STRUCTURAL CHEMISTRY

ISSN 2053-2296

Synthesis and characterization of the 'Japanese rice-ball'-shaped Molybdenum Blue $Na_4[Mo_2O_2(OH)_4(C_6H_4NO_2)_2]_2[Mo_{120}Ce_6O_{366}H_{12}(OH)_2(H_2O)_{76}]{\sim}200H_2O$

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Received 13 February 2022
Accepted 24 March 2022

Edited by A. R. Kennedy, University of Strathclyde, United Kingdom

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Keywords: polyoxomolybdate; cerium; hybrid organic–inorganic; nanocluster; crystal structure; Molybdenum Blue.

CCDC reference: 2161749

Supporting information: this article has supporting information at journals.iucr.org/c

The hybridized lanthanide-containing molybdenum blue (**Ln-MB**) wheel $Na_4[Mo_2O_2(OH)_4(C_6H_4NO_2)_2]_2[Mo_{120}Ce_6O_{366}H_{12}(OH)_2(H_2O)_{76}]{\sim}200H_2O$ ($\{Mo_2(C_6H_4NO_2)_2\}_2\{Mo_{120}Ce_6\}$) was assembled in an aqueous one-pot synthesis. The **Ln-MB** was hybridized with 2-picolinic acid through the generation of the organometallic counter-ion $[Mo_2O_2(OH)_4(C_6H_4NO_2)_2]^{2+}$. Control experiments demonstrated that the position of the carboxylic acid group (2-position to the N atom) in the hybridization component is critical in yielding single crystals of **Ln-MB**. In addition to single-crystal X-ray diffraction (XRD) analysis, which revealed a 'Japanese rice-ball'-shaped **Ln-MB** as the anion, elemental analyses, IR spectroscopy, and thermogravimetric analysis (TGA) were performed to confirm its structure and composition. Bond-valence-sum calculations (BVS) revealed that $\{Mo_2(C_6H_4NO_2)_2\}_2\{Mo_{120}Ce_6\}$ is composed of a 24-electron reduced anionic ring, which was confirmed by Vis–NIR spectroscopy.

1. Introduction

Polyoxometalates (POMs) are polynuclear oxo-bridged metal oxide clusters primarily composed of early transition metals in their highest oxidation states (Pope, 1987; Gumerova & Rompel, 2020). The early transition-metal ions (M^{n+}) are commonly $Mo^{V/VI}$, $W^{V/VI}$, $V^{IV/V}$, Nb^V, or Ta^V, which form $\{MO_x\}$ (x = 4–7) polyhedra that are typically linked together *via* corner- and edge-shared O atoms (Pope, 1987). Their structural diversity (size, shape, and composition) and unique properties give rise to a plethora of potential applications from medicine (Stephan *et al.*, 2013; Yamase, 2005; Bijelic *et al.*, 2019; Tanuhadi *et al.*, 2020) to catalysis (Al-Sayed *et al.*, 2021; Chen *et al.*, 2021) and macromolecular crystallography (Bijelic *et al.*, 2015; Mauracher *et al.*, 2014*a*,*b*; Breibeck *et al.*, 2019).

Molybdenum Blues (**MB**s) are giant POMs with the general formula $[X_aY_bH_cMo^{VI}{}_xMo^{V}{}_yO_z(H_2O)_v]^{n-}$ (a = number of organic ligands; b = number of metallic heteroelements; c = degree of protonation; x and y = number of unreduced and reduced molybdenum, respectively; z = number of O atoms; v = number of coordinated water; n = resulting charge of the nanosized scaffold) (Al-Sayed & Rompel, 2022), with versatile topologies and high structural flexibility. **MB**s are commonly constructed by generating and combining the virtual building blocks $\{MoO_6\}$ ($\{Mo_1\}$) and $\{Mo_2O_{11}\}$ ($\{Mo_2\}$), and the fundamental building block $\{Mo_8O_{35}\}$ ($\{Mo_8\}$) with the pentagonal unit $\{MoO_7Mo_5O_{20}\}$ ($\{Mo(Mo)_5\}$) (Müller & Gouzerh, 2012). $\{Mo_1\}$, $\{Mo_2\}$, and $\{Mo_8\}$ are formed upon acidification

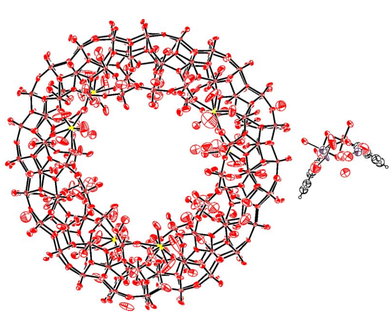

Table 1
List of purely inorganic and hybridized inorganic–organic lanthanide-containing Molybdenum Blue wheels exhibiting a 'Japanese rice-ball' shape [based on the Inorganic Crystal Structure Database (FIZ, Karlsruhe; http://www.fiz-informationsdienste.de/DB/icsd/www-recherche.htm) and the Cambridge Structural Database (CSD; Groom *et al.*, 2016), January 2022].

Formula	Building blocks of the 'Japanese rice-ball'	Reference
$Na_6[Mo_{120}O_{366}(H_2O)_{48}H_{12}\{Pr(H_2O)_5\}_6]$	12 $\{Mo_1\}$, 6 $\{Mo_2\}$, 12 $\{Mo_8\}$, 6 {Pr}	Müller *et al.* (2000)
$Na_6[Mo_{120}Ce_6O_{366}H_{12}(H_2O)_{78}]$	12 $\{Mo_1\}$, 6 $\{Mo_2\}$, 12 $\{Mo_8\}$, 6 {Ce}	Duros *et al.* (2017)
$[NH_4]_4[Mo_{120}O_{366}H_{14}(H_2O)_{48}\{La(H_2O)_5\}_6]$	12 $\{Mo_1\}$, 6 $\{Mo_2\}$, 12 $\{Mo_8\}$, 6 {La}	Yamase *et al.* (2006)
$(C_5H_{14}N_2O_2)_2[\{Mo_8O_{26}\}_{0.5}\subset H_{12}Mo_{124}Ce_4O_{376}(H_2O)_{60}$-$(C_5H_{13}N_2O_2)_6]$	12 $\{Mo_1\}$, 8 $\{Mo_2\}$, 12 $\{Mo_8\}$, 4 {Ce}	Xuan *et al.* (2019)
$Na_2(C_{10}H_{17}N_5O_4)[Mo_{122}Ce_5O_{371}(H_2O)_{69}H_{12}(C_{10}H_{16}N_5O_4)_3]$	12 $\{Mo_1\}$, 7 $\{Mo_2\}$, 12 $\{Mo_8\}$, 5 {Ce}	She *et al.* (2021)

(pH $\leq$ 4.5) (Shishido & Ozeki, 2008) of an orthomolybdate ($[MoO_4]^{2-}$) solution ($\sim$20–30 m*M* for lanthanide-containing MBs in a one-pot synthesis approach) and subsequent addition of a reducing agent (*e.g.* N_2H_4 with $c \sim 1$ m*M*) (Müller & Roy, 2002).

