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 $\beta$ -Nd<sub>2</sub>Mo<sub>4</sub>O<sub>15</sub>

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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{Mo}-\text{O}) = 0.007$  Å;  $R$  factor = 0.046;  $wR$  factor = 0.128; data-to-parameter ratio = 12.5.

The title compound, dineodymium(III) tetramolybdate(VI), has been prepared by a flux technique and is the second polymorph of composition Nd<sub>2</sub>Mo<sub>4</sub>O<sub>15</sub>. The crystal structure is isotypic with those of Ce<sub>2</sub>Mo<sub>4</sub>O<sub>15</sub> and Pr<sub>2</sub>Mo<sub>4</sub>O<sub>15</sub>. It features a three-dimensional network composed of distorted edge- and corner-sharing NdO<sub>7</sub> polyhedra, NdO<sub>8</sub> polyhedra, MoO<sub>4</sub> tetrahedra and MoO<sub>6</sub> octahedra.

## Related literature

For background to molybdates with rare earth (*RE*) cations, see: Borchardt & Bierstedt (1966); Ouwerkerk *et al.* (1982). For the  $\alpha$ -polymorph of Nd<sub>2</sub>Mo<sub>4</sub>O<sub>15</sub>, see: Naruke & Yamase (2003). Structures isotypic with  $\beta$ -Nd<sub>2</sub>Mo<sub>4</sub>O<sub>15</sub> were reported for the Ce (Fallon & Gatehouse, 1982) and Pr (Efremov *et al.*, 1988*a*) analogues. For the crystal structures, properties and applications of other molybdates with general formula  $RE_2\text{Mo}_4\text{O}_{15}$ , see:  $RE = \text{La}$  (Dubois *et al.*, 2001); Tb (Naruke & Yamase, 2001); La, Nd, Sm (Naruke & Yamase, 2003); Ho (Efremov *et al.*, 1988*b*).

## Experimental

## Crystal data

Nd<sub>2</sub>Mo<sub>4</sub>O<sub>15</sub> $M_r = 912.24$ Triclinic,  $P\bar{1}$ 

$a = 7.4000$  (6) Å  
 $b = 7.4992$  (6) Å  
 $c = 11.7291$  (9) Å  
 $\alpha = 88.916$  (2)°  
 $\beta = 83.957$  (1)°  
 $\gamma = 84.196$  (2)°

 $V = 643.94$  (9) Å<sup>3</sup> $Z = 2$ Mo  $K\alpha$  radiation $\mu = 11.77$  mm<sup>-1</sup> $T = 293$  K

0.15 × 0.15 × 0.05 mm

## Data collection

Bruker SMART 1K CCD diffractometer  
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)  
 $T_{\min} = 0.271$ ,  $T_{\max} = 0.591$

3620 measured reflections  
2390 independent reflections  
2268 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.040$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$   
 $wR(F^2) = 0.128$   
 $S = 1.05$   
2390 reflections

191 parameters  
 $\Delta\rho_{\max} = 3.38$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -2.54$  e Å<sup>-3</sup>

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2004); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2425).

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**supplementary materials**

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## $\beta$ -Nd<sub>2</sub>Mo<sub>4</sub>O<sub>15</sub>

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### Comment

Rare-earth molybdate compounds have been intensively studied due to their diversity and excellent chemical stabilities, as well as their potential applications as laser host phosphors, or as ferroelectric and ferroelastic materials (Borchardt & Bierstedt, 1966; Ouwerkerk *et al.*, 1982). Previous studies of the family of RE<sub>2</sub>Mo<sub>4</sub>O<sub>15</sub> (RE is a rare earth metal cation) compounds show that they adopt different structure types, such as monoclinic La<sub>2</sub>Mo<sub>4</sub>O<sub>15</sub> with  $Z = 4$  (Dubois *et al.*, 2001; Naruke & Yamase, 2003); Tb<sub>2</sub>Mo<sub>4</sub>O<sub>15</sub> (Naruke & Yamase, 2001) and Ho<sub>2</sub>Mo<sub>4</sub>O<sub>15</sub> (Efremov *et al.*, 1988*b*) with  $Z = 2$ , or triclinic Nd<sub>2</sub>Mo<sub>4</sub>O<sub>15</sub> (Naruke & Yamase, 2003) with  $Z = 3$ . In this paper, we present synthesis and crystal structure of the  $\beta$ -phase of compound Nd<sub>2</sub>Mo<sub>4</sub>O<sub>15</sub> which is structurally different from the first ( $\alpha$ -) Nd<sub>2</sub>Mo<sub>4</sub>O<sub>15</sub> polymorph (Naruke & Yamase, 2003), but is isotypic with Ce<sub>2</sub>Mo<sub>4</sub>O<sub>15</sub> (Fallon & Gatehouse, 1982) and Pr<sub>2</sub>Mo<sub>4</sub>O<sub>15</sub> (Efremov *et al.*, 1988*a*) with  $Z = 2$ .

