

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Neodymium(III) molybdenum(VI) borate,
NdBO₂MoO₄Peter Held,* Benjamin van der Wolf, Ladislav Bohatý and
Petra BeckerInstitut für Kristallographie, Universität zu Köln, Greinstrasse 6, D-50939 Köln,
Germany

Correspondence e-mail: peter.held@uni-koeln.de

Received 15 April 2011; accepted 11 May 2011

Key indicators: single-crystal X-ray study; $T = 292$ K; mean $\sigma(\text{O}-\text{B}) = 0.006$ Å;
 R factor = 0.025; wR factor = 0.063; data-to-parameter ratio = 16.2.

Single crystals of NdBO₂MoO₄ were obtained from a molybdenum oxide–boron oxide flux under an air atmosphere. The structure features double chains of edge- and face-sharing distorted [NdO₁₀] bicapped square-antiprisms, which are linked by rows of isolated [MoO₄] tetrahedra and by zigzag chains of corner-sharing [BO₃] groups, all of them running along the b axis. The chains of [NdO₁₀], chains of [BO₃] and rows of [MoO₄] groups are arranged in layers parallel to the bc plane.

Related literature

A rough investigation of subsolidus phase relations in the pseudo-ternary system Nd₂O₃ – B₂O₃ – MoO₃ has been reported by Lysanova *et al.* (1983) and Dzhurinskii & Lysanova (1998). X-ray powder diffraction data of LnBO₂MoO₄ ($Ln = \text{La, Ce, Pr, Nd}$) are given by Lysanova *et al.* (1983). The occurrence of a structural phase transition of LaBO₂MoO₄ was reported by Becker *et al.* (2008). For determinations of related structures, see: Palkina *et al.* (1979); Zhao *et al.* (2008, 2009) for LaBO₂MoO₄; Zhao *et al.* (2008) for CeBO₂MoO₄.

Experimental

Crystal data

NdMoBO₆
 $M_r = 346.99$ Monoclinic, $P2_1/c$
 $a = 10.1218$ (19) Å $b = 4.1420$ (5) Å
 $c = 11.896$ (3) Å
 $\beta = 116.897$ (14)°
 $V = 444.78$ (16) Å³
 $Z = 4$ Mo $K\alpha$ radiation
 $\mu = 14.30$ mm⁻¹
 $T = 292$ K
 $0.30 \times 0.20 \times 0.15$ mm

Data collection

Enraf–Nonius CAD-4/MACH3
diffractometer
Absorption correction: ψ scan
(*MolEN*; Fair, 1990)
 $T_{\min} = 0.487$, $T_{\max} = 0.998$
5004 measured reflections1344 independent reflections
1268 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.035$
3 standard reflections every 100
reflections
intensity decay: 2.1%

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.025$
 $wR(F^2) = 0.063$
 $S = 1.22$
1344 reflections83 parameters
 $\Delta\rho_{\max} = 2.24$ e Å⁻³
 $\Delta\rho_{\min} = -1.61$ e Å⁻³

Data collection: *MACH3* (Enraf–Nonius, 1993); cell refinement: *MACH3*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ATOMS* (Dowty, 2002); software used to prepare material for publication: *pubCIF* (Westrip, 2010).

This work was supported by the Deutsche Forschungsgemeinschaft (DFG) under projects BO 1017/5–2 and BE 2147/6–2.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2107).

