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 NdO(NO₃)

Ya-Feng Li,* Li Jin, Dan-Ping Li and Long Zhang

School of Chemical Engineering, Changchun University of Technology, Changchun 130012, People's Republic of China

Correspondence e-mail: fly012345@sohu.com

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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{O}-\text{N}) = 0.007$ Å; R factor = 0.024; wR factor = 0.068; data-to-parameter ratio = 12.1.

The title compound, neodymium(III) oxide nitrate, which is isostructural with LaO(NO₃), arose from a solvothermal reaction. The Nd ion (site symmetry m) is ten-coordinated by eight O atoms of NO₃ groups and two μ_2 -oxide ions. A three-dimensional structure is constructed by the interconnection of NdO₁₀ polyhedra. The oxide ion and the N atom and one of the nitrate O atoms possess site symmetry m .

Related literature

For background, see: Gobichon *et al.* (1997); Guillou *et al.* (1994). For an isostructural compound, see: Zhang *et al.* (2004).

Experimental

Crystal data

NdO(NO ₃)	$V = 338.46$ (11) Å ³
$M_r = 222.25$	$Z = 4$
Orthorhombic, $Pnma$	Mo $K\alpha$ radiation
$a = 7.5233$ (15) Å	$\mu = 15.19$ mm ⁻¹
$b = 5.1618$ (10) Å	$T = 293$ (2) K
$c = 8.7157$ (17) Å	$0.16 \times 0.14 \times 0.12$ mm

Data collection

Rigaku R-Axis RAPID diffractometer	2962 measured reflections
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	410 independent reflections
$T_{\min} = 0.107$, $T_{\max} = 0.158$	405 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.034$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$	34 parameters
$wR(F^2) = 0.068$	30 restraints
$S = 1.81$	$\Delta\rho_{\text{max}} = 1.02$ e Å ⁻³
410 reflections	$\Delta\rho_{\text{min}} = -1.42$ e Å ⁻³

Table 1

Selected bond lengths (Å).

Nd1—O2 ⁱ	2.434 (5)	Nd1—O1	2.694 (3)
Nd1—O2	2.458 (5)	Nd1—O1 ⁱⁱⁱ	2.719 (4)
Nd1—O3 ⁱⁱ	2.6362 (12)	Nd1—O1 ⁱⁱ	2.826 (4)

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

Data collection: *PROCESS-AUTO* (Rigaku, 2002); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2000); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2833).

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supplementary materials

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NdO(NO₃)

Y.-F. Li, L. Jin, D.-P. Li and L. Zhang

Comment

The lanthanide nitrates are not only applied for separation of the lanthanide elements but also widely utilized as the precursor of organic or inorganic synthesis. Thus, a large number of lanthanide nitrates are structurally determined besides a few anhydrous examples (Guillou, *et al.*, 1994; Zhang, *et al.*, 2004; Gobichon, *et al.*, 1997). In this work, the title compound, (I), an anhydrous neodymium oxide nitrate, was unexpectedly obtained under solvothermal conditions in a mixed solvent of H₂O and DMF.

The asymmetric unit of (I) is consisted of 0.5 Nd, 0.5 O and 0.5 NO₃ (Fig. 1). All oxygen atoms of NO₃ group are coordinated to the Nd ions. Two oxygen atoms of nitrate group (O1 and O1^{vi}) are coordinated to three different Nd ions with Nd—O distances in the range of 2.694–2.826 Å, and the last one (O3) is coordinated to two different Nd ions with Nd—O distance of 2.636 Å (Table 1). A μ₂-O (O2) exists in the structure of (I) with Nd—O distances of 2.434 and 2.458 Å and corresponding Nd—O—Nd bond angles of 110.72°. These two Nd—O distances are significantly shorter than the others Nd—O distances. Then, the linkages of two adjacent Nd ions are in two modes, of which one is *via* Nd—μ₂-O—Nd bonds with Nd—Nd distance of 4.0254 (8) Å and the other *via* Nd—O(NO₃)-Nd bonds. A three-dimensional framework constructed by the interconnections of NdO₁₀ polyhedra is shown in Fig. 2.

There are two different structures with the same molecular formula of LnONO₃, such as LnONO₃ (Ln=Y, La) in the *P4/mmm* space group and LaONO₃ in *Pnma* space group. In this work, NdONO₃ is the isostructural compound of the reported LaONO₃ (Zhang, *et al.*, 2004).