The coordinative attachment of organic ligands onto $\{Mo_2\}$ building blocks, the $\{Mo_2\}$ substitution by metal ions of suitable size, such as lanthanide ions (**Ln^{III}**), and the incorporation of long-chain organic surfactants as charge-balancing cations enable structural modifications and changes in the physical properties (*e.g.* solubility) of the MB cluster. The modifications include organically functionalized nanocavities, which allow the stabilization of anionic templates in their centre *via* hydrogen bonds, as well as the construction of molecular shapes ('Japanese rice-ball', 'egg' and ellipsoid) that deviate from the $\{Mo_{154-x}\}$ (x = number of defect sites) wheels (circle-shaped) (Al-Sayed & Rompel, 2022). The introduction of long-chain organic surfactants (*e.g.*, didodecyldimethylammonium, DDMA) increases the hydrophobicity and allows the polarity of the cluster to be modulated (Polarz *et al.*, 2001; Jing *et al.*, 2013). The **Ln-MB** crystal structure library is rather small, with about 30 crystal structures of **Ln-MB** ring systems (of which five are 'Japanese rice-ball'-shaped **Ln-MB**s; Table 1) reported to date (as of January 2022).

Previously, tryptophan has been utilized as a hybridizing ligand for functionalizing the inner ring of an ellipsoidal **Ln-MB**, yielding the cluster $\{Mo_{124}Ce_4(\text{tryptophan})_4\}$, featuring unprecedented kynurenine counter-cations as a result of tryptophan oxidation (Xuan *et al.*, 2018) that occurred *in situ* during the self-assembly of $\{Mo_{124}Ce_4(\text{tryptophan})_4\}$. Following the kynurenine pathway (Tan *et al.*, 2012), which is a metabolic pathway and starts with the oxidation of tryptophan, the catabolite 2-picolinic acid was identified as a bidentate chelating agent. Herein 2-picolinic acid is utilized as an $\{Mo_2\}$-hybridizing ligand, yielding the isolation of the new **Ln-MB** $Na_4[Mo_2O_2(OH)_4(C_6H_4NO_2)_2]_2[Mo_{120}Ce_6O_{366}H_{12}(OH)_2(H_2O)_{76}]\sim 200H_2O$ featuring the organometallic counter-cation $[Mo_2O_2(OH)_4(C_6H_4NO_2)_2]^{2+}$.

2. Experimental

2.1. Synthesis and crystallization

25 ml of a 3.6 m*M* Ce^{III} stock solution [0.9 mmol $CeCl_3\cdot 7H_2O$ (0.335 g) dissolved in 250 ml H_2O] were combined with 25 ml of a 40 m*M* $[MoO_4]^{2-}$ stock solution [10 mmol $Na_2MoO_4\cdot 2H_2O$ (2.42 g) dissolved in 250 ml H_2O]. Following the addition of 2-picolinic acid (0.14 mmol, 0.0172 g), the solution was reduced with 0.5 ml of an aqueous hydrazine ($[N_2H_4]\cdot 2HCl$) solution (0.1 *M*), acidified with 4.5 ml $HClO_4$ (1 *M*) to pH $\sim$1.4, and subsequently heated between 85–90 °C for 1.5 h in an Erlenmeyer flask covered with a watch glass. The resulting clear deep-blue solution was left to crystallize in the open Erlenmeyer flask for two weeks at room temperature. Deep-blue block-shaped crystals were filtered off, washed with ice-cold H_2O and air-dried (yield: 45 mg, 22.5%, based on Mo). Elemental analysis calculated (%): C 1.18, H 2.44, N 0.23, Na 0.38, Mo 48.77, Ce 3.45; found: C 1.37, H 1.45, N 0.39, Na 0.35, Mo 51.5, Ce 4.0. FT–IR (cm^{-1}): 3252 (*br*), 1606 (*m*), 1411 (*m*), 1092 (*m*), 967 (*m*), 904 (*m*), 866 (*m*), 806 (*s*), 746 (*s*), 620 (*s*), 528 (*s*).

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. C—H bond lengths were constrained to 0.95 Å for pyridine-2-carboxylate C—H groups and refined in riding modes, with U_{iso}(H) values set to $1.2U_{eq}$(C). SADI (equal distance) restraints were applied to the C—N and C—C bonds of one pyridine-2-carboxylate ring (N2—C7, C8—C7, C9—C8, C10—C9, C10—C11 and N2—C11) and to the C—O bonds C12—O224 and C6—O225. The bond between the aromatic carbon C1 and the carboxylate carbon C6 (C1—C6) was restrained to 1.43 (2) Å. In addition, all C atoms and some O atoms of the nanoring had to be refined using the constraint of equivalent anisotropic displacement parameters (EADP). One of two sodium ions in the asymmetric unit was refined with two positions (Na2 and Na3), each with 0.5 occupation factor. The refining of (disordered) H_2O molecules with positioned H atoms proved unachievable due to the high number of (disordered) H_2O molecules. Residual electron density arising from disordered H_2O molecules could be identified during crystal structure refinement. Considering the disorder of the H_2O molecules preventing a satisfactory refinement the corresponding electron densities were described employing a solvent mask to stabilize the refinement, and the quantity of H_2O molecules determined with TGA was entered into the CIF file.

2.3. Elemental analyses

The content of C/H/N/O was determined using an EA 1108 CHNS-O elemental analyzer from Carlo Erba Instruments at

Table 2
Experimental details.

Crystal data	
Chemical formula	$Na_4[Mo_2O_2(OH)_4(C_6H_4NO_2)_2]_2$-$[Mo_{120}Ce_6O_{366}H_{12}(OH)_2$-$(H_2O)_{76}]$~$200H_2O$
M_r	24391.76
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	200
a, *b*, *c* (Å)	54.272 (10), 38.896 (7), 31.734 (6)
β (°)	112.145 (4)
V (Å^3)	62047 (19)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	2.97
Crystal size (mm)	0.18 × 0.15 × 0.08
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.583, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	373860, 32484, 23243
R_{int}	0.101
θ_{max} (°)	20.9
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.502
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.083, 0.234, 1.07
No. of reflections	32484
No. of parameters	2814
No. of restraints	239
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	3.03, −2.19

Computer programs: *APEX2* (Bruker, 2016), *SAINT* (Bruker, 2016), *SHELXT2018* (Sheldrick, 2015*a*), *PLATON* (Spek, 2020), *SHELXL2018* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009), *DIAMOND* (Brandenburg, 2006) and *shelXle* (Hübschle *et al.*, 2011).

the Mikroanalytisches Laboratorium, Faculty of Chemistry, University of Vienna. The determination of Na/Mo/Ce was performed by Technische Universität Hamburg, Zentrallabor Chemische Analytik, Hamburg, Germany.

2.4. Vis–NIR spectroscopy

Vis–NIR spectroscopy was carried out at 298 K on a Shimadzu UV-2401PC spectrophotometer using a quartz cuvette with a 1.0 cm optical path length.

2.5. Thermogravimetric analysis (TGA)

TGA was conducted using a thermal analyzer (TA instruments model Q50, USA). The sample, having an initial mass of ~15 mg, was subjected to a temperature range of 298–1173 K at a heating rate of 5 K min^{-1}.

2.6. Attenuated total reflectance Fourier-transform infrared spectroscopy (ATR FT–IR)

All FT–IR spectra were recorded on a Bruker Vertex 70 IR spectrometer equipped with a single-reflection diamond ATR unit. Frequencies are given in cm^{-1} and intensities are denoted as *w* = weak, *m* = medium, *s* = strong, and *br* = broad.

