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The pyrochlore-type molybdate $Pr_{1.37}Ca_{0.63}Mo_2O_7$

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ(Mo–O) = 0.001 Å; disorder in main residue; R factor = 0.027; wR factor = 0.086; data-to-parameter ratio = 22.2.

Praseodymium calcium dimolybdenum heptaoxide, $Pr_{1.37}Ca_{0.63}Mo_2O_7$, crystallizes in the cubic pyrochlore-type structure. In the crystal structure, MoO_6 octahedra are linked together by common corners, forming a three-dimensional $[Mo_2O_6]$ network. The Pr and Ca atoms and the remaining O atoms are located in the voids of the $[Mo_2O_6]$ network. The Pr and Ca atoms are distributed statistically over the same 16c crystallographic position with site-occupancy factors of 0.684 (3) and 0.316 (3), respectively. They are surrounded by eight O atoms forming a ditrigonal scalenohedron. All atoms lie on special positions. The (Pr, Ca) and Mo atoms are, respectively in the 16*c* and 16*d* positions with $\bar{3}m$ symmetry, and the O atoms in the 48*f* or 8*a* positions with *mm* or $\bar{4}3m$ site symmetry, respectively.

Related literature

For related literature, see: Hubert (1974); Subramanian *et al.* (1983); American Chemical Society (2007); Gougeon *et al.* (2003); Kerihuel & Gougeon (1995).

Experimental

Crystal data

$Pr_{1.37}Ca_{0.63}Mo_2O_7$ M_r = 522.18
Cubic, $Fd\bar{3}m$
a = 10.4329 (3) Å
V = 1135.57 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 16.45 mm^{-1}
T = 293 (2) K
0.16 × 0.14 × 0.12 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: analytical (de Meulenaer & Tompa, 1965)
T_{min} = 0.093, T_{max} = 0.125
771 measured reflections
266 independent reflections
167 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.086
S = 1.11
266 reflections
12 parameters
$\Delta\rho_{max}$ = 2.51 e Å^{-3}
$\Delta\rho_{min}$ = −1.55 e Å^{-3}

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 on the Nonius KappaCCD X-ray diffactometer system of 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: PK2092).

References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
American Chemical Society (2007). SciFinder Scholar. http://www.cas.org/SCIFINDER/SCHOLAR.
Brandenburg, K. (2001). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Duisenberg, A. J. M., Kroon-Batenburg, L. M. J. & Schreurs, A. M. M. (2003). *J. Appl. Cryst.* **36**, 220–229.
Gougeon, P., Gall, P., Halet, J.-F. & Gautier, R. (2003). *Acta Cryst.* B**59**, 472–478.
Hubert, Ph. H. (1974). *Bull. Soc. Chim. Fr.* **11**, 2385–2386.
Kerihuel, G. & Gougeon, P. (1995). *Acta Cryst.* C**51**, 1475–1478.
Meulenaer, J. de & Tompa, H. (1965). *Acta Cryst.* **19**, 1014–1018.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Subramanian, M. A., Aravamudan, G. & Subba Rao, G. V. (1983). *Prog. Solid State Chem.* **15**, 55–143.

supporting information

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The pyrochlore-type molybdate $Pr_{1.37}Ca_{0.63}Mo_2O_7$

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S1. Comment

An attempt to synthesize $PrCaMo_{16}O_{28}$, a compound with the $PrMo_8O_{14}$ type structure (Kerihuel & Gougeon, 1995), was unsuccessful, resulting in a multiphase product. However, the formation of the new compound, $Pr_{1.37}Ca_{0.63}Mo_2O_7$ was achieved. A survey of the literature related to the rare earth molybdates $R_2Mo_2O_7$ with the database SciFinder Scholar (American Chemical Society, 2007) shows that these compounds only form for the rare-earths from Nd to Lu. To our knowledge, no quaternary molybdate pyrochlore has thus far been reported.

