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The pyrochlore-type molybdate $Pr_2Mo_{1.73}Sc_{0.27}O_7$

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ(Pr–O) = 0.001 Å; disorder in main residue; R factor = 0.018; wR factor = 0.047; data-to-parameter ratio = 25.1.

Dipraseodymium molybdenum scandium heptaoxide, $Pr_2Mo_{1.73}Sc_{0.27}O_7$, crystallizes in the cubic pyrochlore-type structure. In the crystal, $(Mo,Sc)O_6$ octahedra are linked together by common corners, forming a three-dimensional $[(Mo,Sc)_2O_6]$ framework. The Pr atom and another O atom atom are located in the voids of this framework. The Mo and the Sc atom are distributed statistically over the same 16d crystallographic position, with site-occupancy factors of 0.867 (3) and 0.133 (3), respectively. The Pr^{3+} ions are surrounded by six O atoms from the MoO_6 octahedra and by two other O atoms, forming a ditrigonal scalenohedron. All atoms lie on special positions. The Pr and the statistically distributed (Mo,Sc) sites are in the 16c and 16d positions with $.\bar{3}m$ symmetry, and two O atoms are in 48f and 8a positions with $2.mm$ and $\bar{4}3m$ site symmetry, respectively.

Related literature

For pyrochlore-type molybdates, see, for example: Hubert (1974); Subramanian *et al.* (1983); Gall & Gougeon (2008). For the physical properties of some rare-earth molybdate pyrochlores, see: Hill *et al.* (1989); Ali *et al.* (1989); Miyoshi *et al.* (2001, 2003). An attempt to synthesize $ScPr_9Mo_{16}O_{35}$, a compound with the $LiNd_9Mo_{16}O_{35}$ type structure (Gougeon *et al.*, 2011), was unsuccessful, resulting in a multiphase product with $Pr_2Mo_{1.73}Sc_{0.27}O_7$ and $Pr_{16}Mo_{21}O_{56}$ (Gougeon & Gall, 2011) as predominant phases.

Experimental

Crystal data

$Pr_2Mo_{1.73}Sc_{0.27}O_7$
M_r = 571.69
Cubic, $Fd\bar{3}m$
a = 10.5271 (3) Å
V = 1166.61 (6) $Å^3$
Z = 8
Mo $K\alpha$ radiation
μ = 20.33 mm^{-1}
T = 293 K
0.10 × 0.06 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: analytical (de Meulenaar & Tompa, 1965)
T_{min} = 0.302, T_{max} = 0.461
9208 measured reflections
326 independent reflections
269 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.018$
$wR(F^2) = 0.047$
S = 1.33
326 reflections
13 parameters
$\Delta\rho_{max}$ = 0.79 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.81 e $Å^{-3}$

Table 1
Selected bond lengths (Å).

Pr1—O2	2.2792	Mo1—$O1^{ii}$	2.0440 (8)
Pr1—$O1^{i}$	2.5795 (13)		

Symmetry codes: (i) $z-\frac{1}{4}, x-\frac{1}{4}, -y$; (ii) $x, y+\frac{1}{2}, z+\frac{1}{2}$.

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, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *SHELXL97*.

Intensity data were collected at the Centre de diffractométrie de l'Université de Rennes I (www.cdifx.univ-rennes1.fr).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RU2045).

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supporting information

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The pyrochlore-type molybdate $Pr_2Mo_{1.73}Sc_{0.27}O_7$

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S1. Comment

An attempt to synthesize $ScPr_9Mo_{16}O_{35}$, a compound with the $LiNd_9Mo_{16}O_{35}$ type structure (Gougeon *et al.*, 2011), was unsuccessful, resulting in a multiphase product. However, the formation of the new compound, $Pr_2Mo_{1.73}Sc_{0.27}O_7$ was achieved. Recently, we presented the crystal structure of the pseudo-quaternary pyrochlore $Pr_{1.37}Ca_{0.63}Mo_2O_7$ (Gall & Gougeon, 2008) in which the Pr and Ca toms occupy statistically the A site. The existence of the latter two phases clearly suggests the unknown $Pr_2Mo_2O_7$ could be synthesized. However, our attempts to obtain a single- phase powder sample as well as single-crystals of $Pr_2Mo_2O_7$ were unsuccessful up to now.

