

## Dipraseodymium(III) pyroborate molybdate(VI), Pr<sub>2</sub>(B<sub>2</sub>O<sub>5</sub>)(MoO<sub>4</sub>)

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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 Pr<sub>2</sub>(B<sub>2</sub>O<sub>5</sub>)(MoO<sub>4</sub>) were prepared from an incongruently melting flux in the system Pr<sub>2</sub>O<sub>3</sub>–MoO<sub>3</sub>–B<sub>2</sub>O<sub>3</sub> in a platinum crucible in an atmosphere of air. In the crystal structure, distorted edge-sharing [PrO<sub>8</sub>] square antiprisms form a three-dimensional framework. These are further linked by isolated [MoO<sub>4</sub>] tetrahedra and isolated pyroborate groups [B<sub>2</sub>O<sub>5</sub>], the latter consisting of two independent trigonal [BO<sub>3</sub>] groups sharing one O atom. The [MoO<sub>4</sub>] tetrahedra and the [B<sub>2</sub>O<sub>5</sub>] groups are arranged in alternating layers parallel to the *ab* plane.

### Related literature

A rough investigation of the ternary systems RE<sub>2</sub>O<sub>3</sub>–B<sub>2</sub>O<sub>3</sub>–MoO<sub>3</sub> (*RE* = rare earth element) has been reported by Lysanova *et al.* (1983) and Dzhurinskii & Lysanova (1998). X-ray powder diffraction data of RE<sub>2</sub>(B<sub>2</sub>O<sub>5</sub>)(MoO<sub>4</sub>) compounds with *RE* = Pr, Nd, Sm, Eu, Gd and Tb were reported by Lysanova *et al.* (1983). Geometric parameters of [BO<sub>3</sub>] groups were reviewed by Zobetz (1982).

### Experimental

#### Crystal data

 Pr<sub>2</sub>(B<sub>2</sub>O<sub>5</sub>)(MoO<sub>4</sub>)

 $M_r = 543.38$ 

 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) Å<sup>3</sup>
 $Z = 2$ 

 Mo *K*α radiation

 $\mu = 15.20$  mm<sup>-1</sup>
 $T = 291$  (2) K

 $0.20 \times 0.15 \times 0.12$  mm

#### Data collection

Enraf–Nonius CAD-4 diffractometer

 Absorption correction:  $\psi$  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<sup>-3</sup>
 $\Delta\rho_{\text{min}} = -1.73$  e Å<sup>-3</sup>
**Table 1**

Selected bond lengths (Å).

Pr1–O4	2.370 (3)	Pr2–O3 <sup>vii</sup>	2.585 (3)
Pr1–O3 <sup>i</sup>	2.430 (3)	Pr2–O1 <sup>viii</sup>	2.585 (3)
Pr1–O1 <sup>i</sup>	2.450 (3)	Pr2–O6 <sup>ix</sup>	2.645 (4)
Pr1–O5 <sup>ii</sup>	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 <sup>iii</sup>	2.557 (3)	Mo–O2 <sup>x</sup>	1.803 (3)
Pr1–O6 <sup>iv</sup>	2.610 (3)	B1–O8	1.345 (6)
Pr2–O8	2.364 (3)	B1–O4	1.370 (6)
Pr2–O8 <sup>v</sup>	2.375 (3)	B1–O9	1.387 (6)
Pr2–O4 <sup>vi</sup>	2.456 (3)	B2–O9 <sup>xi</sup>	1.373 (6)
Pr2–O3	2.506 (3)	B2–O1 <sup>xi</sup>	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).

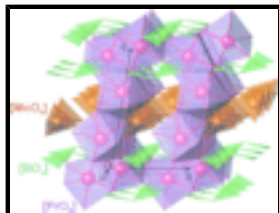
### References

- 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*. OpenVMS. 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.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Westrip, S. P. (2008). *pubCIF*. In preparation.
- Zobetz, E. (1982). *Z. Kristallogr.* **160**, 81–92.

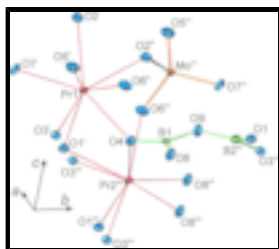




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