

Dipraseodymium(III) pyroborate molybdate(VI), Pr₂(B₂O₅)(MoO₄)

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 Key indicators: single-crystal X-ray study; $T = 291$ K; mean $\sigma(\text{O}-\text{B}) = 0.007$ Å; R factor = 0.031; wR factor = 0.083; data-to-parameter ratio = 17.0.

Single crystals of triclinic Pr₂(B₂O₅)(MoO₄) were prepared from an incongruently melting flux in the system Pr₂O₃–MoO₃–B₂O₃ in a platinum crucible in an atmosphere of air. In the crystal structure, distorted edge-sharing [PrO₈] square antiprisms form a three-dimensional framework. These are further linked by isolated [MoO₄] tetrahedra and isolated pyroborate groups [B₂O₅], the latter consisting of two independent trigonal [BO₃] groups sharing one O atom. The [MoO₄] tetrahedra and the [B₂O₅] groups are arranged in alternating layers parallel to the *ab* plane.

Related literature

A rough investigation of the ternary systems RE₂O₃–B₂O₃–MoO₃ (*RE* = rare earth element) has been reported by Lysanova *et al.* (1983) and Dzhurinskii & Lysanova (1998). X-ray powder diffraction data of RE₂(B₂O₅)(MoO₄) compounds with *RE* = Pr, Nd, Sm, Eu, Gd and Tb were reported by Lysanova *et al.* (1983). Geometric parameters of [BO₃] groups were reviewed by Zobetz (1982).

Experimental

Crystal data

 Pr₂(B₂O₅)(MoO₄)

 $M_r = 543.38$

 Triclinic, *P*1

 $a = 5.2806$ (5) Å

 $b = 7.0278$ (5) Å

 $c = 10.5824$ (9) Å

 $\alpha = 74.557$ (6)°

 $\beta = 76.307$ (7)°

 $\gamma = 73.065$ (6)°

 $V = 356.69$ (5) Å³
 $Z = 2$

 Mo *K*α radiation

 $\mu = 15.20$ mm⁻¹
 $T = 291$ (2) K

0.20 × 0.15 × 0.12 mm

Data collection

Enraf–Nonius CAD-4 diffractometer

 Absorption correction: ψ scan (*MolEN*; Fair, 1990)

 $T_{\min} = 0.296$, $T_{\max} = 0.999$ (expected range = 0.048–0.161)

4733 measured reflections

2155 independent reflections

 1983 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.019$

3 standard reflections

every 100 reflections intensity decay: 1.7%

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.082$
 $S = 1.13$

2155 reflections

127 parameters

 $\Delta\rho_{\text{max}} = 2.55$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.73$ e Å⁻³
Table 1

Selected bond lengths (Å).

Pr1–O4	2.370 (3)	Pr2–O3 ^{vii}	2.585 (3)
Pr1–O3 ⁱ	2.430 (3)	Pr2–O1 ^{viii}	2.585 (3)
Pr1–O1 ⁱ	2.450 (3)	Pr2–O6 ^{ix}	2.645 (4)
Pr1–O5 ⁱⁱ	2.461 (3)	Mo–O5	1.748 (3)
Pr1–O7	2.480 (3)	Mo–O7	1.748 (3)
Pr1–O2	2.529 (3)	Mo–O6	1.782 (4)
Pr1–O2 ⁱⁱⁱ	2.557 (3)	Mo–O2 ^x	1.803 (3)
Pr1–O6 ^{iv}	2.610 (3)	B1–O8	1.345 (6)
Pr2–O8	2.364 (3)	B1–O4	1.370 (6)
Pr2–O8 ^v	2.375 (3)	B1–O9	1.387 (6)
Pr2–O4 ^{vi}	2.456 (3)	B2–O9 ^{xi}	1.373 (6)
Pr2–O3	2.506 (3)	B2–O1 ^{xi}	1.378 (6)
Pr2–O1	2.513 (3)	B2–O3	1.384 (6)

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

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, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2175).