Experimental

Isonicotine (0.123 g, 1.0 mmol) was added to a mixed solution of 5 ml H₂O/3 ml DMF. After being stirred for 5 h, the isonicotine was partially dissolved with pH = 6.0. Then, Nd(NO₃)₃·6H₂O (0.220 g, 0.5 mmol) was added and stirred for 7 h. The molar ratio of Nd(NO₃)₃·6H₂O: isonicotine was 1:2. Finally, the solution with pH = 7.0 was sealed into 23 ml autoclave and heated up to 438 K for 4 days. After naturally cooling to room temperature, colourless prisms of (I) were obtained.

Figures

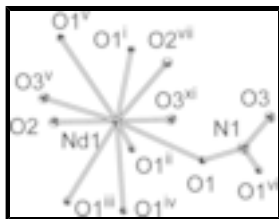


Fig. 1. A fragment of the structure of (I), showing the Nd coordination sphere and displacement ellipsoids at the 50% probability level. [Symmetry codes: (i) $-1/2 + x, y, 1.5 - z$; (ii) $x, 0.5 - y, z$; (iii) $1 - x, 1/2 + y, 2 - z$; (iv) $1 - x, -y, 2 - z$; (v) $-1/2 + x, 0.5 - y, 1.5 - z$; (vi) $x, -0.5 - y, z$; (vii) $1/2 + x, 0.5 - y, 1.5 - z$.]

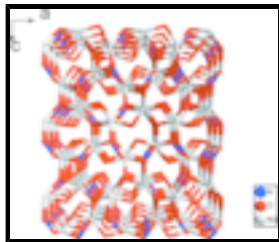


Fig. 2. A packing diagram for (I), viewed along [010].

neodymium(III) oxide nitrate

Crystal data

NdO(NO₃)

$M_r = 222.25$

Orthorhombic, *Pnma*

Hall symbol: -P 2ac 2n

$a = 7.5233$ (15) Å

$b = 5.1618$ (10) Å

$c = 8.7157$ (17) Å

$V = 338.46$ (11) Å³

$Z = 4$

$F_{000} = 396$

$D_x = 4.362$ Mg m⁻³

Mo *K*α radiation

$\lambda = 0.71073$ Å

Cell parameters from 2000 reflections

$\theta = 3.6$ – 27.0°

$\mu = 15.19$ mm⁻¹

$T = 293$ (2) K

Prism, colourless

$0.16 \times 0.14 \times 0.12$ mm

Data collection

Rigaku R-Axis RAPID
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 10.00 pixels mm⁻¹

$T = 293$ (2) K

ω scans

Absorption correction: multi-scan
(ABSCOR; Higashi, 1995)

$T_{\min} = 0.107$, $T_{\max} = 0.158$

2962 measured reflections

410 independent reflections

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

$R_{\text{int}} = 0.034$

$\theta_{\text{max}} = 27.0^\circ$

$\theta_{\text{min}} = 3.6^\circ$

$h = -9 \rightarrow 8$

$k = -5 \rightarrow 6$

$l = -11 \rightarrow 11$

Refinement

Refinement on F^2

Least-squares matrix: full

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

$wR(F^2) = 0.068$

$S = 1.81$

410 reflections

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$w = 1/[\sigma^2(F_o^2) + (0.0285P)^2]$

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

$(\Delta/\sigma)_{\text{max}} = 0.002$

$\Delta\rho_{\text{max}} = 1.02$ e Å⁻³

$\Delta\rho_{\text{min}} = -1.42$ e Å⁻³

34 parameters
30 restraints

Extinction correction: none

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Nd1	0.35352 (4)	0.2500	0.83222 (4)	0.0055 (2)
O1	0.6501 (4)	-0.0288 (7)	0.8846 (4)	0.0047 (7)
O2	0.0359 (6)	0.2500	0.8985 (6)	0.0080 (10)
O3	0.7902 (7)	-0.2500	0.6964 (6)	0.0088 (10)
N1	0.6934 (10)	-0.2500	0.8195 (7)	0.0120 (13)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.0051 (3)	0.0052 (3)	0.0061 (3)	0.000	0.00018 (11)	0.000
O1	0.0054 (10)	0.0043 (10)	0.0045 (10)	0.0002 (7)	0.0004 (7)	-0.0001 (8)
O2	0.0072 (12)	0.0091 (12)	0.0076 (13)	0.000	-0.0001 (9)	0.000
O3	0.0091 (13)	0.0088 (13)	0.0086 (12)	0.000	0.0022 (9)	0.000
N1	0.0121 (15)	0.0120 (15)	0.0121 (15)	0.000	-0.0005 (9)	0.000

