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$Nd_3Mo_4SiO_{14}$

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ(Si–O) = 0.006 Å; disorder in main residue; R factor = 0.037; wR factor = 0.085; data-to-parameter ratio = 25.9.

The title compound, trineodymium silicotetramolybdate, is isotypic with $La_3Mo_4SiO_{14}$. The crystal structure contains ribbons made of chains of triangular Mo_3O_{13} units and chains of edge-sharing MoO_6 octahedra. The ribbons are separated from each other by the Nd^{3+} and Si^{4+} cations. The three distinct Nd^{3+} cations are surrounded by eight to ten O atoms, and the Si^{4+} is tetrahedrally coordinated. Except for two Mo and four O sites, all other sites (three Nd, one Mo, one Si and six O) are located on mirror planes.

Related literature

For the isotypic $La_3Mo_4SiO_{14}$, see Betteridge *et al.* (1984). The structure contains edge-sharing MoO_6 octahedra similar to those found in MoO_2 (Brandt & Skapski, 1967). The oxidation states of Mo atoms were estimated using the data given by Brown & Wu (1976). Besides the title compound, crystals of $NdMo_5O_8$ (Gougeon *et al.*, 2003) were also obtained.

Experimental

Crystal data

$Nd_3Mo_4SiO_{14}$
M_r = 1068.56
Orthorhombic, *Pnma*
a = 17.5348 (15) Å
b = 5.6159 (3) Å
c = 10.8542 (11) Å
V = 1068.85 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 19.04 mm^{-1}
T = 293 (2) K
0.16 × 0.02 × 0.02 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: analytical (de Meulenaer & Tompa, 1965)
T_{min} = 0.272, T_{max} = 0.710
30670 measured reflections
3131 independent reflections
2619 reflections with $I > 2\sigma(I)$
R_{int} = 0.063

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.085
S = 1.38
3131 reflections
121 parameters
$\Delta\rho_{max}$ = 2.32 e Å^{-3}
$\Delta\rho_{min}$ = −3.72 e Å^{-3}

Table 1
Selected bond lengths (Å).

Nd1—O4^{i}	2.321 (4)	Mo1—Mo2	2.5351 (8)
Nd1—O3^{ii}	2.444 (6)	Mo2—O3	1.988 (4)
Nd1—O9^{iii}	2.520 (5)	Mo2—O5	2.023 (4)
Nd1—O5	2.524 (4)	Mo2—O7	2.029 (5)
Nd1—O7	2.651 (7)	Mo2—O2	2.072 (4)
Nd2—O9^{iv}	2.422 (5)	Mo2—O8	2.084 (5)
Nd2—O1^{iv}	2.461 (4)	Mo2—O1	2.127 (4)
Nd2—O4^{v}	2.465 (4)	Mo2—Mo2^{xi}	2.5498 (9)
Nd2—O6^{v}	2.580 (7)	Mo2—Mo2^{xii}	3.0661 (9)
Nd2—O10^{vi}	2.896 (8)	Mo3—O2^{iii}	1.925 (6)
Nd3—O10	2.368 (7)	Mo3—O9^{xi}	1.941 (5)
Nd3—O5^{vii}	2.476 (4)	Mo3—O9^{iv}	1.966 (5)
Nd3—O4^{viii}	2.503 (4)	Mo3—O7	2.047 (6)
Nd3—O8^{ix}	2.544 (6)	Mo3—O9	2.160 (5)
Nd3—O1^{x}	2.760 (5)	Mo3—O9^{iii}	2.187 (5)
Nd3—O6^{viii}	2.8617 (13)	Mo3—Mo3^{xiii}	2.503 (4)
Mo1—O4	1.944 (5)	Mo3—Mo3^{iii}	3.145 (4)
Mo1—O5	2.030 (4)	Si—O10	1.620 (7)
Mo1—O8	2.055 (6)	Si—O6^{xiv}	1.626 (7)
Mo1—O6	2.122 (6)	Si—O1	1.649 (4)

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

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *COLLECT*; data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Bergerhoff, 1996); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2113).

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supplementary materials

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$Nd_3Mo_4SiO_{14}$

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Comment

The title compound is isotypic with $La_3Mo_4SiO_{14}$ (Betteridge *et al.*, 1984). The crystal structure contains chains of triangular Mo_3O_{13} units and chains of edge-sharing MoO_6 octahedra similar to those found in MoO_2 (Brandt & Skapski, 1967). Both chains run parallel to the *b* axis (Fig. 1). Each single Mo chain is linked through O2 and O7 atoms to two Mo_3 chains to form ribbons (Fig. 2). The Mo—Mo distances within the Mo_3 triangles are 2.5351 (8) and 2.5498 (9) Å and the shortest distance between adjacent Mo_3 clusters is 3.0661 (9) Å. In the single Mo chains, the Mo—Mo distances are alternately 2.503 (4) and 3.145 (4) Å. The Mo—O distances of Mo1 and Mo2 forming the Mo_3 cluster unit range from 1.944 (5) to 2.127 (4) Å, while those of the Mo3 atom forming the Mo_2 dimer vary between 1.925 (6) and 2.187 (5) Å. From the lengths of the Mo—O bonds, we can estimate the oxidation states of each independent Mo atom by using the empirical bond length-bond strength relationship developed by Brown and Wu (1976). The calculations result in valence sums of +3.99 (6), +3.59 (6) and +3.92 (6) for Mo1, Mo2 and Mo3, respectively. Consequently, in $Nd_3Mo_4SiO_{14}$ the number of electrons per Mo_3 cluster is evaluated to 7, and to 2 per Mo atom in the single Mo chains. The Si site is tetrahedrally coordinated by O atoms with Si—O distances ranging from 1.620 (7) to 1.649 (9) Å. The bond length-bond strength calculation shows an oxidation state of +3.86 (5), in good agreement with the expected value of +4. The Nd atoms are surrounded by 8 to 10 O atoms forming considerably distorted polyhedra with Nd—O distances ranging from 2.321 (4) to 2.896 (8) Å (Table 1).