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supplementary materials

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Dipraseodymium(III) pyroborate molybdate(VI), Pr₂(B₂O₅)(MoO₄)

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Comment

The existence of several compounds in the systems RE₂O₃—B₂O₃—MoO₃ (RE = rare earth element) has been studied by Lysanova *et al.* (1983) by means of X-ray powder diffraction data and was partly corroborated by Dzhurinskii & Lysanova (1998). Among these pseudo-ternary compounds, rare earth pyroborate molybdates of the type RE₂(B₂O₅)(MoO₄) were reported for RE = Pr - Tb (excluding *Pm*) (Lysanova *et al.*, 1983), all with incongruent melting behaviour. However, no structural information about these compounds has been given so far. In the course of our investigations of the systems RE₂O₃—B₂O₃—MO₃ (M = Mo, W) we grew single crystals of the Pr-compound Pr₂(B₂O₅)(MoO₄), (I), as a representative of the rare earth pyroborate molybdate series.

In the crystal structure of (I) the two symmetrically non-equivalent Pr atoms show a distinct eightfold coordination by oxygen atoms, both with a slightly distorted square antiprismatic coordination polyhedron, and with Pr—O bond lengths ranging from 2.370 (3) Å to 2.610 (3) Å for Pr1, and from 2.364 (3) Å to 2.645 (4) Å for Pr2 (Fig. 2). The [PrO₈] polyhedra are connected *via* common edges, where Pr2 is connected to six neighbouring [PrO₈] polyhedra with Pr—Pr distances ranging from 3.9237 (5) Å to 4.1242 (5) Å, while Pr1 is connected to only four [PrO₈] polyhedra with Pr—Pr distances between 3.9702 (6) Å and 4.1583 (6) Å. From the different connection schemes of the two Pr atoms a three-dimensional framework of [PrO₈] polyhedra with interstitial voids results (Fig. 1). In these voids nearly undistorted and isolated [MoO₄] tetrahedra, that are arranged in layers parallel to the *ab* plane are positioned (Fig. 1).

The two crystallographically different B atoms are threefold coordinated by O atoms. The two [BO₃] groups are linked by a common oxygen ligand O9 (see Fig. 2), thus forming isolated pyroborate groups [B₂O₅]. The pyroborate groups are bent with an angle (B1—O9—B2) of 125.1 (4)°, while the individual [BO₃] groups show no unusual distortions (Zobetz, 1982). The oxygen ligands of the pyroborate group (apart from the bridging oxygen O9, see Fig. 2) each belong either to two different [PrO₈] polyhedra (being simultaneously ligands of B1) or to three different [PrO₈] polyhedra (being simultaneously ligands of B2). All [B₂O₅] groups are arranged in double layers that extend parallel to the *ab*-plane and alternate with layers of [MoO₄] tetrahedra (see Fig. 1).

Experimental

Single crystals of (I) were obtained by growth from the melt. A homogenized powder mixture of Pr₄O₁₁ (99.9%, Alfa Aesar), B₂O₃ (99.98%, Alfa Aesar) and MoO₃ (99.95%, Alfa Aesar) in a molar ratio of 1: 3.33̄: 7 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, light-green prismatic single crystals of the title compound were separated mechanically from the fine-grained praseodymium borate molybdate matrix.

Refinement

The final difference Fourier map indicated a positive maximum at a distance of 0.76 Å from Pr1 and a negative maximum at a distance of 0.85 Å from the same atom.

Figures

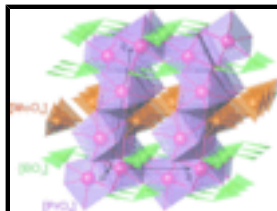


Fig. 1. : View of the structure of (I) approximately along the *a*-axis, emphasizing coordination surroundings of the cations. Pr atoms are shown as large red spheres, Mo atoms as smaller orange spheres, and B atoms as small green spheres. O atoms are indicated by the corners of the coordination polyhedra and are not drawn.

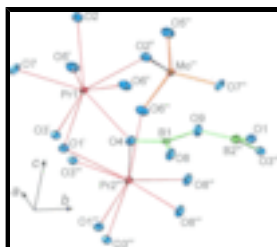


Fig. 2. : Fraction of the structure of (I) with atomic labelling scheme in a projection approximately along the *a*-axis. The atoms are drawn as displacement ellipsoids at the 50% probability level. [Symmetry codes: (i) $x, y + 1, z$; (ii) $-x + 1, -y + 1, -z - 1$; (iii) $-x + 1, -y$, (iv) $x, y - 1, z; -z - 1$; (x) $-x, -y, -z$; (xii) $x + 1, y, z$; (xiii) $x + 1, y + 1, z$; (xiv) $-x + 1, -y - 1, -z$; (xv) $x + 1, y - 1, z$.]