Geometric parameters (\AA , $^\circ$)

Nd1—O2 ⁱ	2.434 (5)	Nd1—Nd1 ⁱⁱ	4.0254 (8)
Nd1—O2	2.458 (5)	Nd1—Nd1 ⁱ	4.0254 (8)
Nd1—O3 ⁱⁱ	2.6362 (12)	O1—N1	1.316 (5)
Nd1—O3 ⁱⁱⁱ	2.6362 (12)	O1—Nd1 ^{vi}	2.719 (4)
Nd1—O1 ^{iv}	2.694 (3)	O1—Nd1 ⁱ	2.826 (4)
Nd1—O1	2.694 (3)	O2—Nd1 ⁱⁱ	2.434 (5)
Nd1—O1 ^v	2.719 (4)	O3—N1	1.297 (8)
Nd1—O1 ^{vi}	2.719 (4)	O3—Nd1 ⁱ	2.6362 (12)
Nd1—O1 ⁱⁱ	2.826 (4)	O3—Nd1 ^{viii}	2.6362 (12)
Nd1—O1 ^{vii}	2.826 (4)	N1—O1 ^{ix}	1.316 (5)
O2 ⁱ —Nd1—O2	137.90 (13)	O3 ⁱⁱ —Nd1—O1 ⁱⁱ	48.73 (13)

supplementary materials

O2 ⁱ —Nd1—O3 ⁱⁱ	91.36 (11)	O3 ⁱⁱⁱ —Nd1—O1 ⁱⁱ	109.73 (13)
O2—Nd1—O3 ⁱⁱ	81.18 (12)	O1 ^{iv} —Nd1—O1 ⁱⁱ	146.51 (6)
O2 ⁱ —Nd1—O3 ⁱⁱⁱ	91.36 (11)	O1—Nd1—O1 ⁱⁱ	106.85 (12)
O2—Nd1—O3 ⁱⁱⁱ	81.18 (12)	O1 ^v —Nd1—O1 ⁱⁱ	144.63 (7)
O3 ⁱⁱ —Nd1—O3 ⁱⁱⁱ	156.5 (2)	O1 ^{vi} —Nd1—O1 ⁱⁱ	112.81 (4)
O2 ⁱ —Nd1—O1 ^{iv}	70.92 (12)	O2 ⁱ —Nd1—O1 ^{vii}	75.69 (11)
O2—Nd1—O1 ^{iv}	139.92 (10)	O2—Nd1—O1 ^{vii}	68.33 (11)
O3 ⁱⁱ —Nd1—O1 ^{iv}	133.51 (14)	O3 ⁱⁱ —Nd1—O1 ^{vii}	109.73 (13)
O3 ⁱⁱⁱ —Nd1—O1 ^{iv}	69.06 (14)	O3 ⁱⁱⁱ —Nd1—O1 ^{vii}	48.73 (13)
O2 ⁱ —Nd1—O1	70.92 (12)	O1 ^{iv} —Nd1—O1 ^{vii}	106.85 (12)
O2—Nd1—O1	139.92 (10)	O1—Nd1—O1 ^{vii}	146.51 (6)
O3 ⁱⁱ —Nd1—O1	69.06 (14)	O1 ^v —Nd1—O1 ^{vii}	112.81 (4)
O3 ⁱⁱⁱ —Nd1—O1	133.51 (14)	O1 ^{vi} —Nd1—O1 ^{vii}	144.63 (7)
O1 ^{iv} —Nd1—O1	64.57 (15)	O1 ⁱⁱ —Nd1—O1 ^{vii}	61.23 (15)
O2 ⁱ —Nd1—O1 ^v	139.04 (10)	Nd1 ⁱⁱ —Nd1—Nd1 ⁱ	138.29 (2)
O2—Nd1—O1 ^v	77.12 (12)	N1—O1—Nd1	126.5 (4)
O3 ⁱⁱ —Nd1—O1 ^v	119.67 (13)	N1—O1—Nd1 ^{vi}	91.7 (3)
O3 ⁱⁱⁱ —Nd1—O1 ^v	70.90 (13)	Nd1—O1—Nd1 ^{vi}	111.71 (11)
O1 ^{iv} —Nd1—O1 ^v	68.29 (11)	N1—O1—Nd1 ⁱ	91.1 (3)
O1—Nd1—O1 ^v	94.51 (7)	Nd1—O1—Nd1 ⁱ	93.62 (12)
O2 ⁱ —Nd1—O1 ^{vi}	139.04 (10)	Nd1 ^{vi} —O1—Nd1 ⁱ	145.72 (12)
O2—Nd1—O1 ^{vi}	77.12 (12)	Nd1 ⁱⁱ —O2—Nd1	110.73 (19)
O3 ⁱⁱ —Nd1—O1 ^{vi}	70.90 (13)	N1—O3—Nd1 ⁱ	100.35 (11)
O3 ⁱⁱⁱ —Nd1—O1 ^{vi}	119.67 (13)	N1—O3—Nd1 ^{viii}	100.35 (11)
O1 ^{iv} —Nd1—O1 ^{vi}	94.51 (7)	Nd1 ⁱ —O3—Nd1 ^{viii}	156.5 (2)
O1—Nd1—O1 ^{vi}	68.29 (11)	O3—N1—O1	119.7 (3)
O1 ^v —Nd1—O1 ^{vi}	49.66 (16)	O3—N1—O1 ^{ix}	119.7 (3)
O2 ⁱ —Nd1—O1 ⁱⁱ	75.69 (11)	O1—N1—O1 ^{ix}	120.4 (6)
O2—Nd1—O1 ⁱⁱ	68.33 (12)		