References

- Becker, P., van der Wolf, B., Bohatý, L., Dong, J. & Kaminskii, A. A. (2008). *Laser Phys. Lett.* **5**, 737–745.
- Dowty, E. (2002). *ATOMS*. Shape Software, Kingsport, Tennessee, USA.
- Dzhurinskii, B. F. & Lysanova, G. V. (1998). *Russ. J. Inorg. Chem.* **43**, 1931–1940.
- Enraf–Nonius (1993). *MACH3 Server Software*. Enraf–Nonius, Delft, The Netherlands.
- Fair, C. K. (1990). *MolEN*. Enraf–Nonius, Delft, The Netherlands.
- Lysanova, G. V., Dzhurinskii, B. F., Komova, M. G. & Tananaev, I. V. (1983). *Russ. J. Inorg. Chem.* **28**, 1344–1349.
- Palkina, K. K., Saifuddinov, V. Z., Kuznetsov, V. G., Dzhurinskii, B. F., Lysanova, G. V. & Reznik, E. M. (1979). *Russ. J. Inorg. Chem.* **24**, 663–666.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
- Zhao, D., Cheng, W.-D., Zhang, H., Hang, S.-P. & Fang, M. (2008). *Dalton Trans.* pp. 3709–3714.
- Zhao, W., Zhang, L., Wang, G., Song, M., Huang, Y. & Wang, G. (2009). *Opt. Mater.* **31**, 849–853.

supporting information

Acta Cryst. (2011). E67, i36 [doi:10.1107/S1600536811017806]

Neodymium(III) molybdenum(VI) borate, NdBO₂MoO₄

Peter Held, Benjamin van der Wolf, Ladislav Bohatý and Petra Becker

S1. Comment

In the family of lanthanide compounds LnBO₂MoO₄ the crystal structure of LaBO₂MoO₄ was first described by Palkina *et al.* (1979), giving the polar space group $P2_1$ and lattice constants $a = 5.964$ (1) Å, $b = 4.147$ (1) Å, $c = 9.373$ (3) Å, $\beta = 99.28$ (2)°. On the basis of X-ray powder diffraction data, Lysanova *et al.* (1983) claimed the isomorphism of the compounds LnBO₂MoO₄ with Ln = La, Ce, Pr, Nd. The structure of LaBO₂MoO₄ was redetermined by Zhao *et al.* (2008), who reported a centrosymmetric structure with space group symmetry $P2_1/c$ with lattice constants $a = 10.2968$ (8) Å, $b = 4.1636$ (3) Å, $c = 23.8587$ (15) Å, $\beta = 115.367$ (3)°. These results were corroborated by Zhao *et al.* (2009), who, however, attributed this crystal structure to a high-temperature modification of LaBO₂MoO₄. The occurrence of a structural phase transition of LaBO₂MoO₄ was reported by Becker *et al.* (2008). Zhao *et al.* (2008) also presented the crystal structure of the related cerium compound, CeBO₂MoO₄, with space group $P2_1/c$ and lattice constants $a = 10.2404$ (15) Å, $b = 4.1495$ (4) Å, $c = 11.9286$ (14) Å, $\beta = 116.100$ (9)°, and thus showed, that the presumed isomorphism of the lanthanum and the cerium compound is not correct. However, the crystal structures are closely related, with an unit cell of LaBO₂MoO₄ which is doubled with respect to the unit cell of CeBO₂MoO₄. The result of the present study shows, that also NdBO₂MoO₄ is not isomorphic to LaBO₂MoO₄, but is isomorphic to CeBO₂MoO₄.