Diprasedymium(III) pyroborate molybdate(VI)

Crystal data

$\text{Pr}_2(\text{B}_2\text{O}_5)(\text{MoO}_4)$

$M_r = 543.38$

Triclinic, $P\bar{1}$

$a = 5.2806$ (5) Å

$b = 7.0278$ (5) Å

$c = 10.5824$ (9) Å

$\alpha = 74.557$ (6)°

$\beta = 76.307$ (7)°

$\gamma = 73.065$ (6)°

$V = 356.69$ (5) Å³

$Z = 2$

$F_{000} = 484$

$D_x = 5.059$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 25 reflections

$\theta = 20.8\text{--}24.2^\circ$

$\mu = 15.20$ mm⁻¹

$T = 291$ (2) K

Prism, light green

$0.20 \times 0.15 \times 0.12$ mm

Data collection

Enraf-Nonius CAD-4
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 291$ (2) K

$\omega/2\theta$ scans

Absorption correction: ψ scan
(MolEN; Fair, 1990)

$R_{\text{int}} = 0.019$

$\theta_{\text{max}} = 30.4^\circ$

$\theta_{\text{min}} = 3.1^\circ$

$h = -7 \rightarrow 7$

$k = -10 \rightarrow 10$

$l = -15 \rightarrow 15$

$T_{\min} = 0.296$, $T_{\max} = 0.999$
 4733 measured reflections
 2155 independent reflections
 1983 reflections with $I > 2\sigma(I)$

3 standard reflections
 every 100 reflections
 intensity decay: 1.7%

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.082$
 $S = 1.13$
 2155 reflections
 127 parameters
 Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
 $w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 1.1726P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 2.55 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -1.73 \text{ e } \text{\AA}^{-3}$
 Extinction correction: SHELXL97 (Sheldrick, 2008),
 $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.0319 (13)

Special details

Experimental. A suitable single-crystal was carefully selected under a polarizing microscope and mounted in a glass capillary.

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Pr1	0.37016 (5)	0.07689 (4)	-0.31461 (2)	0.00706 (11)
Pr2	0.15410 (5)	-0.79427 (4)	0.04666 (2)	0.00693 (11)
Mo	0.03514 (8)	0.70782 (6)	-0.41958 (4)	0.00758 (12)
O7	0.1449 (8)	0.4427 (5)	-0.3778 (4)	0.0144 (7)
O5	0.2335 (7)	0.7903 (6)	-0.5706 (3)	0.0152 (7)
O6	0.0805 (7)	0.8248 (6)	-0.2991 (4)	0.0141 (7)
O2	0.3079 (7)	0.1829 (5)	-0.5554 (3)	0.0111 (6)
B1	0.4573 (10)	-0.4118 (7)	-0.1373 (5)	0.0077 (8)
O4	0.4775 (7)	-0.2184 (5)	-0.1465 (3)	0.0114 (6)
O8	0.2350 (7)	-0.4758 (5)	-0.0732 (3)	0.0114 (6)
O9	0.6870 (7)	-0.5435 (5)	-0.1886 (4)	0.0121 (7)
B2	-0.2634 (10)	-0.7520 (8)	-0.1570 (5)	0.0091 (8)
O1	0.5437 (7)	-0.8575 (5)	-0.1392 (3)	0.0094 (6)
O3	-0.0094 (7)	-0.8664 (5)	-0.1355 (3)	0.0086 (6)