S2. Experimental

Single crystals of $Pr_2Mo_{1.73}Sc_{0.27}O_7$ were prepared from a mixture of Pr_6O_{11} (Rhone Poulenc, 99.99%), Sc_2O_3 (Strem Chemicals, 99.99%), MoO_3 (Cerac, 99.95%) and Mo (Plansee, 99.9999%) with the nominal composition $ScPr_9Mo_{16}O_{35}$. Before use, Mo powder was reduced under H_2 flowing gas at 1273 K during ten hours in order to eliminate any trace of oxygen. 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 2223 K, temperature which was held for 5 min., then cooled at 100 K/h down to 1373 K and finally furnace cooled. The final product was multiphasic with $Pr_2Mo_{1.73}Sc_{0.27}O_7$ and $Pr_{16}Mo_{21}O_{56}$ (Gougeon & Gall, 2011), as predominant phases. The crystals thus obtained were of irregular shape.

S3. Refinement

The structure was solved by direct method using *SIR97*. The second setting, with the origin at $\bar{3}$ m of the Fd3m space group, was chosen. The first refinements taking into account a full occupancy of the Pr1 and Mo1 sites resulted in a *R* factor of about 0.033. Refinements of the site-occupancy factors of the Pr1 and Mo1 atoms show that the first site was fully occupied while the second one was slightly deficiency. As qualitative microanalyses using a Jeol JSM-35 CF scanning electron microscope equipped with a Tracor energy- dispersive-type X-ray spectrometer indicated the presence of scandium in the crystals, we could expect that the deficiency observed on the Mo1 site results from the presence of scandium. Refinements taking into account an occupation of the deficient Mo1 site simultaneously by Mo and Sc atoms with no constraint on the site-occupancy factors of the Mo1 and Sc1 atoms led to an occupation of 1.03 (9) of the 16 d position. Consequently, the sum of the site occupancy factors was constrained to the unity, and the ADPs of the Mo1 and Sc1 atoms were constrained to be equal. Refinement of the occupancy factor of the O2 atom in 8a position which frequently exhibits partial or total deficiency, indicates a quasi-full occupation of this position (0.97 (2) %).

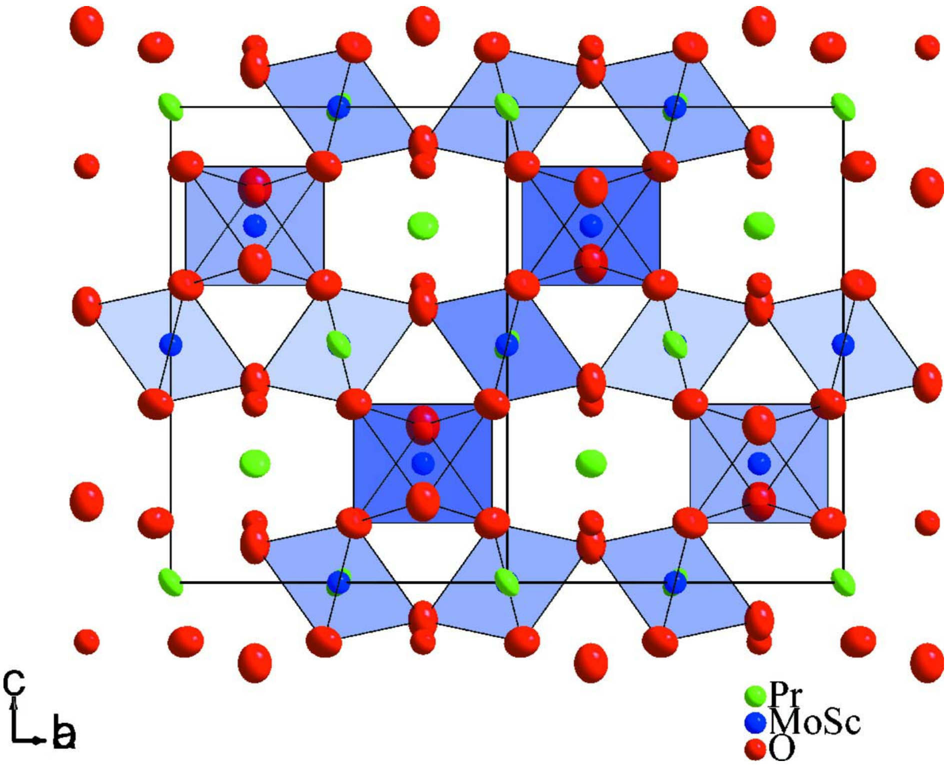

Figure 1

View of $Pr_2Mo_{1.73}Sc_{0.27}O_7$ along the [1$\bar{1}$0] direction. Displacement ellipsoids are drawn at the 97% probability level.