The crystal structure of NdBO₂MoO₄ consists of groups [BO₃] and [MoO₄] and tenfold coordinated neodymium atoms. The [BO₃] groups are connected *via* common oxygen ligands to zigzag chains [B₂O₄]_∞ along the *b* axis, with a periodicity of two [BO₃] groups. The planar [BO₃] groups are slightly distorted with O—B—O angles of 114.4 (4)°, 117.4 (4)° and 128.1 (4)°. They are linked by the common oxygen atom O1 with a bond angle B—O1—B of 125.6 (3)° (see Fig. 1). The O1 ligands are connected to two boron atoms and one Nd atom, each, while the O2 ligands of the [BO₃] groups are linked to three Nd atoms and one B, each. Mo atoms are tetrahedrally coordinated by the oxygen atoms O3, O4, O5 and O6 (see Fig. 1), with Mo—O distances ranging from 1.740 (4) Å (Mo—O3) to 1.816 (3) Å (Mo—O4) and angles O—Mo—O ranging from 96.3 (2)° (O4—Mo—O3) to 117.5 (2)° (O4—Mo—O6). The [MoO₄] tetrahedra are arranged in rows that run parallel the *b* axis. Within a single row the [MoO₄] tetrahedra are aligned with their Mo—O3 bonding directions pointing in the same direction approximately parallel to the *b* axis. Rows with opposite Mo—O3 bonding direction (*+b* and *-b*) alternate along the *c* axis, as shown in Fig. 2. Within a row the distance of a Mo atom to the O3 ligand of the neighbouring tetrahedron amounts 2.419 (3) Å. (Note that in Zhao *et al.* (2008) a distorted trigonal bipyramid is preferred as description of the coordination surrounding of Mo in CeBO₂MoO₄.) The oxygen atoms O3 and O5 serve as ligands of one Mo and one Nd atom, each, while the oxygen atoms O6 and O4 act as ligands for one Mo and two Nd atoms, each. The tenfold coordination of neodymium atoms in NdBO₂MoO₄ can be described as distorted bicapped square antiprism with Nd—O bonding distances ranging between 2.364 (3) Å (Nd—O2) and 2.981 (4) Å (Nd—O6). [NdO₁₀] polyhedra are connected along the *b* axis by sharing three common oxygen ligands, namely O2, O6 and O4 (Fig. 1), with each neighbouring polyhedron, thus forming chains along the *b* axis. Two parallel chains are linked *via* edges (formed by two common O2 atoms) of the Nd coordination polyhedra, resulting in a double chain along *b*, see Fig. 2.

S2. Experimental

NdBO₂MoO₄ melts incongruently, therefore, single crystals of NdBO₂MoO₄ were grown from a melt with a composition differing from the crystal stoichiometry. A homogenized powder mixture of Nd₂O₃ (99.9%, Alfa Aesar), B₂O₃ (99.98%, Alfa Aesar) and MoO₃ (99.95%, Alfa Aesar) in a molar ratio of 1: 1.375: 2.625 was heated in a covered platinum crucible in air atmosphere to 1423 K and subsequently cooled at a rate of 3 K h⁻¹ to 1173 K. Transparent violet prismatic crystals of the title compound were separated mechanically from the surrounding flux. A suitable single-crystal was carefully selected using a polarizing microscope and mounted in a glass capillary.

S3. Refinement

The final difference maps indicate a maximum of 2.235 e Å⁻³ at a distance of 0.66 Å from Nd and a minimum of -1.611 e Å⁻³ at a distance of 1.06 Å of Nd.