supplementary materials

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pr1	0.00931 (15)	0.00715 (15)	0.00456 (15)	-0.00225 (10)	-0.00160 (10)	-0.00032 (10)
Pr2	0.00839 (16)	0.00662 (15)	0.00584 (15)	-0.00215 (10)	-0.00193 (10)	-0.00046 (9)
Mo	0.0094 (2)	0.0072 (2)	0.00587 (19)	-0.00159 (14)	-0.00209 (14)	-0.00082 (13)
O7	0.0190 (18)	0.0082 (15)	0.0112 (15)	-0.0002 (12)	-0.0023 (14)	0.0025 (12)
O5	0.0167 (17)	0.0188 (17)	0.0100 (15)	-0.0069 (14)	0.0023 (13)	-0.0039 (13)
O6	0.0165 (17)	0.0179 (17)	0.0109 (15)	-0.0060 (13)	-0.0036 (13)	-0.0052 (13)
O2	0.0110 (15)	0.0136 (16)	0.0096 (15)	-0.0016 (12)	-0.0034 (12)	-0.0038 (12)
B1	0.011 (2)	0.008 (2)	0.0034 (19)	-0.0022 (16)	-0.0003 (16)	-0.0011 (15)
O4	0.0159 (16)	0.0096 (15)	0.0101 (15)	-0.0046 (12)	-0.0044 (13)	-0.0008 (11)
O8	0.0093 (15)	0.0086 (14)	0.0130 (16)	-0.0015 (11)	0.0004 (13)	0.0005 (12)
O9	0.0120 (16)	0.0075 (15)	0.0142 (17)	-0.0020 (12)	0.0011 (13)	-0.0012 (12)
B2	0.009 (2)	0.009 (2)	0.008	-0.0028 (16)	-0.0004 (17)	-0.0010 (16)
O1	0.0099 (15)	0.0107 (15)	0.0088 (14)	-0.0036 (12)	-0.0030 (12)	-0.0017 (11)
O3	0.0076 (14)	0.0106 (15)	0.0071 (14)	-0.0025 (11)	0.0007 (11)	-0.0024 (11)

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

Pr1—O4	2.370 (3)	Pr2—O1 ^{ix}	2.585 (3)
Pr1—O3 ⁱ	2.430 (3)	Pr2—O6 ^x	2.645 (4)
Pr1—O1 ⁱ	2.450 (3)	Pr2—B2 ^{viii}	3.021 (5)
Pr1—O5 ⁱⁱ	2.461 (3)	Pr2—Pr2 ^{vii}	3.9237 (6)
Pr1—O7	2.480 (3)	Pr2—Pr1 ^{vi}	3.9702 (5)
Pr1—O2	2.529 (3)	Pr2—Pr1 ^{iv}	3.9893 (5)
Pr1—O2 ⁱⁱⁱ	2.557 (3)	Mo—O5	1.748 (3)
Pr1—O6 ^{iv}	2.610 (3)	Mo—O7	1.748 (3)
Pr1—Mo ^v	3.6714 (6)	Mo—O6	1.782 (4)
Pr1—Pr2 ^{vi}	3.9702 (5)	Mo—O2 ^v	1.803 (3)
Pr1—Pr2 ⁱ	3.9893 (5)	Mo—Pr1 ^v	3.6714 (6)
Pr1—Pr2 ^{vii}	4.0171 (5)	B1—O8	1.345 (6)
Pr2—O8	2.364 (3)	B1—O4	1.370 (6)
Pr2—O8 ^{vii}	2.375 (3)	B1—O9	1.387 (6)
Pr2—O4 ^{vi}	2.456 (3)	B2—O9 ^{xi}	1.373 (6)
Pr2—O3	2.506 (3)	B2—O1 ^{xi}	1.378 (6)
Pr2—O1	2.513 (3)	B2—O3	1.384 (6)
Pr2—O3 ^{viii}	2.585 (3)	B2—Pr2 ^{viii}	3.021 (5)
O4—Pr1—O3 ⁱ	77.59 (12)	O4 ^{vi} —Pr2—O1 ^{ix}	64.22 (10)
O4—Pr1—O1 ⁱ	67.58 (11)	O3—Pr2—O1 ^{ix}	102.94 (11)
O3 ⁱ —Pr1—O1 ⁱ	73.79 (11)	O1—Pr2—O1 ^{ix}	75.10 (12)
O4—Pr1—O5 ⁱⁱ	112.06 (12)	O3 ^{viii} —Pr2—O1 ^{ix}	54.11 (11)
O3 ⁱ —Pr1—O5 ⁱⁱ	139.81 (11)	O8—Pr2—O6 ^x	117.87 (11)