S2. Experimental

Single crystals of $Pr_{1.37}Ca_{0.63}Mo_2O_7$ were prepared from a mixture of Pr_6O_{11} (Rhone Poulenc, 99.99%), $CaMoO_4$, MoO_3 (Cerac, 99.95%) and Mo (Plansee, 99.9999%) with the nominal composition $PrCaMo_{16}O_{28}$. Before use, Mo powder was reduced under a flow of H_2 gas at 1273 K for ten hours in order to eliminate any trace of oxygen. $CaMoO_4$ was prepared by heating a stoichiometric mixture of $CaCO_3$ and MoO_3 in an open porcelain crucible at 1073 K for 24 h. 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 a rate of 300 K/h up to 2223 K, and the temperature was held for 5 min., then cooled at 100 K/h to 1373 K and finally furnace cooled. The final product was multiphasic with $Pr_{1.37}Ca_{0.63}Mo_2O_7$ and $Pr_{1-x}Ca_xMo_{10}O_{16}$, isomorphous with the RMo_5O_8 compounds (R = La to Gd; Gougeon *et al.*, 2003), as predominant phases. The crystals thus obtained were of irregular shape.

S3. Refinement

The structure was solved by direct methods using *SIR97* (Altomare *et al.*, 1999). The second setting, with the origin at $\bar{3}$ m of the Fd3m space group, was chosen. Initial refinement with full occupancy for the Pr1 site resulted in an R factor of about 0.30. Refinement of the site-occupancy factor of the Pr1 atoms lowered the R factor to 0.0274 with an occupation factor of 0.74. 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 calcium in the crystals, we surmised that the deficiency observed on the Pr1 site resulted from the presence of calcium. Refinements taking into account an occupation of the deficient Pr1 site simultaneously by Pr and Ca atoms with no constraint on the site-occupancy factors of the Pr1 and Ca1 atoms led to an over-occupation of the 16 d position. Consequently, the sum of the site occupancy factors was constrained to unity, and the ADPs of the Pr1 and Ca1 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 full occupation of this position.

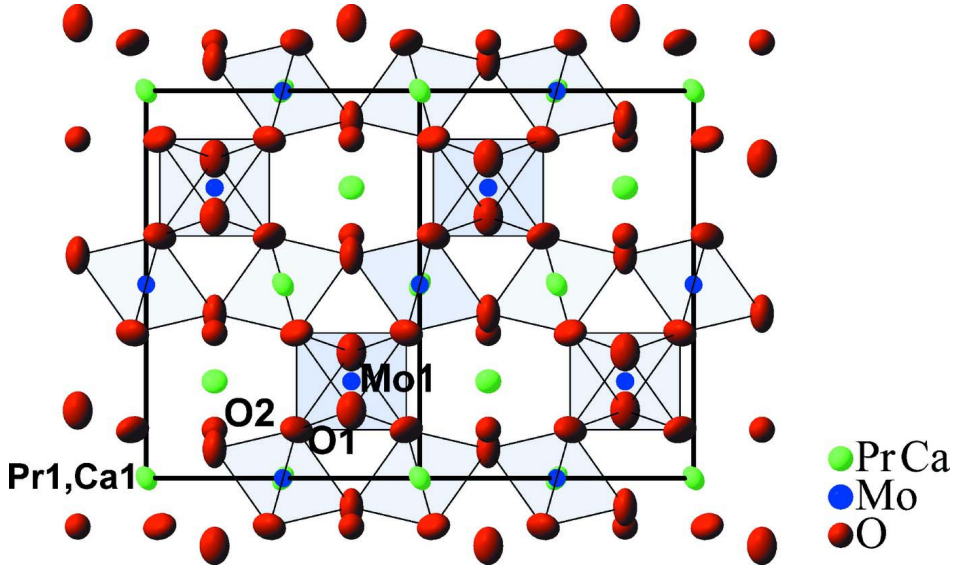

Figure 1

View of $Pr_{1.37}Ca_{0.63}Mo_2O_7$ along the [1$\bar{1}$0] direction. Displacement ellipsoids are drawn at the 97% probability level.

