0.070 (4)	0.000	0.000
O3	0.0224 (12)	0.0121 (13)	0.0284 (13)	0.0055 (10)	−0.0016 (10)	0.0001 (10)
O4	0.0188 (11)	0.0131 (14)	0.0329 (14)	−0.0039 (10)	−0.0022 (10)	−0.0029 (10)
O5	0.0128 (11)	0.0165 (13)	0.0284 (13)	0.0006 (9)	0.0027 (10)	0.0008 (10)
OW1	0.0280 (13)	0.0159 (13)	0.0255 (13)	−0.0007 (11)	0.0012 (11)	−0.0012 (10)
OW2	0.0171 (12)	0.0357 (17)	0.0254 (13)	−0.0010 (11)	0.0007 (10)	0.0006 (12)
OW3	0.0303 (15)	0.050 (2)	0.0228 (13)	−0.0153 (14)	0.0008 (11)	−0.0011 (13)
OW4	0.089 (3)	0.077 (3)	0.059 (3)	−0.028 (3)	0.035 (2)	−0.029 (2)

Geometric parameters (Å, º)

Nd1—O5	2.491 (2)	Nd2—O5	2.513 (2)
Nd1—O5^{i}	2.491 (2)	Nd2—O1^{iv}	2.514 (2)
Nd1—O3^{i}	2.492 (2)	Nd2—O1	2.514 (2)
Nd1—O3	2.492 (2)	Nd2—OW3^{iv}	2.591 (3)
Nd1—OW1^{i}	2.581 (3)	Nd2—OW3	2.591 (3)
Nd1—OW1	2.581 (3)	Nd2—O3^{ii}	2.759 (3)
Nd1—OW2	2.582 (3)	Nd2—O3^{v}	2.759 (3)
Nd1—OW2^{i}	2.582 (3)	Nd2—C1	2.953 (6)
Nd1—O4^{ii}	2.762 (3)	Nd2—C2^{iv}	3.040 (3)
Nd1—O4^{iii}	2.762 (3)	C1—O2	1.243 (8)
Nd1—C2	3.051 (3)	C1—O1	1.291 (4)
Nd1—C2^{i}	3.051 (3)	C1—O1^{iv}	1.291 (4)
Nd2—O4	2.499 (3)	C2—O4^{ii}	1.263 (4)
Nd2—O4^{iv}	2.499 (3)	C2—O3^{ii}	1.272 (4)
Nd2—O5^{iv}	2.513 (2)	C2—O5	1.300 (4)

O5—Nd1—O5^{i}	145.15 (12)	O4^{iv}—Nd2—O5	109.18 (8)
O5—Nd1—O3^{i}	111.28 (8)	O5^{iv}—Nd2—O5	169.43 (12)
O5^{i}—Nd1—O3^{i}	78.92 (8)	O4—Nd2—O1^{iv}	72.75 (8)
O5—Nd1—O3	78.92 (8)	O4^{iv}—Nd2—O1^{iv}	76.70 (8)
O5^{i}—Nd1—O3	111.28 (8)	O5^{iv}—Nd2—O1^{iv}	71.64 (8)
O3^{i}—Nd1—O3	146.88 (12)	O5—Nd2—O1^{iv}	118.74 (8)