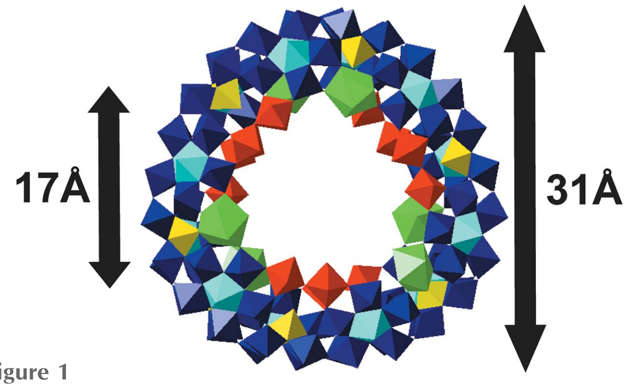

Figure 1
Polyhedral representation [and inner (left) and outer (right) diameters of the respective ring/rim] of the 'Japanese rice-ball' in $\{Mo_2(C_5H_5N)_2\}_2$-$\{Mo_{120}Ce_6\}$. Colour code: $\{MoO_6\}$ yellow, $\{Mo_2O_{11}\}$ red, $\{Mo_8O_{35}\}$ blue, with the central $\{MoO_7\}$ unit in cyan, and $\{CeO_9\}$ green.

3. Results and discussion

The 2-picolinic acid/Ce/Mo ratio (0.14/0.9/1) was critical for producing single crystals of $Na_4[Mo_2O_2(OH)_4(C_6H_4NO_2)_2]_2$-$[Mo_{120}Ce_6O_{366}H_{12}(OH)_2(H_2O)_{76}]$~$200H_2O$ ($\{Mo_2(C_6H_4NO_2)_2\}_2$-$\{Mo_{120}Ce_6\}$). When the concentration of 2-picolinic acid was lower (0.03–0.12 mol equivalents), either small weakly scattering crystals formed or the reaction solution remained clear with no crystals forming. $\{Mo_2(C_6H_4NO_2)_2\}_2\{Mo_{120}Ce_6\}$ is a 'Japanese rice-ball'-shaped complete **Ln-MB** ring system, which crystallizes in the space group *C*2/*c*. The inner and outer

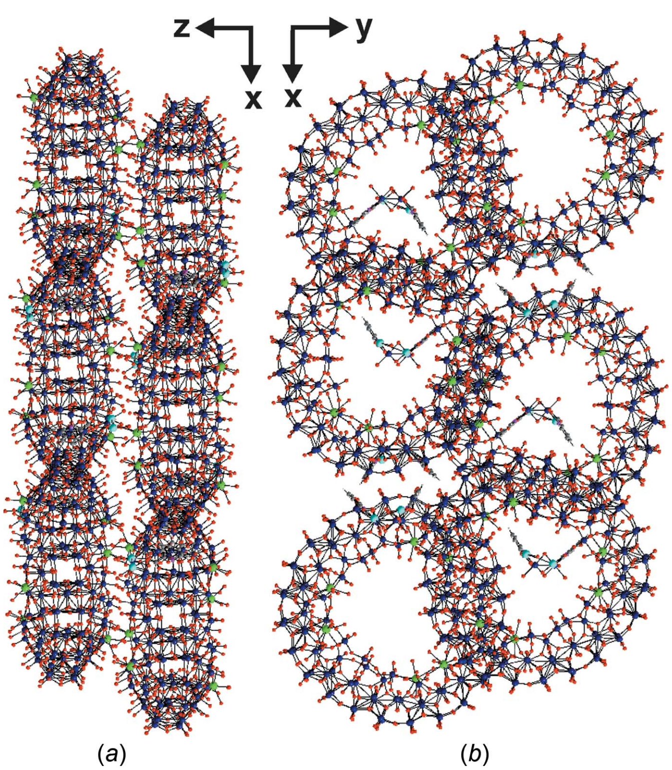

Figure 2
Ball-and-stick representation of the packing mode of $\{Mo_2(C_6H_4$-$NO_2)_2\}_2\{Mo_{120}Ce_6\}$ along the (*a*) *y* axis and (*b*) *z* axis. Colour code: Mo blue, Ce green, O red, Na turquoise, C grey, and N pink.

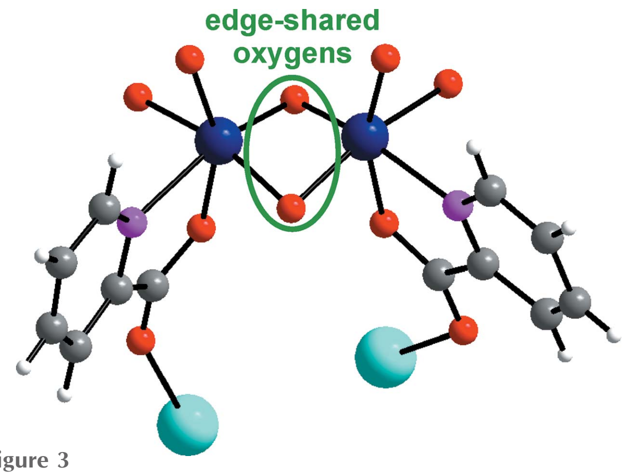

Figure 3
Ball-and-stick representation of the charge-balancing cation $[Mo_2O_2(OH)_4(C_6H_4NO_2)_2]^{2+}$ ($\{Mo_2(C_6H_4NO_2)_2\}^{2+}$) coordinated to Na^+ ions. Colour code: Mo dark blue, C grey, N pink, O red, H white, and Na turquoise.

diameters of the **Ln-MB** anion $\{Mo_{120}Ce_6\}$ are ∼17 and ∼31 Å, respectively (Fig. 1). The $\{Mo_{124}Ce_6\}$ scaffold is composed of 12 $\{Mo_1\}$, 6 $\{Mo_2\}$, 12 $\{Mo_8\}$, and 6 {Ce} (= $\{Ce^{III}O_9\}$) building units. In the 'Japanese rice-ball' $\{Mo_2(C_6H_4NO_2)_2\}_2\{Mo_{120}Ce_6\}$, six $\{Mo_2\}$ groups are replaced by six $\{Ce^{III}\}$ groups. The average size of the incorporated $\{Ce^{III}\}$ in the inner ring (O—Ce^{III}—O) is 4.8 Å, while the corner-sharing $\{Mo_2\}$ units (O—Mo—O—Mo—O) are 7.3 Å, forcing the cluster into a 'more contracted' architecture exhibiting an irregular ring shape and a lower symmetry (D_3) compared to that of the ideal circular parent structure $\{Mo_{154}\}$ (D_{7d}) (Müller *et al.*, 1996). All cerium ions on both the upper and lower surfaces of $\{Mo_{120}Ce_6\}$ are trivalent and exhibit tricapped trigonal prismatic coordination spheres (Fig. 1). Each Ce^{III} ion is coordinated by five water molecules ($\{Ce^{III}(H_2O)_5\}$) and is linked to the **Ln-MB** scaffold *via* six μ_2-O atoms. The negative charge of 8− of the 'Japanese rice-ball' is balanced by two $[Mo_2O_2(OH)_4(C_6H_4NO_2)_2]^{2+}$ ($\{Mo_2(C_6H_4NO_2)_2\}^{2+}$) organometallic cations and four Na^+ ions (Fig. 2), which are located in the outer shell of the cluster. In $\{Mo_2(C_6H_4NO_2)_2\}^{2+}$, two 2-picolinic acid molecules are coordinated equatorially and axially onto both Mo^{VI} ions, which are linked together *via* monoprotonated edge-shared O atoms (Fig. 3). Control experiments revealed that neither nicotinic acid nor isonicotinic acid (both isomers of 2-picolinic acid) can yield hybridized **Ln-MB** frameworks under otherwise identical synthetic conditions.

