

LiCe₉Mo₁₆O₃₅

Patrick Gougeon* and Philippe Gall

Sciences Chimiques de Rennes, UMR CNRS No. 6226, Université de Rennes 1 - INSA
Rennes, Avenue du Général Leclerc, 35042 Rennes CEDEX, France
Correspondence e-mail: Patrick.Gougeon@univ-rennes1.fr

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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{Ce}-\text{O}) = 0.002$ Å;
R factor = 0.016; wR factor = 0.033; data-to-parameter ratio = 22.2.

The structure of lithium nonacerium hexadecamolybdenum pentatridecaoxide, LiCe₉Mo₁₆O₃₅, is isotopic with LiNd₉Mo₁₆O₃₅ [Gougeon Gall, Cuny, Gautier, Le Polles, Delevoye & Trebosc (2011). *Chem. Eur. J.* **17**, 13806–13813]. It is characterized by Mo₁₆O₂₆ⁱO₁₀^a units (where $i = \text{inner}$ and $a = \text{apical}$) containing Mo₁₆ clusters that share some of their O atoms to form infinite molybdenum cluster chains running parallel to the b axis and separated by Li⁺ and Ce³⁺ cations. The Mo₁₆ cluster units are centred at Wyckoff positions $2c$ and have point-group symmetry $2/m$. The Li⁺ atom, in a flattened octahedron of O atoms, is in a $2a$ Wyckoff position with $2/m$ symmetry. The Ce³⁺ cations have coordination numbers to the O atoms of 6, 9 or 10. Two Ce, two Mo and five O atoms lie on sites with m symmetry (Wyckoff site $4i$), and one Ce and one O atom on sites with $2/m$ symmetry (Wyckoff sites $2b$ and $2d$, respectively).

Related literature

For the crystal structure of the LiNd₉Mo₁₆O₃₅ compound, see: Gougeon *et al.* (2011). For details of the i - and a -type ligand notation, see: Schäfer & von Schnering (1964). For compounds containing Mo₁₀ clusters, see: Hibble *et al.* (1988); Dronskowski & Simon (1989); Gougeon *et al.* (1990, 1991, 2003, 2007); Dronskowski *et al.* (1991); Gall *et al.* (1993, 1995, 1999); Gall & Gougeon (1993, 1994*a,b*, 1998); Gougeon & Gall (2002). The oxidation states of the Mo, Ce and Li atoms were estimated using the data given by Brown & Wu (1976).

Experimental

Crystal data

LiCe ₉ Mo ₁₆ O ₃₅	$V = 1516.46$ (3) Å ³
$M_r = 3363.06$	$Z = 2$
Monoclinic, $C2/m$	Mo $K\alpha$ radiation
$a = 18.3000$ (2) Å	$\mu = 19.66$ mm ⁻¹
$b = 8.6326$ (1) Å	$T = 293$ K
$c = 9.8172$ (1) Å	$0.15 \times 0.12 \times 0.06$ mm
$\beta = 102.0953$ (7)°	

Data collection

Nonius KappaCCD diffractometer	21270 measured reflections
Absorption correction: multi-scan (PLATON; Spek, 2009)	3511 independent reflections
$T_{\min} = 0.190$, $T_{\max} = 0.418$	3383 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.016$	158 parameters
$wR(F^2) = 0.033$	$\Delta\rho_{\max} = 1.13$ e Å ⁻³
$S = 1.29$	$\Delta\rho_{\min} = -1.33$ e Å ⁻³
3511 reflections	

Table 1

Selected bond lengths (Å).

Li—O7	1.861 (3)	Mo1—O2	1.9759 (16)
Li—O10	2.4135 (16)	Mo1—O2 ^v	1.9759 (16)
Ce1—O3 ⁱ	2.3603 (16)	Mo1—O4 ^v	2.0332 (17)
Ce1—O12	2.3916 (16)	Mo1—O4	2.0332 (17)
Ce1—O1 ⁱⁱ	2.4055 (5)	Mo1—O1	2.045 (3)
Ce1—O8	2.4159 (16)	Mo1—Mo3	2.7003 (3)
Ce1—O10 ⁱⁱⁱ	2.5499 (19)	Mo1—Mo2	2.7129 (3)
Ce1—O4 ⁱⁱ	2.7161 (18)	Mo2—O3 ^{ix}	2.0277 (16)
Ce1—O2 ⁱⁱ	2.874 (2)	Mo2—O2	2.077 (2)
Ce1—O11	2.8865 (16)	Mo2—O7	2.0773 (16)
Ce1—O7 ^{iv}	2.8959 (17)	Mo2—O5	2.0985 (16)
Ce2—O12	2.337 (3)	Mo2—O10	2.0997 (19)
Ce2—O3 ^v	2.3829 (19)	Mo2—Mo4 ⁱⁱ	2.6412 (3)
Ce2—O3	2.3829 (19)	Mo2—Mo5 ^{xiii}	2.7691 (3)
Ce2—O1 ^{iv}	2.622 (2)	Mo2—Mo3	2.7739 (2)
Ce2—O2 ^{vi}	2.6352 (17)	Mo2—Mo2 ^v	2.7851 (4)
Ce2—O2 ^{iv}	2.6352 (17)	Mo3—O8	2.0315 (16)
Ce2—O5 ⁱⁱ	2.8054 (16)	Mo3—O5	2.0688 (16)
Ce2—O5 ^{vii}	2.8054 (16)	Mo3—O11	2.0795 (16)
Ce2—O2 ^{vii}	2.9625 (17)	Mo3—O4	2.0860 (19)
Ce2—O2 ⁱⁱ	2.9625 (17)	Mo3—Mo3 ^v	2.7338 (4)
Ce3—O8	2.3670 (17)	Mo3—Mo4 ⁱⁱ	2.7375 (3)
Ce3—O8 ^{viii}	2.3670 (17)	Mo3—Mo5	2.7405 (3)
Ce3—O4 ⁱⁱ	2.5309 (18)	Mo3—Mo4 ^{xiii}	2.8391 (3)
Ce3—O4 ^{ix}	2.5309 (18)	Mo3—Mo5 ^{xii}	2.8928 (3)
Ce3—O5 ^{viii}	2.7980 (17)	Mo4—O6	2.0145 (14)
Ce3—O5	2.7980 (17)	Mo4—O8 ^{xiv}	2.0758 (19)
Ce3—O4 ^{vii}	3.0001 (17)	Mo4—O5 ⁱⁱ	2.0797 (19)
Ce3—O4	3.0001 (17)	Mo4—O10 ⁱⁱ	2.0857 (16)
Ce3—O11 ⁱⁱ	3.089 (3)	Mo4—O9	2.1141 (2)
Ce4—O6 ^x	2.280 (2)	Mo4—Mo4 ^{xv}	2.7958 (3)
Ce4—O6	2.280 (2)	Mo5—O11	2.078 (3)
Ce4—O3	2.4244 (19)	Mo5—O10 ^{xii}	2.0950 (16)
Ce4—O3 ^x	2.4244 (19)	Mo5—O10 ⁱⁱⁱ	2.0950 (16)
Ce4—O3 ^v	2.4244 (19)	Mo5—Mo5 ^{xii}	2.9030 (5)
Ce4—O3 ^{xi}	2.4244 (19)		

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

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 (Bergerhoff, 1996); software used to prepare material for publication: SHELXL97.

Intensity data were collected on the Nonius KappaCCD X-ray diffractometer system of the 'Centre de diffractométrie de l'Université de Rennes I'.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RU2029).

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.
- Bergerhoff, G. (1996). *DIAMOND*. University of Bonn, Germany.
- Brown, I. D. & Wu, K. K. (1976). *Acta Cryst.* **B32**, 1957–1959.
- Dronskowski, R. & Simon, A. (1989). *Angew. Chem. Int. Ed. Engl.* **28**, 758–760.
- Dronskowski, R., Simon, A. & Mertin, W. (1991). *Z. Anorg. Allg. Chem.* **602**, 49–63.
- Duisenberg, A. J. M., Kroon-Batenburg, L. M. J. & Schreurs, A. M. M. (2003). *J. Appl. Cryst.* **36**, 220–229.
- Gall, P., Gautier, R., Halet, J.-F. & Gougeon, P. (1999). *Inorg. Chem.* **38**, 4455–4461.
- Gall, P. & Gougeon, P. (1993). *Acta Cryst.* **C49**, 659–663.
- Gall, P. & Gougeon, P. (1994a). *Acta Cryst.* **C50**, 7–9.
- Gall, P. & Gougeon, P. (1994b). *Acta Cryst.* **C50**, 1183–1185.
- Gall, P. & Gougeon, P. (1998). *Z. Kristallogr. New Cryst. Struct.* **213**, 1–2.
- Gall, P., Gougeon, P., Greenblatt, M., Jones, E. B., Mc Carroll, W. H. & Ramanujachary, K. V. (1995). *Croat. Chem. Acta*, **68**, 849–860.
- Gall, P., Noel, H. & Gougeon, P. (1993). *Mater. Res. Bull.* **28**, 1225–1231.
- Gougeon, P. & Gall, P. (2002). *Acta Cryst.* **E58**, i65–i67.
- Gougeon, P., Gall, P., Cuny, J., Gautier, R., Le Polles, L., Delevoye, L. & Trebosc, J. (2011). *Chem. Eur. J.* **17**, 13806–13813.
- Gougeon, P., Gall, P., Halet, J.-F. & Gautier, R. (2003). *Acta Cryst.* **B59**, 472–478.
- Gougeon, P., Gall, P. & McCarroll, W. H. (2007). *Acta Cryst.* **E63**, i119–i121.
- Gougeon, P., Gall, P. & Sergent, M. (1991). *Acta Cryst.* **C47**, 421–423.
- Gougeon, P., Potel, M. & Sergent, M. (1990). *Acta Cryst.* **C46**, 1188–1190.
- Hibble, S. J., Cheetham, A. K., Bogle, A. R. L., Wakerley, H. R. & Cox, D. E. (1988). *J. Am. Chem. Soc.* **110**, 3295–3296.
- Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
- Schäfer, H. & von Schnering, H. G. (1964). *Angew. Chem.* **76**, 833–845.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

supplementary materials

Acta Cryst. (2012). E68, i21–i22 [doi:10.1107/S160053681200801X]