Dipraseodymium molybdenum scandium heptaoxide

Crystal data

$Pr_2Mo_{1.73}Sc_{0.27}O_7$
$M_r = 571.69$
Cubic, $Fd\bar{3}m$
$a = 10.5271$ (3) Å
$V = 1166.61$ (6) Å^3
$Z = 8$
$F(000) = 2018$
$D_x = 6.510$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71070$ Å
Cell parameters from 5283 reflections
$\theta = 5.5$–50°
$\mu = 20.33$ mm^{-1}
$T = 293$ K
Irregular block, black
0.1 × 0.06 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Horizontally mounted graphite crystal monochromator
Detector resolution: 9 pixels mm^{-1}
φ scans ($\kappa = 0$) + additional ω scans
Absorption correction: analytical (de Meulenaar & Tompa, 1965)
$T_{min} = 0.302$, $T_{max} = 0.461$
9208 measured reflections
326 independent reflections
269 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$
$\theta_{max} = 50.0°$, $\theta_{min} = 5.5°$
$h = -19 \rightarrow 22$
$k = -12 \rightarrow 22$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0144P)^2 + 3.2607P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.018$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.047$	$\Delta\rho_{max} = 0.79$ e Å^{-3}
$S = 1.33$	$\Delta\rho_{min} = -0.81$ e Å^{-3}
326 reflections	Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
13 parameters	Extinction coefficient: 0.00067 (7)
0 restraints	
Primary atom site location: structure-invariant direct methods	

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Pr1	0.0000	0.0000	0.0000	0.00874 (8)	
Mo1	0.5000	0.5000	0.5000	0.00591 (13)	0.867 (6)
Sc1	0.5000	0.5000	0.5000	0.00591 (13)	0.133 (6)
O1	0.41969 (18)	0.1250	0.1250	0.0132 (3)	
O2	0.1250	0.1250	0.1250	0.0072 (6)	0.972 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pr1	0.00874 (8)	0.00874 (8)	0.00874 (8)	−0.00193 (2)	−0.00193 (2)	−0.00193 (2)
Mo1	0.00591 (13)	0.00591 (13)	0.00591 (13)	−0.00007 (4)	−0.00007 (4)	−0.00007 (4)
Sc1	0.00591 (13)	0.00591 (13)	0.00591 (13)	−0.00007 (4)	−0.00007 (4)	−0.00007 (4)
O1	0.0175 (7)	0.0110 (4)	0.0110 (4)	0.000	0.000	−0.0014 (5)
O2	0.0072 (6)	0.0072 (6)	0.0072 (6)	0.000	0.000	0.000

Geometric parameters (Å, º)

Pr1—O2^{i}	2.2792	Mo1—O1^{xiii}	2.0440 (8)
Pr1—O2	2.2792	Mo1—O1^{xiv}	2.0440 (8)
Pr1—O1^{ii}	2.5795 (13)	Mo1—O1^{xv}	2.0440 (8)
Pr1—O1^{iii}	2.5795 (13)	Mo1—O1^{xvi}	2.0440 (8)
Pr1—O1^{iv}	2.5795 (13)	O1—Sc1^{xvii}	2.0440 (8)
Pr1—O1^{v}	2.5795 (13)	O1—Mo1^{xvii}	2.0440 (8)
Pr1—O1^{vi}	2.5795 (13)	O1—Sc1^{xviii}	2.0440 (8)
Pr1—O1^{vii}	2.5795 (13)	O1—Mo1^{xviii}	2.0440 (8)