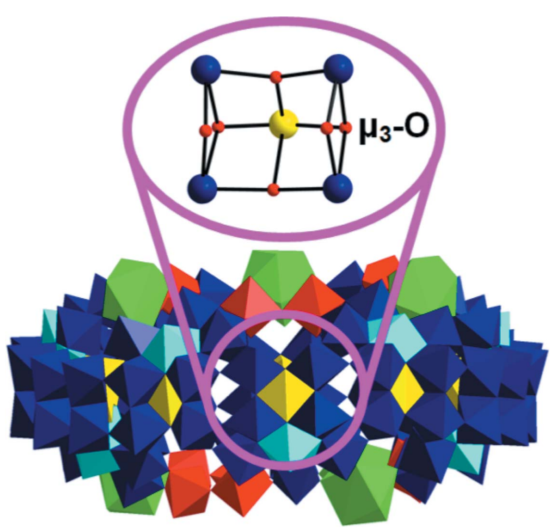

Figure 4
Polyhedral representation of $\{Mo_2(C_5H_5N)_2\}_2\{Mo_{120}Ce_6\}$, with one of 12 $\{Mo_5O_6\}$-incomplete double-cubane-type compartments highlighted in a ball-and-stick representation. Colour code: $\{MoO_6\}$ yellow, $\{Mo_2O_{11}\}$ red, $\{Mo_8O_{35}\}$ blue, with the central $\{MoO_7\}$ unit in cyan, $\{CeO_9\}$ green, Mo blue and yellow spheres, and O red spheres.

The sum formula of $\{Mo_2(C_6H_4NO_2)_2\}_2\{Mo_{120}Ce_6\}$ was determined based on single-crystal X-ray diffraction (XRD), elemental, bond-valence-sum (BVS; Brown, 1981), and thermogravimetric (TGA) analysis. Furthermore, BVS was carried out to calculate the number of Mo^V centres within the **Ln-MB** and UV–Vis–NIR spectroscopy was performed to determine the contribution of each Mo^V centre to the overall reduction state of the nanocluster. Due to the low water solubility of $\{Mo_2(C_6H_4NO_2)_2\}_2\{Mo_{120}Ce_6\}$, which is a frequently encountered problem in the case of hybridized **Ln-MB**s (Xuan *et al.*, 2019; She *et al.*, 2021), redox titration to determine the number of reduced electrons in $\{Mo_2(C_6H_4NO_2)_2\}_2\{Mo_{120}Ce_6\}$ was not feasible.

BVS calculations revealed that $\{Mo_2(C_6H_4NO_2)_2\}_2\{Mo_{120}Ce_6\}$ is constructed of a 24-electron reduced wheel containing 14 mono- and 76 diprotonated O atoms. 12 monoprotonated O atoms are the μ_3-O of the 12 $\{Mo_5O_6\}$-incomplete double-cubane-type compartments in the equatorial plane of the wheel (Fig. 4). They exhibit an average BVS value of 1.2 (= monoprotonation), consistent with previous work (Müller & Serain, 2000; Xuan *et al.*, 2018). The average BVS value of the Mo centres in the equatorial plane of the wheel spanning the 12 $\{Mo_5O_6\}$ compartments is 5.6, demonstrating the presence of two 4*d* electrons delocalized in each compartment, which is in accordance with previous work (Müller & Serain, 2000; Xuan *et al.*, 2018).

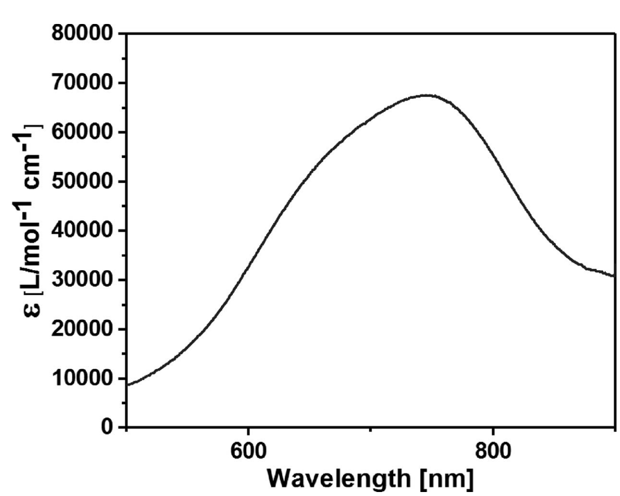

Figure 5
Vis–NIR spectrum of $\{Mo_2(C_6H_4NO_2)_2\}_2\{Mo_{120}Ce_6\}$ in 0.5 *M* H_2SO_4 (c = 1.56×10^{-5} mol l^{-1}).

Table 3
Summary of the main vibrational bands observed for $\{Mo_2(C_6H_4NO_2)_2\}_2\{Mo_{120}Ce_6\}$.

Intensities are denoted as: *w* = weak, *m* = medium, *s* = strong, and *br* = broad.

Wavenumber (cm^{-1})	Assignment
3252 (*br*)	ν(O—H) of H_2O
1606 (*m*)	δ(O—H) of H_2O
1411 (*m*)	ν(C═N) 2-picolinic acid
1092 (*m*)	ν(C—N) 2-picolinic acid
967 (*m*)	ν(Mo═O) of **Ln-MB**
904 (*m*)	ν(Mo—O—Mo) of **Ln-MB**
866 (*m*)	ν(Mo—O—Mo) of **Ln-MB**
806 (*s*)	ν(Mo—O—Mo) of **Ln-MB**
746 (*s*)	ν(Mo—O—Mo) of **Ln-MB**
620 (*s*)	ν(Mo—O—Mo) of **Ln-MB**
528 (*s*)	ν(Mo—O—Mo) of **Ln-MB**

The molar extinction coefficient (ε_M) of **Ln-MB**s around 750 nm (in aqueous medium) is associated with the total number of reduced Mo^V centres present in the nanocluster (Müller & Gouzerh, 2012). The ε_M of $\{Mo_2(C_6H_4NO_2)_2\}_2\{Mo_{120}Ce_6\}$ was determined to be 6.76×10^4 l mol^{-1} cm^{-1} (in a 0.5 *M* H_2SO_4 solution to ensure complete dissolution) which is in the range typical for 'Japanese rice-ball'-shaped **Ln-MB**s with 24 Mo^V centres (2.6–14.4×10^4 l mol^{-1} cm^{-1}) (Yamase, 2005; Duros *et al.*, 2017). Consequently, the average contribution to the determined ε_M is approximately 2.82×10^3 l mol^{-1} cm^{-1} per Mo^V centre at 745 nm (Fig. 5), which corresponds to the intervalence charge transfer between Mo^{VI} and Mo^V.