Experimental

In an attempt to prepare $Nd_{16}Mo_{20}SiO_{56}$, single crystals of $Nd_3Mo_4SiO_{14}$ were obtained by the reaction of Nd_2O_3, MoO_3, SiO_2 and Mo in the molar ratio 8:10:1:10. The initial mixture (*ca* 5 g) was cold pressed and loaded into a molybdenum crucible, which was sealed under a low argon pressure using an arc welding system. The charge was heated at the rate of 300 K/h up to 1873 K, the temperature which was held for 48 h, then cooled at 100 K/h down to 1373 K and finally cooled to room temperature by turning off the furnace. X-ray powder diffraction measurements using Cu $K\alpha_1$ radiation and a INEL CPS-120 curved position sensitive detector showed that the dominant products were $NdMo_5O_8$ (Gougeon *et al.*, 2003) and $Nd_3Mo_4SiO_{14}$.

Refinement

In the final refinement cycles the site occupancy factor for the Mo3 atom was constrained to 0.5. Because of the disorder of the Mo3 atom, we made reciprocal space reconstructions of different planes as well as long-exposure rotations along the three axes on the Kappa CCD diffractometer. In both cases, we did not observed any superlattice reflections or diffuse lines. The highest peak and the deepest hole in the final Fourier map are located 1.75Å from O5 and 1.43Å from Mo2, respectively.

Figures

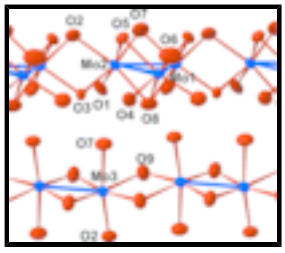

Fig. 1. : Fragment of the chains of triangular Mo_3O_{13} units and edge sharing MoO_6 octahedra in $Nd_3Mo_4SiO_{14}$. Displacement ellipsoids are drawn at the 97% probability level.

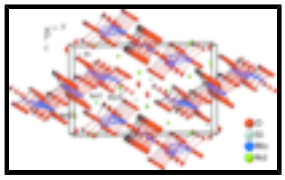

Fig. 2. : View of $Nd_3Mo_4SiO_{14}$ along [010]. Displacement ellipsoids are drawn at the 97% probability level. Symmetry codes: (i) $x, y-1, z$; (ii) $x+1/2, -y+1/2, -z+1/2$.

trineodymium silicotetramolybdate

Crystal data

$Nd_3Mo_4SiO_{14}$	F_{000} = 1896
M_r = 1068.56	D_x = 6.640 Mg m^{-3}
Orthorhombic, *Pnma*	Mo $K\alpha$ radiation λ = 0.71069 Å
Hall symbol: -P 2ac 2n	Cell parameters from 4003 reflections
a = 17.5348 (15) Å	θ = 3.8–38.0°
b = 5.6159 (3) Å	μ = 19.04 mm^{-1}
c = 10.8542 (11) Å	T = 293 (2) K
V = 1068.85 (15) Å^3	Needle, black
Z = 4	0.16 × 0.02 × 0.02 mm

Data collection

Nonius KappaCCD diffractometer	3131 independent reflections
Radiation source: fine-focus sealed tube	2619 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.063
T = 293(2) K	θ_{max} = 38.0°
φ scans (κ = 0) + additional ω scans	θ_{min} = 3.8°
Absorption correction: analytical (de Meulenaer & Tompa, 1965)	h = −30→29
T_{min} = 0.272, T_{max} = 0.710	k = −8→9
30670 measured reflections	l = −18→17

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map

$R[F^2 > 2\sigma(F^2)] = 0.037$

$wR(F^2) = 0.085$

$S = 1.38$

3131 reflections

121 parameters

$w = 1/[\sigma^2(F_o^2) + 19.2566P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 2.32$ e Å^{-3}