The structure of  $\beta$ -Nd<sub>2</sub>Mo<sub>4</sub>O<sub>15</sub> features a three-dimensional framework composed of distorted NdO<sub>7</sub>, NdO<sub>8</sub>, MoO<sub>4</sub> and MoO<sub>6</sub> polyhedra, as shown in Fig. 1. There are four crystallographically different Mo atoms in the asymmetric unit. Mo(1), Mo(2), Mo(3) atoms are surrounded by four oxygen atoms within a tetrahedral coordination, while the Mo(4) atom is surrounded by six oxygen atoms within a considerably distorted octahedral coordination. Two adjacent Mo(4)O<sub>6</sub> octahedra are connected through edge-sharing, forming Mo<sub>2</sub>O<sub>10</sub> units. These Mo<sub>2</sub>O<sub>10</sub> units are interconnected by Mo(1)O<sub>4</sub> tetrahedra *via* corner-sharing to form an infinite Mo<sub>4</sub>O<sub>14</sub> chain parallel to [100]. The distorted environments of the two Nd atoms Nd(1) and Nd(2) are different. While Nd(1) is coordinated by seven oxygen atoms, Nd(2) is coordinated by eight oxygen atoms. The Mo<sub>4</sub>O<sub>14</sub> chains are linked perpendicularly to the chain direction into a three-dimensional framework *via* isolated Mo(2)O<sub>4</sub> and Mo(3)O<sub>4</sub> tetrahedra and by Nd(1)O<sub>7</sub> and Nd(2)O<sub>8</sub> polyhedra sharing edges and corners (Fig. 2).

### Experimental

The finely ground reagents K<sub>2</sub>CO<sub>3</sub>, Nd<sub>2</sub>O<sub>3</sub>, and MoO<sub>3</sub> were mixed in the molar ratio K: Nd: Mo = 3: 2: 6, were placed in a Pt crucible, and heated at 573 K for 4 h. The mixture was then re-ground and heated at 1273 K for 20 h, then cooled to 673 K at a rate of 3 K h<sup>-1</sup>, and finally quenched to room temperature. A few light-red crystals of the title compound with prismatic shape were obtained.

### Refinement

The highest peak in the difference electron density map equals to 3.38 e/Å<sup>3</sup> at the distance of 0.92 Å from the Nd(1) site while the deepest hole equals to -2.54 e/Å<sup>3</sup> at the distance of 1.22 Å from the Nd(2) site.

Figures

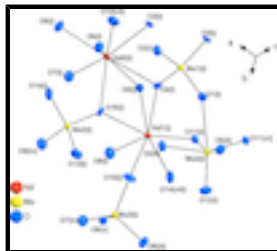


Fig. 1. The expanded asymmetric unit of  $\beta\text{-Nd}_2\text{Mo}_4\text{O}_{15}$  showing the coordination environments of the Mo and Nd atoms. [Symmetry codes: (i)  $x, y, z$ ; (ii)  $1 - x, 1 - y, 1 - z$ ; (iii)  $-1 + x, 1 + y, z$ ; (iv)  $1 - x, 1 - y, -z$ ; (v)  $x, 1 + y, z$ ; (vi)  $-x, 1 - y, 1 - z$ ; (vii)  $x, -1 + y, z$ ; (viii)  $-1 + x, y, z$ .]