LiCe₉Mo₁₆O₃₅**Patrick Gougeon and Philippe Gall****Comment**

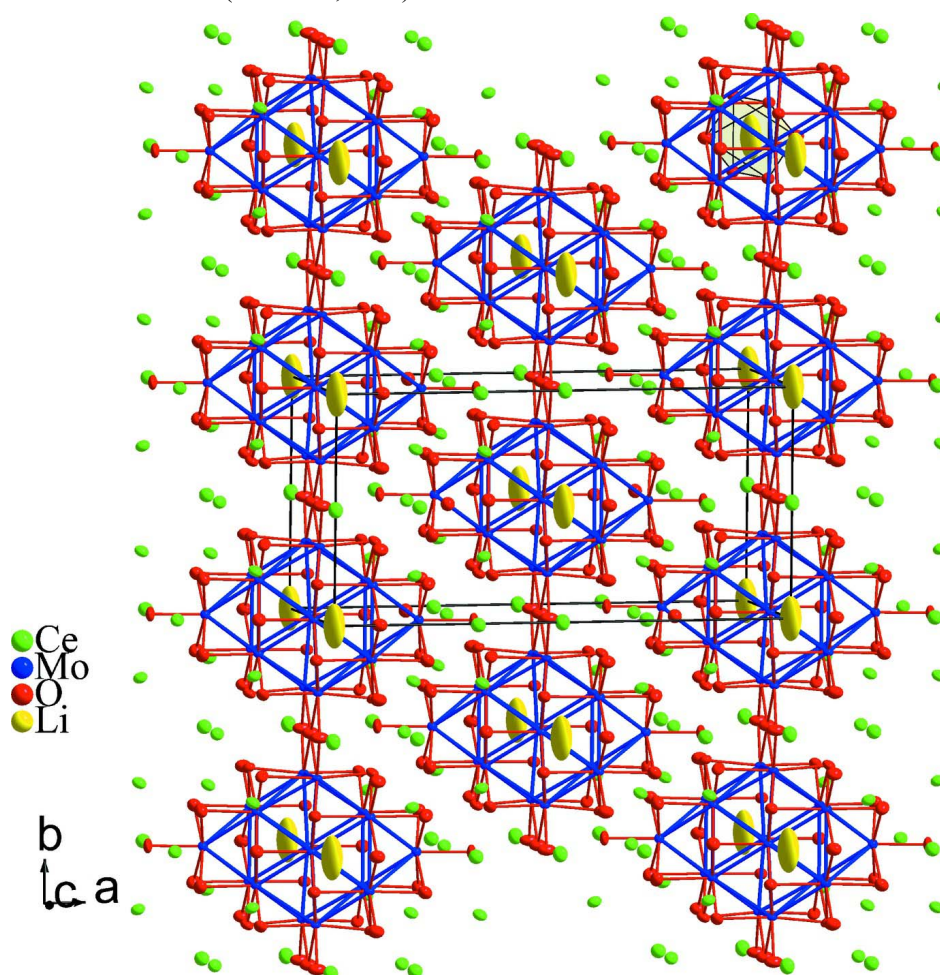
LiCe₉Mo₁₆O₃₅ is isotopic with the LiNd₉Mo₁₆O₃₅ (Gougeon *et al.*, 2011) structure type. The crystal structure (Fig. 1) is based on Mo₁₆O₂₆ⁱO₁₀^a cluster units (Fig. 2) sharing two Oⁱ or four O^a ligands (for details of the i- and a-type ligand notation, see Schäfer & von Schnering (1964)) to form infinite molybdenum cluster chains running parallel to the b axis. The Mo₁₆ core of the Mo₁₆O₂₆ⁱO₁₀^a unit can be seen as resulting of the fusion of two bioctahedral Mo₁₀ clusters through the sharing of three edges per Mo₁₀ cluster. The Mo₁₀ cluster results itself from metal edge-sharing of two Mo₆ octahedra and was first observed forming infinite chains in the MMo₅O₈ (M = Ca, Sr, Sn, Pb, La–Gd) compounds (Hibble *et al.*, 1988; Dronskowski & Simon, 1989; Gougeon *et al.*, 1990, 1991, 2003, 2007; Dronskowski *et al.*, 1991; Gall *et al.*, 1993, 1995; Gall & Gougeon, 1994*a,b*; Gougeon & Gall, 2002) and more later as isolated cluster in the R₁₆Mo₂₁O₅₆ (R = La, Ce, Pr, and Nd) series (Gall & Gougeon, 1993, 1998; Gall *et al.*, 1999). The Mo₁₆O₂₆ⁱO₁₀^a cluster is centered on 2b position and thus has point-group symmetry 2/m. The Mo—Mo distances lie between 2.6412 (3) and 2.9030 (5) Å compared to 2.725 Å in the Mo metal and the Mo—O distances between 1.9759 (16) and 2.11407 (18) Å. The Mo—O chains, which have the connectivity formula Mo₁₆O₂₄ⁱO₂₂ⁱ⁻ⁱO₆^aO₄₂^{a-a} are separated by the Li⁺ and Ce³⁺ cations. The Li⁺ cation occupies a highly tetragonally distorted octahedral site of O atoms of symmetry 2/m centered at the origin of the unit cell. The Li—O distances in the equatorial plane are 2.4135 (16) Å [Li—O10] and the two trans Li—O7 bonds are 1.861 (3) Å. The coordination numbers of the Ce ions are 6, 9 or 10 with Ce—O distances spreading over a wide range [2.280 (2) to 3.089 (3) Å]. By using the bond-length–bond-strength formula (Brown & Wu, 1976) for the Mo—O, Ce—O and Li—O bonds ($s = [d(\text{Mo—O})/1.882]^{-6}$, $s = [d(\text{Ce—O})/2.160]^{-6.5}$ and $s = [d(\text{Li—O})/1.378]^{-4.065}$), an assignment of oxidation states to the Mo, Ce and Li atoms was made. The valence of each independent Mo atom was determined as follows: Mo(1) +3.36, Mo(2) +2.78, Mo(3) +2.29, Mo(4) + 2.81, and Mo(5) + 1.6. From these values, we could deduce an average Mo oxidation state of + 2.60 which is close to that based on the stoichiometry, + 2.625, when considering all the Ce ions as trivalent and the Li ion monovalent. Bond-valence sums of the Ce—O bonds was +3.08, +3.11, +3.09, and +3.30 for Ce1, Ce2, Ce3, and Ce4, respectively. For the Li atom, a value of +1.00 was found. It is interesting to note that for the total valence sum $\Sigma(\text{Mo—O}) + \Sigma(\text{Ce—O}) + \Sigma(\text{Li—O})$, we obtained a value of 70.5 per formula unit, which is in very good agreement with the theoretical value of 70 based on the 35 O atoms.

Experimental

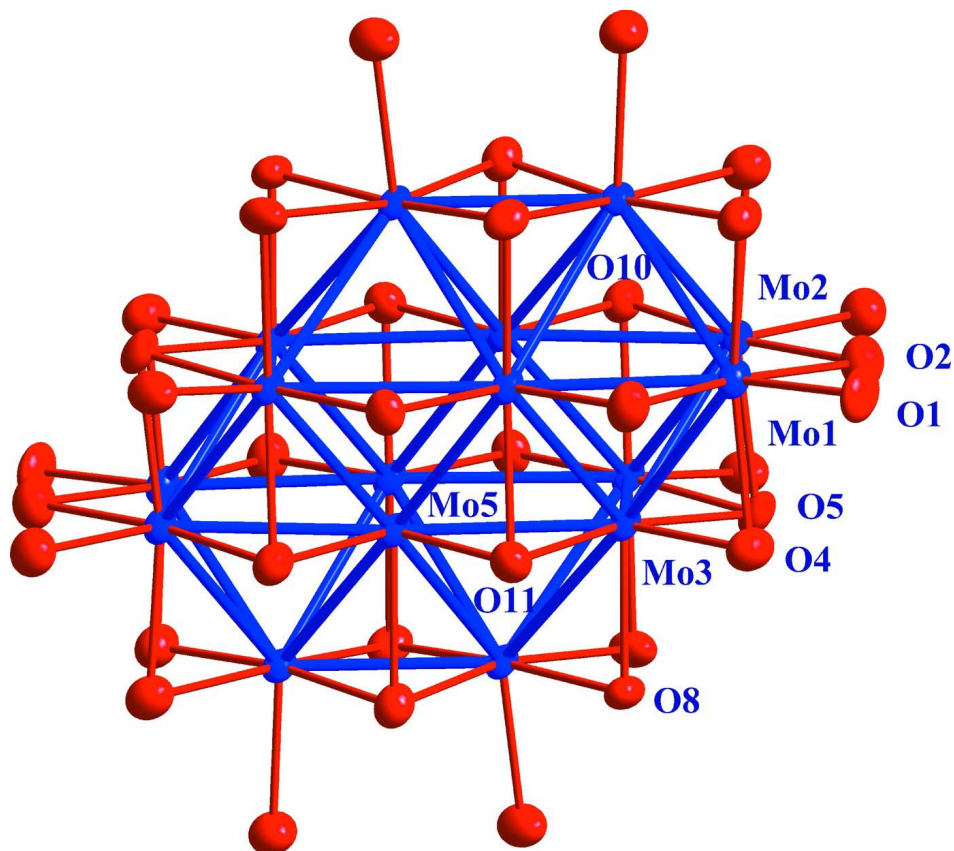
Single crystals of LiCe₉Mo₁₆O₃₅ were obtained from a mixture of Li₂MoO₄, CeO₂, MoO₃, and Mo with the nominal composition Li₂CeMo₆O₁₂. Before use, Mo powder was reduced under H₂ flowing gas at 1273 K during 10 h in order to eliminate any trace of oxygen. The initial mixture (ca 4 g) was cold pressed and 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 2000 K, temperature which was held for 18 h, then cooled at 100 K/h down to 1373 K and finally furnace cooled.

Computing details

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *COLLECT* (Nonius, 1998); 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* (Bergerhoff, 1996); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

**Figure 1**

View of the crystal structure of $\text{LiCe}_9\text{Mo}_{16}\text{O}_{35}$ (Displacement ellipsoids are drawn at the 97% probability level).


Figure 2

Plot showing the atom-numbering scheme of the $\text{Mo}_{16}\text{O}_{26}\text{O}_{10}^a$ units. Displacement ellipsoids are drawn at the 97% probability level.

lithium nonacerium hexadecamolybdenum pentatridecaoxide

Crystal data

$\text{LiCe}_9\text{Mo}_{16}\text{O}_{35}$

$M_r = 3363.06$

Monoclinic, $C2/m$

$a = 18.3000$ (2) Å

$b = 8.6326$ (1) Å

$c = 9.8172$ (1) Å

$\beta = 102.0953$ (7)°

$V = 1516.46$ (3) Å³

$Z = 2$

$F(000) = 2954$

$D_x = 7.365$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å

Cell parameters from 21270 reflections

$\theta = 0.9\text{--}35.0^\circ$

$\mu = 19.66$ mm⁻¹

$T = 293$ K

Multi-faceted fragment, black

$0.15 \times 0.12 \times 0.06$ mm

Data collection

Nonius KappaCCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ scans ($\kappa = 0$) and additional ω scans

Absorption correction: multi-scan

(*PLATON*; Spek, 2009)

$T_{\min} = 0.190$, $T_{\max} = 0.418$

21270 measured reflections

3511 independent reflections

3383 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\max} = 35.0^\circ$, $\theta_{\min} = 3.5^\circ$

$h = -26 \rightarrow 29$

$k = -13 \rightarrow 13$

$l = -15 \rightarrow 10$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.016$

$wR(F^2) = 0.033$

$S = 1.29$

3511 reflections

158 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

$w = 1/[\sigma^2(F_o^2) + (0.P)^2 + 6.2844P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.004$

$\Delta\rho_{\max} = 1.13 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -1.33 \text{ e } \text{\AA}^{-3}$