$\Delta\rho_{min} = -3.72$ e Å^{-3}

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 $F^2 > 2$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}	Occ. (<1)
Nd1	0.16358 (3)	0.7500	0.63158 (4)	0.00610 (8)	
Nd2	0.03477 (3)	1.2500	0.79944 (4)	0.00879 (8)	
Nd3	−0.15474 (3)	0.2500	0.00583 (4)	0.00702 (8)	
Mo1	0.28501 (4)	0.7500	0.36147 (6)	0.00450 (11)	
Mo2	0.16265 (3)	0.52298 (8)	0.32043 (4)	0.00428 (8)	
Mo3	−0.00732 (5)	0.7788 (4)	0.50698 (9)	0.0047 (4)	0.50
Si	0.06365 (13)	0.2500	0.1039 (2)	0.0052 (4)	
O1	0.0800 (3)	0.5018 (8)	0.1775 (4)	0.0077 (7)	
O2	0.1004 (4)	0.2500	0.4002 (6)	0.0076 (10)	
O3	0.2135 (3)	0.2500	0.2377 (5)	0.0051 (9)	
O4	0.3506 (3)	0.4958 (8)	0.3020 (4)	0.0084 (7)	
O5	0.2315 (2)	0.5069 (7)	0.4697 (4)	0.0060 (7)	
O6	0.3766 (4)	0.7500	0.4892 (6)	0.0121 (12)	
O7	0.0941 (4)	0.7500	0.4146 (6)	0.0089 (10)	
O8	0.2217 (3)	0.7500	0.2021 (6)	0.0074 (10)	
O9	−0.0452 (3)	0.5027 (8)	0.3826 (4)	0.0107 (8)	
O10	−0.0224 (4)	0.2500	0.0497 (7)	0.0141 (13)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Nd1	0.00569 (17)	0.00825 (17)	0.00435 (17)	0.000	−0.00015 (12)	0.000
Nd2	0.00467 (17)	0.01261 (18)	0.0091 (2)	0.000	−0.00054 (13)	0.000
Nd3	0.00575 (17)	0.00927 (17)	0.00606 (17)	0.000	−0.00034 (13)	0.000
Mo1	0.0037 (2)	0.0056 (2)	0.0041 (3)	0.000	−0.00002 (19)	0.000

Mo2	0.00411 (18)	0.00450 (16)	0.00421 (18)	0.00031 (13)	0.00010 (13)	−0.00078 (13)
Mo3	0.0042 (3)	0.0057 (12)	0.0040 (3)	0.0002 (3)	0.0001 (2)	−0.0002 (3)
Si	0.0045 (9)	0.0073 (9)	0.0037 (9)	0.000	−0.0002 (7)	0.000
O1	0.0079 (18)	0.0077 (16)	0.0075 (18)	0.0002 (13)	−0.0015 (13)	−0.0036 (14)
O2	0.006 (2)	0.009 (2)	0.008 (3)	0.000	0.0023 (19)	0.000
O3	0.006 (2)	0.003 (2)	0.006 (2)	0.000	0.0009 (18)	0.000
O4	0.0075 (18)	0.0094 (16)	0.0083 (18)	−0.0028 (14)	0.0002 (13)	−0.0014 (14)
O5	0.0067 (17)	0.0062 (15)	0.0050 (17)	0.0005 (13)	−0.0001 (13)	0.0018 (12)
O6	0.006 (3)	0.021 (3)	0.009 (3)	0.000	−0.004 (2)	0.000
O7	0.005 (2)	0.011 (3)	0.010 (3)	0.000	0.003 (2)	0.000
O8	0.004 (2)	0.012 (2)	0.007 (3)	0.000	0.0003 (18)	0.000
O9	0.010 (2)	0.0061 (17)	0.016 (2)	0.0008 (14)	0.0043 (15)	−0.0003 (15)
O10	0.006 (3)	0.019 (3)	0.018 (3)	0.000	−0.002 (2)	0.000

Geometric parameters (Å, °)

Nd1—O4^{i}	2.321 (4)	Mo2—O2	2.072 (4)
Nd1—O4^{ii}	2.321 (4)	Mo2—O8	2.084 (5)
Nd1—O3^{ii}	2.444 (6)	Mo2—O1	2.127 (4)
Nd1—O9^{iii}	2.520 (5)	Mo2—Mo2^{v}	2.5498 (9)
Nd1—O9^{iv}	2.520 (5)	Mo2—Mo2^{xvii}	3.0661 (9)
Nd1—O5^{v}	2.524 (4)	Mo3—Mo3^{v}	0.323 (4)
Nd1—O5	2.524 (4)	Mo3—O2^{iii}	1.925 (6)
Nd1—O7	2.651 (7)	Mo3—O9^{v}	1.941 (5)
Nd1—Mo3	3.2916 (11)	Mo3—O9^{iv}	1.966 (5)
Nd1—Mo3^{v}	3.2916 (11)	Mo3—O7	2.047 (6)
Nd1—Mo2	3.6099 (7)	Mo3—O9	2.160 (5)
Nd1—Mo2^{v}	3.6099 (7)	Mo3—O9^{iii}	2.187 (5)
Nd2—O9^{iv}	2.422 (5)	Mo3—Mo3^{vi}	2.503 (4)
Nd2—O9^{vi}	2.422 (5)	Mo3—Mo3^{iv}	2.8237 (2)
Nd2—O1^{iv}	2.461 (4)	Mo3—Mo3^{xviii}	2.8237 (2)
Nd2—O1^{vi}	2.461 (4)	Mo3—Mo3^{iii}	3.145 (4)
Nd2—O4^{vii}	2.465 (4)	Si—O10	1.620 (7)
Nd2—O4^{i}	2.465 (4)	Si—O6^{xix}	1.626 (7)
Nd2—O6^{vii}	2.580 (7)	Si—O1	1.649 (4)
Nd2—O10^{viii}	2.896 (8)	Si—O1^{xvii}	1.649 (4)
Nd2—Mo1^{vii}	3.2310 (9)	Si—Nd2^{xx}	3.343 (2)
Nd2—Si^{viii}	3.343 (2)	Si—Nd3^{xi}	3.4428 (14)
Nd2—Mo3^{vi}	3.3645 (11)	Si—Nd3^{xxi}	3.4428 (14)
Nd2—Mo3^{iv}	3.3645 (11)	Si—Nd2^{iii}	3.4590 (14)
Nd3—O10	2.368 (7)	Si—Nd2^{vi}	3.4590 (14)
Nd3—O5^{ix}	2.476 (4)	O1—Nd2^{vi}	2.461 (4)
Nd3—O5^{x}	2.476 (4)	O1—Nd3^{xi}	2.760 (5)
Nd3—O4^{x}	2.503 (4)	O2—Mo3^{iii}	1.925 (6)