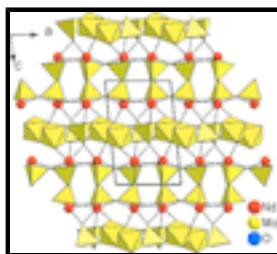


Fig. 2. View of the crystal structure of  $\beta\text{-Nd}_2\text{Mo}_4\text{O}_{15}$  along  $[0\bar{1}0]$ . MoO<sub>4</sub> and MoO<sub>6</sub> units are given in the polyhedral representation.

dineodymium(III) tetramolybdate(VI)

Crystal data

$\text{Nd}_2\text{Mo}_4\text{O}_{15}$	$Z = 2$
$M_r = 912.24$	$F(000) = 816$
Triclinic, $P\bar{1}$	$D_x = 4.705 \text{ Mg m}^{-3}$
Hall symbol: $-P 1$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 7.4000 (6) \text{ \AA}$	Cell parameters from 487 reflections
$b = 7.4992 (6) \text{ \AA}$	$\theta = 2.1\text{--}23.0^\circ$
$c = 11.7291 (9) \text{ \AA}$	$\mu = 11.77 \text{ mm}^{-1}$
$\alpha = 88.916 (2)^\circ$	$T = 293 \text{ K}$
$\beta = 83.957 (1)^\circ$	Prism, light-red
$\gamma = 84.196 (2)^\circ$	$0.15 \times 0.15 \times 0.05 \text{ mm}$
$V = 643.94 (9) \text{ \AA}^3$	

Data collection

Bruker SMART 1K CCD diffractometer	2390 independent reflections
Radiation source: fine-focus sealed tube graphite	2268 reflections with $I > 2\sigma(I)$
$\omega$ scans	$R_{\text{int}} = 0.040$
Absorption correction: multi-scan (SADABS; Bruker, 1997)	$\theta_{\text{max}} = 25.7^\circ, \theta_{\text{min}} = 1.8^\circ$
$T_{\text{min}} = 0.271, T_{\text{max}} = 0.591$	$h = -9 \rightarrow 8$
3620 measured reflections	$k = -9 \rightarrow 6$
	$l = -14 \rightarrow 14$

Refinement

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.046$	$w = 1/[\sigma^2(F_o^2) + (0.0986P)^2 + 6.3644P]$
$wR(F^2) = 0.128$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{\max} < 0.001$
2390 reflections	$\Delta\rho_{\max} = 3.38 \text{ e } \text{\AA}^{-3}$
191 parameters	$\Delta\rho_{\min} = -2.54 \text{ e } \text{\AA}^{-3}$
0 restraints	Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.0080 (7)

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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Nd1	0.24478 (7)	0.41215 (6)	0.22477 (4)	0.0090 (2)
Nd2	0.67891 (6)	0.09060 (6)	0.22360 (4)	0.0081 (2)
Mo1	0.43929 (11)	0.25334 (11)	0.52879 (7)	0.0093 (3)
Mo2	0.72798 (11)	0.57014 (10)	0.12800 (7)	0.0081 (3)
Mo3	0.22775 (11)	0.92862 (10)	0.12894 (7)	0.0084 (3)
Mo4	0.09418 (11)	0.67225 (10)	0.52795 (7)	0.0090 (3)
O11	0.0842 (9)	0.4745 (9)	0.4032 (6)	0.0122 (14)
O2	0.6680 (10)	0.2917 (10)	0.5608 (6)	0.0180 (15)
O15	0.5756 (9)	0.4080 (9)	0.1806 (6)	0.0124 (14)
O8	0.3544 (9)	0.0941 (9)	0.1872 (6)	0.0116 (14)
O1	0.2954 (10)	0.4305 (9)	0.5914 (6)	0.0161 (15)
O5	0.8677 (10)	0.2270 (10)	0.3442 (7)	0.0183 (15)
O7	0.7035 (11)	0.0974 (11)	0.0170 (7)	0.0209 (17)
O12	-0.0335 (11)	0.8313 (10)	0.4610 (7)	0.0217 (16)
O4	0.4229 (10)	0.2652 (9)	0.3798 (6)	0.0153 (15)
O6	0.9983 (10)	0.0078 (11)	0.1526 (7)	0.0231 (17)
O9	0.2747 (11)	0.4070 (11)	0.0191 (7)	0.0227 (17)
O10	0.2620 (11)	0.7197 (10)	0.1964 (6)	0.0200 (16)

## supplementary materials

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O13	0.6638 (11)	0.7841 (10)	0.1853 (7)	0.0207 (16)
O14	0.9451 (11)	0.4864 (12)	0.1581 (7)	0.0253 (18)
O3	0.3788 (10)	0.0521 (9)	0.5944 (6)	0.0150 (14)