TGA was carried out to determine the number of crystal, coordinated, and structural water molecules in $\{Mo_2(C_6H_4NO_2)_2\}_2\{Mo_{120}Ce_6\}$. The obtained TG curve shows three main steps (I, II, and IV) of weight losses and one step (III) of weight increase in the range between 25 and 900 °C (Fig. 6). The first weight loss (∼13%) occurs between 25 and 110 °C, corresponding to ∼172 crystalline H_2O. The second weight loss (∼10%) takes place between 110 and 473 °C, which can be assigned to ∼104 H_2O (= 76 coordinated H_2O + 28 structure H_2O), and ∼4 2-picolinic acid ligands. The third step (III) emerges between 473 and 630 °C, and represents an increase in weight (∼1.75%) attributed to the oxidation of ∼3 2-picolinic acid ligands to 2-picolinic acid *N*-oxide by $\{Mo_2(C_6H_4NO_2)_2\}_2\{Mo_{120}Ce_6\}$, which is consistent with previous observations made for $Mo^{VI/V}$-containing POMs of the Keplerate archetype as catalysts for the conversion of picolinic acid derivatives to the corresponding *N*-oxides in excellent yields (Yang *et al.*, 2015). The fourth and last weight loss (∼75%) occurs between 635 and 900 °C, and is related to the decomposition of the metal oxide framework of **Ln-MB**.

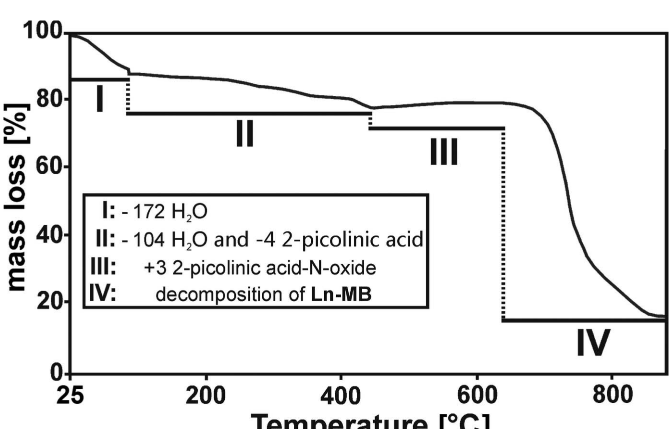

Figure 6
Thermogravimetric curve of $\{Mo_2(C_5H_5N)_2\}_2\{Mo_{120}Ce_6\}$, exhibiting three steps (I, II and IV) of weight loss and one step (III) of weight increase.

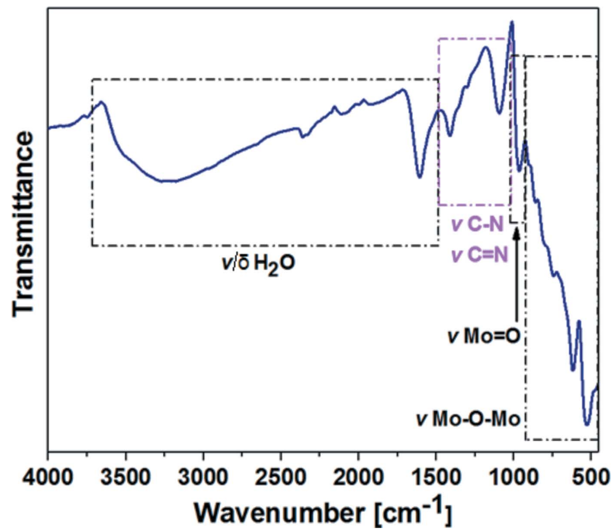

Figure 7
FT–IR spectrum of $\{Mo_2(C_6H_4NO_2)_2\}_2\{Mo_{120}Ce_6\}$ in the region between 4000 and 450 cm^{-1}.

The FT–IR spectrum of $\{Mo_2(C_6H_4NO_2)_2\}_2\{Mo_{120}Ce_6\}$ is depicted in Fig. 7, with the main vibrational bands listed in Table 3. The sharp and broad bands in the region between 1606 and 3252 cm^{-1} correspond to the stretching and bending vibrations ν/δ(O—H) of H_2O. The vibrational bands ν(C—N) and ν(C═N) of 2-picolinic acid emerge between 1092 and 1411 cm^{-1}, which are missing in a pure inorganic cerium-containing 'Japanese rice-ball' (Duros *et al.*, 2017). The vibrational bands ν(C═C) (∼1600 cm^{-1}) and ν(═C—H) (∼3000 cm^{-1}) of 2-picolinic acid are obscured as they are likely overlaid by the water bands in this particular region. The vibrational band at 967 cm^{-1}, which is very sharp and characteristic for molybdenum-based POM structures, is attributed to terminal Mo═O groups. All bands appearing below 967 cm^{-1} correspond to the deformation vibrations ν(Mo—O—Mo) of the Mo—O—Mo bridging units.

4. Conclusion

The successful construction of $\{Mo_2(C_5H_5N)_2\}_2\{Mo_{120}Ce_6\}$ enlarged the sparse crystal structure library of 'Japanese rice-ball'-shaped **Ln-MB**s. As $\{Mo_2\}$-type building blocks, resulting from the self-assembly process of **Ln-MB** clusters, are organically modifiable, grafting organic ligands onto them yields unique hybridized inorganic–organic **Ln-MB** frameworks. $\{Mo_2(C_5H_5N)_2\}_2\{Mo_{120}Ce_6\}$ is the first reported 'Japanese rice-ball'-shaped **Ln-MB** containing a metal–organic charge-balancing unit complexed aromatically with 2-picolinic acid in the outer shell.

Acknowledgements

The authors thank Mag. Johannes Theiner (Mikroanalytisches Laboratorium Universität Wien) and Dr Magnus Bo-Elfers (Technische Universität Hamburg, Zentrallabor Chemische Analytik, Hamburg, Germany) for elemental analyses. TGA measurements were carried out at the Institute of Materials Chemistry, Faculty of Chemistry, University of Vienna. ET and AR acknowledge the University of Vienna for awarding an Uni:docs fellowship.

Funding information

Funding for this research was provided by: Austrian Science Fund FWF (award No. P33089 to AR).

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supporting information

Acta Cryst. (2022). C**78**, 299-304 [https://doi.org/10.1107/S2053229622003369]

Synthesis and characterization of the `Japanese rice-ball′-shaped Molybdenum Blue $Na_4[Mo_2O_2(OH)_4(C_6H_4NO_2)_2]_2[Mo_{120}Ce_6O_{366}H_{12}(OH)_2(H_2O)_{76}]$~$200H_2O$

Emir Al-Sayed, Elias Tanuhadi, Gerald Giester and Annette Rompel

Computing details

Data collection: *APEX2* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: SHELXT2018 (Sheldrick, 2015*a*); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015*b*); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009), *DIAMOND* (Brandenburg, 2006) and *shelXle* (Hübschle *et al.*, 2011); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

(I)

Crystal data

$Ce_6Mo_{120}O_{444}\cdot 2(C_{12}H_8Mo_2N_2Na_2O_{10.5})\cdot 36(O)$
M_r = 24391.76
Monoclinic, $C2/c$
a = 54.272 (10) Å
b = 38.896 (7) Å
c = 31.734 (6) Å
β = 112.145 (4)°
V = 62047 (19) Å^3
Z = 4
$F(000)$ = 46688
D_x = 2.611 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9572 reflections
θ = 2.2–20.5°
μ = 2.97 mm^{-1}
T = 200 K
Block, dark blue
0.18 × 0.15 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed X-ray tube, Incoatec IuS
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.583, T_{max} = 0.745
373860 measured reflections
32484 independent reflections
23243 reflections with $I > 2\sigma(I)$
R_{int} = 0.101
θ_{max} = 20.9°, θ_{min} = 1.1°
h = −54→54
k = −38→38
l = −31→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.083
$wR(F^2)$ = 0.234
S = 1.07
32484 reflections
2814 parameters
239 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0756P)^2 + 9956.6523P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 3.03 e Å^{-3}
$\Delta\rho_{min}$ = −2.19 e Å^{-3}