Extinction correction: *SHELXL97* (Sheldrick,
2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.00166 (3)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Li	-0.5000	-0.5000	1.0000	0.038 (4)
Ce1	-0.345982 (8)	-0.273486 (15)	0.201055 (12)	0.00556 (3)
Ce2	-0.191529 (11)	-0.5000	0.071345 (17)	0.00625 (4)
Ce3	-0.298077 (11)	0.0000	0.534154 (17)	0.00582 (4)
Ce4	0.0000	-0.5000	0.0000	0.00664 (5)
Mo1	-0.290730 (16)	-0.5000	0.74596 (2)	0.00368 (5)
Mo2	-0.401044 (12)	-0.33869 (2)	0.828637 (17)	0.00338 (4)
Mo3	-0.388827 (11)	-0.34166 (2)	0.551746 (17)	0.00319 (4)
Mo4	-0.000772 (11)	-0.31629 (2)	0.357312 (17)	0.00311 (4)
Mo5	-0.490663 (16)	-0.5000	0.35678 (2)	0.00316 (5)
O1	-0.17701 (15)	-0.5000	0.8112 (2)	0.0070 (4)
O2	-0.28523 (11)	-0.3349 (2)	0.88711 (16)	0.0064 (3)
O3	-0.10014 (11)	-0.6759 (2)	0.02198 (16)	0.0062 (3)
O4	-0.27246 (11)	-0.3355 (2)	0.60863 (16)	0.0059 (3)
O5	-0.38352 (11)	-0.1616 (2)	0.69257 (16)	0.0051 (3)
O6	0.00695 (16)	-0.5000	0.2346 (2)	0.0066 (4)
O7	-0.40015 (16)	-0.5000	0.9860 (2)	0.0067 (4)
O8	-0.38482 (10)	-0.1769 (2)	0.40574 (15)	0.0050 (3)
O9	0.0000	-0.5000	0.5000	0.0059 (6)
O10	-0.51815 (10)	-0.33622 (19)	0.79643 (16)	0.0050 (3)
O11	-0.37455 (15)	-0.5000	0.3998 (2)	0.0052 (4)
O12	-0.26903 (15)	-0.5000	0.2327 (2)	0.0063 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Li	0.007 (6)	0.070 (12)	0.037 (7)	0.000	0.005 (5)	0.000
Ce1	0.00563 (6)	0.00466 (5)	0.00630 (5)	0.00095 (4)	0.00106 (4)	0.00077 (3)
Ce2	0.00587 (9)	0.00703 (8)	0.00639 (6)	0.000	0.00251 (5)	0.000
Ce3	0.00568 (9)	0.00564 (7)	0.00553 (6)	0.000	-0.00025 (5)	0.000
Ce4	0.00575 (12)	0.00932 (11)	0.00530 (9)	0.000	0.00216 (7)	0.000
Mo1	0.00269 (12)	0.00349 (10)	0.00447 (9)	0.000	-0.00012 (7)	0.000
Mo2	0.00339 (9)	0.00276 (7)	0.00372 (6)	0.00000 (6)	0.00011 (5)	-0.00036 (5)
Mo3	0.00291 (9)	0.00265 (7)	0.00385 (6)	-0.00007 (6)	0.00036 (5)	0.00014 (5)
Mo4	0.00306 (9)	0.00221 (7)	0.00386 (6)	-0.00005 (6)	0.00029 (5)	-0.00010 (5)
Mo5	0.00309 (12)	0.00254 (10)	0.00372 (9)	0.000	0.00047 (7)	0.000
O1	0.0034 (11)	0.0067 (10)	0.0095 (9)	0.000	-0.0014 (7)	0.000
O2	0.0061 (8)	0.0056 (7)	0.0068 (6)	0.0004 (6)	-0.0004 (5)	-0.0021 (5)
O3	0.0073 (8)	0.0050 (7)	0.0063 (6)	0.0000 (6)	0.0010 (5)	0.0013 (5)
O4	0.0038 (8)	0.0062 (7)	0.0077 (6)	-0.0006 (6)	0.0010 (5)	0.0006 (5)
O5	0.0044 (8)	0.0043 (7)	0.0062 (6)	-0.0001 (6)	0.0006 (5)	0.0000 (5)
O6	0.0110 (12)	0.0039 (10)	0.0047 (8)	0.000	0.0013 (7)	0.000
O7	0.0089 (12)	0.0051 (10)	0.0058 (8)	0.000	0.0011 (7)	0.000
O8	0.0039 (8)	0.0051 (7)	0.0055 (6)	-0.0001 (6)	0.0000 (5)	0.0009 (5)
O9	0.0100 (17)	0.0036 (13)	0.0041 (11)	0.000	0.0014 (10)	0.000
O10	0.0037 (8)	0.0041 (7)	0.0073 (6)	-0.0001 (6)	0.0013 (5)	0.0000 (5)
O11	0.0046 (11)	0.0060 (10)	0.0053 (8)	0.000	0.0017 (7)	0.000
O12	0.0063 (12)	0.0063 (10)	0.0060 (8)	0.000	0.0002 (7)	0.000

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

Li—O7 ⁱ	1.861 (3)	Mo3—O11	2.0795 (16)
Li—O7	1.861 (3)	Mo3—O4	2.0860 (19)
Li—O10 ⁱⁱ	2.4135 (16)	Mo3—Mo3 ⁱⁱ	2.7338 (4)
Li—O10 ⁱⁱⁱ	2.4135 (16)	Mo3—Mo4 ^v	2.7375 (3)
Li—O10 ⁱ	2.4135 (16)	Mo3—Mo5	2.7405 (3)
Li—O10	2.4135 (16)	Mo3—Mo4 ^{xv}	2.8391 (3)
Ce1—O3 ^{iv}	2.3603 (16)	Mo3—Mo5 ^{xiv}	2.8928 (3)
Ce1—O12	2.3916 (16)	Mo4—O6	2.0145 (14)
Ce1—O1 ^v	2.4055 (5)	Mo4—O8 ^{xvi}	2.0758 (19)
Ce1—O8	2.4159 (16)	Mo4—O5 ^v	2.0797 (19)
Ce1—O10 ^{vi}	2.5499 (19)	Mo4—O10 ^v	2.0857 (16)
Ce1—O4 ^v	2.7161 (18)	Mo4—O9	2.1141 (2)
Ce1—O2 ^v	2.874 (2)	Mo4—Mo2 ^v	2.6412 (3)
Ce1—O11	2.8865 (16)	Mo4—Mo5 ^{xvii}	2.7367 (2)
Ce1—O7 ^{vii}	2.8959 (17)	Mo4—Mo3 ^v	2.7375 (3)
Ce2—O12	2.337 (3)	Mo4—Mo4 ^{xviii}	2.7958 (3)
Ce2—O3 ⁱⁱ	2.3829 (19)	Mo4—Mo3 ^{xvi}	2.8391 (3)
Ce2—O3	2.3829 (19)	Mo4—Mo4 ⁱⁱ	3.1718 (4)
Ce2—O1 ^{vii}	2.622 (2)	Mo5—O11	2.078 (3)
Ce2—O2 ^{viii}	2.6352 (17)	Mo5—O10 ^{xiv}	2.0950 (16)
Ce2—O2 ^{vii}	2.6352 (17)	Mo5—O10 ^{vi}	2.0950 (16)
Ce2—O5 ^v	2.8054 (16)	Mo5—Mo4 ^{xix}	2.7367 (2)

Ce2—O5 ^{ix}	2.8054 (16)	Mo5—Mo4 ^{xv}	2.7367 (2)
Ce2—O2 ^{ix}	2.9625 (17)	Mo5—Mo3 ⁱⁱ	2.7405 (3)
Ce2—O2 ^v	2.9625 (17)	Mo5—Mo2 ^{xiv}	2.7691 (3)
Ce3—O12 ^v	2.360 (2)	Mo5—Mo2 ^{vi}	2.7691 (3)
Ce3—O8	2.3670 (17)	Mo5—Mo3 ^{xiv}	2.8928 (3)
Ce3—O8 ^x	2.3670 (17)	Mo5—Mo3 ^{vi}	2.8928 (3)
Ce3—O4 ^v	2.5309 (18)	Mo5—Mo5 ^{xiv}	2.9030 (5)
Ce3—O4 ^{xi}	2.5309 (18)	O1—Ce1 ^v	2.4055 (5)
Ce3—O5 ^x	2.7980 (17)	O1—Ce1 ^{ix}	2.4055 (5)
Ce3—O5	2.7980 (17)	O1—Ce2 ^{xx}	2.622 (2)
Ce3—O4 ^x	3.0001 (17)	O1—Ce3 ^v	3.325 (2)
Ce3—O4	3.0001 (17)	O2—Ce2 ^{xx}	2.6352 (17)
Ce3—O11 ^v	3.089 (3)	O2—Ce1 ^v	2.874 (2)
Ce4—O6 ^{xii}	2.280 (2)	O2—Ce2 ^v	2.9625 (17)
Ce4—O6	2.280 (2)	O3—Mo2 ^{ix}	2.0277 (16)
Ce4—O3	2.4244 (19)	O3—Ce1 ^{xxi}	2.3603 (16)
Ce4—O3 ^{xii}	2.4244 (19)	O4—Ce3 ^v	2.5309 (18)
Ce4—O3 ⁱⁱ	2.4244 (19)	O4—Ce1 ^v	2.7161 (18)
Ce4—O3 ^{xiii}	2.4244 (19)	O5—Mo4 ^v	2.0797 (19)
Mo1—O2	1.9759 (16)	O5—Ce2 ^v	2.8054 (16)
Mo1—O2 ⁱⁱ	1.9759 (16)	O6—Mo4 ⁱⁱ	2.0145 (14)
Mo1—O4 ⁱⁱ	2.0332 (17)	O7—Mo2 ⁱⁱ	2.0773 (16)
Mo1—O4	2.0332 (17)	O7—Ce1 ^{xx}	2.8959 (17)
Mo1—O1	2.045 (3)	O7—Ce1 ^{xxii}	2.8959 (17)
Mo1—Mo3 ⁱⁱ	2.7003 (3)	O8—Mo4 ^{xv}	2.0758 (19)
Mo1—Mo3	2.7003 (3)	O9—Mo4 ⁱⁱ	2.1141 (2)
Mo1—Mo2 ⁱⁱ	2.7129 (3)	O9—Mo4 ^{xviii}	2.1141 (2)
Mo1—Mo2	2.7129 (3)	O9—Mo4 ^{xxiii}	2.1141 (2)
Mo2—O3 ^{xi}	2.0277 (16)	O9—Ce3 ^v	3.6397 (2)
Mo2—O2	2.077 (2)	O9—Ce3 ^{xxiv}	3.6397 (2)
Mo2—O7	2.0773 (16)	O10—Mo4 ^v	2.0857 (16)
Mo2—O5	2.0985 (16)	O10—Mo5 ^{xiv}	2.0950 (16)
Mo2—O10	2.0997 (19)	O10—Ce1 ^{vi}	2.5499 (19)
Mo2—Mo4 ^v	2.6412 (3)	O11—Mo3 ⁱⁱ	2.0795 (16)
Mo2—Mo5 ^{xiv}	2.7691 (3)	O11—Ce1 ⁱⁱ	2.8865 (16)
Mo2—Mo3	2.7739 (2)	O11—Ce3 ^v	3.089 (3)
Mo2—Mo2 ⁱⁱ	2.7851 (4)	O12—Ce3 ^v	2.360 (2)
Mo3—O8	2.0315 (16)	O12—Ce1 ⁱⁱ	2.3916 (16)
Mo3—O5	2.0688 (16)		
O7 ⁱ —Li—O7	180.0	O2 ⁱⁱ —Mo1—Mo2	95.29 (6)
O7 ⁱ —Li—O10 ⁱⁱ	95.41 (7)	O4 ⁱⁱ —Mo1—Mo2	142.46 (6)
O7—Li—O10 ⁱⁱ	84.59 (7)	O4—Mo1—Mo2	94.36 (5)
O7 ⁱ —Li—O10 ⁱⁱⁱ	84.59 (7)	O1—Mo1—Mo2	132.72 (5)
O7—Li—O10 ⁱⁱⁱ	95.41 (7)	Mo3 ⁱⁱ —Mo1—Mo2	92.568 (10)
O10 ⁱⁱ —Li—O10 ⁱⁱⁱ	180.0	Mo3—Mo1—Mo2	61.651 (7)
O7 ⁱ —Li—O10 ⁱ	84.59 (7)	Mo2 ⁱⁱ —Mo1—Mo2	61.767 (10)
O7—Li—O10 ⁱ	95.41 (7)	O2—Mo1—Ce2 ^{xx}	52.36 (5)
O10 ⁱⁱ —Li—O10 ⁱ	108.28 (8)	O2 ⁱⁱ —Mo1—Ce2 ^{xx}	52.36 (5)