Nd3—O4^{ix}	2.503 (4)	O2—Mo3^{xviii}	1.925 (6)
Nd3—O8^{xi}	2.544 (6)	O2—Mo2^{xvii}	2.072 (4)
Nd3—O1^{xii}	2.760 (5)	O3—Mo2^{xvii}	1.988 (4)
Nd3—O1^{xi}	2.760 (5)	O3—Nd1^{xix}	2.444 (6)
Nd3—O6^{x}	2.8617 (13)	O4—Nd1^{xix}	2.321 (4)
Nd3—O6^{xiii}	2.8617 (13)	O4—Nd2^{xiv}	2.465 (4)
Nd3—Mo1^{x}	3.3280 (5)	O4—Nd3^{xvi}	2.503 (4)
Nd3—Mo1^{xiii}	3.3280 (5)	O5—Nd3^{xvi}	2.476 (4)
Mo1—O4^{v}	1.944 (5)	O6—Si^{ii}	1.626 (7)
Mo1—O4	1.944 (5)	O6—Nd2^{xiv}	2.580 (7)
Mo1—O5	2.030 (4)	O6—Nd3^{xvi}	2.8617 (13)
Mo1—O5^{v}	2.030 (4)	O6—Nd3^{xv}	2.8617 (13)
Mo1—O8	2.055 (6)	O7—Mo2^{v}	2.029 (5)
Mo1—O6	2.122 (6)	O7—Mo3^{v}	2.047 (6)
Mo1—Mo2	2.5351 (8)	O8—Mo2^{v}	2.084 (5)
Mo1—Mo2^{v}	2.5351 (8)	O8—Nd3^{xi}	2.544 (6)
Mo1—Nd2^{xiv}	3.2310 (9)	O9—Mo3^{v}	1.941 (5)
Mo1—Nd3^{xv}	3.3280 (5)	O9—Mo3^{xviii}	1.966 (5)
Mo1—Nd3^{xvi}	3.3280 (5)	O9—Mo3^{iii}	2.187 (5)
Mo2—O3	1.988 (4)	O9—Nd2^{vi}	2.422 (5)
Mo2—O5	2.023 (4)	O9—Nd1^{iii}	2.520 (5)
Mo2—O7	2.029 (5)	O10—Nd2^{xx}	2.896 (8)
O4^{i}—Nd1—O4^{ii}	73.0 (2)	O5—Mo2—Mo2^{v}	92.56 (12)
O4^{i}—Nd1—O3^{ii}	73.68 (16)	O7—Mo2—Mo2^{v}	51.08 (11)
O4^{ii}—Nd1—O3^{ii}	73.68 (16)	O2—Mo2—Mo2^{v}	137.73 (13)
O4^{i}—Nd1—O9^{iii}	107.18 (16)	O8—Mo2—Mo2^{v}	52.29 (10)
O4^{ii}—Nd1—O9^{iii}	68.00 (16)	O1—Mo2—Mo2^{v}	93.21 (12)
O3^{ii}—Nd1—O9^{iii}	139.08 (13)	Mo1—Mo2—Mo2^{v}	59.808 (13)
O4^{i}—Nd1—O9^{iv}	68.00 (16)	O3—Mo2—Mo2^{xvii}	39.53 (13)
O4^{ii}—Nd1—O9^{iv}	107.18 (16)	O5—Mo2—Mo2^{xvii}	87.44 (12)
O3^{ii}—Nd1—O9^{iv}	139.08 (13)	O7—Mo2—Mo2^{xvii}	128.92 (11)
O9^{iii}—Nd1—O9^{iv}	68.6 (2)	O2—Mo2—Mo2^{xvii}	42.27 (13)
O4^{i}—Nd1—O5^{v}	106.48 (15)	O8—Mo2—Mo2^{xvii}	127.71 (10)
O4^{ii}—Nd1—O5^{v}	157.96 (15)	O1—Mo2—Mo2^{xvii}	86.79 (12)
O3^{ii}—Nd1—O5^{v}	84.93 (15)	Mo1—Mo2—Mo2^{xvii}	120.192 (13)
O9^{iii}—Nd1—O5^{v}	130.62 (15)	Mo2^{v}—Mo2—Mo2^{xvii}	180.00 (6)
O9^{iv}—Nd1—O5^{v}	92.40 (14)	O3—Mo2—Nd1	133.87 (17)
O4^{i}—Nd1—O5	157.96 (15)	O5—Mo2—Nd1	42.60 (12)
O4^{ii}—Nd1—O5	106.48 (14)	O7—Mo2—Nd1	46.31 (19)
O3^{ii}—Nd1—O5	84.93 (15)	O2—Mo2—Nd1	82.68 (16)