Praseodymium calcium dimolybdenum heptaoxide

Crystal data

$Pr_{1.37}Ca_{0.63}Mo_2O_7$
M_r = 522.18
Cubic, $Fd\bar{3}m$
Hall symbol: -F 4vw 2vw
a = 10.4329 (3) Å
V = 1135.57 (6) Å^3
Z = 8
F(000) = 1867.4
D_x = 6.109 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71070 Å
Cell parameters from 1172 reflections
θ = 3.4–45.3°
μ = 16.45 mm^{-1}
T = 293 K
Irregular block, black
0.16 × 0.14 × 0.12 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 (κ = 0) + additional ω scans
Absorption correction: analytical (de Meulenaer & Tompa, 1965)
T_{min} = 0.093, T_{max} = 0.125
771 measured reflections
266 independent reflections
167 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 45.3°, θ_{min} = 3.4°
h = 1→20
k = 0→14
l = 0→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.086
S = 1.12
266 reflections
12 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0207P)^2 + 4.885P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 2.51 e Å^{-3}

$\Delta\rho_{min} = -1.55$ e Å^{-3}

Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00256 (19)

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	0.00947 (18)	0.685 (3)
Ca1	0.0000	0.0000	0.0000	0.00947 (18)	0.315 (3)
Mo1	0.5000	0.5000	0.5000	0.00539 (19)	
O1	0.4247 (3)	0.1250	0.1250	0.0160 (5)	
O2	0.1250	0.1250	0.1250	0.0100 (8)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pr1	0.00947 (18)	0.00947 (18)	0.00947 (18)	−0.00154 (5)	−0.00154 (5)	−0.00154 (5)
Ca1	0.00947 (18)	0.00947 (18)	0.00947 (18)	−0.00154 (5)	−0.00154 (5)	−0.00154 (5)
Mo1	0.00539 (19)	0.00539 (19)	0.00539 (19)	−0.00013 (5)	−0.00013 (5)	−0.00013 (5)
O1	0.0239 (14)	0.0120 (6)	0.0120 (6)	0.000	0.000	−0.0026 (8)
O2	0.0100 (8)	0.0100 (8)	0.0100 (8)	0.000	0.000	0.000

Geometric parameters (Å, º)

Pr1—O2^{i}	2.2588	Mo1—Ca1^{xvii}	3.6886 (1)
Pr1—O2	2.2588	Mo1—Ca1^{xviii}	3.6886 (1)
Pr1—O1^{ii}	2.5930 (18)	Mo1—Ca1^{xix}	3.6886 (1)
Pr1—O1^{iii}	2.5930 (18)	Mo1—Ca1^{xx}	3.6886 (1)
Pr1—O1^{iv}	2.5930 (18)	Mo1—Ca1^{xxi}	3.6886 (1)
Pr1—O1^{v}	2.5930 (18)	Mo1—Ca1^{xxii}	3.6886 (1)
Pr1—O1^{vi}	2.5930 (18)	O1—Mo1^{xxiii}	2.0046 (10)
Pr1—O1^{vii}	2.5930 (18)	O1—Mo1^{xxiv}	2.0046 (10)
Pr1—Pr1^{vii}	3.6886 (1)	O1—Pr1^{vii}	2.5930 (18)
Pr1—Ca1^{viii}	3.6886 (1)	O1—Ca1^{vii}	2.5930 (18)
Pr1—Ca1^{ix}	3.6886 (1)	O1—Ca1^{xxv}	2.5930 (18)
Pr1—Ca1^{x}	3.6886 (1)	O1—Pr1^{xxv}	2.5930 (18)
Mo1—O1^{xi}	2.0046 (10)	O2—Ca1^{xxv}	2.2588
Mo1—O1^{xii}	2.0046 (10)	O2—Pr1^{vii}	2.2588
Mo1—O1^{xiii}	2.0046 (10)	O2—Pr1^{ix}	2.2588