Pr1—Pr1$^{\mathrm{v}}$	3.7219 (1)	O1—Pr1$^{\mathrm{v}}$	2.5795 (13)
Pr1—Pr1$^{\mathrm{viii}}$	3.7219 (1)	O1—Pr1$^{\mathrm{viii}}$	2.5795 (13)
Pr1—Pr1$^{\mathrm{ix}}$	3.7219 (1)	O2—Pr1$^{\mathrm{viii}}$	2.2792
Pr1—Pr1$^{\mathrm{x}}$	3.7219 (1)	O2—Pr1$^{\mathrm{v}}$	2.2792
Mo1—O1$^{\mathrm{xi}}$	2.0440 (8)	O2—Pr1$^{\mathrm{x}}$	2.2792
Mo1—O1$^{\mathrm{xii}}$	2.0440 (8)		
O2$^{\mathrm{i}}$—Pr1—O2	180.0	O1$^{\mathrm{vi}}$—Pr1—Pr1$^{\mathrm{ix}}$	43.83 (3)
O2$^{\mathrm{i}}$—Pr1—O1$^{\mathrm{ii}}$	79.09 (3)	O1$^{\mathrm{vii}}$—Pr1—Pr1$^{\mathrm{ix}}$	136.17 (3)
O2—Pr1—O1$^{\mathrm{ii}}$	100.91 (3)	Pr1$^{\mathrm{v}}$—Pr1—Pr1$^{\mathrm{ix}}$	180.0
O2$^{\mathrm{i}}$—Pr1—O1$^{\mathrm{iii}}$	100.91 (3)	Pr1$^{\mathrm{viii}}$—Pr1—Pr1$^{\mathrm{ix}}$	120.0
O2—Pr1—O1$^{\mathrm{iii}}$	79.09 (3)	O2$^{\mathrm{i}}$—Pr1—Pr1$^{\mathrm{x}}$	144.7
O1$^{\mathrm{ii}}$—Pr1—O1$^{\mathrm{iii}}$	180.00 (6)	O2—Pr1—Pr1$^{\mathrm{x}}$	35.3
O2$^{\mathrm{i}}$—Pr1—O1$^{\mathrm{iv}}$	79.09 (3)	O1$^{\mathrm{ii}}$—Pr1—Pr1$^{\mathrm{x}}$	82.59 (3)
O2—Pr1—O1$^{\mathrm{iv}}$	100.91 (3)	O1$^{\mathrm{iii}}$—Pr1—Pr1$^{\mathrm{x}}$	97.41 (3)
O1$^{\mathrm{ii}}$—Pr1—O1$^{\mathrm{iv}}$	116.506 (19)	O1$^{\mathrm{iv}}$—Pr1—Pr1$^{\mathrm{x}}$	136.17 (3)
O1$^{\mathrm{iii}}$—Pr1—O1$^{\mathrm{iv}}$	63.494 (19)	O1$^{\mathrm{v}}$—Pr1—Pr1$^{\mathrm{x}}$	43.83 (3)
O2$^{\mathrm{i}}$—Pr1—O1$^{\mathrm{v}}$	100.91 (3)	O1$^{\mathrm{vi}}$—Pr1—Pr1$^{\mathrm{x}}$	82.59 (3)
O2—Pr1—O1$^{\mathrm{v}}$	79.09 (3)	O1$^{\mathrm{vii}}$—Pr1—Pr1$^{\mathrm{x}}$	97.41 (3)
O1$^{\mathrm{ii}}$—Pr1—O1$^{\mathrm{v}}$	63.494 (19)	Pr1$^{\mathrm{v}}$—Pr1—Pr1$^{\mathrm{x}}$	60.0
O1$^{\mathrm{iii}}$—Pr1—O1$^{\mathrm{v}}$	116.506 (19)	Pr1$^{\mathrm{viii}}$—Pr1—Pr1$^{\mathrm{x}}$	60.0
O1$^{\mathrm{iv}}$—Pr1—O1$^{\mathrm{v}}$	180.00 (6)	Pr1$^{\mathrm{ix}}$—Pr1—Pr1$^{\mathrm{x}}$	120.0
O2$^{\mathrm{i}}$—Pr1—O1$^{\mathrm{vi}}$	79.09 (3)	O1$^{\mathrm{xi}}$—Mo1—O1$^{\mathrm{xii}}$	83.22 (6)
O2—Pr1—O1$^{\mathrm{vi}}$	100.91 (3)	O1$^{\mathrm{xi}}$—Mo1—O1$^{\mathrm{xiii}}$	96.78 (6)
O1$^{\mathrm{ii}}$—Pr1—O1$^{\mathrm{vi}}$	116.506 (19)	O1$^{\mathrm{xii}}$—Mo1—O1$^{\mathrm{xiii}}$	180.0
O1$^{\mathrm{iii}}$—Pr1—O1$^{\mathrm{vi}}$	63.494 (19)	O1$^{\mathrm{xi}}$—Mo1—O1$^{\mathrm{xiv}}$	83.22 (6)