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. 1. Fixed U_{iso} At 1.2 times of: All C(H) groups 2. Restrained distances C6—C1 1.43 with σ of 0.02 O224—C12 ~ O225—C6 with σ of 0.02 N2—C7 ~ C8—C7 ~ C9—C8 ~ C10—C9 ~ C10—C11 ~ N2—C11 with σ of 0.02 3. U_{iso}/Uaniso restraints and constraints Uanis(Na1) ~ U_{eq}: with σ of 0.01 and σ for terminal atoms of 0.02 Uanis(O223) ~ U_{eq}, Uanis(O233) ~ U_{eq}, Uanis(O234) ~ U_{eq}, Uanis(O236) ~ U_{eq}, Uanis(O225) ~ U_{eq}, Uanis(O156) ~ U_{eq}, Uanis(O195) ~ U_{eq}: with σ of 0.01 and σ for terminal atoms of 0.02 Uanis(Na3) ~ U_{eq}: with σ of 0.01 and σ for terminal atoms of 0.02 Uanis(O230) ~ U_{eq}, Uanis(Mo61) ~ U_{eq}: with σ of 0.01 and σ for terminal atoms of 0.02 Uanis(C11) ~ U_{eq}, Uanis(C10) ~ U_{eq}, Uanis(C9) ~ U_{eq}, Uanis(C8) ~ U_{eq}, Uanis(C7) ~ U_{eq}, Uanis(C1) ~ U_{eq}, Uanis(C2) ~ U_{eq}, Uanis(C3) ~ U_{eq}, Uanis(C5) ~ U_{eq}, Uanis(C4) ~ U_{eq}, Uanis(N1) ~ U_{eq}, Uanis(N2) ~ U_{eq}, Uanis(C6) ~ U_{eq}, Uanis(C12) ~ U_{eq}: with σ of 0.001 and σ for terminal atoms of 0.002 Uanis(O13) ~ U_{eq}, Uanis(O244) ~ U_{eq}, Uanis(O241) ~ U_{eq}, Uanis(O42) ~ U_{eq}, Uanis(O54) ~ U_{eq}, Uanis(O5) ~ U_{eq}, Uanis(O184) ~ U_{eq}, Uanis(O120) ~ U_{eq}, Uanis(O146) ~ U_{eq}, Uanis(O202) ~ U_{eq}, Uanis(O188) ~ U_{eq}: with σ of 0.001 and σ for terminal atoms of 0.002 Uanis(O239) ~ U_{eq}: with σ of 0.01 and σ for terminal atoms of 0.02 Uanis(C6) = Uanis(C1) = Uanis(C2) Uanis(O63) = Uanis(O39) = Uanis(O67) Uanis(O228) = Uanis(O229) = Uanis(O230) = Uanis(O224) Uanis(O207) = Uanis(O206) = Uanis(O205) = Uanis(O215) Uanis(O66) = Uanis(O42) Uanis(O86) = Uanis(O65) = Uanis(O122) Uanis(O180) = Uanis(O157) = Uanis(O200) Uanis(O58) = Uanis(O40) Uanis(O231) = Uanis(O230) = Uanis(O227) Uanis(O231) = Uanis(O186) Uanis(O227) = Uanis(O226) Uanis(O226) = Uanis(O227) Uanis(C7) = Uanis(C8) = Uanis(C10) = Uanis(C9) Uanis(C2) = Uanis(C3) Uanis(C11) = Uanis(C12) Uanis(O169) = Uanis(O171) Uanis(Na2) = Uanis(Na1) Uanis(C4) = Uanis(C5) Uanis(O192) = Uanis(O187) Uanis(O212) = Uanis(O193) = Uanis(O178) Uanis(C10) = Uanis(C11) = Uanis(C12) Uanis(O161) = Uanis(O149) 4. Others Fixed Sof: Na2 (1/2) O226 (1/2) O227 (1/2) O234 (1/2) Na3 (1/2) O239 (1/2) 5.a Aromatic/amide H refined with riding coordinates: C2(H2), C3(H3), C4(H4), C5(H5), C7(H7), C8(H8), C9(H9), C10(H10)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ce1	0.58639 (3)	0.53787 (5)	0.43521 (7)	0.0564 (5)	
Ce2	0.37593 (3)	0.82743 (4)	0.45086 (7)	0.0531 (5)	
Ce3	0.33459 (3)	0.93214 (4)	0.06681 (7)	0.0516 (5)	
Mo1	0.48296 (4)	0.38871 (6)	0.31290 (10)	0.0447 (7)	
Mo2	0.46586 (5)	0.46146 (6)	0.13819 (10)	0.0447 (7)	
Mo3	0.50700 (5)	0.52694 (8)	0.41985 (12)	0.0698 (10)	
Mo4	0.47504 (4)	0.45473 (6)	0.37199 (9)	0.0401 (6)	
Mo5	0.44633 (4)	0.46080 (5)	0.25719 (9)	0.0380 (6)	
Mo6	0.46397 (5)	0.58890 (7)	0.45056 (12)	0.0624 (9)	
Mo7	0.43043 (5)	0.51227 (7)	0.37419 (11)	0.0530 (8)	
Mo8	0.41478 (4)	0.42171 (5)	0.32228 (10)	0.0431 (7)	
Mo9	0.38857 (4)	0.41868 (6)	0.20919 (10)	0.0441 (7)	
Mo10	0.37651 (5)	0.50004 (6)	0.14689 (11)	0.0533 (8)	
Mo11	0.33248 (4)	0.47067 (6)	0.21197 (10)	0.0454 (7)	
Mo12	0.36170 (4)	0.48004 (6)	0.32547 (10)	0.0439 (7)	
Mo13	0.35384 (5)	0.55385 (6)	0.26393 (10)	0.0444 (7)	
Mo14	0.31214 (4)	0.55032 (6)	0.31881 (10)	0.0421 (7)	
Mo15	0.34715 (5)	0.62961 (6)	0.37026 (11)	0.0517 (8)	
Mo16	0.41840 (6)	0.65631 (8)	0.43334 (18)	0.1126 (18)	
Mo17	0.34891 (5)	0.58405 (7)	0.08514 (10)	0.0535 (8)	
Mo18	0.32257 (4)	0.53989 (6)	0.14878 (9)	0.0418 (7)	
Mo19	0.32522 (6)	0.67426 (7)	0.06394 (12)	0.0620 (9)	