O5—Nd1—OW1^{i}	139.03 (8)	O4—Nd2—O1	76.70 (8)
O5^{i}—Nd1—OW1^{i}	75.53 (8)	O4^{iv}—Nd2—O1	72.75 (8)
O3^{i}—Nd1—OW1^{i}	72.68 (8)	O5^{iv}—Nd2—O1	118.74 (8)
O3—Nd1—OW1^{i}	79.45 (8)	O5—Nd2—O1	71.64 (8)
O5—Nd1—OW1	75.53 (8)	O1^{iv}—Nd2—O1	51.48 (11)
O5^{i}—Nd1—OW1	139.03 (8)	O4—Nd2—OW3^{iv}	141.63 (9)
O3^{i}—Nd1—OW1	79.45 (8)	O4^{iv}—Nd2—OW3^{iv}	72.13 (9)
O3—Nd1—OW1	72.68 (8)	O5^{iv}—Nd2—OW3^{iv}	69.98 (9)
OW1^{i}—Nd1—OW1	64.96 (12)	O5—Nd2—OW3^{iv}	101.07 (10)
O5—Nd1—OW2	67.38 (8)	O1^{iv}—Nd2—OW3^{iv}	135.64 (9)
O5^{i}—Nd1—OW2	83.13 (9)	O1—Nd2—OW3^{iv}	139.06 (9)
O3^{i}—Nd1—OW2	139.15 (9)	O4—Nd2—OW3	72.13 (9)
O3—Nd1—OW2	73.95 (8)	O4^{iv}—Nd2—OW3	141.63 (9)
OW1^{i}—Nd1—OW2	136.78 (8)	O5^{iv}—Nd2—OW3	101.07 (10)
OW1—Nd1—OW2	133.78 (8)	O5—Nd2—OW3	69.98 (9)
O5—Nd1—OW2^{i}	83.13 (9)	O1^{iv}—Nd2—OW3	139.06 (9)
O5^{i}—Nd1—OW2^{i}	67.38 (8)	O1—Nd2—OW3	135.64 (9)
O3^{i}—Nd1—OW2^{i}	73.95 (8)	OW3^{iv}—Nd2—OW3	70.59 (13)
O3—Nd1—OW2^{i}	139.15 (9)	O4—Nd2—O3^{ii}	120.36 (9)
OW1^{i}—Nd1—OW2^{i}	133.78 (8)	O4^{iv}—Nd2—O3^{ii}	62.32 (9)
OW1—Nd1—OW2^{i}	136.78 (8)	O5^{iv}—Nd2—O3^{ii}	130.16 (8)
OW2—Nd1—OW2^{i}	65.29 (12)	O5—Nd2—O3^{ii}	48.87 (7)
O5—Nd1—O4^{ii}	48.95 (8)	O1^{iv}—Nd2—O3^{ii}	116.91 (8)
O5^{i}—Nd1—O4^{ii}	127.62 (8)	O1—Nd2—O3^{ii}	70.95 (8)
O3^{i}—Nd1—O4^{ii}	62.36 (9)	OW3^{iv}—Nd2—O3^{ii}	74.51 (9)
O3—Nd1—O4^{ii}	120.53 (9)	OW3—Nd2—O3^{ii}	98.79 (9)
OW1^{i}—Nd1—O4^{ii}	119.54 (8)	O4—Nd2—O3^{v}	62.32 (9)
OW1—Nd1—O4^{ii}	68.74 (8)	O4^{iv}—Nd2—O3^{v}	120.36 (9)
OW2—Nd1—O4^{ii}	103.32 (8)	O5^{iv}—Nd2—O3^{v}	48.87 (7)
OW2^{i}—Nd1—O4^{ii}	68.87 (8)	O5—Nd2—O3^{v}	130.16 (8)
O5—Nd1—O4^{iii}	127.62 (8)	O1^{iv}—Nd2—O3^{v}	70.95 (8)
O5^{i}—Nd1—O4^{iii}	48.95 (8)	O1—Nd2—O3^{v}	116.91 (8)
O3^{i}—Nd1—O4^{iii}	120.53 (9)	OW3^{iv}—Nd2—O3^{v}	98.79 (9)
O3—Nd1—O4^{iii}	62.36 (9)	OW3—Nd2—O3^{v}	74.51 (9)
OW1^{i}—Nd1—O4^{iii}	68.74 (8)	O3^{ii}—Nd2—O3^{v}	171.97 (11)
OW1—Nd1—O4^{iii}	119.54 (8)	O2—C1—O1	122.2 (2)
OW2—Nd1—O4^{iii}	68.87 (8)	O2—C1—O1^{iv}	122.2 (2)
OW2^{i}—Nd1—O4^{iii}	103.32 (8)	O1—C1—O1^{iv}	115.5 (5)
O4^{ii}—Nd1—O4^{iii}	171.14 (11)	O4^{ii}—C2—O3^{ii}	125.6 (3)
O4—Nd2—O4^{iv}	146.01 (13)	O4^{ii}—C2—O5	117.4 (3)
O4—Nd2—O5^{iv}	109.18 (8)	O3^{ii}—C2—O5	117.0 (3)
O4^{iv}—Nd2—O5^{iv}	74.05 (8)	O4^{ii}—C2—O1	113.5 (2)
O4—Nd2—O5	74.05 (8)		

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

Hydrogen-bond geometry (Å)

D—H···*A*	*D*···*A*
O*W*1···O1	2.645 (4)

O*W*1···O*W*1^{i}	2.772 (5)
O*W*1···O*W*4^{vi}	2.792 (5)
O*W*1···O*W*3^{ii}	2.795 (4)
O*W*2···O1^{vii}	2.645 (3)
O*W*2···O*W*2^{i}	2.786 (5)
O*W*2···O5	2.815 (4)
O*W*2···O*W*4^{i}	2.833 (5)
O*W*3···O2^{viii}	2.626 (5)
O*W*3···O*W*1^{vii}	2.795 (4)
O*W*3···O5	2.928 (4)
O*W*3···O*W*3^{iv}	2.994 (6)
O*W*4···O*W*1^{ix}	2.792 (5)
O*W*4···O*W*2^{i}	2.833 (5)
O*W*4···O*W*4^{x}	2.909 (9)
O*W*4···O*W*2^{i}	3.231 (6)

Symmetry codes: (i) −*x*+1/2, −*y*+1/2, *z*; (ii) *x*+1/2, −*y*+1, −*z*+1/2; (iv) −*x*+1/2, −*y*+3/2, *z*; (vi) −*x*+1/2, *y*, *z*−1/2; (vii) *x*−1/2, −*y*+1, −*z*+1/2; (viii) *x*, −*y*+3/2, *z*+1/2; (ix) −*x*+1/2, *y*, *z*+1/2; (x) −*x*+1, −*y*+1, −*z*+1.