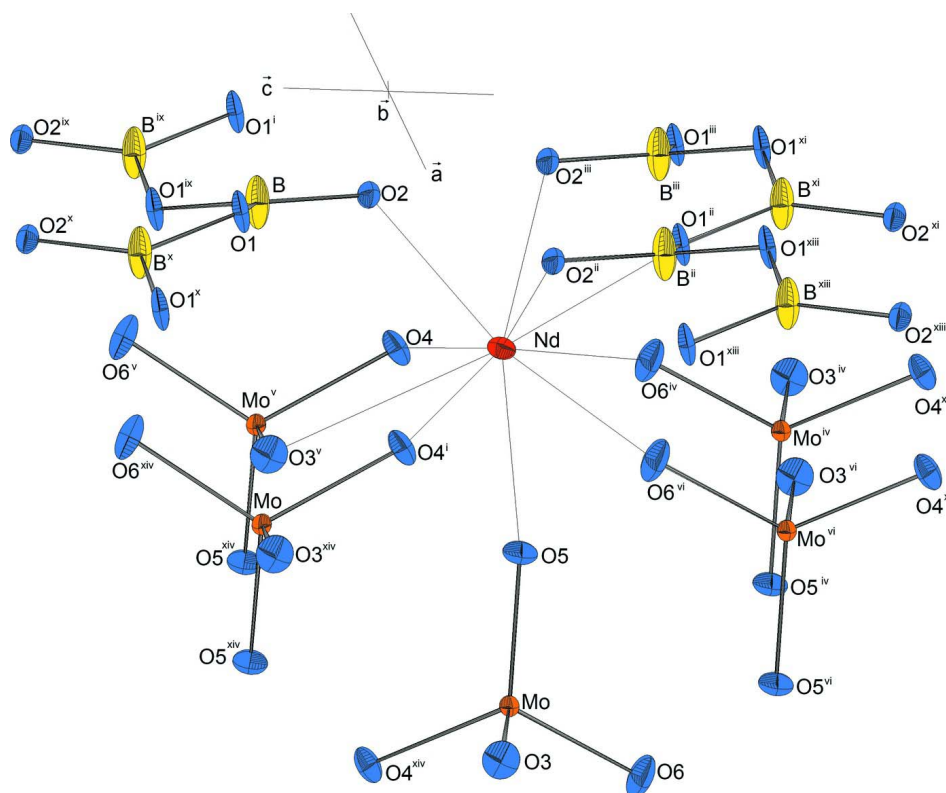
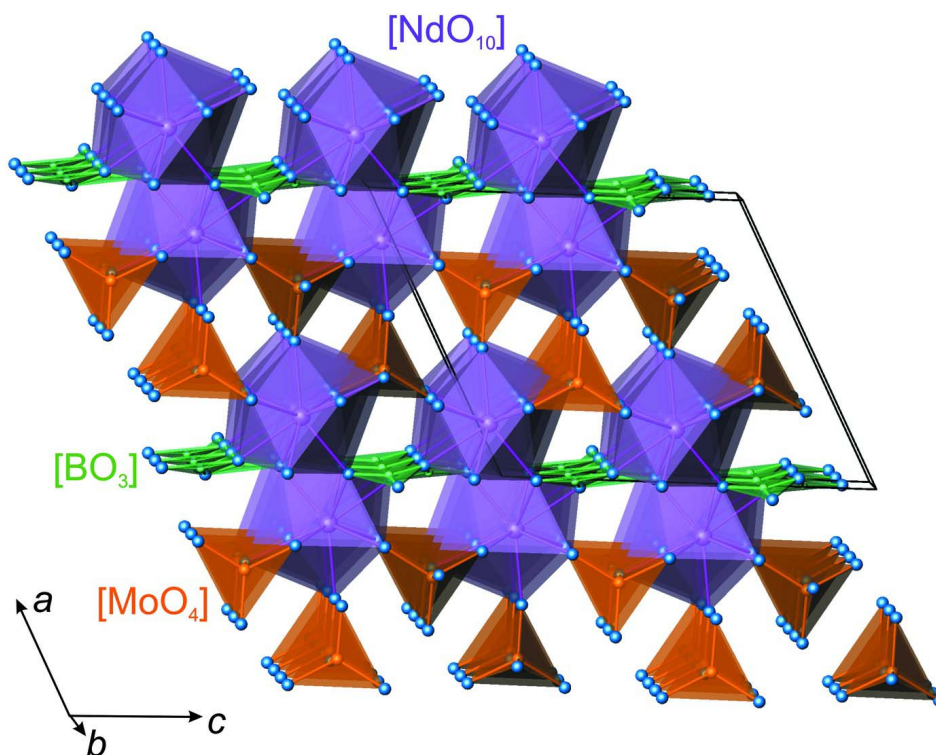


Figure 1

The structural units in NdBO₂MoO₄ with atomic numbering scheme (projection approximately along the *b*-axis). Atoms are drawn as 50% probability ellipsoids. Symmetry codes: (i) $x, y + 1, z$; (ii) $-x, -y + 1, -z - 1$; (iii) $-x, -y, -z - 1$; (iv) $-x + 1, -y, -z - 1$; (v) $-x + 1, y - 1/2, -z - 1/2$; (vi) $-x + 1, -y + 1, -z - 1$; (vii) $-x + 1, y + 1/2, -z - 1/2$; (viii) $x, y - 1, z$; (ix) $-x, y - 1/2, -z - 1/2$; (x) $-x, y + 1/2, -z - 1/2$; (xi) $x, -y + 1/2, z + 1/2$; (xii) $x, -y - 1/2, z - 1/2$; (xiii) $x, 3/2 - y, z - 1/2$; (xiv) $1 - x, 1/2 + y, z - 1/2$.