Mo20	0.30069 (5)	0.62060 (6)	0.14146 (10)	0.0453 (7)
Mo21	0.28350 (4)	0.54493 (6)	0.20562 (10)	0.0406 (7)
Mo22	0.36674 (5)	0.72166 (7)	0.42358 (12)	0.0656 (9)
Mo23	0.30514 (5)	0.69365 (6)	0.36306 (10)	0.0448 (7)
Mo24	0.27051 (4)	0.62775 (6)	0.30685 (9)	0.0413 (7)
Mo25	0.28993 (5)	0.69528 (7)	0.24715 (9)	0.0462 (7)
Mo26	0.25062 (4)	0.62957 (6)	0.19340 (9)	0.0398 (7)
Mo27	0.30972 (7)	0.76071 (7)	0.07165 (16)	0.0874 (13)
Mo28	0.22752 (4)	0.72193 (6)	0.18720 (9)	0.0396 (6)
Mo29	0.24555 (5)	0.72256 (6)	0.30090 (9)	0.0407 (6)
Mo30	0.30721 (5)	0.77945 (6)	0.36368 (10)	0.0494 (7)
Mo31	0.26313 (5)	0.77581 (6)	0.13315 (10)	0.0440 (7)
Mo32	0.28757 (6)	0.85009 (7)	0.07493 (11)	0.0625 (9)
Mo33	0.24964 (4)	0.85937 (6)	0.13618 (8)	0.0354 (6)
Mo34	0.21771 (4)	0.81624 (5)	0.18884 (9)	0.0341 (6)
Mo35	0.28025 (4)	0.85296 (6)	0.25091 (8)	0.0366 (6)
Mo36	0.24181 (4)	0.81733 (6)	0.30209 (9)	0.0365 (6)
Mo37	0.28546 (5)	0.93025 (6)	0.14007 (9)	0.0400 (6)
Mo38	0.23420 (4)	0.91839 (6)	0.19742 (8)	0.0332 (6)
Mo39	0.25943 (4)	0.91098 (6)	0.31070 (8)	0.0337 (6)
Mo40	0.33192 (5)	0.90835 (6)	0.37620 (9)	0.0435 (7)
Mo41	0.40553 (5)	0.92635 (7)	0.43683 (11)	0.0560 (8)
Mo42	0.36042 (4)	0.98506 (6)	0.37853 (8)	0.0362 (6)
Mo43	0.29565 (4)	0.99238 (6)	0.32119 (8)	0.0359 (6)
Mo44	0.33865 (5)	0.98235 (6)	0.26297 (8)	0.0366 (6)
Mo45	0.27164 (4)	0.99897 (6)	0.20771 (8)	0.0343 (6)
Mo46	0.40470 (5)	0.98770 (7)	0.08821 (11)	0.0576 (8)
Mo47	0.35881 (5)	1.01721 (6)	0.14717 (9)	0.0434 (7)
Mo48	0.32473 (4)	1.06065 (6)	0.21232 (9)	0.0362 (6)
Mo49	0.35294 (4)	1.05953 (6)	0.32562 (8)	0.0356 (6)
Mo50	0.41901 (4)	1.00861 (6)	0.37680 (9)	0.0378 (6)
Mo51	0.47009 (5)	0.93991 (7)	0.42472 (11)	0.0569 (8)
Mo52	0.53362 (5)	0.96248 (7)	0.42945 (11)	0.0575 (8)
Mo53	0.41628 (4)	1.09388 (6)	0.32479 (9)	0.0375 (6)
Mo54	0.44274 (5)	1.04829 (6)	0.26279 (9)	0.0427 (7)
Mo55	0.38572 (4)	1.10226 (6)	0.21162 (9)	0.0377 (6)
Mo56	0.41179 (4)	1.06105 (6)	0.14759 (9)	0.0382 (6)
Mo57	0.47011 (5)	1.04304 (6)	0.14118 (10)	0.0459 (7)
Mo58	0.51767 (4)	1.11376 (6)	0.18527 (9)	0.0381 (6)
Mo59	0.45386 (4)	1.12096 (5)	0.20209 (9)	0.0361 (6)
Mo60	0.45209 (4)	0.38932 (5)	0.19988 (10)	0.0436 (7)
O1	0.3270 (3)	1.0754 (4)	0.2713 (7)	0.048 (5)
O2	0.4357 (3)	1.1524 (4)	0.1668 (6)	0.048 (5)
O253	0.4968 (3)	1.0761 (5)	0.1486 (6)	0.049 (5)
O4	0.4519 (4)	1.0740 (5)	0.0737 (6)	0.053 (5)
O5	0.4743 (4)	1.0119 (5)	0.1067 (6)	0.049 (5)
O6	0.4486 (3)	1.0796 (4)	0.1616 (6)	0.033 (4)
O7	0.4818 (4)	1.0241 (5)	0.1930 (8)	0.061 (6)

O8	0.4723 (3)	1.0745 (4)	0.2572 (6)	0.036 (4)
O9	0.3978 (3)	1.0894 (5)	0.1059 (6)	0.048 (5)
O10	0.4302 (3)	1.0295 (4)	0.1203 (6)	0.048 (5)
O11	0.3775 (3)	1.1370 (4)	0.1780 (7)	0.052 (6)
O12	0.4217 (3)	1.0940 (4)	0.2040 (6)	0.045 (5)
O13	0.4017 (3)	1.1209 (4)	0.2693 (5)	0.029 (4)
O14	0.4494 (3)	1.0871 (4)	0.3108 (6)	0.044 (5)
O15	0.4272 (3)	1.1262 (4)	0.3635 (6)	0.043 (5)
O16	0.4574 (4)	1.0157 (4)	0.2992 (6)	0.051 (5)
O17	0.4072 (3)	1.0560 (4)	0.2658 (6)	0.033 (4)
O18	0.4317 (3)	1.0290 (4)	0.2097 (6)	0.045 (5)
O19	0.3812 (3)	1.0630 (4)	0.1682 (6)	0.034 (4)
O20	0.3882 (3)	1.0209 (4)	0.1217 (6)	0.045 (5)
O21	0.4282 (4)	0.9680 (5)	0.1631 (7)	0.059 (6)
O22	0.3883 (4)	1.0063 (5)	0.0353 (6)	0.052 (5)
O23	0.3831 (4)	0.9552 (4)	0.0870 (6)	0.046 (5)
O24	0.3395 (4)	1.0546 (6)	0.0852 (7)	0.065 (6)
O25	0.3780 (3)	0.9936 (5)	0.1931 (8)	0.064 (6)
O26	0.3540 (3)	1.0899 (4)	0.2165 (6)	0.038 (5)
O27	0.3810 (3)	1.0844 (4)	0.3233 (5)	0.033 (4)
O28	0.4268 (3)	1.0518 (4)	0.3626 (6)	0.045 (5)
O29	0.5204 (5)	0.9415 (8)	0.3612 (8)	0.103 (9)
O30	0.5678 (4)	0.9666 (6)	0.4201 (8)	0.074 (7)
O31	0.5460 (7)	0.9880 (7)	0.4803 (10)	0.139 (14)
O32	0.5410 (4)	0.9215 (5)	0.4524 (8)	0.065 (6)
O33	0.4983 (4)	0.9660 (5)	0.4187 (9)	0.075 (7)
O34	0.4213 (4)	1.0379 (6)	0.4421 (8)	0.079 (7)
O35	0.4491 (3)	0.9903 (5)	0.4121 (6)	0.043 (5)
O36	0.4847 (4)	0.9653 (5)	0.4956 (8)	0.071 (7)
O37	0.4885 (4)	0.9044 (6)	0.4511 (9)	0.081 (8)
O38	0.4121 (4)	0.9888 (5)	0.3268 (7)	0.055 (5)
O39	0.3452 (3)	1.0804 (4)	0.3652 (6)	0.040 (3)
O40	0.3787 (3)	1.0244 (4)	0.3609 (6)	0.039 (3)
O41	0.5844 (6)	0.4902 (8)	0.4852 (11)	0.129 (12)
O42	0.3577 (3)	1.0258 (4)	0.2665 (5)	0.032 (3)
O43	0.3336 (3)	1.0346 (4)	0.1659 (5)	0.034 (4)
O44	0.2976 (3)	1.0824 (4)	0.1792 (7)	0.050 (5)
O45	0.3417 (4)	0.9865 (5)	0.1067 (6)	0.054 (6)
O46	0.3371 (6)	0.9719 (8)	0.0059 (9)	0.133 (13)
O47	0.3294 (11)	0.9012 (9)	−0.0065 (15)	0.21 (2)
O48	0.2892 (6)	0.9450 (14)	0.0084 (10)	0.20 (2)
O49	0.3668 (6)	0.8833 (7)	0.0810 (12)	0.127 (12)
O50	0.3563 (5)	0.9172 (6)	0.1522 (9)	0.091 (8)
O51	0.3086 (3)	1.0165 (4)	0.2216 (6)	0.036 (4)
O52	0.3444 (3)	0.9609 (4)	0.2215 (6)	0.043 (5)
O53	0.3599 (3)	0.9629 (4)	0.3140 (5)	0.027 (4)
O54	0.3325 (3)	1.0138 (4)	0.3246 (6)	0.038 (4)
O55	0.4550 (5)	0.9273 (5)	0.3705 (9)	0.084 (8)