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Nd1	0.0097 (3)	0.0080 (3)	0.0089 (3)	0.0000 (2)	0.0000 (2)	0.0003 (2)
Nd2	0.0096 (3)	0.0058 (3)	0.0091 (3)	-0.0022 (2)	-0.0012 (2)	-0.0003 (3)
Mo1	0.0098 (4)	0.0084 (4)	0.0101 (4)	-0.0026 (3)	-0.0019 (3)	0.0022 (3)
Mo2	0.0086 (4)	0.0075 (4)	0.0084 (4)	-0.0030 (3)	0.0001 (3)	0.0001 (3)
Mo3	0.0089 (4)	0.0080 (4)	0.0088 (4)	-0.0025 (3)	-0.0011 (3)	-0.0016 (3)
Mo4	0.0083 (4)	0.0079 (4)	0.0113 (4)	-0.0026 (3)	-0.0011 (3)	-0.0023 (3)
O11	0.013 (3)	0.013 (3)	0.011 (3)	-0.004 (3)	-0.001 (3)	0.000 (3)
O2	0.017 (4)	0.023 (4)	0.015 (4)	-0.006 (3)	0.000 (3)	0.002 (3)
O15	0.006 (3)	0.011 (3)	0.020 (4)	-0.001 (2)	0.003 (3)	-0.006 (3)
O8	0.010 (3)	0.008 (3)	0.017 (3)	-0.006 (3)	-0.002 (3)	-0.002 (3)
O1	0.019 (4)	0.009 (3)	0.019 (4)	-0.003 (3)	0.000 (3)	-0.001 (3)
O5	0.016 (4)	0.016 (4)	0.024 (4)	-0.004 (3)	-0.001 (3)	-0.004 (3)
O7	0.026 (4)	0.024 (4)	0.012 (4)	-0.001 (3)	0.000 (3)	-0.006 (3)
O12	0.023 (4)	0.016 (4)	0.027 (4)	0.003 (3)	-0.008 (3)	0.000 (3)
O4	0.015 (3)	0.009 (3)	0.019 (4)	0.005 (3)	0.001 (3)	-0.001 (3)
O6	0.012 (4)	0.030 (5)	0.026 (4)	0.002 (3)	0.001 (3)	-0.002 (3)
O9	0.026 (4)	0.027 (4)	0.016 (4)	-0.005 (3)	-0.001 (3)	-0.003 (3)
O10	0.032 (4)	0.015 (4)	0.016 (4)	-0.005 (3)	-0.013 (3)	0.004 (3)
O13	0.031 (4)	0.011 (4)	0.021 (4)	-0.006 (3)	-0.006 (3)	-0.001 (3)
O14	0.015 (4)	0.039 (5)	0.021 (4)	-0.007 (3)	0.003 (3)	0.007 (4)
O3	0.017 (3)	0.008 (3)	0.019 (4)	-0.002 (3)	0.000 (3)	0.008 (3)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

Nd1—O11	2.326 (7)	Mo2—O15	1.798 (7)
Nd1—O10	2.339 (7)	Mo3—O6 <sup>v</sup>	1.737 (7)
Nd1—O9	2.400 (8)	Mo3—O7 <sup>iv</sup>	1.742 (8)
Nd1—O14 <sup>i</sup>	2.437 (8)	Mo3—O10	1.749 (7)
Nd1—O15	2.446 (6)	Mo3—O8 <sup>vi</sup>	1.814 (6)
Nd1—O8	2.472 (7)	Mo4—O12	1.680 (8)
Nd1—O4	2.528 (7)	Mo4—O5 <sup>vii</sup>	1.753 (7)
Nd1—Nd2	3.8158 (7)	Mo4—O11 <sup>viii</sup>	1.909 (7)
Nd2—O13 <sup>ii</sup>	2.366 (7)	Mo4—O2 <sup>vii</sup>	1.989 (7)
Nd2—O3 <sup>iii</sup>	2.387 (7)	Mo4—O11	2.115 (7)
Nd2—O5	2.399 (7)	Mo4—O1	2.386 (7)
Nd2—O7	2.411 (8)	Mo4—Mo4 <sup>viii</sup>	3.1674 (15)
Nd2—O6	2.444 (7)	O11—Mo4 <sup>viii</sup>	1.909 (7)
Nd2—O8	2.480 (7)	O2—Mo4 <sup>vii</sup>	1.989 (7)
Nd2—O15	2.484 (7)	O8—Mo3 <sup>ii</sup>	1.814 (6)