Mo1—O1^{xiv}	2.0046 (10)	O2—Pr1^{xxv}	2.2588
Mo1—O1^{xv}	2.0046 (10)	O2—Ca1^{vii}	2.2588
Mo1—O1^{xvi}	2.0046 (10)	O2—Ca1^{ix}	2.2588
O2^{i}—Pr1—O2	180.0	O1^{xii}—Mo1—Ca1^{xvii}	42.51 (5)
O2^{i}—Pr1—O1^{ii}	79.93 (4)	O1^{xiii}—Mo1—Ca1^{xvii}	137.49 (5)
O2—Pr1—O1^{ii}	100.07 (4)	O1^{xiv}—Mo1—Ca1^{xvii}	90.0
O2^{i}—Pr1—O1^{iii}	79.93 (4)	O1^{xv}—Mo1—Ca1^{xvii}	137.49 (5)
O2—Pr1—O1^{iii}	100.07 (4)	O1^{xvi}—Mo1—Ca1^{xvii}	42.51 (5)
O1^{ii}—Pr1—O1^{iii}	117.01 (2)	O1^{xi}—Mo1—Ca1^{xviii}	42.51 (5)
O2^{i}—Pr1—O1^{iv}	79.93 (4)	O1^{xii}—Mo1—Ca1^{xviii}	90.0
O2—Pr1—O1^{iv}	100.07 (4)	O1^{xiii}—Mo1—Ca1^{xviii}	137.49 (5)
O1^{ii}—Pr1—O1^{iv}	117.01 (2)	O1^{xiv}—Mo1—Ca1^{xviii}	137.49 (5)
O1^{iii}—Pr1—O1^{iv}	117.01 (2)	O1^{xv}—Mo1—Ca1^{xviii}	90.0
O2^{i}—Pr1—O1^{v}	100.07 (4)	O1^{xvi}—Mo1—Ca1^{xviii}	42.51 (5)
O2—Pr1—O1^{v}	79.93 (4)	Ca1^{xvii}—Mo1—Ca1^{xviii}	60.0
O1^{ii}—Pr1—O1^{v}	180.00 (8)	O1^{xi}—Mo1—Ca1^{xix}	42.51 (5)
O1^{iii}—Pr1—O1^{v}	62.99 (2)	O1^{xii}—Mo1—Ca1^{xix}	137.49 (5)
O1^{iv}—Pr1—O1^{v}	62.99 (2)	O1^{xiii}—Mo1—Ca1^{xix}	90.0
O2^{i}—Pr1—O1^{vi}	100.07 (4)	O1^{xiv}—Mo1—Ca1^{xix}	137.49 (5)
O2—Pr1—O1^{vi}	79.93 (4)	O1^{xv}—Mo1—Ca1^{xix}	42.51 (5)
O1^{ii}—Pr1—O1^{vi}	62.99 (2)	O1^{xvi}—Mo1—Ca1^{xix}	90.0
O1^{iii}—Pr1—O1^{vi}	180.00 (8)	Ca1^{xvii}—Mo1—Ca1^{xix}	120.0
O1^{iv}—Pr1—O1^{vi}	62.99 (2)	Ca1^{xviii}—Mo1—Ca1^{xix}	60.0
O1^{v}—Pr1—O1^{vi}	117.01 (2)	O1^{xi}—Mo1—Ca1^{xx}	137.49 (5)
O2^{i}—Pr1—O1^{vii}	100.07 (4)	O1^{xii}—Mo1—Ca1^{xx}	90.0
O2—Pr1—O1^{vii}	79.93 (4)	O1^{xiii}—Mo1—Ca1^{xx}	42.51 (5)
O1^{ii}—Pr1—O1^{vii}	62.99 (2)	O1^{xiv}—Mo1—Ca1^{xx}	42.51 (5)
O1^{iii}—Pr1—O1^{vii}	62.99 (2)	O1^{xv}—Mo1—Ca1^{xx}	90.0
O1^{iv}—Pr1—O1^{vii}	180.00 (8)	O1^{xvi}—Mo1—Ca1^{xx}	137.49 (5)
O1^{v}—Pr1—O1^{vii}	117.01 (2)	Ca1^{xvii}—Mo1—Ca1^{xx}	120.0
O1^{vi}—Pr1—O1^{vii}	117.01 (2)	Ca1^{xviii}—Mo1—Ca1^{xx}	180.0
O2^{i}—Pr1—Pr1^{vii}	144.7	Ca1^{xix}—Mo1—Ca1^{xx}	120.0
O2—Pr1—Pr1^{vii}	35.3	O1^{xi}—Mo1—Ca1^{xxi}	90.0
O1^{ii}—Pr1—Pr1^{vii}	135.34 (4)	O1^{xii}—Mo1—Ca1^{xxi}	137.49 (5)
O1^{iii}—Pr1—Pr1^{vii}	81.87 (4)	O1^{xiii}—Mo1—Ca1^{xxi}	42.51 (5)
O1^{iv}—Pr1—Pr1^{vii}	81.87 (4)	O1^{xiv}—Mo1—Ca1^{xxi}	90.0
O1^{v}—Pr1—Pr1^{vii}	44.66 (4)	O1^{xv}—Mo1—Ca1^{xxi}	42.51 (5)
O1^{vi}—Pr1—Pr1^{vii}	98.13 (4)	O1^{xvi}—Mo1—Ca1^{xxi}	137.49 (5)
O1^{vii}—Pr1—Pr1^{vii}	98.13 (4)	Ca1^{xvii}—Mo1—Ca1^{xxi}	180.0
O2^{i}—Pr1—Ca1^{viii}	35.3	Ca1^{xviii}—Mo1—Ca1^{xxi}	120.0
O2—Pr1—Ca1^{viii}	144.7	Ca1^{xix}—Mo1—Ca1^{xxi}	60.0
O1^{ii}—Pr1—Ca1^{viii}	44.66 (4)	Ca1^{xx}—Mo1—Ca1^{xxi}	60.0
O1^{iii}—Pr1—Ca1^{viii}	98.13 (4)	O1^{xi}—Mo1—Ca1^{xxii}	137.49 (5)
O1^{iv}—Pr1—Ca1^{viii}	98.13 (4)	O1^{xii}—Mo1—Ca1^{xxii}	42.51 (5)
O1^{v}—Pr1—Ca1^{viii}	135.34 (4)	O1^{xiii}—Mo1—Ca1^{xxii}	90.0
O1^{vi}—Pr1—Ca1^{viii}	81.87 (4)	O1^{xiv}—Mo1—Ca1^{xxii}	42.51 (5)
O1^{vii}—Pr1—Ca1^{viii}	81.87 (4)	O1^{xv}—Mo1—Ca1^{xxii}	137.49 (5)