O9^{iii}—Nd1—O5	92.40 (14)	O8—Mo2—Nd1	110.98 (14)
O9^{iv}—Nd1—O5	130.62 (15)	O1—Mo2—Nd1	134.87 (12)
O5^{v}—Nd1—O5	65.47 (19)	Mo1—Mo2—Nd1	69.77 (2)
O4^{i}—Nd1—O7	131.17 (14)	Mo2^{v}—Mo2—Nd1	69.319 (8)
O4^{ii}—Nd1—O7	131.17 (14)	Mo2^{xvii}—Mo2—Nd1	110.681 (8)
O3^{ii}—Nd1—O7	145.5 (2)	Mo3^{v}—Mo3—O2^{iii}	85.19 (7)
O9^{iii}—Nd1—O7	64.33 (15)	Mo3^{v}—Mo3—O9^{v}	129.21 (15)
O9^{iv}—Nd1—O7	64.33 (15)	O2^{iii}—Mo3—O9^{v}	97.3 (2)
O5^{v}—Nd1—O7	66.35 (14)	Mo3^{v}—Mo3—O9^{iv}	129.78 (15)
O5—Nd1—O7	66.35 (14)	O2^{iii}—Mo3—O9^{iv}	97.6 (2)
O9^{iv}—Nd2—O9^{vi}	70.0 (2)	O9^{v}—Mo3—O9^{iv}	100.3 (2)
O9^{iv}—Nd2—O1^{iv}	79.63 (15)	Mo3^{v}—Mo3—O7	85.48 (6)
O9^{vi}—Nd2—O1^{iv}	118.00 (15)	O2^{iii}—Mo3—O7	170.39 (14)
O9^{iv}—Nd2—O1^{vi}	118.00 (15)	O9^{v}—Mo3—O7	90.4 (2)
O9^{vi}—Nd2—O1^{vi}	79.63 (15)	O9^{iv}—Mo3—O7	86.7 (2)
O1^{iv}—Nd2—O1^{vi}	69.0 (2)	Mo3^{v}—Mo3—O9	44.14 (14)
O9^{iv}—Nd2—O4^{vii}	106.24 (15)	O2^{iii}—Mo3—O9	90.35 (19)
O9^{vi}—Nd2—O4^{vii}	67.40 (15)	O9^{v}—Mo3—O9	85.1 (3)
O1^{iv}—Nd2—O4^{vii}	173.48 (15)	O9^{iv}—Mo3—O9	169.71 (13)
O1^{vi}—Nd2—O4^{vii}	109.73 (15)	O7—Mo3—O9	84.51 (19)
O9^{iv}—Nd2—O4^{i}	67.40 (15)	Mo3^{v}—Mo3—O9^{iii}	43.71 (13)
O9^{vi}—Nd2—O4^{i}	106.24 (15)	O2^{iii}—Mo3—O9^{iii}	90.55 (19)
O1^{iv}—Nd2—O4^{i}	109.73 (15)	O9^{v}—Mo3—O9^{iii}	169.09 (14)
O1^{vi}—Nd2—O4^{i}	173.48 (15)	O9^{iv}—Mo3—O9^{iii}	86.1 (3)
O4^{vii}—Nd2—O4^{i}	70.8 (2)	O7—Mo3—O9^{iii}	81.12 (18)
O9^{iv}—Nd2—O6^{vii}	127.30 (15)	O9—Mo3—O9^{iii}	87.3 (2)
O9^{vi}—Nd2—O6^{vii}	127.30 (15)	Mo3^{v}—Mo3—Mo3^{vi}	173.16 (4)
O1^{iv}—Nd2—O6^{vii}	114.28 (15)	O2^{iii}—Mo3—Mo3^{vi}	101.65 (9)
O1^{vi}—Nd2—O6^{vii}	114.28 (15)	O9^{v}—Mo3—Mo3^{vi}	50.60 (15)
O4^{vii}—Nd2—O6^{vii}	60.01 (15)	O9^{iv}—Mo3—Mo3^{vi}	49.73 (15)
O4^{i}—Nd2—O6^{vii}	60.01 (15)	O7—Mo3—Mo3^{vi}	87.69 (6)
O9^{iv}—Nd2—O10^{viii}	142.32 (12)	O9—Mo3—Mo3^{vi}	134.93 (14)
O9^{vi}—Nd2—O10^{viii}	142.32 (12)	O9^{iii}—Mo3—Mo3^{vi}	135.05 (14)
O1^{iv}—Nd2—O10^{viii}	67.74 (15)	Mo3^{v}—Mo3—Mo3^{iv}	173.94 (4)
O1^{vi}—Nd2—O10^{viii}	67.74 (15)	O2^{iii}—Mo3—Mo3^{iv}	100.87 (8)
O4^{vii}—Nd2—O10^{viii}	105.78 (15)	O9^{v}—Mo3—Mo3^{iv}	50.59 (15)
O4^{i}—Nd2—O10^{viii}	105.78 (15)	O9^{iv}—Mo3—Mo3^{iv}	49.75 (15)
O6^{vii}—Nd2—O10^{viii}	57.3 (2)	O7—Mo3—Mo3^{iv}	88.47 (7)
O10—Nd3—O5^{ix}	140.12 (12)	O9—Mo3—Mo3^{iv}	135.08 (14)
O10—Nd3—O5^{x}	140.12 (12)	O9^{iii}—Mo3—Mo3^{iv}	135.23 (14)
O5^{ix}—Nd3—O5^{x}	71.3 (2)	Mo3^{vi}—Mo3—Mo3^{iv}	0.780 (13)

