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$NdO(NO_3)$

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ(O–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 $LaO(NO_3)$, arose from a solvothermal reaction. The Nd ion (site symmetry m) is ten-coordinated by eight O atoms of NO_3 groups and two μ_2-oxide ions. A three-dimensional structure is constructed by the interconnection of NdO_{10} 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

$NdO(NO_3)$
M_r = 222.25
Orthorhombic, *Pnma*
a = 7.5233 (15) Å
b = 5.1618 (10) Å
c = 8.7157 (17) Å
V = 338.46 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 15.19 mm^{-1}
T = 293 (2) K
0.16 × 0.14 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
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_{int} = 0.034

Refinement

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

References

Brandenburg, K. (2000). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Gobichon, A. E., Auffrédic, J. P. & Louër, D. (1997). *Solid State Ionics*, **93**, 51–64.
Guillou, N., Auffrédic, J. P. & Louër, D. (1994). *J. Solid State Chem.* **112**, 45–52.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Rigaku (2002). *PROCESS-AUTO* and *CrystalStructure*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhang, Q., Lu, C., Yang, W., Chen, S. & Yu, Y. (2004). *Inorg. Chem. Commun.* **7**, 889–892.

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S1. 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 determinated 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 H_2O and DMF.

The asymmetric unit of (I) is consisted of 0.5 N d, 0.5 O and 0.5 NO_3 (Fig. 1). All oxygen atoms of NO_3 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 A°, and the last one (O3) is coordinated to two different Nd ions with Nd—O distance of 2.636 A° (Table 1). A μ_2-O (O2) exists in the structure of (I) with Nd—O distances of 2.434 and 2.458 A° and corresponding Nd—O2—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-μ_2-O—Nd bonds with Nd—Nd distance of 4.0254 (8)A° and the other *via* Nd—O(NO_3)-Nd bonds. A three-dimensional framework constructed by the interconnections of NdO_{10} polyhedra is shown in Fig. 2.

There are two different structures with the same molecular formula of $LnONO_3$, such as $LnONO_3$(Ln=Y, La) in the P_4/mmm space group and $LaONO_3$ in *Pnma* space group. In this work, $NdONO_3$ is the isostructural compound of the reported $LaONO_3$ (Zhang, *et al.*, 2004).

S2. Experimental

Isonicotine (0.123 g, 1.0 mmol) was added to a mixed solution of 5 ml H_2O/3 ml DMF. After being stirred for 5 h, the isonicotine was partially dissovled with pH = 6.0. Then, $Nd(NO_3)_3{\cdot}6H_2O$ (0.220 g, 0.5 mmol) was added and stirred for 7 h. The molar ratio of $Nd(NO_3)_3{\cdot}6H_2O$: 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.