O10 ⁱⁱⁱ —Li—O10 ⁱ	71.72 (8)	O4 ⁱⁱ —Mo1—Ce2 ^{xx}	120.27 (5)
O7 ⁱ —Li—O10	95.41 (7)	O4—Mo1—Ce2 ^{xx}	120.27 (5)
O7—Li—O10	84.59 (7)	O1—Mo1—Ce2 ^{xx}	52.01 (7)
O10 ⁱⁱ —Li—O10	71.72 (8)	Mo3 ⁱⁱ —Mo1—Ce2 ^{xx}	145.707 (6)
O10 ⁱⁱⁱ —Li—O10	108.28 (8)	Mo3—Mo1—Ce2 ^{xx}	145.707 (6)
O10 ⁱ —Li—O10	180.000 (1)	Mo2 ⁱⁱ —Mo1—Ce2 ^{xx}	90.187 (8)
O7 ⁱ —Li—Mo2	138.20 (5)	Mo2—Mo1—Ce2 ^{xx}	90.187 (8)
O7—Li—Mo2	41.80 (5)	O2—Mo1—Ce1 ^v	57.59 (6)
O10 ⁱⁱ —Li—Mo2	78.79 (4)	O2 ⁱⁱ —Mo1—Ce1 ^v	117.78 (5)
O10 ⁱⁱⁱ —Li—Mo2	101.21 (4)	O4 ⁱⁱ —Mo1—Ce1 ^v	111.62 (5)
O10 ⁱ —Li—Mo2	136.78 (4)	O4—Mo1—Ce1 ^v	53.03 (5)
O10—Li—Mo2	43.22 (4)	O1—Mo1—Ce1 ^v	44.290 (8)
O7 ⁱ —Li—Mo2 ⁱ	41.80 (5)	Mo3 ⁱⁱ —Mo1—Ce1 ^v	144.943 (9)
O7—Li—Mo2 ⁱ	138.20 (5)	Mo3—Mo1—Ce1 ^v	96.635 (6)
O10 ⁱⁱ —Li—Mo2 ⁱ	101.21 (4)	Mo2 ⁱⁱ —Mo1—Ce1 ^v	151.707 (9)
O10 ⁱⁱⁱ —Li—Mo2 ⁱ	78.79 (4)	Mo2—Mo1—Ce1 ^v	99.651 (5)
O10 ⁱ —Li—Mo2 ⁱ	43.22 (4)	Ce2 ^{xx} —Mo1—Ce1 ^v	67.487 (5)
O10—Li—Mo2 ⁱ	136.78 (4)	O2—Mo1—Ce1 ^{ix}	117.78 (5)
Mo2—Li—Mo2 ⁱ	180.000 (6)	O2 ⁱⁱ —Mo1—Ce1 ^{ix}	57.59 (6)
O7 ⁱ —Li—Mo2 ⁱⁱ	138.20 (5)	O4 ⁱⁱ —Mo1—Ce1 ^{ix}	53.03 (5)
O7—Li—Mo2 ⁱⁱ	41.80 (5)	O4—Mo1—Ce1 ^{ix}	111.62 (5)
O10 ⁱⁱ —Li—Mo2 ⁱⁱ	43.22 (4)	O1—Mo1—Ce1 ^{ix}	44.290 (8)
O10 ⁱⁱⁱ —Li—Mo2 ⁱⁱ	136.78 (4)	Mo3 ⁱⁱ —Mo1—Ce1 ^{ix}	96.635 (6)
O10 ⁱ —Li—Mo2 ⁱⁱ	101.21 (4)	Mo3—Mo1—Ce1 ^{ix}	144.943 (9)
O10—Li—Mo2 ⁱⁱ	78.79 (4)	Mo2 ⁱⁱ —Mo1—Ce1 ^{ix}	99.651 (5)
Mo2—Li—Mo2 ⁱⁱ	54.260 (7)	Mo2—Mo1—Ce1 ^{ix}	151.707 (9)
Mo2 ⁱ —Li—Mo2 ⁱⁱ	125.740 (7)	Ce2 ^{xx} —Mo1—Ce1 ^{ix}	67.487 (5)
O7 ⁱ —Li—Mo2 ⁱⁱⁱ	41.80 (5)	Ce1 ^v —Mo1—Ce1 ^{ix}	87.964 (8)
O7—Li—Mo2 ⁱⁱⁱ	138.20 (5)	O3 ^{xi} —Mo2—O2	86.18 (7)
O10 ⁱⁱ —Li—Mo2 ⁱⁱⁱ	136.78 (4)	O3 ^{xi} —Mo2—O7	85.95 (6)
O10 ⁱⁱⁱ —Li—Mo2 ⁱⁱⁱ	43.22 (4)	O2—Mo2—O7	87.51 (9)
O10 ⁱ —Li—Mo2 ⁱⁱⁱ	78.79 (4)	O3 ^{xi} —Mo2—O5	88.61 (7)
O10—Li—Mo2 ⁱⁱⁱ	101.21 (4)	O2—Mo2—O5	83.17 (7)
Mo2—Li—Mo2 ⁱⁱⁱ	125.740 (7)	O7—Mo2—O5	169.50 (9)
Mo2 ⁱ —Li—Mo2 ⁱⁱⁱ	54.260 (7)	O3 ^{xi} —Mo2—O10	87.58 (7)
Mo2 ⁱⁱ —Li—Mo2 ⁱⁱⁱ	180.0	O2—Mo2—O10	172.63 (6)
O7 ⁱ —Li—Ce1 ^{xx}	128.23 (5)	O7—Mo2—O10	88.14 (9)
O7—Li—Ce1 ^{xx}	51.77 (5)	O5—Mo2—O10	100.61 (7)
O10 ⁱⁱ —Li—Ce1 ^{xx}	135.89 (4)	O3 ^{xi} —Mo2—Mo4 ^v	92.95 (5)
O10 ⁱⁱⁱ —Li—Ce1 ^{xx}	44.11 (4)	O2—Mo2—Mo4 ^v	133.64 (5)
O10 ⁱ —Li—Ce1 ^{xx}	84.80 (4)	O7—Mo2—Mo4 ^v	138.74 (8)
O10—Li—Ce1 ^{xx}	95.20 (4)	O5—Mo2—Mo4 ^v	50.48 (5)
Mo2—Li—Ce1 ^{xx}	64.780 (4)	O10—Mo2—Mo4 ^v	50.64 (4)
Mo2 ⁱ —Li—Ce1 ^{xx}	115.220 (4)	O3 ^{xi} —Mo2—Mo1	132.54 (6)
Mo2 ⁱⁱ —Li—Ce1 ^{xx}	93.573 (4)	O2—Mo2—Mo1	46.41 (5)
Mo2 ⁱⁱⁱ —Li—Ce1 ^{xx}	86.427 (4)	O7—Mo2—Mo1	89.31 (7)
O7 ⁱ —Li—Ce1 ^{xiv}	51.77 (5)	O5—Mo2—Mo1	87.76 (5)
O7—Li—Ce1 ^{xiv}	128.23 (5)	O10—Mo2—Mo1	139.47 (5)
O10 ⁱⁱ —Li—Ce1 ^{xiv}	44.11 (4)	Mo4 ^v —Mo2—Mo1	119.623 (9)

O10 ⁱⁱⁱ —Li—Ce1 ^{xiv}	135.89 (4)	O3 ^{xi} —Mo2—Mo5 ^{xiv}	136.18 (6)
O10 ⁱ —Li—Ce1 ^{xiv}	95.20 (4)	O2—Mo2—Mo5 ^{xiv}	137.57 (5)
O10—Li—Ce1 ^{xiv}	84.80 (4)	O7—Mo2—Mo5 ^{xiv}	92.57 (6)
Mo2—Li—Ce1 ^{xiv}	115.220 (4)	O5—Mo2—Mo5 ^{xiv}	97.57 (5)
Mo2 ⁱ —Li—Ce1 ^{xiv}	64.780 (4)	O10—Mo2—Mo5 ^{xiv}	48.62 (4)
Mo2 ⁱⁱ —Li—Ce1 ^{xiv}	86.427 (4)	Mo4 ^v —Mo2—Mo5 ^{xiv}	60.718 (6)
Mo2 ⁱⁱⁱ —Li—Ce1 ^{xiv}	93.573 (4)	Mo1—Mo2—Mo5 ^{xiv}	91.153 (9)
Ce1 ^{xx} —Li—Ce1 ^{xiv}	180.000 (3)	O3 ^{xi} —Mo2—Mo3	136.41 (5)
O3 ^{iv} —Ce1—O12	122.15 (7)	O2—Mo2—Mo3	89.08 (4)
O3 ^{iv} —Ce1—O1 ^v	69.32 (7)	O7—Mo2—Mo3	137.13 (4)
O12—Ce1—O1 ^v	134.79 (8)	O5—Mo2—Mo3	47.81 (4)
O3 ^{iv} —Ce1—O8	120.66 (6)	O10—Mo2—Mo3	98.15 (4)
O12—Ce1—O8	116.24 (7)	Mo4 ^v —Mo2—Mo3	60.674 (7)
O1 ^v —Ce1—O8	77.76 (7)	Mo1—Mo2—Mo3	58.951 (7)
O3 ^{iv} —Ce1—O10 ^{vi}	82.31 (6)	Mo5 ^{xiv} —Mo2—Mo3	62.917 (8)
O12—Ce1—O10 ^{vi}	111.96 (7)	O3 ^{xi} —Mo2—Mo2 ⁱⁱ	133.86 (5)
O1 ^v —Ce1—O10 ^{vi}	112.96 (7)	O2—Mo2—Mo2 ⁱⁱ	90.91 (5)
O8—Ce1—O10 ^{vi}	66.91 (6)	O7—Mo2—Mo2 ⁱⁱ	47.91 (4)
O3 ^{iv} —Ce1—O4 ^v	129.24 (6)	O5—Mo2—Mo2 ⁱⁱ	136.76 (4)
O12—Ce1—O4 ^v	80.26 (6)	O10—Mo2—Mo2 ⁱⁱ	90.58 (5)
O1 ^v —Ce1—O4 ^v	64.64 (7)	Mo4 ^v —Mo2—Mo2 ⁱⁱ	120.433 (6)
O8—Ce1—O4 ^v	68.88 (6)	Mo1—Mo2—Mo2 ⁱⁱ	59.117 (5)
O10 ^{vi} —Ce1—O4 ^v	134.92 (5)	Mo5 ^{xiv} —Mo2—Mo2 ⁱⁱ	59.809 (5)
O3 ^{iv} —Ce1—O2 ^v	79.48 (6)	Mo3—Mo2—Mo2 ⁱⁱ	89.470 (5)
O12—Ce1—O2 ^v	78.39 (7)	O3 ^{xi} —Mo2—Li	80.52 (5)
O1 ^v —Ce1—O2 ^v	59.97 (7)	O2—Mo2—Li	122.93 (5)
O8—Ce1—O2 ^v	123.24 (5)	O7—Mo2—Li	36.66 (8)
O10 ^{vi} —Ce1—O2 ^v	161.79 (5)	O5—Mo2—Li	150.49 (5)
O4 ^v —Ce1—O2 ^v	59.85 (5)	O10—Mo2—Li	51.92 (4)
O3 ^{iv} —Ce1—O11	140.28 (7)	Mo4 ^v —Mo2—Li	102.456 (8)
O12—Ce1—O11	62.84 (7)	Mo1—Mo2—Li	119.677 (7)
O1 ^v —Ce1—O11	139.21 (6)	Mo5 ^{xiv} —Mo2—Li	72.991 (7)
O8—Ce1—O11	62.94 (5)	Mo3—Mo2—Li	135.603 (8)
O10 ^{vi} —Ce1—O11	62.26 (6)	Mo2 ⁱⁱ —Mo2—Li	62.870 (4)
O4 ^v —Ce1—O11	90.07 (6)	O3 ^{xi} —Mo2—Ce2 ^v	43.12 (5)
O2 ^v —Ce1—O11	134.84 (6)	O2—Mo2—Ce2 ^v	59.43 (5)
O3 ^{iv} —Ce1—O7 ^{vii}	63.38 (5)	O7—Mo2—Ce2 ^v	115.69 (5)
O12—Ce1—O7 ^{vii}	69.19 (7)	O5—Mo2—Ce2 ^v	55.05 (4)
O1 ^v —Ce1—O7 ^{vii}	131.52 (6)	O10—Mo2—Ce2 ^v	117.60 (5)
O8—Ce1—O7 ^{vii}	136.39 (7)	Mo4 ^v —Mo2—Ce2 ^v	89.410 (7)
O10 ^{vi} —Ce1—O7 ^{vii}	71.23 (7)	Mo1—Mo2—Ce2 ^v	99.782 (8)
O4 ^v —Ce1—O7 ^{vii}	146.86 (6)	Mo5 ^{xiv} —Mo2—Ce2 ^v	149.571 (7)
O2 ^v —Ce1—O7 ^{vii}	100.38 (6)	Mo3—Mo2—Ce2 ^v	98.774 (7)
O11—Ce1—O7 ^{vii}	87.29 (5)	Mo2 ⁱⁱ —Mo2—Ce2 ^v	148.794 (4)
O3 ^{iv} —Ce1—Mo1 ^v	92.59 (5)	Li—Mo2—Ce2 ^v	123.174 (6)
O12—Ce1—Mo1 ^v	98.83 (5)	O8—Mo3—O5	86.67 (6)
O1 ^v —Ce1—Mo1 ^v	36.42 (6)	O8—Mo3—O11	85.73 (6)
O8—Ce1—Mo1 ^v	88.19 (4)	O5—Mo3—O11	167.88 (8)
O10 ^{vi} —Ce1—Mo1 ^v	146.49 (4)	O8—Mo3—O4	89.16 (7)