**Figure 2**

View of the crystal structure of $\text{NdBO}_2\text{MoO}_4$ along the b axis, showing chains of corner-sharing $[\text{BO}_3]$ groups (green), double-chains of face- and edge-sharing $[\text{NdO}_{10}]$ polyhedra (purple), and rows of isolated $[\text{MoO}_4]$ tetrahedra (orange), all of them running along the b axis. In a single row, $[\text{MoO}_4]$ tetrahedra are arranged with identical orientation, thus giving a polarity $+b$ or $-b$ to the row. Note the alternating polarity of the arrangement of $[\text{MoO}_4]$ tetrahedra rows along the c axis.

Neodymium(III) molybdenum(VI) borate

Crystal data

NdMoBO_6
 $M_r = 346.99$
 Monoclinic, $P2_1/c$
 Hall symbol: $-P\ 2ybc$
 $a = 10.1218\ (19)\ \text{\AA}$
 $b = 4.1420\ (5)\ \text{\AA}$
 $c = 11.896\ (3)\ \text{\AA}$
 $\beta = 116.897\ (14)^\circ$
 $V = 444.78\ (16)\ \text{\AA}^3$
 $Z = 4$

$F(000) = 620$
 $D_x = 5.182\ \text{Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$
 Cell parameters from 25 reflections
 $\theta = 12.1\text{--}21.2^\circ$
 $\mu = 14.30\ \text{mm}^{-1}$
 $T = 292\ \text{K}$
 Prism, light violet
 $0.30 \times 0.20 \times 0.15\ \text{mm}$

Data collection

Enraf–Nonius CAD4/MACH3
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 $\omega/2\theta$ scans
 Absorption correction: ψ scan
 (*MoIEN*; Fair, 1990)

$T_{\min} = 0.487$, $T_{\max} = 0.998$
 5004 measured reflections
 1344 independent reflections
 1268 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.035$
 $\theta_{\max} = 30.4^\circ$, $\theta_{\min} = 2.3^\circ$
 $h = -14 \rightarrow 14$

$k = -5 \rightarrow 5$
 $l = -16 \rightarrow 16$

3 standard reflections every 100 reflections
 intensity decay: 2.1%

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.025$
 $wR(F^2) = 0.063$
 $S = 1.22$
 1344 reflections
 83 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 $w = 1/[\sigma^2(F_o^2) + (0.0304P)^2 + 1.8082P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 2.24 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -1.61 \text{ e } \text{\AA}^{-3}$
 Extinction correction: *SHELXL97* (Sheldrick,
 2008), $F_c^* = kFc[1 + 0.001x Fc^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.0428 (13)

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 is done 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 $F^2 > 2\sigma(F^2)$ 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	$U_{\text{iso}}^*/U_{\text{eq}}$
Nd	0.19204 (2)	0.21132 (6)	-0.47183 (2)	0.00919 (11)
Mo	0.64536 (4)	0.30466 (8)	-0.31742 (3)	0.00668 (12)
B	-0.0028 (7)	0.3290 (12)	-0.3083 (5)	0.0182 (10)
O1	-0.0326 (4)	0.6580 (8)	-0.3013 (3)	0.0120 (6)
O2	-0.0035 (3)	0.2247 (7)	-0.4150 (3)	0.0099 (5)
O3	0.6616 (4)	0.7223 (8)	-0.3016 (4)	0.0173 (7)
O4	0.2605 (4)	-0.2856 (7)	-0.3501 (3)	0.0124 (6)
O5	0.4556 (4)	0.2256 (9)	-0.3956 (3)	0.0156 (6)
O6	0.7424 (4)	0.2194 (9)	-0.4084 (4)	0.0190 (7)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd	0.00733 (14)	0.00900 (16)	0.00992 (14)	-0.00094 (6)	0.00274 (10)	-0.00205 (7)
Mo	0.00602 (17)	0.0087 (2)	0.00546 (17)	-0.00022 (10)	0.00270 (13)	-0.00094 (10)
B	0.040 (3)	0.007 (2)	0.013 (2)	0.0020 (19)	0.017 (2)	-0.0003 (17)
O1	0.0259 (16)	0.0056 (13)	0.0050 (12)	-0.0010 (11)	0.0074 (12)	-0.0004 (10)
O2	0.0108 (13)	0.0118 (14)	0.0084 (13)	-0.0018 (10)	0.0055 (11)	-0.0021 (10)
O3	0.0203 (16)	0.0125 (15)	0.0199 (16)	0.0003 (12)	0.0099 (14)	-0.0002 (12)
O4	0.0173 (15)	0.0091 (14)	0.0067 (13)	-0.0007 (10)	0.0018 (12)	-0.0017 (10)
O5	0.0066 (12)	0.0235 (17)	0.0137 (15)	-0.0009 (11)	0.0019 (11)	-0.0008 (12)
O6	0.0271 (18)	0.0192 (17)	0.0207 (17)	-0.0024 (13)	0.0197 (15)	-0.0039 (13)