O1$^{\mathrm{iv}}$—Pr1—O1$^{\mathrm{vi}}$	116.506 (19)	O1$^{\mathrm{xii}}$—Mo1—O1$^{\mathrm{xiv}}$	96.78 (6)
O1$^{\mathrm{v}}$—Pr1—O1$^{\mathrm{vi}}$	63.494 (19)	O1$^{\mathrm{xiii}}$—Mo1—O1$^{\mathrm{xiv}}$	83.22 (6)
O2$^{\mathrm{i}}$—Pr1—O1$^{\mathrm{vii}}$	100.91 (3)	O1$^{\mathrm{xi}}$—Mo1—O1$^{\mathrm{xv}}$	96.78 (6)
O2—Pr1—O1$^{\mathrm{vii}}$	79.09 (3)	O1$^{\mathrm{xii}}$—Mo1—O1$^{\mathrm{xv}}$	83.22 (6)
O1$^{\mathrm{ii}}$—Pr1—O1$^{\mathrm{vii}}$	63.494 (19)	O1$^{\mathrm{xiii}}$—Mo1—O1$^{\mathrm{xv}}$	96.78 (6)
O1$^{\mathrm{iii}}$—Pr1—O1$^{\mathrm{vii}}$	116.506 (19)	O1$^{\mathrm{xiv}}$—Mo1—O1$^{\mathrm{xv}}$	180.0
O1$^{\mathrm{iv}}$—Pr1—O1$^{\mathrm{vii}}$	63.494 (19)	O1$^{\mathrm{xi}}$—Mo1—O1$^{\mathrm{xvi}}$	180.0
O1$^{\mathrm{v}}$—Pr1—O1$^{\mathrm{vii}}$	116.506 (19)	O1$^{\mathrm{xii}}$—Mo1—O1$^{\mathrm{xvi}}$	96.78 (6)
O1$^{\mathrm{vi}}$—Pr1—O1$^{\mathrm{vii}}$	180.00 (6)	O1$^{\mathrm{xiii}}$—Mo1—O1$^{\mathrm{xvi}}$	83.22 (6)
O2$^{\mathrm{i}}$—Pr1—Pr1$^{\mathrm{v}}$	144.7	O1$^{\mathrm{xiv}}$—Mo1—O1$^{\mathrm{xvi}}$	96.78 (6)
O2—Pr1—Pr1$^{\mathrm{v}}$	35.3	O1$^{\mathrm{xv}}$—Mo1—O1$^{\mathrm{xvi}}$	83.22 (6)
O1$^{\mathrm{ii}}$—Pr1—Pr1$^{\mathrm{v}}$	82.59 (3)	Sc1$^{\mathrm{xvii}}$—O1—Mo1$^{\mathrm{xvii}}$	0.0
O1$^{\mathrm{iii}}$—Pr1—Pr1$^{\mathrm{v}}$	97.41 (3)	Sc1$^{\mathrm{xvii}}$—O1—Sc1$^{\mathrm{xviii}}$	131.13 (9)
O1$^{\mathrm{iv}}$—Pr1—Pr1$^{\mathrm{v}}$	82.59 (3)	Mo1$^{\mathrm{xvii}}$—O1—Sc1$^{\mathrm{xviii}}$	131.13 (9)
O1$^{\mathrm{v}}$—Pr1—Pr1$^{\mathrm{v}}$	97.41 (3)	Sc1$^{\mathrm{xvii}}$—O1—Mo1$^{\mathrm{xviii}}$	131.13 (9)
O1$^{\mathrm{vi}}$—Pr1—Pr1$^{\mathrm{v}}$	136.17 (3)	Mo1$^{\mathrm{xvii}}$—O1—Mo1$^{\mathrm{xviii}}$	131.13 (9)
O1$^{\mathrm{vii}}$—Pr1—Pr1$^{\mathrm{v}}$	43.83 (3)	Sc1$^{\mathrm{xviii}}$—O1—Mo1$^{\mathrm{xviii}}$	0.0
O2$^{\mathrm{i}}$—Pr1—Pr1$^{\mathrm{viii}}$	144.7	Sc1$^{\mathrm{xvii}}$—O1—Pr1$^{\mathrm{v}}$	106.64 (2)
O2—Pr1—Pr1$^{\mathrm{viii}}$	35.3	Mo1$^{\mathrm{xvii}}$—O1—Pr1$^{\mathrm{v}}$	106.64 (2)
O1$^{\mathrm{ii}}$—Pr1—Pr1$^{\mathrm{viii}}$	136.17 (3)	Sc1$^{\mathrm{xviii}}$—O1—Pr1$^{\mathrm{v}}$	106.64 (2)
O1$^{\mathrm{iii}}$—Pr1—Pr1$^{\mathrm{viii}}$	43.83 (3)	Mo1$^{\mathrm{xviii}}$—O1—Pr1$^{\mathrm{v}}$	106.64 (2)
O1$^{\mathrm{iv}}$—Pr1—Pr1$^{\mathrm{viii}}$	82.59 (3)	Sc1$^{\mathrm{xvii}}$—O1—Pr1$^{\mathrm{viii}}$	106.64 (2)