O1 ⁱ —Pr1—O5 ⁱⁱ	74.69 (11)	O8 ^{vii} —Pr2—O6 ^x	68.69 (12)
O4—Pr1—O7	149.37 (12)	O4 ^{vi} —Pr2—O6 ^x	79.69 (11)
O3 ⁱ —Pr1—O7	75.46 (11)	O3—Pr2—O6 ^x	126.73 (10)
O1 ⁱ —Pr1—O7	90.93 (12)	O1—Pr2—O6 ^x	154.52 (11)
O5 ⁱⁱ —Pr1—O7	80.77 (12)	O3 ^{viii} —Pr2—O6 ^x	69.74 (10)
O4—Pr1—O2	141.05 (11)	O1 ^{ix} —Pr2—O6 ^x	82.67 (11)
O3 ⁱ —Pr1—O2	121.14 (11)	O8—Pr2—Pr2 ^{vii}	34.21 (8)
O1 ⁱ —Pr1—O2	146.59 (11)	O8 ^{vii} —Pr2—Pr2 ^{vii}	34.03 (8)
O5 ⁱⁱ —Pr1—O2	76.77 (11)	O4 ^{vi} —Pr2—Pr2 ^{vii}	97.53 (8)
O7—Pr1—O2	67.53 (11)	O3—Pr2—Pr2 ^{vii}	93.69 (8)
O4—Pr1—O2 ⁱⁱⁱ	76.63 (11)	O1—Pr2—Pr2 ^{vii}	103.65 (8)
O3 ⁱ —Pr1—O2 ⁱⁱⁱ	145.67 (11)	O3 ^{viii} —Pr2—Pr2 ^{vii}	140.80 (7)
O1 ⁱ —Pr1—O2 ⁱⁱⁱ	115.72 (11)	O1 ^{ix} —Pr2—Pr2 ^{vii}	161.72 (7)
O5 ⁱⁱ —Pr1—O2 ⁱⁱⁱ	71.93 (11)	O6 ^x —Pr2—Pr2 ^{vii}	93.54 (8)
O7—Pr1—O2 ⁱⁱⁱ	133.79 (11)	B2 ^{viii} —Pr2—Pr2 ^{vii}	166.65 (10)
O2—Pr1—O2 ⁱⁱⁱ	70.32 (12)	O8—Pr2—Pr1 ^{vi}	113.11 (9)
O4—Pr1—O6 ^{iv}	69.35 (11)	O8 ^{vii} —Pr2—Pr1 ^{vi}	125.58 (9)
O3 ⁱ —Pr1—O6 ^{iv}	72.69 (11)	O4 ^{vi} —Pr2—Pr1 ^{vi}	33.96 (8)
O1 ⁱ —Pr1—O6 ^{iv}	129.69 (11)	O3—Pr2—Pr1 ^{vi}	139.70 (8)
O5 ⁱⁱ —Pr1—O6 ^{iv}	147.48 (12)	O1—Pr2—Pr1 ^{vi}	90.73 (8)
O7—Pr1—O6 ^{iv}	115.17 (12)	O3 ^{viii} —Pr2—Pr1 ^{vi}	79.17 (7)
O2—Pr1—O6 ^{iv}	83.51 (11)	O1 ^{ix} —Pr2—Pr1 ^{vi}	36.78 (7)
O2 ⁱⁱⁱ —Pr1—O6 ^{iv}	77.21 (11)	O6 ^x —Pr2—Pr1 ^{vi}	63.84 (8)
O4—Pr1—Pr2 ^{vi}	35.36 (8)	B2 ^{viii} —Pr2—Pr1 ^{vi}	57.28 (10)
O3 ⁱ —Pr1—Pr2 ^{vi}	89.53 (8)	Pr2 ^{vii} —Pr2—Pr1 ^{vi}	126.063 (11)
O1 ⁱ —Pr1—Pr2 ^{vi}	39.18 (8)	O8—Pr2—Pr1 ^{iv}	82.46 (9)
O5 ⁱⁱ —Pr1—Pr2 ^{vi}	81.40 (9)	O8 ^{vii} —Pr2—Pr1 ^{iv}	115.15 (9)
O7—Pr1—Pr2 ^{vi}	129.95 (9)	O4 ^{vi} —Pr2—Pr1 ^{iv}	115.41 (8)
O2—Pr1—Pr2 ^{vi}	149.14 (8)	O3—Pr2—Pr1 ^{iv}	35.45 (7)
O2 ⁱⁱⁱ —Pr1—Pr2 ^{vi}	82.37 (8)	O1—Pr2—Pr1 ^{iv}	35.98 (7)
O6 ^{iv} —Pr1—Pr2 ^{vi}	104.66 (8)	O3 ^{viii} —Pr2—Pr1 ^{iv}	88.62 (7)
Mo ^v —Pr1—Pr2 ^{vi}	173.822 (12)	O1 ^{ix} —Pr2—Pr1 ^{iv}	89.26 (7)
O4—Pr1—Pr2 ⁱ	68.51 (8)	O6 ^x —Pr2—Pr1 ^{iv}	157.63 (7)
O3 ⁱ —Pr1—Pr2 ⁱ	36.74 (8)	B2 ^{viii} —Pr2—Pr1 ^{iv}	87.02 (10)
O1 ⁱ —Pr1—Pr2 ⁱ	37.06 (8)	Pr2 ^{vii} —Pr2—Pr1 ^{iv}	100.262 (11)
O5 ⁱⁱ —Pr1—Pr2 ⁱ	108.19 (8)	Pr1 ^{vi} —Pr2—Pr1 ^{iv}	118.956 (9)
O7—Pr1—Pr2 ⁱ	81.16 (8)	O5—Mo—O7	107.10 (17)
O2—Pr1—Pr2 ⁱ	147.30 (8)	O5—Mo—O6	107.70 (16)
O2 ⁱⁱⁱ —Pr1—Pr2 ⁱ	142.36 (8)	O7—Mo—O6	111.77 (17)
O6 ^{iv} —Pr1—Pr2 ⁱ	102.41 (8)	O5—Mo—O2 ^v	105.62 (17)
Mo ^v —Pr1—Pr2 ⁱ	124.637 (12)	O7—Mo—O2 ^v	118.20 (16)