Geometric parameters (Å, °)

Nd—O2	2.364 (3)	B—O2	1.338 (6)
Nd—O5	2.399 (3)	B—O1 ^{ix}	1.381 (6)
Nd—O4	2.431 (3)	B—O1	1.406 (6)
Nd—O4 ⁱ	2.452 (3)	B—Nd ⁱⁱ	3.099 (6)
Nd—O1 ⁱⁱ	2.498 (3)	B—Nd ⁱⁱⁱ	3.315 (6)
Nd—O2 ⁱⁱⁱ	2.528 (3)	O1—B ^x	1.381 (6)
Nd—O6 ^{iv}	2.551 (3)	O1—Nd ⁱⁱ	2.498 (3)
Nd—O3 ^v	2.901 (4)	O2—Nd ⁱⁱⁱ	2.528 (3)
Nd—O2 ⁱⁱ	2.930 (3)	O2—Nd ⁱⁱ	2.930 (3)
Nd—O6 ^{vi}	2.981 (4)	O3—Mo ⁱ	2.419 (3)
Mo—O3	1.740 (4)	O3—Nd ^{vii}	2.901 (4)
Mo—O5	1.745 (3)	O4—Mo ^v	1.816 (3)
Mo—O6	1.795 (3)	O4—Nd ^{viii}	2.452 (3)
Mo—O4 ^{vii}	1.816 (3)	O6—Nd ^{iv}	2.551 (3)
Mo—O3 ^{viii}	2.419 (3)	O6—Nd ^{vi}	2.981 (4)
Mo—Nd ^{vii}	3.5017 (8)		
O2—Nd—O5	145.40 (12)	O4 ^{vii} —Mo—Nd ^{vi}	128.02 (11)
O2—Nd—O4	84.21 (11)	O3 ^{viii} —Mo—Nd ^{vi}	120.27 (9)
O5—Nd—O4	80.04 (12)	Nd ^{vii} —Mo—Nd ^{vi}	103.052 (17)
O2—Nd—O4 ⁱ	81.98 (11)	Nd ^v —Mo—Nd ^{vi}	135.816 (15)
O5—Nd—O4 ⁱ	77.71 (12)	O3—Mo—Nd	99.98 (12)
O4—Nd—O4 ⁱ	116.06 (13)	O5—Mo—Nd	7.61 (12)
O2—Nd—O1 ⁱⁱ	95.08 (11)	O6—Mo—Nd	121.06 (13)
O5—Nd—O1 ⁱⁱ	117.89 (12)	O4 ^{vii} —Mo—Nd	113.32 (11)
O4—Nd—O1 ⁱⁱ	134.27 (11)	O3 ^{viii} —Mo—Nd	87.93 (9)
O4 ⁱ —Nd—O1 ⁱⁱ	109.02 (10)	Nd ^{vii} —Mo—Nd	114.650 (15)
O2—Nd—O2 ⁱⁱⁱ	68.97 (12)	Nd ^v —Mo—Nd	105.813 (15)
O5—Nd—O2 ⁱⁱⁱ	131.40 (11)	Nd ^{vi} —Mo—Nd	116.653 (16)
O4—Nd—O2 ⁱⁱⁱ	69.84 (11)	O3—Mo—Nd ^{iv}	122.17 (12)
O4 ⁱ —Nd—O2 ⁱⁱⁱ	149.91 (11)	O5—Mo—Nd ^{iv}	102.87 (12)
O1 ⁱⁱ —Nd—O2 ⁱⁱⁱ	67.44 (11)	O6—Mo—Nd ^{iv}	20.25 (12)
O2—Nd—O6 ^{iv}	129.71 (11)	O4 ^{vii} —Mo—Nd ^{iv}	113.64 (11)
O5—Nd—O6 ^{iv}	72.70 (12)	O3 ^{viii} —Mo—Nd ^{iv}	60.20 (9)
O4—Nd—O6 ^{iv}	70.40 (12)	Nd ^{vii} —Mo—Nd ^{iv}	134.533 (16)
O4 ⁱ —Nd—O6 ^{iv}	148.09 (12)	Nd ^v —Mo—Nd ^{iv}	94.773 (16)
O1 ⁱⁱ —Nd—O6 ^{iv}	75.67 (12)	Nd ^{vi} —Mo—Nd ^{iv}	60.259 (12)
O2 ⁱⁱⁱ —Nd—O6 ^{iv}	61.79 (10)	Nd—Mo—Nd ^{iv}	110.359 (15)
O2—Nd—O3 ^v	75.40 (11)	O2—B—O1 ^{ix}	128.1 (4)
O5—Nd—O3 ^v	70.07 (11)	O2—B—O1	117.4 (4)
O4—Nd—O3 ^v	58.78 (10)	O1 ^{ix} —B—Nd ⁱⁱ	155.4 (4)
O4 ⁱ —Nd—O3 ^v	57.31 (10)	O1 ^{ix} —B—Nd ⁱⁱⁱ	102.0 (3)
O1 ⁱⁱ —Nd—O3 ^v	163.84 (10)	O1—B—Nd ⁱⁱⁱ	129.6 (4)
O2 ⁱⁱⁱ —Nd—O3 ^v	119.20 (10)	Nd ⁱⁱ —B—Nd ⁱⁱⁱ	80.37 (14)
O6 ^{iv} —Nd—O3 ^v	120.47 (11)	O1 ^{ix} —B—Nd	120.0 (3)
O2—Nd—O2 ⁱⁱ	69.96 (11)	O1—B—Nd	111.8 (3)