O4 ^v —Ce1—Mo1 ^v	36.73 (4)	O5—Mo3—O4	84.24 (7)
O2 ^v —Ce1—Mo1 ^v	35.48 (3)	O11—Mo3—O4	86.22 (9)
O11—Ce1—Mo1 ^v	126.78 (5)	O8—Mo3—Mo1	137.36 (5)
O7 ^{vii} —Ce1—Mo1 ^v	135.15 (5)	O5—Mo3—Mo1	88.70 (5)
O3 ^{iv} —Ce1—Mo4 ^{xv}	96.09 (5)	O11—Mo3—Mo1	90.50 (6)
O12—Ce1—Mo4 ^{xv}	128.25 (6)	O4—Mo3—Mo1	48.20 (5)
O1 ^v —Ce1—Mo4 ^{xv}	88.36 (6)	O8—Mo3—Mo3 ⁱⁱ	134.44 (5)
O8—Ce1—Mo4 ^{xv}	34.03 (4)	O5—Mo3—Mo3 ⁱⁱ	138.70 (4)
O10 ^{vi} —Ce1—Mo4 ^{xv}	34.97 (4)	O11—Mo3—Mo3 ⁱⁱ	48.91 (4)
O4 ^v —Ce1—Mo4 ^{xv}	102.68 (4)	O4—Mo3—Mo3 ⁱⁱ	91.45 (5)
O2 ^v —Ce1—Mo4 ^{xv}	147.69 (3)	Mo1—Mo3—Mo3 ⁱⁱ	59.590 (5)
O11—Ce1—Mo4 ^{xv}	65.48 (4)	O8—Mo3—Mo4 ^v	91.12 (5)
O7 ^{vii} —Ce1—Mo4 ^{xv}	106.14 (6)	O5—Mo3—Mo4 ^v	48.88 (5)
Mo1 ^v —Ce1—Mo4 ^{xv}	114.039 (6)	O11—Mo3—Mo4 ^v	140.67 (7)
O3 ^{iv} —Ce1—Mo2 ^{vii}	31.40 (4)	O4—Mo3—Mo4 ^v	132.99 (5)
O12—Ce1—Mo2 ^{vii}	92.04 (5)	Mo1—Mo3—Mo4 ^v	116.662 (9)
O1 ^v —Ce1—Mo2 ^{vii}	96.68 (5)	Mo3 ⁱⁱ —Mo3—Mo4 ^v	119.873 (6)
O8—Ce1—Mo2 ^{vii}	145.48 (4)	O8—Mo3—Mo5	88.64 (5)
O10 ^{vi} —Ce1—Mo2 ^{vii}	84.91 (3)	O5—Mo3—Mo5	140.47 (5)
O4 ^v —Ce1—Mo2 ^{vii}	139.49 (4)	O11—Mo3—Mo5	48.74 (7)
O2 ^v —Ce1—Mo2 ^{vii}	79.64 (3)	O4—Mo3—Mo5	134.94 (5)
O11—Ce1—Mo2 ^{vii}	121.66 (4)	Mo1—Mo3—Mo5	119.660 (8)
O7 ^{vii} —Ce1—Mo2 ^{vii}	34.91 (3)	Mo3 ⁱⁱ —Mo3—Mo5	60.081 (5)
Mo1 ^v —Ce1—Mo2 ^{vii}	107.584 (6)	Mo4 ^v —Mo3—Mo5	92.056 (9)
Mo4 ^{xv} —Ce1—Mo2 ^{vii}	112.839 (6)	O8—Mo3—Mo2	135.01 (5)
O12—Ce2—O3 ⁱⁱ	133.58 (5)	O5—Mo3—Mo2	48.73 (4)
O12—Ce2—O3	133.58 (5)	O11—Mo3—Mo2	139.20 (4)
O3 ⁱⁱ —Ce2—O3	79.20 (9)	O4—Mo3—Mo2	91.42 (4)
O12—Ce2—O1 ^{vii}	149.28 (9)	Mo1—Mo3—Mo2	59.398 (8)
O3 ⁱⁱ —Ce2—O1 ^{vii}	65.37 (6)	Mo3 ⁱⁱ —Mo3—Mo2	90.530 (5)
O3—Ce2—O1 ^{vii}	65.37 (6)	Mo4 ^v —Mo3—Mo2	57.266 (7)
O12—Ce2—O2 ^{viii}	93.73 (7)	Mo5—Mo3—Mo2	120.425 (10)
O3 ⁱⁱ —Ce2—O2 ^{viii}	126.07 (5)	O8—Mo3—Mo4 ^{xv}	46.92 (5)
O3—Ce2—O2 ^{viii}	84.21 (6)	O5—Mo3—Mo4 ^{xv}	90.84 (5)
O1 ^{vii} —Ce2—O2 ^{viii}	61.04 (6)	O11—Mo3—Mo4 ^{xv}	90.85 (6)
O12—Ce2—O2 ^{vii}	93.73 (7)	O4—Mo3—Mo4 ^{xv}	136.07 (5)
O3 ⁱⁱ —Ce2—O2 ^{vii}	84.21 (6)	Mo1—Mo3—Mo4 ^{xv}	175.622 (10)
O3—Ce2—O2 ^{vii}	126.07 (5)	Mo3 ⁱⁱ —Mo3—Mo4 ^{xv}	118.702 (5)
O1 ^{vii} —Ce2—O2 ^{vii}	61.04 (6)	Mo4 ^v —Mo3—Mo4 ^{xv}	60.145 (7)
O2 ^{viii} —Ce2—O2 ^{vii}	65.50 (7)	Mo5—Mo3—Mo4 ^{xv}	58.713 (6)
O12—Ce2—O5 ^v	72.64 (6)	Mo2—Mo3—Mo4 ^{xv}	117.351 (9)
O3 ⁱⁱ —Ce2—O5 ^v	66.93 (5)	O8—Mo3—Mo5 ^{xiv}	133.82 (5)
O3—Ce2—O5 ^v	104.01 (6)	O5—Mo3—Mo5 ^{xiv}	94.57 (5)
O1 ^{vii} —Ce2—O5 ^v	132.27 (6)	O11—Mo3—Mo5 ^{xiv}	97.51 (6)
O2 ^{viii} —Ce2—O5 ^v	166.30 (5)	O4—Mo3—Mo5 ^{xiv}	136.95 (5)
O2 ^{vii} —Ce2—O5 ^v	115.69 (5)	Mo1—Mo3—Mo5 ^{xiv}	88.790 (9)
O12—Ce2—O5 ^{ix}	72.64 (6)	Mo3 ⁱⁱ —Mo3—Mo5 ^{xiv}	61.803 (5)
O3 ⁱⁱ —Ce2—O5 ^{ix}	104.01 (6)	Mo4 ^v —Mo3—Mo5 ^{xiv}	58.087 (6)
O3—Ce2—O5 ^{ix}	66.93 (5)	Mo5—Mo3—Mo5 ^{xiv}	61.970 (9)