O1^{v}—Pr1—Pr1^{viii}	97.41 (3)	Mo1^{xvii}—O1—Pr1^{viii}	106.64 (2)
O1^{vi}—Pr1—Pr1^{viii}	82.59 (3)	Sc1^{xviii}—O1—Pr1^{viii}	106.64 (2)
O1^{vii}—Pr1—Pr1^{viii}	97.41 (3)	Mo1^{xviii}—O1—Pr1^{viii}	106.64 (2)
Pr1^{v}—Pr1—Pr1^{viii}	60.0	Pr1^{v}—O1—Pr1^{viii}	92.34 (6)
O2^{i}—Pr1—Pr1^{ix}	35.3	Pr1—O2—Pr1^{viii}	109.5
O2—Pr1—Pr1^{ix}	144.7	Pr1—O2—Pr1^{v}	109.5
O1^{ii}—Pr1—Pr1^{ix}	97.41 (3)	Pr1^{viii}—O2—Pr1^{v}	109.5
O1^{iii}—Pr1—Pr1^{ix}	82.59 (3)	Pr1—O2—Pr1^{x}	109.5
O1^{iv}—Pr1—Pr1^{ix}	97.41 (3)	Pr1^{viii}—O2—Pr1^{x}	109.5
O1^{v}—Pr1—Pr1^{ix}	82.59 (3)	Pr1^{v}—O2—Pr1^{x}	109.5

Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) *z*−1/4, *x*−1/4, −*y*; (iii) −*z*+1/4, −*x*+1/4, *y*; (iv) *x*−1/4, *y*−1/4, −*z*; (v) −*x*+1/4, −*y*+1/4, *z*; (vi) −*y*, *z*−1/4, *x*−1/4; (vii) *y*, −*z*+1/4, −*x*+1/4; (viii) *y*+1/4, −*x*, *z*+1/4; (ix) −*x*−1/4, −*y*−1/4, *z*; (x) *x*, −*y*+1/4, −*z*+1/4; (xi) −*y*+1/2, −*z*+1/2, −*x*+1; (xii) *x*, *y*+1/2, *z*+1/2; (xiii) −*x*+1, −*y*+1/2, −*z*+1/2; (xiv) *z*+1/2, *x*, *y*+1/2; (xv) −*z*+1/2, −*x*+1, −*y*+1/2; (xvi) *y*+1/2, *z*+1/2, *x*; (xvii) *x*, −*y*+3/4, −*z*+3/4; (xviii) *x*, *y*−1/2, *z*−1/2.