O10—Nd3—O4^{x}	78.21 (18)	Mo3^{v}—Mo3—Mo3^{xviii}	6.06 (4)
O5^{ix}—Nd3—O4^{x}	105.19 (14)	O2^{iii}—Mo3—Mo3^{xviii}	91.24 (7)
O5^{x}—Nd3—O4^{x}	67.62 (14)	O9^{v}—Mo3—Mo3^{xviii}	128.49 (16)
O10—Nd3—O4^{ix}	78.21 (18)	O9^{iv}—Mo3—Mo3^{xviii}	128.78 (15)
O5^{ix}—Nd3—O4^{ix}	67.62 (14)	O7—Mo3—Mo3^{xviii}	79.42 (7)
O5^{x}—Nd3—O4^{ix}	105.19 (14)	O9—Mo3—Mo3^{xviii}	44.01 (13)
O4^{x}—Nd3—O4^{ix}	66.9 (2)	O9^{iii}—Mo3—Mo3^{xviii}	43.31 (13)
O10—Nd3—O8^{xi}	129.1 (2)	Mo3^{vi}—Mo3—Mo3^{xviii}	167.10 (8)
O5^{ix}—Nd3—O8^{xi}	73.97 (14)	Mo3^{iv}—Mo3—Mo3^{xviii}	167.88 (7)
O5^{x}—Nd3—O8^{xi}	73.97 (14)	Mo3^{v}—Mo3—Mo3^{iii}	5.44 (3)
O4^{x}—Nd3—O8^{xi}	139.17 (13)	O2^{iii}—Mo3—Mo3^{iii}	90.62 (8)
O4^{ix}—Nd3—O8^{xi}	139.17 (13)	O9^{v}—Mo3—Mo3^{iii}	128.59 (15)
O10—Nd3—O1^{xii}	71.33 (18)	O9^{iv}—Mo3—Mo3^{iii}	128.91 (15)
O5^{ix}—Nd3—O1^{xii}	99.53 (13)	O7—Mo3—Mo3^{iii}	80.04 (6)
O5^{x}—Nd3—O1^{xii}	138.96 (13)	O9—Mo3—Mo3^{iii}	43.99 (13)
O4^{x}—Nd3—O1^{xii}	149.47 (14)	O9^{iii}—Mo3—Mo3^{iii}	43.32 (13)
O4^{ix}—Nd3—O1^{xii}	107.72 (13)	Mo3^{vi}—Mo3—Mo3^{iii}	167.73 (7)
O8^{xi}—Nd3—O1^{xii}	65.13 (14)	Mo3^{iv}—Mo3—Mo3^{iii}	168.51 (7)
O10—Nd3—O1^{xi}	71.33 (18)	Mo3^{xviii}—Mo3—Mo3^{iii}	0.621 (8)
O5^{ix}—Nd3—O1^{xi}	138.96 (13)	O10—Si—O6^{xix}	108.8 (4)
O5^{x}—Nd3—O1^{xi}	99.53 (13)	O10—Si—O1	109.7 (2)
O4^{x}—Nd3—O1^{xi}	107.72 (13)	O6^{xix}—Si—O1	105.0 (2)
O4^{ix}—Nd3—O1^{xi}	149.47 (14)	O10—Si—O1^{xvii}	109.7 (2)
O8^{xi}—Nd3—O1^{xi}	65.13 (14)	O6^{xix}—Si—O1^{xvii}	105.0 (2)
O1^{xii}—Nd3—O1^{xi}	60.67 (17)	O1—Si—O1^{xvii}	118.0 (3)
O10—Nd3—O6^{x}	78.94 (13)	Si—O1—Mo2	121.3 (2)
O5^{ix}—Nd3—O6^{x}	136.43 (16)	Si—O1—Nd2^{vi}	113.1 (2)
O5^{x}—Nd3—O6^{x}	65.21 (16)	Mo2—O1—Nd2^{vi}	116.82 (18)
O4^{x}—Nd3—O6^{x}	55.67 (17)	Si—O1—Nd3^{xi}	99.6 (2)
O4^{ix}—Nd3—O6^{x}	121.22 (17)	Mo2—O1—Nd3^{xi}	100.03 (16)
O8^{xi}—Nd3—O6^{x}	96.04 (14)	Nd2^{vi}—O1—Nd3^{xi}	100.11 (15)
O1^{xii}—Nd3—O6^{x}	114.70 (16)	Mo3^{iii}—O2—Mo2^{xvii}	127.12 (13)
O1^{xi}—Nd3—O6^{x}	55.02 (16)	Mo3^{xviii}—O2—Mo2^{xvii}	136.69 (16)
O10—Nd3—O6^{xiii}	78.94 (13)	Mo3^{iii}—O2—Mo2	136.69 (16)
O5^{ix}—Nd3—O6^{xiii}	65.21 (16)	Mo3^{xviii}—O2—Mo2	127.12 (13)
O5^{x}—Nd3—O6^{xiii}	136.43 (16)	Mo2^{xvii}—O2—Mo2	95.5 (3)
O4^{x}—Nd3—O6^{xiii}	121.22 (17)	Mo2—O3—Mo2^{xvii}	100.9 (3)
O4^{ix}—Nd3—O6^{xiii}	55.67 (17)	Mo2—O3—Nd1^{xix}	127.47 (15)
O8^{xi}—Nd3—O6^{xiii}	96.04 (14)	Mo2^{xvii}—O3—Nd1^{xix}	127.47 (15)
O1^{xii}—Nd3—O6^{xiii}	55.02 (16)	Mo1—O4—Nd1^{xix}	129.6 (2)
O1^{xi}—Nd3—O6^{xiii}	114.70 (16)	Mo1—O4—Nd2^{xiv}	93.50 (17)