Pr1^{vii}—Pr1—Ca1^{viii}	180.0	O1^{xvi}—Mo1—Ca1^{xxii}	90.0
O2^{i}—Pr1—Ca1^{ix}	144.7	Ca1^{xvii}—Mo1—Ca1^{xxii}	60.0
O2—Pr1—Ca1^{ix}	35.3	Ca1^{xviii}—Mo1—Ca1^{xxii}	120.0
O1^{ii}—Pr1—Ca1^{ix}	81.87 (4)	Ca1^{xix}—Mo1—Ca1^{xxii}	180.0
O1^{iii}—Pr1—Ca1^{ix}	81.87 (4)	Ca1^{xx}—Mo1—Ca1^{xxii}	60.0
O1^{iv}—Pr1—Ca1^{ix}	135.34 (4)	Ca1^{xxi}—Mo1—Ca1^{xxii}	120.0
O1^{v}—Pr1—Ca1^{ix}	98.13 (4)	Mo1^{xxiii}—O1—Mo1^{xxiv}	133.86 (14)
O1^{vi}—Pr1—Ca1^{ix}	98.13 (4)	Mo1^{xxiii}—O1—Pr1^{vii}	105.99 (3)
O1^{vii}—Pr1—Ca1^{ix}	44.66 (4)	Mo1^{xxiv}—O1—Pr1^{vii}	105.99 (3)
Pr1^{vii}—Pr1—Ca1^{ix}	60.0	Mo1^{xxiii}—O1—Ca1^{vii}	105.99 (3)
Ca1^{viii}—Pr1—Ca1^{ix}	120.0	Mo1^{xxiv}—O1—Ca1^{vii}	105.99 (3)
O2^{i}—Pr1—Ca1^{x}	35.3	Mo1^{xxiii}—O1—Ca1^{xxv}	105.99 (3)
O2—Pr1—Ca1^{x}	144.7	Mo1^{xxiv}—O1—Ca1^{xxv}	105.99 (3)
O1^{ii}—Pr1—Ca1^{x}	98.13 (4)	Pr1^{vii}—O1—Ca1^{xxv}	90.68 (8)
O1^{iii}—Pr1—Ca1^{x}	98.13 (4)	Ca1^{vii}—O1—Ca1^{xxv}	90.68 (8)
O1^{iv}—Pr1—Ca1^{x}	44.66 (4)	Mo1^{xxiii}—O1—Pr1^{xxv}	105.99 (3)
O1^{v}—Pr1—Ca1^{x}	81.87 (4)	Mo1^{xxiv}—O1—Pr1^{xxv}	105.99 (3)
O1^{vi}—Pr1—Ca1^{x}	81.87 (4)	Pr1^{vii}—O1—Pr1^{xxv}	90.68 (8)
O1^{vii}—Pr1—Ca1^{x}	135.34 (4)	Ca1^{vii}—O1—Pr1^{xxv}	90.68 (8)
Pr1^{vii}—Pr1—Ca1^{x}	120.0	Pr1—O2—Ca1^{xxv}	109.5
Ca1^{viii}—Pr1—Ca1^{x}	60.0	Pr1—O2—Pr1^{vii}	109.5
Ca1^{ix}—Pr1—Ca1^{x}	180.0	Ca1^{xxv}—O2—Pr1^{vii}	109.5
O1^{xi}—Mo1—O1^{xii}	94.97 (9)	Pr1—O2—Pr1^{ix}	109.5
O1^{xi}—Mo1—O1^{xiii}	94.97 (9)	Ca1^{xxv}—O2—Pr1^{ix}	109.5
O1^{xii}—Mo1—O1^{xiii}	94.97 (9)	Pr1^{vii}—O2—Pr1^{ix}	109.5
O1^{xi}—Mo1—O1^{xiv}	180.0	Pr1—O2—Pr1^{xxv}	109.5
O1^{xii}—Mo1—O1^{xiv}	85.03 (9)	Pr1^{vii}—O2—Pr1^{xxv}	109.5
O1^{xiii}—Mo1—O1^{xiv}	85.03 (9)	Pr1^{ix}—O2—Pr1^{xxv}	109.5
O1^{xi}—Mo1—O1^{xv}	85.03 (9)	Pr1—O2—Ca1^{vii}	109.5
O1^{xii}—Mo1—O1^{xv}	180.0	Ca1^{xxv}—O2—Ca1^{vii}	109.5
O1^{xiii}—Mo1—O1^{xv}	85.03 (9)	Pr1^{ix}—O2—Ca1^{vii}	109.5
O1^{xiv}—Mo1—O1^{xv}	94.97 (9)	Pr1^{xxv}—O2—Ca1^{vii}	109.5
O1^{xi}—Mo1—O1^{xvi}	85.03 (9)	Pr1—O2—Ca1^{ix}	109.5
O1^{xii}—Mo1—O1^{xvi}	85.03 (9)	Ca1^{xxv}—O2—Ca1^{ix}	109.5
O1^{xiii}—Mo1—O1^{xvi}	180.0	Pr1^{vii}—O2—Ca1^{ix}	109.5
O1^{xiv}—Mo1—O1^{xvi}	94.97 (9)	Pr1^{xxv}—O2—Ca1^{ix}	109.5
O1^{xv}—Mo1—O1^{xvi}	94.97 (9)	Ca1^{vii}—O2—Ca1^{ix}	109.5
O1^{xi}—Mo1—Ca1^{xvii}	90.0		