Nd2—O4	2.742 (7)	O5—Mo4 <sup>vii</sup>	1.753 (7)
Mo1—O1	1.739 (7)	O7—Mo3 <sup>iv</sup>	1.742 (8)
Mo1—O3	1.758 (7)	O6—Mo3 <sup>ix</sup>	1.737 (7)
Mo1—O4	1.764 (7)	O9—Mo2 <sup>iv</sup>	1.733 (8)
Mo1—O2	1.823 (7)	O13—Nd2 <sup>vi</sup>	2.366 (7)
Mo2—O9 <sup>iv</sup>	1.733 (8)	O14—Nd1 <sup>x</sup>	2.437 (8)
Mo2—O14	1.734 (8)	O3—Nd2 <sup>iii</sup>	2.387 (7)
Mo2—O13	1.753 (7)		
O11—Nd1—O10	88.8 (3)	O4—Nd2—Nd1	41.44 (15)
O11—Nd1—O9	153.3 (3)	O1—Mo1—O3	108.8 (3)
O10—Nd1—O9	83.4 (3)	O1—Mo1—O4	107.4 (3)
O11—Nd1—O14 <sup>i</sup>	82.8 (3)	O3—Mo1—O4	114.5 (3)
O10—Nd1—O14 <sup>i</sup>	82.1 (3)	O1—Mo1—O2	105.5 (3)
O9—Nd1—O14 <sup>i</sup>	70.9 (3)	O3—Mo1—O2	109.3 (3)
O11—Nd1—O15	125.3 (2)	O4—Mo1—O2	110.9 (3)
O10—Nd1—O15	81.3 (3)	O9 <sup>iv</sup> —Mo2—O14	109.3 (4)
O9—Nd1—O15	78.7 (3)	O9 <sup>iv</sup> —Mo2—O13	106.3 (4)
O14 <sup>i</sup> —Nd1—O15	146.7 (3)	O14—Mo2—O13	112.1 (4)
O11—Nd1—O8	116.2 (2)	O9 <sup>iv</sup> —Mo2—O15	109.1 (4)
O10—Nd1—O8	152.5 (3)	O14—Mo2—O15	107.0 (3)
O9—Nd1—O8	78.6 (3)	O13—Mo2—O15	113.0 (3)
O14 <sup>i</sup> —Nd1—O8	110.8 (3)	O6 <sup>v</sup> —Mo3—O7 <sup>iv</sup>	111.1 (4)
O15—Nd1—O8	75.0 (2)	O6 <sup>v</sup> —Mo3—O10	109.0 (4)
O11—Nd1—O4	70.6 (2)	O7 <sup>iv</sup> —Mo3—O10	108.4 (4)
O10—Nd1—O4	116.3 (2)	O6 <sup>v</sup> —Mo3—O8 <sup>vi</sup>	106.6 (4)
O9—Nd1—O4	135.5 (2)	O7 <sup>iv</sup> —Mo3—O8 <sup>vi</sup>	109.7 (3)
O14 <sup>i</sup> —Nd1—O4	146.5 (2)	O10—Mo3—O8 <sup>vi</sup>	112.0 (3)
O15—Nd1—O4	66.7 (2)	O12—Mo4—O5 <sup>vii</sup>	104.3 (4)
O8—Nd1—O4	66.3 (2)	O12—Mo4—O11 <sup>viii</sup>	102.4 (4)
O11—Nd1—Nd2	116.20 (17)	O5 <sup>vii</sup> —Mo4—O11 <sup>viii</sup>	95.7 (3)
O10—Nd1—Nd2	120.5 (2)	O12—Mo4—O2 <sup>vii</sup>	97.0 (4)
O9—Nd1—Nd2	89.6 (2)	O5 <sup>vii</sup> —Mo4—O2 <sup>vii</sup>	97.9 (3)
O14 <sup>i</sup> —Nd1—Nd2	148.9 (2)	O11 <sup>viii</sup> —Mo4—O2 <sup>vii</sup>	152.7 (3)
O15—Nd1—Nd2	39.66 (16)	O12—Mo4—O11	94.5 (3)
O8—Nd1—Nd2	39.68 (15)	O5 <sup>vii</sup> —Mo4—O11	160.8 (3)
O4—Nd1—Nd2	45.87 (15)	O11 <sup>viii</sup> —Mo4—O11	76.3 (3)
O13 <sup>ii</sup> —Nd2—O3 <sup>iii</sup>	73.9 (3)	O2 <sup>vii</sup> —Mo4—O11	83.4 (3)
O13 <sup>ii</sup> —Nd2—O5	129.8 (3)	O12—Mo4—O1	170.4 (3)
O3 <sup>iii</sup> —Nd2—O5	75.9 (3)	O5 <sup>vii</sup> —Mo4—O1	83.9 (3)
O13 <sup>ii</sup> —Nd2—O7	79.6 (3)	O11 <sup>viii</sup> —Mo4—O1	81.3 (3)
O3 <sup>iii</sup> —Nd2—O7	153.0 (3)	O2 <sup>vii</sup> —Mo4—O1	76.7 (3)
O5—Nd2—O7	126.9 (3)	O11—Mo4—O1	77.7 (3)