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

Fig. 1

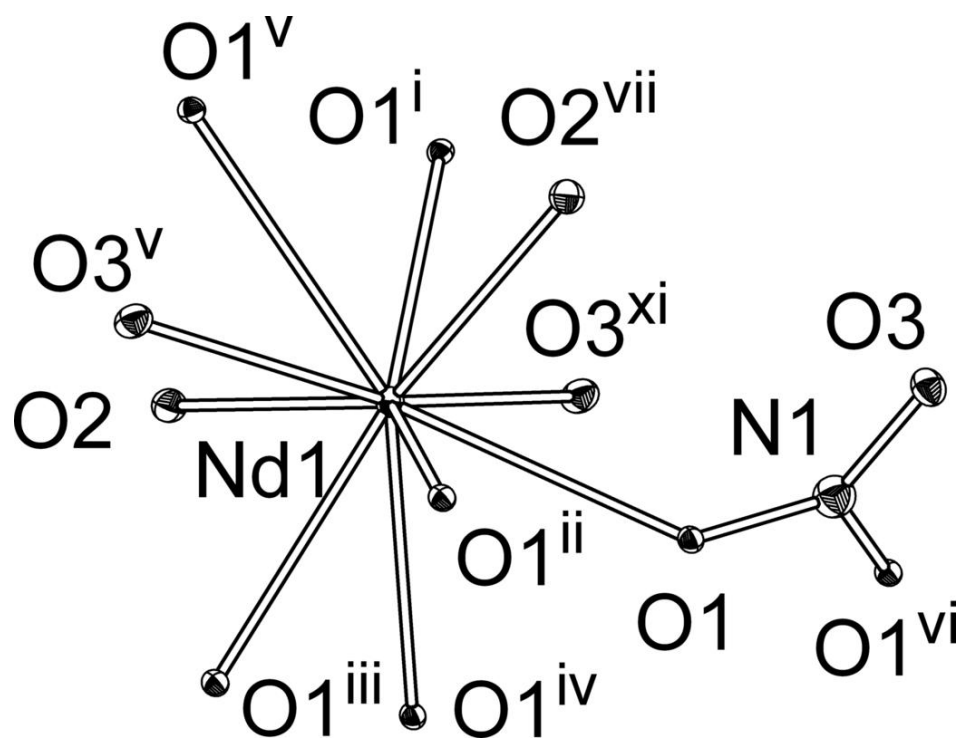


Fig. 2