O1 ^{vii} —Ce2—O5 ^{ix}	132.27 (6)	Mo2—Mo3—Mo5 ^{xiv}	58.461 (7)
O2 ^{viii} —Ce2—O5 ^{ix}	115.69 (5)	Mo4 ^{xv} —Mo3—Mo5 ^{xiv}	86.906 (8)
O2 ^{vii} —Ce2—O5 ^{ix}	166.30 (5)	O8—Mo3—Ce3	42.95 (5)
O5 ^v —Ce2—O5 ^{ix}	59.64 (7)	O5—Mo3—Ce3	55.13 (5)
O12—Ce2—O2 ^{ix}	77.39 (4)	O11—Mo3—Ce3	113.38 (5)
O3 ⁱⁱ —Ce2—O2 ^{ix}	140.99 (6)	O4—Mo3—Ce3	60.69 (5)
O3—Ce2—O2 ^{ix}	62.17 (6)	Mo1—Mo3—Ce3	102.416 (8)
O1 ^{vii} —Ce2—O2 ^{ix}	100.42 (3)	Mo3 ⁱⁱ —Mo3—Ce3	149.964 (5)
O2 ^{viii} —Ce2—O2 ^{ix}	58.34 (6)	Mo4 ^v —Mo3—Ce3	89.212 (7)
O2 ^{vii} —Ce2—O2 ^{ix}	122.06 (3)	Mo5—Mo3—Ce3	131.587 (7)
O5 ^v —Ce2—O2 ^{ix}	115.54 (5)	Mo2—Mo3—Ce3	100.481 (7)
O5 ^{ix} —Ce2—O2 ^{ix}	57.35 (5)	Mo4 ^{xv} —Mo3—Ce3	80.844 (7)
O12—Ce2—O2 ^v	77.39 (4)	Mo5 ^{xiv} —Mo3—Ce3	146.743 (8)
O3 ⁱⁱ —Ce2—O2 ^v	62.17 (6)	O6—Mo4—O8 ^{xvi}	85.31 (9)
O3—Ce2—O2 ^v	140.99 (6)	O6—Mo4—O5 ^v	89.00 (9)
O1 ^{vii} —Ce2—O2 ^v	100.42 (3)	O8 ^{xvi} —Mo4—O5 ^v	173.10 (7)
O2 ^{viii} —Ce2—O2 ^v	122.06 (3)	O6—Mo4—O10 ^v	91.20 (7)
O2 ^{vii} —Ce2—O2 ^v	58.34 (6)	O8 ^{xvi} —Mo4—O10 ^v	82.35 (7)
O5 ^v —Ce2—O2 ^v	57.35 (5)	O5 ^v —Mo4—O10 ^v	101.70 (7)
O5 ^{ix} —Ce2—O2 ^v	115.54 (5)	O6—Mo4—O9	79.29 (5)
O2 ^{ix} —Ce2—O2 ^v	154.73 (7)	O8 ^{xvi} —Mo4—O9	87.84 (5)
O12—Ce2—Mo1 ^{vii}	111.35 (6)	O5 ^v —Mo4—O9	87.27 (4)
O3 ⁱⁱ —Ce2—Mo1 ^{vii}	94.00 (4)	O10 ^v —Mo4—O9	166.89 (5)
O3—Ce2—Mo1 ^{vii}	94.00 (4)	O6—Mo4—Mo2 ^v	96.21 (6)
O1 ^{vii} —Ce2—Mo1 ^{vii}	37.93 (6)	O8 ^{xvi} —Mo4—Mo2 ^v	133.42 (5)
O2 ^{viii} —Ce2—Mo1 ^{vii}	36.42 (4)	O5 ^v —Mo4—Mo2 ^v	51.11 (4)
O2 ^{vii} —Ce2—Mo1 ^{vii}	36.42 (4)	O10 ^v —Mo4—Mo2 ^v	51.11 (5)
O5 ^v —Ce2—Mo1 ^{vii}	150.15 (3)	O9—Mo4—Mo2 ^v	138.338 (10)
O5 ^{ix} —Ce2—Mo1 ^{vii}	150.15 (3)	O6—Mo4—Mo5 ^{xvii}	140.45 (5)
O2 ^{ix} —Ce2—Mo1 ^{vii}	93.84 (3)	O8 ^{xvi} —Mo4—Mo5 ^{xvii}	87.85 (5)
O2 ^v —Ce2—Mo1 ^{vii}	93.84 (3)	O5 ^v —Mo4—Mo5 ^{xvii}	99.03 (5)
O12—Ce2—Mo2 ^v	98.05 (3)	O10 ^v —Mo4—Mo5 ^{xvii}	49.26 (5)
O3 ⁱⁱ —Ce2—Mo2 ^v	35.57 (4)	O9—Mo4—Mo5 ^{xvii}	139.345 (9)
O3—Ce2—Mo2 ^v	106.07 (5)	Mo2 ^v —Mo4—Mo5 ^{xvii}	61.952 (8)
O1 ^{vii} —Ce2—Mo2 ^v	97.73 (3)	O6—Mo4—Mo3 ^v	137.41 (8)
O2 ^{viii} —Ce2—Mo2 ^v	150.68 (4)	O8 ^{xvi} —Mo4—Mo3 ^v	136.74 (4)
O2 ^{vii} —Ce2—Mo2 ^v	86.93 (4)	O5 ^v —Mo4—Mo3 ^v	48.54 (5)
O5 ^v —Ce2—Mo2 ^v	37.81 (3)	O10 ^v —Mo4—Mo3 ^v	99.64 (5)
O5 ^{ix} —Ce2—Mo2 ^v	93.48 (4)	O9—Mo4—Mo3 ^v	93.467 (8)
O2 ^{ix} —Ce2—Mo2 ^v	150.67 (3)	Mo2 ^v —Mo4—Mo3 ^v	62.060 (7)
O2 ^v —Ce2—Mo2 ^v	37.12 (4)	Mo5 ^{xvii} —Mo4—Mo3 ^v	63.801 (8)
Mo1 ^{vii} —Ce2—Mo2 ^v	114.434 (4)	O6—Mo4—Mo4 ^{xviii}	127.74 (5)
O12 ^v —Ce3—O8	132.16 (5)	O8 ^{xvi} —Mo4—Mo4 ^{xviii}	88.58 (4)
O12 ^v —Ce3—O8 ^x	132.16 (5)	O5 ^v —Mo4—Mo4 ^{xviii}	91.83 (4)
O8—Ce3—O8 ^x	80.35 (8)	O10 ^v —Mo4—Mo4 ^{xviii}	139.18 (4)
O12 ^v —Ce3—O4 ^v	108.37 (7)	O9—Mo4—Mo4 ^{xviii}	48.606 (5)
O8—Ce3—O4 ^v	72.90 (6)	Mo2 ^v —Mo4—Mo4 ^{xviii}	123.722 (10)
O8 ^x —Ce3—O4 ^v	115.46 (5)	Mo5 ^{xvii} —Mo4—Mo4 ^{xviii}	90.884 (6)
O12 ^v —Ce3—O4 ^{xi}	108.37 (7)	Mo3 ^v —Mo4—Mo4 ^{xviii}	61.730 (7)

O8—Ce3—O4 ^{xi}	115.46 (5)	O6—Mo4—Mo3 ^{xvi}	130.47 (8)
O8 ^x —Ce3—O4 ^{xi}	72.90 (6)	O8 ^{xvi} —Mo4—Mo3 ^{xvi}	45.63 (4)
O4 ^v —Ce3—O4 ^{xi}	68.25 (8)	O5 ^v —Mo4—Mo3 ^{xvi}	139.29 (4)
O12 ^v —Ce3—O5 ^x	72.46 (7)	O10 ^v —Mo4—Mo3 ^{xvi}	88.72 (5)
O8—Ce3—O5 ^x	103.13 (6)	O9—Mo4—Mo3 ^{xvi}	90.635 (7)
O8 ^x —Ce3—O5 ^x	65.41 (5)	Mo2 ^v —Mo4—Mo3 ^{xvi}	120.793 (9)
O4 ^v —Ce3—O5 ^x	175.45 (6)	Mo5 ^{xvii} —Mo4—Mo3 ^{xvi}	58.843 (8)
O4 ^{xi} —Ce3—O5 ^x	115.94 (5)	Mo3 ^v —Mo4—Mo3 ^{xvi}	91.111 (9)
O12 ^v —Ce3—O5	72.47 (7)	Mo4 ^{xviii} —Mo4—Mo3 ^{xvi}	58.125 (7)
O8—Ce3—O5	65.41 (5)	O6—Mo4—Mo4 ⁱⁱ	38.07 (5)
O8 ^x —Ce3—O5	103.13 (6)	O8 ^{xvi} —Mo4—Mo4 ⁱⁱ	88.38 (5)
O4 ^v —Ce3—O5	115.94 (5)	O5 ^v —Mo4—Mo4 ⁱⁱ	84.74 (5)
O4 ^{xi} —Ce3—O5	175.45 (6)	O10 ^v —Mo4—Mo4 ⁱⁱ	129.14 (5)
O5 ^x —Ce3—O5	59.82 (7)	O9—Mo4—Mo4 ⁱⁱ	41.395 (5)
O12 ^v —Ce3—O4 ^x	74.97 (3)	Mo2 ^v —Mo4—Mo4 ⁱⁱ	120.433 (6)
O8—Ce3—O4 ^x	143.69 (6)	Mo5 ^{xvii} —Mo4—Mo4 ⁱⁱ	176.099 (7)
O8 ^x —Ce3—O4 ^x	63.90 (5)	Mo3 ^v —Mo4—Mo4 ⁱⁱ	119.873 (6)
O4 ^v —Ce3—O4 ^x	127.22 (4)	Mo4 ^{xviii} —Mo4—Mo4 ⁱⁱ	90.0
O4 ^{xi} —Ce3—O4 ^x	61.42 (6)	Mo3 ^{xvi} —Mo4—Mo4 ⁱⁱ	118.702 (5)
O5 ^x —Ce3—O4 ^x	57.32 (5)	O6—Mo4—Ce1 ^{xvi}	75.70 (7)
O5—Ce3—O4 ^x	115.02 (5)	O8 ^{xvi} —Mo4—Ce1 ^{xvi}	40.64 (4)
O12 ^v —Ce3—O4	74.97 (3)	O5 ^v —Mo4—Ce1 ^{xvi}	141.03 (4)
O8—Ce3—O4	63.90 (5)	O10 ^v —Mo4—Ce1 ^{xvi}	44.48 (5)
O8 ^x —Ce3—O4	143.69 (6)	O9—Mo4—Ce1 ^{xvi}	123.412 (8)
O4 ^v —Ce3—O4	61.42 (6)	Mo2 ^v —Mo4—Ce1 ^{xvi}	94.531 (7)
O4 ^{xi} —Ce3—O4	127.22 (3)	Mo5 ^{xvii} —Mo4—Ce1 ^{xvi}	73.927 (8)
O5 ^x —Ce3—O4	115.02 (5)	Mo3 ^v —Mo4—Ce1 ^{xvi}	137.453 (8)
O5—Ce3—O4	57.32 (5)	Mo4 ^{xviii} —Mo4—Ce1 ^{xvi}	125.945 (10)
O4 ^x —Ce3—O4	149.80 (6)	Mo3 ^{xvi} —Mo4—Ce1 ^{xvi}	70.101 (6)
O12 ^v —Ce3—O11 ^v	59.67 (8)	Mo4 ⁱⁱ —Mo4—Ce1 ^{xvi}	102.511 (4)
O8—Ce3—O11 ^v	130.85 (5)	O11—Mo5—O10 ^{xiv}	85.23 (7)
O8 ^x —Ce3—O11 ^v	130.85 (5)	O11—Mo5—O10 ^{vi}	85.23 (7)
O4 ^v —Ce3—O11 ^v	59.89 (5)	O10 ^{xiv} —Mo5—O10 ^{vi}	84.89 (9)
O4 ^{xi} —Ce3—O11 ^v	59.89 (5)	O11—Mo5—Mo4 ^{xix}	93.800 (8)
O5 ^x —Ce3—O11 ^v	123.33 (5)	O10 ^{xiv} —Mo5—Mo4 ^{xix}	48.96 (4)
O5—Ce3—O11 ^v	123.33 (5)	O10 ^{vi} —Mo5—Mo4 ^{xix}	133.64 (5)
O4 ^x —Ce3—O11 ^v	81.27 (4)	O11—Mo5—Mo4 ^{xv}	93.800 (8)
O4—Ce3—O11 ^v	81.27 (4)	O10 ^{xiv} —Mo5—Mo4 ^{xv}	133.64 (5)
O12 ^v —Ce3—O1 ^v	157.12 (8)	O10 ^{vi} —Mo5—Mo4 ^{xv}	48.96 (4)
O8—Ce3—O1 ^v	61.54 (5)	Mo4 ^{xix} —Mo5—Mo4 ^{xv}	172.199 (15)
O8 ^x —Ce3—O1 ^v	61.54 (5)	O11—Mo5—Mo3	48.79 (4)
O4 ^v —Ce3—O1 ^v	53.99 (5)	O10 ^{xiv} —Mo5—Mo3	134.00 (5)
O4 ^{xi} —Ce3—O1 ^v	53.99 (5)	O10 ^{vi} —Mo5—Mo3	91.23 (5)
O5 ^x —Ce3—O1 ^v	126.41 (5)	Mo4 ^{xix} —Mo5—Mo3	122.183 (10)
O5—Ce3—O1 ^v	126.41 (5)	Mo4 ^{xv} —Mo5—Mo3	62.444 (6)
O4 ^x —Ce3—O1 ^v	103.27 (3)	O11—Mo5—Mo3 ⁱⁱ	48.79 (4)
O4—Ce3—O1 ^v	103.27 (3)	O10 ^{xiv} —Mo5—Mo3 ⁱⁱ	91.23 (5)
O11 ^v —Ce3—O1 ^v	97.45 (6)	O10 ^{vi} —Mo5—Mo3 ⁱⁱ	134.00 (5)
O12 ^v —Ce3—Mo3	96.37 (3)	Mo4 ^{xix} —Mo5—Mo3 ⁱⁱ	62.444 (6)