supplementary materials

Pr2 ^{vi} —Pr1—Pr2 ⁱ	61.044 (9)	O6—Mo—O2 ^v	105.89 (16)
O4—Pr1—Pr2 ^{vii}	53.61 (8)	Pr1 ⁱ —O6—Pr2 ^x	99.70 (12)
O3 ⁱ —Pr1—Pr2 ^{vii}	38.13 (7)	Mo ^v —O2—Pr1	114.85 (15)
O1 ⁱ —Pr1—Pr2 ^{vii}	91.90 (8)	Mo ^v —O2—Pr1 ⁱⁱⁱ	122.00 (16)
O5 ⁱⁱ —Pr1—Pr2 ^{vii}	164.08 (9)	Pr1—O2—Pr1 ⁱⁱⁱ	109.68 (12)
O7—Pr1—Pr2 ^{vii}	108.49 (8)	O8—B1—O4	122.1 (4)
O2—Pr1—Pr2 ^{vii}	118.48 (8)	O8—B1—O9	121.5 (4)
O2 ⁱⁱⁱ —Pr1—Pr2 ^{vii}	107.57 (8)	O4—B1—O9	116.2 (4)
O6 ^{iv} —Pr1—Pr2 ^{vii}	40.47 (8)	B1—O4—Pr1	129.0 (3)
Mo ^v —Pr1—Pr2 ^{vii}	97.798 (12)	B1—O4—Pr2 ^{vi}	113.9 (3)
Pr2 ^{vi} —Pr1—Pr2 ^{vii}	82.769 (10)	Pr1—O4—Pr2 ^{vi}	110.68 (12)
Pr2 ⁱ —Pr1—Pr2 ^{vii}	62.010 (9)	B1—O8—Pr2	134.1 (3)
O8—Pr2—O8 ^{vii}	68.24 (13)	B1—O8—Pr2 ^{vii}	113.4 (3)
O8—Pr2—O4 ^{vi}	79.16 (11)	Pr2—O8—Pr2 ^{vii}	111.76 (13)
O8 ^{vii} —Pr2—O4 ^{vi}	113.81 (11)	B2 ^{xii} —O9—B1	125.1 (4)
O8—Pr2—O3	95.79 (11)	O9 ^{xi} —B2—O1 ^{xi}	123.8 (4)
O8 ^{vii} —Pr2—O3	90.33 (12)	O9 ^{xi} —B2—O3	119.3 (4)
O4 ^{vi} —Pr2—O3	150.59 (11)	O1 ^{xi} —B2—O3	116.8 (4)
O8—Pr2—O1	72.10 (11)	Pr1 ^{iv} —O1—Pr2	106.97 (12)
O8 ^{vii} —Pr2—O1	134.09 (11)	B2 ^{xii} —O1—Pr2 ^{ix}	94.4 (3)
O4 ^{vi} —Pr2—O1	79.52 (11)	Pr1 ^{iv} —O1—Pr2 ^{ix}	104.05 (12)
O3—Pr2—O1	71.43 (11)	Pr2—O1—Pr2 ^{ix}	104.90 (12)
O8—Pr2—O3 ^{viii}	167.27 (12)	B2—O3—Pr1 ^{iv}	123.2 (3)
O8 ^{vii} —Pr2—O3 ^{viii}	108.01 (11)	B2—O3—Pr2	114.9 (3)
O4 ^{vi} —Pr2—O3 ^{viii}	113.02 (11)	Pr1 ^{iv} —O3—Pr2	107.81 (12)
O3—Pr2—O3 ^{viii}	71.81 (12)	B2—O3—Pr2 ^{viii}	94.2 (3)
O1—Pr2—O3 ^{viii}	105.54 (10)	Pr1 ^{iv} —O3—Pr2 ^{viii}	106.39 (12)
O8—Pr2—O1 ^{ix}	134.34 (11)	Pr2—O3—Pr2 ^{viii}	108.19 (12)
O8 ^{vii} —Pr2—O1 ^{ix}	150.80 (11)		