Symmetry codes: (i) $-x, -y, -z$; (ii) $-y, z-1/4, x-1/4$; (iii) $z-1/4, x-1/4, -y$; (iv) $x-1/4, y-1/4, -z$; (v) $y, -z+1/4, -x+1/4$; (vi) $-z+1/4, -x+1/4, y$; (vii) $-x+1/4, -y+1/4, z$; (viii) $-x-1/4, -y-1/4, z$; (ix) $x, -y+1/4, -z+1/4$; (x) $x, -y-1/4, -z-1/4$; (xi) $-y+1/2, -z+1/2, -x+1$; (xii) $-z+1/2, -x+1, -y+1/2$; (xiii) $-x+1, -y+1/2, -z+1/2$; (xiv) $y+1/2, z+1/2, x$; (xv) $z+1/2, x, y+1/2$; (xvi) $x, y+1/2, z+1/2$; (xvii) $-x+1/4, -y+3/4, z+1/2$; (xviii) $y+1/4, -x+1/2, z+3/4$; (xix) $x+1/2, -y+1/4, -z+3/4$; (xx) $y+3/4, -x+1/2, z+1/4$; (xxi) $-x+3/4, -y+1/4, z+1/2$; (xxii) $x+1/2, -y+3/4, -z+1/4$; (xxiii) $x, -y+3/4, -z+3/4$; (xxiv) $x, y-1/2, z-1/2$; (xxv) $y+1/4, -x, z+1/4$.