O8—Ce3—Mo3	35.79 (4)	Mo4 ^{xv} —Mo5—Mo3 ⁱⁱ	122.183 (10)
O8 ^x —Ce3—Mo3	107.81 (4)	Mo3—Mo5—Mo3 ⁱⁱ	59.838 (9)
O4 ^v —Ce3—Mo3	81.55 (4)	O11—Mo5—Mo2 ^{xiv}	133.96 (4)
O4 ^{xi} —Ce3—Mo3	145.52 (4)	O10 ^{xiv} —Mo5—Mo2 ^{xiv}	48.76 (5)
O5 ^x —Ce3—Mo3	93.92 (4)	O10 ^{vi} —Mo5—Mo2 ^{xiv}	91.12 (5)
O5—Ce3—Mo3	37.35 (3)	Mo4 ^{xix} —Mo5—Mo2 ^{xiv}	57.330 (6)
O4 ^x —Ce3—Mo3	151.21 (4)	Mo4 ^{xv} —Mo5—Mo2 ^{xiv}	117.621 (10)
O4—Ce3—Mo3	37.32 (4)	Mo3—Mo5—Mo2 ^{xiv}	176.566 (12)
O11 ^v —Ce3—Mo3	118.510 (8)	Mo3 ⁱⁱ —Mo5—Mo2 ^{xiv}	119.773 (6)
O1 ^v —Ce3—Mo3	95.02 (2)	O11—Mo5—Mo2 ^{vi}	133.96 (4)
O12 ^v —Ce3—Mo3 ^x	96.37 (3)	O10 ^{xiv} —Mo5—Mo2 ^{vi}	91.12 (5)
O8—Ce3—Mo3 ^x	107.81 (4)	O10 ^{vi} —Mo5—Mo2 ^{vi}	48.76 (5)
O8 ^x —Ce3—Mo3 ^x	35.79 (4)	Mo4 ^{xix} —Mo5—Mo2 ^{vi}	117.621 (10)
O4 ^v —Ce3—Mo3 ^x	145.52 (4)	Mo4 ^{xv} —Mo5—Mo2 ^{vi}	57.330 (6)
O4 ^{xi} —Ce3—Mo3 ^x	81.55 (4)	Mo3—Mo5—Mo2 ^{vi}	119.773 (6)
O5 ^x —Ce3—Mo3 ^x	37.35 (3)	Mo3 ⁱⁱ —Mo5—Mo2 ^{vi}	176.566 (12)
O5—Ce3—Mo3 ^x	93.92 (4)	Mo2 ^{xiv} —Mo5—Mo2 ^{vi}	60.381 (9)
O4 ^x —Ce3—Mo3 ^x	37.32 (4)	O11—Mo5—Mo3 ^{xiv}	138.63 (4)
O4—Ce3—Mo3 ^x	151.21 (4)	O10 ^{xiv} —Mo5—Mo3 ^{xiv}	94.72 (5)
O11 ^v —Ce3—Mo3 ^x	118.510 (8)	O10 ^{vi} —Mo5—Mo3 ^{xiv}	136.07 (5)
O1 ^v —Ce3—Mo3 ^x	95.02 (2)	Mo4 ^{xix} —Mo5—Mo3 ^{xiv}	58.113 (6)
Mo3—Ce3—Mo3 ^x	119.929 (9)	Mo4 ^{xv} —Mo5—Mo3 ^{xiv}	114.493 (10)
O12 ^v —Ce3—Mo1 ^v	122.20 (7)	Mo3—Mo5—Mo3 ^{xiv}	118.030 (9)
O8—Ce3—Mo1 ^v	87.20 (4)	Mo3 ⁱⁱ —Mo5—Mo3 ^{xiv}	89.919 (9)
O8 ^x —Ce3—Mo1 ^v	87.20 (4)	Mo2 ^{xiv} —Mo5—Mo3 ^{xiv}	58.622 (7)
O4 ^v —Ce3—Mo1 ^v	35.35 (4)	Mo2 ^{vi} —Mo5—Mo3 ^{xiv}	87.395 (10)
O4 ^{xi} —Ce3—Mo1 ^v	35.35 (4)	O11—Mo5—Mo3 ^{vi}	138.63 (4)
O5 ^x —Ce3—Mo1 ^v	148.03 (3)	O10 ^{xiv} —Mo5—Mo3 ^{vi}	136.07 (5)
O5—Ce3—Mo1 ^v	148.03 (3)	O10 ^{vi} —Mo5—Mo3 ^{vi}	94.72 (5)
O4 ^x —Ce3—Mo1 ^v	96.76 (3)	Mo4 ^{xix} —Mo5—Mo3 ^{vi}	114.493 (10)
O4—Ce3—Mo1 ^v	96.76 (3)	Mo4 ^{xv} —Mo5—Mo3 ^{vi}	58.113 (6)
O11 ^v —Ce3—Mo1 ^v	62.53 (4)	Mo3—Mo5—Mo3 ^{vi}	89.919 (9)
O1 ^v —Ce3—Mo1 ^v	34.92 (5)	Mo3 ⁱⁱ —Mo5—Mo3 ^{vi}	118.030 (9)
Mo3—Ce3—Mo1 ^v	110.725 (4)	Mo2 ^{xiv} —Mo5—Mo3 ^{vi}	87.395 (10)
Mo3 ^x —Ce3—Mo1 ^v	110.725 (4)	Mo2 ^{vi} —Mo5—Mo3 ^{vi}	58.622 (7)
O12 ^v —Ce3—O9 ^{xxv}	113.66 (7)	Mo3 ^{xiv} —Mo5—Mo3 ^{vi}	56.395 (9)
O8—Ce3—O9 ^{xxv}	52.86 (4)	O11—Mo5—Mo5 ^{xiv}	97.23 (6)
O8 ^x —Ce3—O9 ^{xxv}	52.86 (4)	O10 ^{xiv} —Mo5—Mo5 ^{xiv}	137.55 (4)
O4 ^v —Ce3—O9 ^{xxv}	125.08 (4)	O10 ^{vi} —Mo5—Mo5 ^{xiv}	137.55 (4)
O4 ^{xi} —Ce3—O9 ^{xxv}	125.08 (4)	Mo4 ^{xix} —Mo5—Mo5 ^{xiv}	88.648 (6)
O5 ^x —Ce3—O9 ^{xxv}	51.42 (4)	Mo4 ^{xv} —Mo5—Mo5 ^{xiv}	88.648 (6)
O5—Ce3—O9 ^{xxv}	51.42 (4)	Mo3—Mo5—Mo5 ^{xiv}	61.593 (9)
O4 ^x —Ce3—O9 ^{xxv}	97.25 (4)	Mo3 ⁱⁱ —Mo5—Mo5 ^{xiv}	61.593 (9)
O4—Ce3—O9 ^{xxv}	97.25 (4)	Mo2 ^{xiv} —Mo5—Mo5 ^{xiv}	115.053 (13)
O11 ^v —Ce3—O9 ^{xxv}	173.33 (4)	Mo2 ^{vi} —Mo5—Mo5 ^{xiv}	115.053 (13)
O1 ^v —Ce3—O9 ^{xxv}	89.22 (5)	Mo3 ^{xiv} —Mo5—Mo5 ^{xiv}	56.437 (9)
Mo3—Ce3—O9 ^{xxv}	60.555 (5)	Mo3 ^{vi} —Mo5—Mo5 ^{xiv}	56.437 (9)
Mo3 ^x —Ce3—O9 ^{xxv}	60.555 (5)	Mo1—O1—Ce1 ^v	99.29 (6)
Mo1 ^v —Ce3—O9 ^{xxv}	124.139 (7)	Mo1—O1—Ce1 ^{ix}	99.29 (6)

O12 ^v —Ce3—Ce1 ^{xi}	36.60 (3)	Ce1 ^v —O1—Ce1 ^{ix}	157.89 (13)
O8—Ce3—Ce1 ^{xi}	168.71 (4)	Mo1—O1—Ce2 ^{xx}	90.06 (9)
O8 ^x —Ce3—Ce1 ^{xi}	108.76 (4)	Ce1 ^v —O1—Ce2 ^{xx}	95.93 (6)
O4 ^v —Ce3—Ce1 ^{xi}	107.70 (4)	Ce1 ^{ix} —O1—Ce2 ^{xx}	95.93 (6)
O4 ^{xi} —Ce3—Ce1 ^{xi}	74.40 (4)	Mo1—O1—Ce3 ^v	76.55 (7)
O5 ^x —Ce3—Ce1 ^{xi}	75.73 (4)	Ce1 ^v —O1—Ce3 ^v	86.38 (6)
O5—Ce3—Ce1 ^{xi}	105.23 (3)	Ce1 ^{ix} —O1—Ce3 ^v	86.38 (6)
O4 ^x —Ce3—Ce1 ^{xi}	44.87 (3)	Ce2 ^{xx} —O1—Ce3 ^v	166.61 (11)
O4—Ce3—Ce1 ^{xi}	106.11 (3)	Mo1—O2—Mo2	84.01 (7)
O11 ^v —Ce3—Ce1 ^{xi}	47.87 (3)	Mo1—O2—Ce2 ^{xx}	91.22 (7)
O1 ^v —Ce3—Ce1 ^{xi}	128.32 (4)	Mo2—O2—Ce2 ^{xx}	131.36 (8)
Mo3—Ce3—Ce1 ^{xi}	132.947 (5)	Mo1—O2—Ce1 ^v	86.94 (6)
Mo3 ^x —Ce3—Ce1 ^{xi}	78.291 (4)	Mo2—O2—Ce1 ^v	142.24 (7)
Mo1 ^v —Ce3—Ce1 ^{xi}	99.649 (6)	Ce2 ^{xx} —O2—Ce1 ^v	85.31 (6)
O9 ^{xxv} —Ce3—Ce1 ^{xi}	127.147 (5)	Mo1—O2—Ce2 ^v	144.38 (7)
O6 ^{xii} —Ce4—O6	180.0	Mo2—O2—Ce2 ^v	83.45 (6)
O6 ^{xii} —Ce4—O3	101.93 (7)	Ce2 ^{xx} —O2—Ce2 ^v	121.66 (6)
O6—Ce4—O3	78.07 (7)	Ce1 ^v —O2—Ce2 ^v	82.93 (5)
O6 ^{xii} —Ce4—O3 ^{xii}	78.07 (7)	Mo2 ^{ix} —O3—Ce1 ^{xxi}	111.27 (8)
O6—Ce4—O3 ^{xii}	101.93 (7)	Mo2 ^{ix} —O3—Ce2	101.31 (7)
O3—Ce4—O3 ^{xii}	180.00 (6)	Ce1 ^{xxi} —O3—Ce2	103.98 (7)
O6 ^{xii} —Ce4—O3 ⁱⁱ	101.93 (7)	Mo2 ^{ix} —O3—Ce4	127.21 (8)
O6—Ce4—O3 ⁱⁱ	78.07 (7)	Ce1 ^{xxi} —O3—Ce4	108.51 (6)
O3—Ce4—O3 ⁱⁱ	77.58 (9)	Ce2—O3—Ce4	101.22 (6)
O3 ^{xii} —Ce4—O3 ⁱⁱ	102.42 (9)	Mo1—O4—Mo3	81.91 (7)
O6 ^{xii} —Ce4—O3 ^{xiii}	78.07 (7)	Mo1—O4—Ce3 ^v	98.59 (7)
O6—Ce4—O3 ^{xiii}	101.93 (7)	Mo3—O4—Ce3 ^v	116.62 (7)
O3—Ce4—O3 ^{xiii}	102.42 (9)	Mo1—O4—Ce1 ^v	90.24 (6)
O3 ^{xii} —Ce4—O3 ^{xiii}	77.58 (9)	Mo3—O4—Ce1 ^v	144.66 (8)
O3 ⁱⁱ —Ce4—O3 ^{xiii}	180.00 (6)	Ce3 ^v —O4—Ce1 ^v	98.58 (6)
O6 ^{xii} —Ce4—Ce2	109.59 (7)	Mo1—O4—Ce3	142.82 (8)
O6—Ce4—Ce2	70.41 (7)	Mo3—O4—Ce3	81.99 (6)
O3—Ce4—Ce2	38.98 (4)	Ce3 ^v —O4—Ce3	118.58 (6)
O3 ^{xii} —Ce4—Ce2	141.02 (4)	Ce1 ^v —O4—Ce3	83.95 (5)
O3 ⁱⁱ —Ce4—Ce2	38.98 (4)	Mo3—O5—Mo4 ^v	82.58 (6)
O3 ^{xiii} —Ce4—Ce2	141.02 (4)	Mo3—O5—Mo2	83.46 (6)
O6 ^{xii} —Ce4—Ce2 ^{xii}	70.41 (7)	Mo4 ^v —O5—Mo2	78.42 (6)
O6—Ce4—Ce2 ^{xii}	109.59 (7)	Mo3—O5—Ce3	87.52 (6)
O3—Ce4—Ce2 ^{xii}	141.02 (4)	Mo4 ^v —O5—Ce3	125.09 (7)
O3 ^{xii} —Ce4—Ce2 ^{xii}	38.98 (4)	Mo2—O5—Ce3	153.48 (9)
O3 ⁱⁱ —Ce4—Ce2 ^{xii}	141.02 (4)	Mo3—O5—Ce2 ^v	150.69 (9)
O3 ^{xiii} —Ce4—Ce2 ^{xii}	38.98 (4)	Mo4 ^v —O5—Ce2 ^v	122.56 (7)
Ce2—Ce4—Ce2 ^{xii}	180.000 (1)	Mo2—O5—Ce2 ^v	87.13 (5)
O6 ^{xii} —Ce4—Ce1 ^{xvi}	113.22 (5)	Ce3—O5—Ce2 ^v	88.70 (5)
O6—Ce4—Ce1 ^{xvi}	66.78 (5)	Mo4—O6—Mo4 ⁱⁱ	103.86 (10)
O3—Ce4—Ce1 ^{xvi}	144.81 (4)	Mo4—O6—Ce4	127.46 (5)
O3 ^{xii} —Ce4—Ce1 ^{xvi}	35.19 (4)	Mo4 ⁱⁱ —O6—Ce4	127.46 (5)
O3 ⁱⁱ —Ce4—Ce1 ^{xvi}	93.18 (4)	Li—O7—Mo2 ⁱⁱ	101.54 (10)
O3 ^{xiii} —Ce4—Ce1 ^{xvi}	86.82 (4)	Li—O7—Mo2	101.54 (10)