## supplementary materials

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O13 <sup>ii</sup> —Nd2—O6	80.7 (3)	O12—Mo4—Mo4 <sup>viii</sup>	100.5 (3)
O3 <sup>iii</sup> —Nd2—O6	107.9 (3)	O5 <sup>vii</sup> —Mo4—Mo4 <sup>viii</sup>	133.6 (3)
O5—Nd2—O6	71.7 (3)	O11 <sup>viii</sup> —Mo4—Mo4 <sup>viii</sup>	40.4 (2)
O7—Nd2—O6	72.0 (3)	O2 <sup>vii</sup> —Mo4—Mo4 <sup>viii</sup>	117.3 (2)
O13 <sup>ii</sup> —Nd2—O8	79.2 (3)	O11—Mo4—Mo4 <sup>viii</sup>	35.83 (18)
O3 <sup>iii</sup> —Nd2—O8	91.6 (2)	O1—Mo4—Mo4 <sup>viii</sup>	76.52 (17)
O5—Nd2—O8	140.7 (2)	Mo4 <sup>viii</sup> —O11—Mo4	103.7 (3)
O7—Nd2—O8	78.5 (3)	Mo4 <sup>viii</sup> —O11—Nd1	122.5 (3)
O6—Nd2—O8	146.8 (3)	Mo4—O11—Nd1	133.7 (3)
O13 <sup>ii</sup> —Nd2—O15	147.6 (2)	Mo1—O2—Mo4 <sup>vii</sup>	136.8 (4)
O3 <sup>iii</sup> —Nd2—O15	124.5 (2)	Mo2—O15—Nd1	135.0 (4)
O5—Nd2—O15	82.5 (2)	Mo2—O15—Nd2	123.6 (3)
O7—Nd2—O15	77.3 (3)	Nd1—O15—Nd2	101.4 (2)
O6—Nd2—O15	112.6 (3)	Mo3 <sup>ii</sup> —O8—Nd1	126.2 (3)
O8—Nd2—O15	74.2 (2)	Mo3 <sup>ii</sup> —O8—Nd2	132.4 (3)
O13 <sup>ii</sup> —Nd2—O4	119.7 (3)	Nd1—O8—Nd2	100.8 (2)
O3 <sup>iii</sup> —Nd2—O4	63.0 (2)	Mo1—O1—Mo4	136.9 (4)
O5—Nd2—O4	78.3 (2)	Mo4 <sup>vii</sup> —O5—Nd2	152.6 (4)
O7—Nd2—O4	129.9 (2)	Mo3 <sup>iv</sup> —O7—Nd2	165.9 (5)
O6—Nd2—O4	150.0 (2)	Mo1—O4—Nd1	144.6 (4)
O8—Nd2—O4	63.0 (2)	Mo1—O4—Nd2	122.6 (3)
O15—Nd2—O4	62.9 (2)	Nd1—O4—Nd2	92.7 (2)
O13 <sup>ii</sup> —Nd2—Nd1	118.7 (2)	Mo3 <sup>ix</sup> —O6—Nd2	168.5 (5)
O3 <sup>iii</sup> —Nd2—Nd1	99.86 (17)	Mo2 <sup>iv</sup> —O9—Nd1	171.6 (5)
O5—Nd2—Nd1	105.23 (18)	Mo3—O10—Nd1	156.8 (4)
O7—Nd2—Nd1	88.49 (19)	Mo2—O13—Nd2 <sup>vi</sup>	159.0 (5)
O6—Nd2—Nd1	150.0 (2)	Mo2—O14—Nd1 <sup>x</sup>	169.8 (5)
O8—Nd2—Nd1	39.53 (15)	Mo1—O3—Nd2 <sup>iii</sup>	143.0 (4)
O15—Nd2—Nd1	38.92 (15)		

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