O6^{x}—Nd3—O6^{xiii}	157.8 (3)	Nd1^{xix}—O4—Nd2^{xiv}	115.01 (18)
O4^{v}—Mo1—O4	94.5 (3)	Mo1—O4—Nd3^{xvi}	96.08 (17)
O4^{v}—Mo1—O5	163.60 (18)	Nd1^{xix}—O4—Nd3^{xvi}	109.39 (17)
O4—Mo1—O5	88.37 (18)	Nd2^{xiv}—O4—Nd3^{xvi}	111.05 (17)
O4^{v}—Mo1—O5^{v}	88.37 (18)	Mo2—O5—Mo1	77.44 (15)
O4—Mo1—O5^{v}	163.60 (18)	Mo2—O5—Nd3^{xvi}	126.38 (19)
O5—Mo1—O5^{v}	84.5 (2)	Mo1—O5—Nd3^{xvi}	94.71 (16)
O4^{v}—Mo1—O8	92.31 (17)	Mo2—O5—Nd1	104.56 (17)
O4—Mo1—O8	92.31 (17)	Mo1—O5—Nd1	104.90 (17)
O5—Mo1—O8	103.72 (17)	Nd3^{xvi}—O5—Nd1	128.36 (17)
O5^{v}—Mo1—O8	103.72 (17)	Si^{ii}—O6—Mo1	170.9 (4)
O4^{v}—Mo1—O6	76.65 (18)	Si^{ii}—O6—Nd2^{xiv}	102.9 (3)
O4—Mo1—O6	76.65 (18)	Mo1—O6—Nd2^{xiv}	86.2 (2)
O5—Mo1—O6	88.36 (18)	Si^{ii}—O6—Nd3^{xvi}	96.28 (14)
O5^{v}—Mo1—O6	88.36 (18)	Mo1—O6—Nd3^{xvi}	82.35 (13)
O8—Mo1—O6	163.5 (3)	Nd2^{xiv}—O6—Nd3^{xvi}	97.50 (14)
O4^{v}—Mo1—Mo2	144.28 (13)	Si^{ii}—O6—Nd3^{xv}	96.28 (14)
O4—Mo1—Mo2	94.20 (13)	Mo1—O6—Nd3^{xv}	82.35 (13)
O5—Mo1—Mo2	51.15 (12)	Nd2^{xiv}—O6—Nd3^{xv}	97.50 (14)
O5^{v}—Mo1—Mo2	92.81 (12)	Nd3^{xvi}—O6—Nd3^{xv}	157.8 (3)
O8—Mo1—Mo2	52.76 (13)	Mo2^{v}—O7—Mo2	77.8 (2)
O6—Mo1—Mo2	139.06 (12)	Mo2^{v}—O7—Mo3	135.39 (13)
O4^{v}—Mo1—Mo2^{v}	94.20 (13)	Mo2—O7—Mo3	144.19 (16)
O4—Mo1—Mo2^{v}	144.28 (13)	Mo2^{v}—O7—Mo3^{v}	144.19 (16)
O5—Mo1—Mo2^{v}	92.81 (12)	Mo2—O7—Mo3^{v}	135.39 (13)
O5^{v}—Mo1—Mo2^{v}	51.15 (12)	Mo2^{v}—O7—Nd1	100.1 (2)
O8—Mo1—Mo2^{v}	52.76 (13)	Mo2—O7—Nd1	100.1 (2)
O6—Mo1—Mo2^{v}	139.06 (12)	Mo3—O7—Nd1	88.0 (2)
Mo2—Mo1—Mo2^{v}	60.38 (3)	Mo3^{v}—O7—Nd1	88.0 (2)
O3—Mo2—O5	93.4 (2)	Mo1—O8—Mo2	75.52 (19)
O3—Mo2—O7	167.96 (18)	Mo1—O8—Mo2^{v}	75.52 (19)
O5—Mo2—O7	88.8 (2)	Mo2—O8—Mo2^{v}	75.4 (2)
O3—Mo2—O2	81.62 (18)	Mo1—O8—Nd3^{xi}	174.8 (3)
O5—Mo2—O2	87.0 (2)	Mo2—O8—Nd3^{xi}	108.5 (2)
O7—Mo2—O2	86.67 (17)	Mo2^{v}—O8—Nd3^{xi}	108.5 (2)
O3—Mo2—O8	88.33 (17)	Mo3^{v}—O9—Mo3^{xviii}	79.7 (2)
O5—Mo2—O8	102.9 (2)	Mo3^{xviii}—O9—Mo3	86.24 (19)
O7—Mo2—O8	102.73 (16)	Mo3^{v}—O9—Mo3^{iii}	86.11 (19)
O2—Mo2—O8	166.3 (2)	Mo3^{v}—O9—Nd2^{vi}	100.32 (19)
O3—Mo2—O1	86.1 (2)	Mo3^{xviii}—O9—Nd2^{vi}	146.0 (2)
O5—Mo2—O1	171.44 (17)	Mo3—O9—Nd2^{vi}	94.31 (17)