Ce2—Ce4—Ce1 ^{xvi}	121.134 (3)	Mo2 ⁱⁱ —O7—Mo2	84.19 (8)
Ce2 ^{xii} —Ce4—Ce1 ^{xvi}	58.866 (3)	Li—O7—Ce1 ^{xx}	97.91 (7)
O6 ^{xii} —Ce4—Ce1 ^{xxi}	66.78 (5)	Mo2 ⁱⁱ —O7—Ce1 ^{xx}	160.55 (13)
O6—Ce4—Ce1 ^{xxi}	113.22 (5)	Mo2—O7—Ce1 ^{xx}	92.16 (3)
O3—Ce4—Ce1 ^{xxi}	35.19 (4)	Li—O7—Ce1 ^{xxii}	97.91 (7)
O3 ^{xii} —Ce4—Ce1 ^{xxi}	144.81 (4)	Mo2 ⁱⁱ —O7—Ce1 ^{xxii}	92.16 (3)
O3 ⁱⁱ —Ce4—Ce1 ^{xxi}	86.82 (4)	Mo2—O7—Ce1 ^{xxii}	160.55 (13)
O3 ^{xiii} —Ce4—Ce1 ^{xxi}	93.18 (4)	Ce1 ^{xx} —O7—Ce1 ^{xxii}	84.94 (6)
Ce2—Ce4—Ce1 ^{xxi}	58.866 (3)	Mo3—O8—Mo4 ^{xv}	87.45 (7)
Ce2 ^{xii} —Ce4—Ce1 ^{xxi}	121.134 (3)	Mo3—O8—Ce3	101.26 (6)
Ce1 ^{xvi} —Ce4—Ce1 ^{xxi}	180.000 (3)	Mo4 ^{xv} —O8—Ce3	132.81 (8)
O6 ^{xii} —Ce4—Ce1 ^{xxiv}	113.22 (5)	Mo3—O8—Ce1	113.93 (8)
O6—Ce4—Ce1 ^{xxiv}	66.78 (5)	Mo4 ^{xv} —O8—Ce1	105.34 (6)
O3—Ce4—Ce1 ^{xxiv}	93.18 (4)	Ce3—O8—Ce1	112.60 (7)
O3 ^{xii} —Ce4—Ce1 ^{xxiv}	86.82 (4)	Mo4 ⁱⁱ —O9—Mo4 ^{xviii}	180.000 (11)
O3 ⁱⁱ —Ce4—Ce1 ^{xxiv}	144.81 (4)	Mo4 ⁱⁱ —O9—Mo4	97.211 (10)
O3 ^{xiii} —Ce4—Ce1 ^{xxiv}	35.19 (4)	Mo4 ^{xviii} —O9—Mo4	82.789 (10)
Ce2—Ce4—Ce1 ^{xxiv}	121.134 (3)	Mo4 ⁱⁱ —O9—Mo4 ^{xxiii}	82.789 (10)
Ce2 ^{xii} —Ce4—Ce1 ^{xxiv}	58.866 (3)	Mo4 ^{xviii} —O9—Mo4 ^{xxiii}	97.211 (10)
Ce1 ^{xvi} —Ce4—Ce1 ^{xxiv}	74.878 (4)	Mo4—O9—Mo4 ^{xxiii}	180.000 (11)
Ce1 ^{xxi} —Ce4—Ce1 ^{xxiv}	105.122 (4)	Mo4 ⁱⁱ —O9—Ce3 ^v	94.201 (6)
O6 ^{xii} —Ce4—Ce1 ^{xxvi}	66.78 (5)	Mo4 ^{xviii} —O9—Ce3 ^v	85.799 (6)
O6—Ce4—Ce1 ^{xxvi}	113.22 (5)	Mo4—O9—Ce3 ^v	94.201 (6)
O3—Ce4—Ce1 ^{xxvi}	86.82 (4)	Mo4 ^{xxiii} —O9—Ce3 ^v	85.799 (6)
O3 ^{xii} —Ce4—Ce1 ^{xxvi}	93.18 (4)	Mo4 ⁱⁱ —O9—Ce3 ^{xxiv}	85.799 (6)
O3 ⁱⁱ —Ce4—Ce1 ^{xxvi}	35.19 (4)	Mo4 ^{xviii} —O9—Ce3 ^{xxiv}	94.201 (6)
O3 ^{xiii} —Ce4—Ce1 ^{xxvi}	144.81 (4)	Mo4—O9—Ce3 ^{xxiv}	85.799 (6)
Ce2—Ce4—Ce1 ^{xxvi}	58.866 (3)	Mo4 ^{xxiii} —O9—Ce3 ^{xxiv}	94.201 (6)
Ce2 ^{xii} —Ce4—Ce1 ^{xxvi}	121.134 (3)	Ce3 ^v —O9—Ce3 ^{xxiv}	180.000 (5)
Ce1 ^{xvi} —Ce4—Ce1 ^{xxvi}	105.122 (4)	Mo4 ^v —O10—Mo5 ^{xiv}	81.78 (6)
Ce1 ^{xxi} —Ce4—Ce1 ^{xxvi}	74.878 (4)	Mo4 ^v —O10—Mo2	78.26 (6)
Ce1 ^{xxiv} —Ce4—Ce1 ^{xxvi}	180.000 (3)	Mo5 ^{xiv} —O10—Mo2	82.62 (6)
O2—Mo1—O2 ⁱⁱ	92.35 (10)	Mo4 ^v —O10—Li	162.57 (9)
O2—Mo1—O4 ⁱⁱ	167.83 (8)	Mo5 ^{xiv} —O10—Li	100.44 (7)
O2 ⁱⁱ —Mo1—O4 ⁱⁱ	88.28 (7)	Mo2—O10—Li	84.86 (6)
O2—Mo1—O4	88.28 (7)	Mo4 ^v —O10—Ce1 ^{vi}	100.54 (7)
O2 ⁱⁱ —Mo1—O4	167.83 (8)	Mo5 ^{xiv} —O10—Ce1 ^{vi}	111.85 (7)
O4 ⁱⁱ —Mo1—O4	88.58 (10)	Mo2—O10—Ce1 ^{vi}	165.29 (8)
O2—Mo1—O1	83.18 (7)	Li—O10—Ce1 ^{vi}	94.68 (6)
O2 ⁱⁱ —Mo1—O1	83.18 (7)	Mo5—O11—Mo3	82.47 (8)
O4 ⁱⁱ —Mo1—O1	84.83 (7)	Mo5—O11—Mo3 ⁱⁱ	82.47 (8)
O4—Mo1—O1	84.83 (7)	Mo3—O11—Mo3 ⁱⁱ	82.19 (8)
O2—Mo1—Mo3 ⁱⁱ	142.09 (6)	Mo5—O11—Ce1 ⁱⁱ	100.65 (7)
O2 ⁱⁱ —Mo1—Mo3 ⁱⁱ	93.36 (5)	Mo3—O11—Ce1 ⁱⁱ	176.28 (11)
O4 ⁱⁱ —Mo1—Mo3 ⁱⁱ	49.89 (5)	Mo3 ⁱⁱ —O11—Ce1 ⁱⁱ	96.162 (13)
O4—Mo1—Mo3 ⁱⁱ	93.59 (5)	Mo5—O11—Ce1	100.65 (7)
O1—Mo1—Mo3 ⁱⁱ	134.71 (5)	Mo3—O11—Ce1	96.162 (13)
O2—Mo1—Mo3	93.36 (5)	Mo3 ⁱⁱ —O11—Ce1	176.28 (11)
O2 ⁱⁱ —Mo1—Mo3	142.09 (6)	Ce1 ⁱⁱ —O11—Ce1	85.28 (6)

O4 ⁱⁱ —Mo1—Mo3	93.59 (5)	Mo5—O11—Ce3 ^v	179.63 (10)
O4—Mo1—Mo3	49.89 (5)	Mo3—O11—Ce3 ^v	97.25 (8)
O1—Mo1—Mo3	134.71 (5)	Mo3 ⁱⁱ —O11—Ce3 ^v	97.25 (8)
Mo3 ⁱⁱ —Mo1—Mo3	60.821 (10)	Ce1 ⁱⁱ —O11—Ce3 ^v	79.62 (6)
O2—Mo1—Mo2 ⁱⁱ	95.29 (6)	Ce1—O11—Ce3 ^v	79.62 (6)
O2 ⁱⁱ —Mo1—Mo2 ⁱⁱ	49.58 (6)	Ce2—O12—Ce3 ^v	113.01 (11)
O4 ⁱⁱ —Mo1—Mo2 ⁱⁱ	94.36 (5)	Ce2—O12—Ce1 ⁱⁱ	109.67 (6)
O4—Mo1—Mo2 ⁱⁱ	142.46 (6)	Ce3 ^v —O12—Ce1 ⁱⁱ	107.36 (6)
O1—Mo1—Mo2 ⁱⁱ	132.72 (5)	Ce2—O12—Ce1	109.67 (6)
Mo3 ⁱⁱ —Mo1—Mo2 ⁱⁱ	61.651 (7)	Ce3 ^v —O12—Ce1	107.36 (6)
Mo3—Mo1—Mo2 ⁱⁱ	92.568 (10)	Ce1 ⁱⁱ —O12—Ce1	109.69 (11)
O2—Mo1—Mo2	49.58 (6)		

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