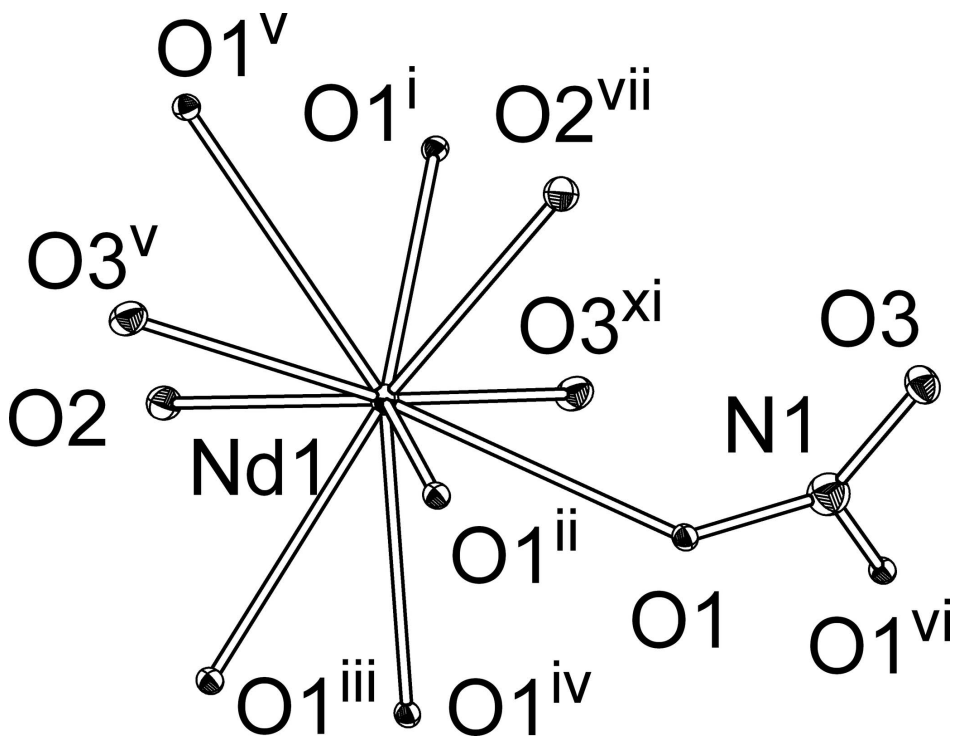

Figure 1

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*.]

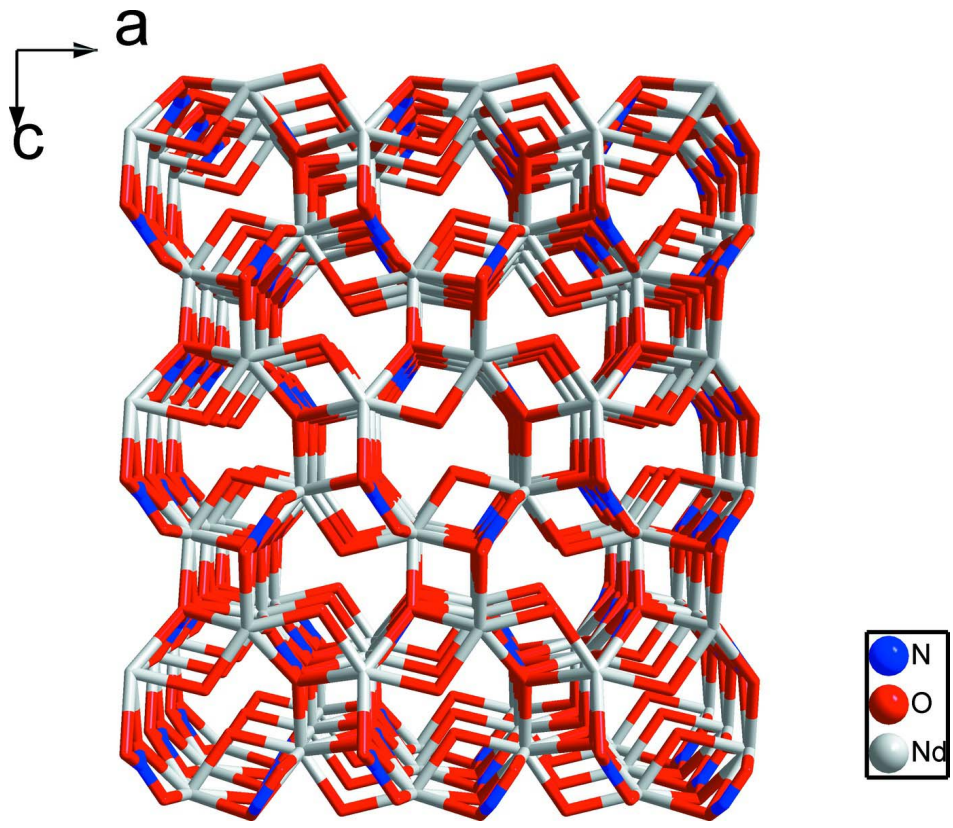

Figure 2

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

neodymium(III) oxide nitrate

Crystal data

$NdO(NO_3)$
$M_r = 222.25$
Orthorhombic, *Pnma*
Hall symbol: -P 2ac 2n
$a = 7.5233\ (15)$ Å
$b = 5.1618\ (10)$ Å
$c = 8.7157\ (17)$ Å
$V = 338.46\ (11)$ Å^3
$Z = 4$
$F(000) = 396$
$D_x = 4.362$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2000 reflections
$\theta = 3.6–27.0°$
$\mu = 15.19$ mm^{-1}
$T = 293$ K
Prism, colourless
0.16 × 0.14 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.00 pixels mm^{-1}
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 $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 27.0°$, $\theta_{min} = 3.6°$
$h = -9\rightarrow8$
$k = -5\rightarrow6$
$l = -11\rightarrow11$

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
34 parameters
30 restraints

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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.02$ e Å^{-3}
$\Delta\rho_{min} = -1.42$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{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 (Å²)

	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 (Å, º)

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)
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) $x, -y-1/2, z$.