O5—Nd—O2 ⁱⁱ	122.40 (10)	Nd ⁱⁱ —B—Nd	84.34 (13)
O4—Nd—O2 ⁱⁱ	154.13 (10)	Nd ⁱⁱⁱ —B—Nd	74.17 (11)
O4 ⁱ —Nd—O2 ⁱⁱ	62.95 (10)	O2—B—Nd ^{xi}	144.1 (4)
O1 ⁱⁱ —Nd—O2 ⁱⁱ	50.40 (10)	O1—B—Nd ^{xi}	90.2 (3)
O2 ⁱⁱⁱ —Nd—O2 ⁱⁱ	98.46 (10)	Nd ⁱⁱ —B—Nd ^{xi}	142.25 (16)
O6 ^{iv} —Nd—O2 ⁱⁱ	125.50 (11)	Nd ⁱⁱⁱ —B—Nd ^{xi}	132.90 (16)
O3 ^v —Nd—O2 ⁱⁱ	113.50 (9)	Nd—B—Nd ^{xi}	117.93 (18)
O2—Nd—O6 ^{vi}	120.96 (10)	B ^x —O1—B	125.6 (3)
O5—Nd—O6 ^{vi}	73.22 (11)	B ^x —O1—Nd ⁱⁱ	132.3 (3)
O4—Nd—O6 ^{vi}	152.84 (11)	B—O1—Nd ⁱⁱ	101.4 (3)
O4 ⁱ —Nd—O6 ^{vi}	62.98 (10)	B ^x —O1—Nd ^{xi}	57.4 (2)
O1 ⁱⁱ —Nd—O6 ^{vi}	59.13 (11)	B—O1—Nd ^{xi}	68.4 (3)
O2 ⁱⁱⁱ —Nd—O6 ^{vi}	126.02 (10)	Nd ⁱⁱ —O1—Nd ^{xi}	169.04 (12)
O6 ^{iv} —Nd—O6 ^{vi}	96.66 (11)	B ^x —O1—Nd	137.1 (3)
O3 ^v —Nd—O6 ^{vi}	114.35 (10)	B—O1—Nd	49.7 (3)
O2 ⁱⁱ —Nd—O6 ^{vi}	52.35 (9)	Nd ⁱⁱ —O1—Nd	78.20 (8)
O3—Mo—O5	105.76 (17)	Nd ^{xi} —O1—Nd	96.89 (8)
O3—Mo—O6	102.12 (17)	B—O2—Nd	129.3 (3)
O5—Mo—O6	114.36 (17)	B—O2—Nd ⁱⁱⁱ	114.5 (3)
O3—Mo—O4 ^{vii}	96.26 (16)	Nd—O2—Nd ⁱⁱⁱ	111.03 (12)
O5—Mo—O4 ^{vii}	116.79 (16)	B—O2—Nd ⁱⁱ	84.3 (3)
O6—Mo—O4 ^{vii}	117.52 (17)	Nd—O2—Nd ⁱⁱ	110.04 (11)
O3—Mo—O3 ^{viii}	169.5 (2)	Nd ⁱⁱⁱ —O2—Nd ⁱⁱ	98.46 (10)
O5—Mo—O3 ^{viii}	82.75 (15)	Mo—O3—Mo ⁱ	169.5 (2)
O6—Mo—O3 ^{viii}	79.30 (15)	Mo—O3—Nd ^{vii}	94.65 (15)
O4 ^{vii} —Mo—O3 ^{viii}	74.10 (13)	Mo ⁱ —O3—Nd ^{vii}	94.88 (12)
O3—Mo—Nd ^{vii}	55.67 (13)	Mo—O3—Nd ^{vi}	92.60 (14)
O5—Mo—Nd ^{vii}	121.91 (12)	Mo ⁱ —O3—Nd ^{vi}	84.42 (10)
O6—Mo—Nd ^{vii}	123.02 (13)	Nd ^{vii} —O3—Nd ^{vi}	131.41 (12)
O4 ^{vii} —Mo—Nd ^{vii}	40.63 (10)	Mo ^v —O4—Nd	110.25 (14)
O3 ^{viii} —Mo—Nd ^{vii}	114.71 (9)	Mo ^v —O4—Nd ^{viii}	133.69 (16)
O3—Mo—Nd ^v	123.03 (13)	Nd—O4—Nd ^{viii}	116.06 (13)
O5—Mo—Nd ^v	105.84 (12)	Mo ^v —O4—Nd ⁱⁱⁱ	117.45 (14)
O6—Mo—Nd ^v	106.15 (13)	Nd—O4—Nd ⁱⁱⁱ	71.19 (8)
O4 ^{vii} —Mo—Nd ^v	26.80 (10)	Nd ^{viii} —O4—Nd ⁱⁱⁱ	78.89 (8)
O3 ^{viii} —Mo—Nd ^v	47.32 (9)	Mo—O5—Nd	166.9 (2)
Nd ^{vii} —Mo—Nd ^v	67.430 (16)	Mo—O6—Nd ^{iv}	145.65 (19)
O3—Mo—Nd ^{vi}	62.27 (12)	Mo—O6—Nd ^{vi}	115.69 (16)
O5—Mo—Nd ^{vi}	114.60 (12)	Nd ^{iv} —O6—Nd ^{vi}	96.66 (11)
O6—Mo—Nd ^{vi}	41.02 (12)		

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