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

Fig. 1

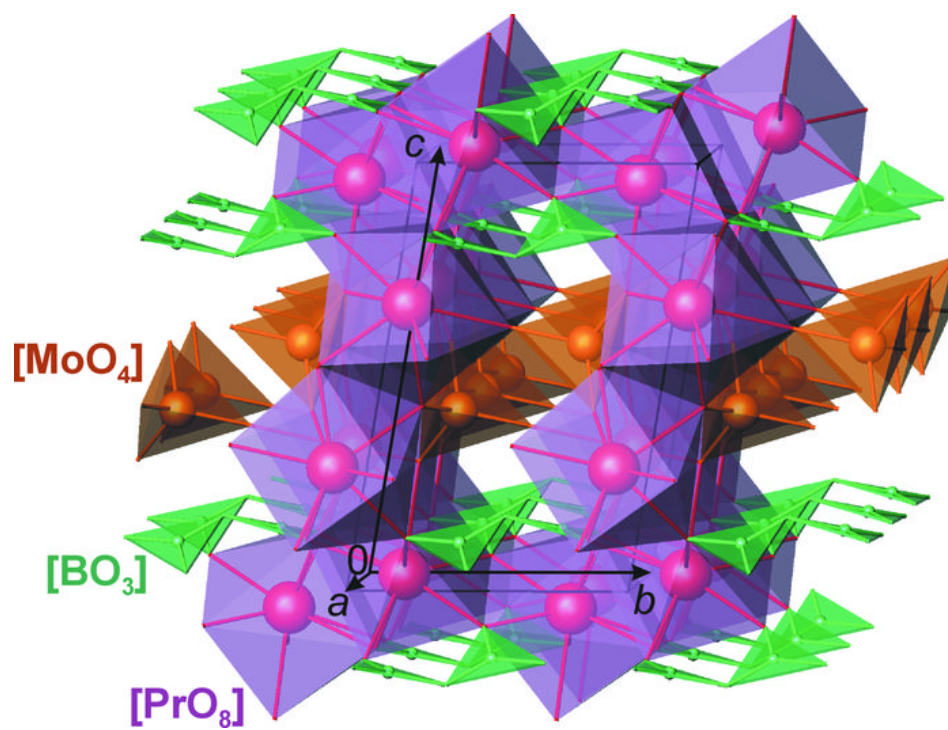


Fig. 2