O7—Mo2—O1	89.9 (2)	$Mo3^{iii}$—O9—$Nd2^{vi}$	146.1 (2)
O2—Mo2—O1	84.5 (2)	$Mo3^{v}$—O9—$Nd1^{iii}$	132.9 (2)
O8—Mo2—O1	85.6 (2)	$Mo3^{xviii}$—O9—$Nd1^{iii}$	93.60 (18)
O3—Mo2—Mo1	95.04 (16)	Mo3—O9—$Nd1^{iii}$	134.1 (2)
O5—Mo2—Mo1	51.41 (12)	$Mo3^{iii}$—O9—$Nd1^{iii}$	88.46 (16)
O7—Mo2—Mo1	95.57 (15)	$Nd2^{vi}$—O9—$Nd1^{iii}$	109.58 (19)
O2—Mo2—Mo1	138.13 (18)	Si—O10—Nd3	170.3 (5)
O8—Mo2—Mo1	51.72 (17)	Si—O10—$Nd2^{xx}$	91.0 (3)
O1—Mo2—Mo1	137.15 (12)	Nd3—O10—$Nd2^{xx}$	98.7 (2)
O3—Mo2—$Mo2^{v}$	140.47 (13)		

Symmetry codes: (i) −*x*+1/2, *y*+1/2, *z*+1/2; (ii) −*x*+1/2, −*y*+1, *z*+1/2; (iii) −*x*, −*y*+1, −*z*+1; (iv) −*x*, *y*+1/2, −*z*+1; (v) *x*, −*y*+3/2, *z*; (vi) −*x*, −*y*+2, −*z*+1; (vii) −*x*+1/2, −*y*+2, *z*+1/2; (viii) *x*, *y*+1, *z*+1; (ix) *x*−1/2, −*y*+1/2, −*z*+1/2; (x) *x*−1/2, *y*, −*z*+1/2; (xi) −*x*, −*y*+1, −*z*; (xii) −*x*, *y*−1/2, −*z*; (xiii) *x*−1/2, *y*−1, −*z*+1/2; (xiv) −*x*+1/2, −*y*+2, *z*−1/2; (xv) *x*+1/2, *y*+1, −*z*+1/2; (xvi) *x*+1/2, *y*, −*z*+1/2; (xvii) *x*, −*y*+1/2, *z*; (xviii) −*x*, *y*−1/2, −*z*+1; (xix) −*x*+1/2, −*y*+1, *z*−1/2; (xx) *x*, *y*−1, *z*−1; (xxi) −*x*, −*y*, −*z*.

Fig. 1

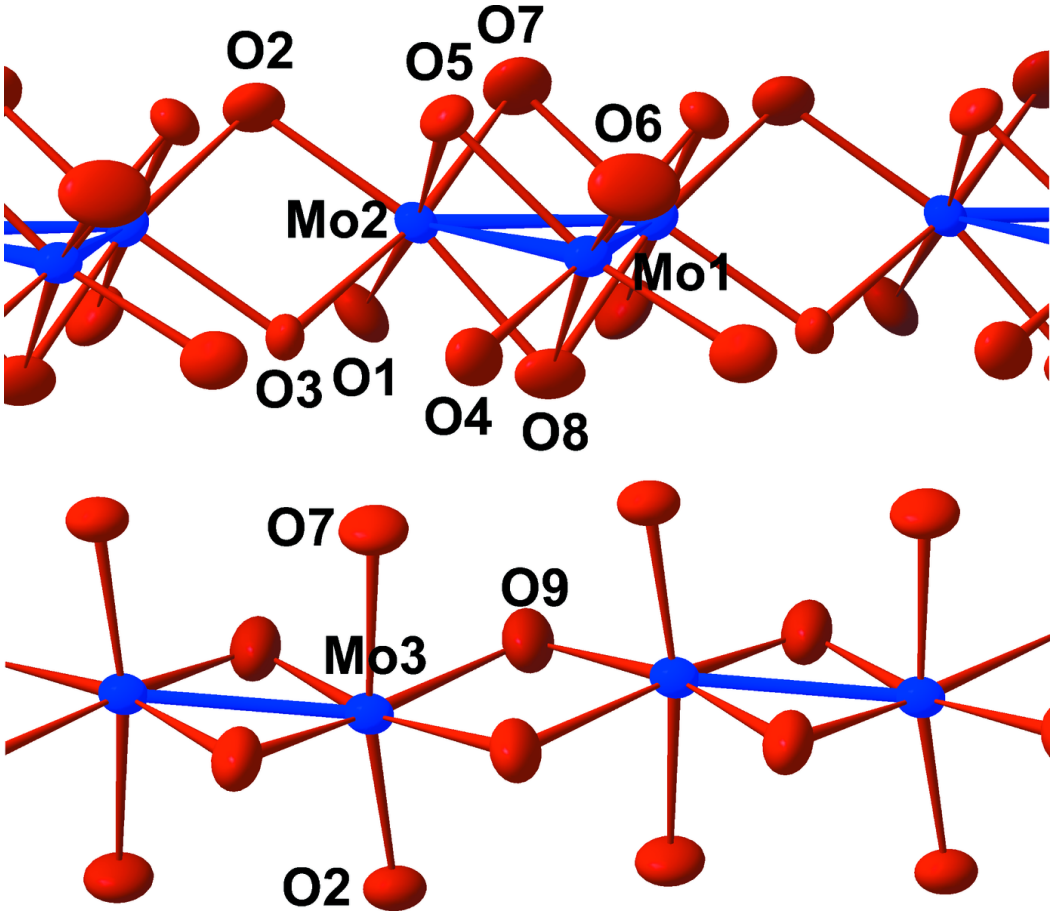

Fig. 2