O56	0.4394 (4)	0.9286 (5)	0.4434 (8)	0.065 (6)
O57	0.3988 (3)	0.9744 (4)	0.4017 (6)	0.046 (5)
O58	0.3569 (3)	1.0068 (4)	0.4219 (6)	0.039 (3)
O59	0.4096 (4)	0.9445 (5)	0.4901 (6)	0.055 (5)
O60	0.3994 (4)	0.9089 (5)	0.3633 (7)	0.061 (6)
O61	0.3995 (3)	0.8853 (5)	0.4424 (7)	0.057 (6)
O62	0.3665 (3)	0.9374 (4)	0.4061 (6)	0.038 (4)
O63	0.2919 (3)	1.0182 (4)	0.3616 (6)	0.040 (3)
O64	0.3248 (3)	0.9610 (4)	0.3580 (6)	0.032 (4)
O65	0.2752 (3)	1.0141 (4)	0.2669 (6)	0.037 (3)
O66	0.3044 (3)	0.9630 (4)	0.2618 (5)	0.032 (3)
O67	0.2527 (3)	1.0305 (4)	0.1754 (6)	0.040 (3)
O68	0.2801 (3)	0.9713 (4)	0.1617 (6)	0.038 (4)
O69	0.3015 (4)	0.9401 (5)	0.1030 (7)	0.052 (5)
O70	0.3104 (5)	0.8790 (6)	0.0684 (9)	0.084 (8)
O71	0.2473 (4)	0.9481 (5)	0.0788 (6)	0.052 (5)
O72	0.3095 (3)	0.9120 (4)	0.1854 (6)	0.047 (5)
O73	0.3228 (4)	0.9307 (5)	0.4360 (7)	0.055 (5)
O74	0.3405 (3)	0.8985 (5)	0.3306 (6)	0.046 (5)
O75	0.2720 (4)	0.9578 (4)	0.3155 (6)	0.046 (5)
O76	0.2469 (3)	0.9638 (4)	0.2047 (6)	0.036 (4)
O77	0.3415 (7)	0.8276 (14)	0.4902 (13)	0.21 (2)
O78	0.3870 (11)	0.7876 (8)	0.5212 (10)	0.21 (2)
O79	0.3887 (6)	0.8617 (5)	0.5235 (8)	0.097 (9)
O80	0.4221 (5)	0.8141 (7)	0.4668 (18)	0.21 (3)
O81	0.3451 (4)	0.8759 (5)	0.4145 (7)	0.050 (5)
O82	0.3760 (6)	0.8317 (7)	0.3702 (9)	0.106 (10)
O83	0.2955 (3)	0.8998 (4)	0.3517 (6)	0.036 (4)
O84	0.2434 (3)	0.9085 (4)	0.3472 (6)	0.044 (5)
O85	0.2774 (3)	0.9032 (4)	0.2540 (6)	0.033 (4)
O86	0.2305 (3)	0.9165 (4)	0.2541 (6)	0.037 (3)
O87	0.2025 (3)	0.9217 (4)	0.1600 (6)	0.041 (5)
O88	0.2534 (3)	0.9085 (4)	0.1573 (6)	0.040 (5)
O89	0.2727 (3)	0.8831 (4)	0.1083 (6)	0.035 (4)
O90	0.3198 (4)	0.8430 (6)	0.1478 (8)	0.083 (7)
O91	0.2607 (5)	0.8535 (6)	0.0235 (7)	0.074 (7)
O92	0.2990 (4)	0.8092 (4)	0.0654 (7)	0.053 (5)
O93	0.2198 (4)	0.8650 (4)	0.0927 (6)	0.047 (5)
O94	0.2666 (4)	0.8252 (4)	0.1111 (6)	0.044 (5)
O95	0.2368 (3)	0.8645 (4)	0.1910 (6)	0.035 (4)
O96	0.2855 (3)	0.8515 (4)	0.1992 (6)	0.034 (4)
O97	0.2592 (3)	0.8615 (5)	0.2936 (6)	0.044 (5)
O98	0.3107 (3)	0.8445 (4)	0.2900 (6)	0.043 (5)
O99	0.3776 (4)	0.7637 (5)	0.4299 (7)	0.062 (6)
O100	0.2950 (5)	0.7702 (6)	0.4263 (7)	0.077 (7)
O101	0.3333 (4)	0.8043 (5)	0.4007 (9)	0.082 (8)
O102	0.2774 (3)	0.8066 (4)	0.3476 (6)	0.042 (5)
O103	0.2263 (3)	0.8313 (4)	0.3369 (6)	0.044 (5)

O104	0.3130 (4)	0.7782 (4)	0.3137 (7)	0.056 (6)
O105	0.2610 (3)	0.8099 (4)	0.2465 (6)	0.045 (5)
O106	0.2137 (4)	0.8238 (4)	0.2440 (6)	0.043 (5)
O107	0.1879 (3)	0.8269 (4)	0.1492 (6)	0.047 (5)
O108	0.2400 (3)	0.8118 (4)	0.1515 (6)	0.033 (4)
O109	0.2769 (6)	0.7543 (8)	0.0071 (8)	0.106 (10)
O110	0.3317 (5)	0.7646 (5)	0.0453 (10)	0.092 (9)
O111	0.2762 (4)	0.7585 (5)	0.0947 (7)	0.060 (6)
O112	0.2233 (4)	0.7799 (6)	0.0681 (7)	0.066 (6)
O113	0.3320 (5)	0.7680 (6)	0.1317 (10)	0.096 (9)
O114	0.2901 (3)	0.7777 (4)	0.1825 (6)	0.048 (5)
O115	0.2156 (3)	0.7692 (5)	0.1895 (6)	0.048 (5)
O116	0.2355 (3)	0.7700 (5)	0.2967 (6)	0.045 (5)
O117	0.3637 (5)	0.7139 (5)	0.4760 (7)	0.073 (7)
O118	0.3279 (3)	0.7343 (4)	0.3893 (6)	0.047 (5)
O119	0.3669 (4)	0.7267 (5)	0.3506 (8)	0.063 (6)
O120	0.2822 (3)	0.7347 (4)	0.3434 (6)	0.042 (5)
O121	0.2309 (4)	0.7057 (4)	0.3339 (8)	0.060 (6)
O122	0.2226 (3)	0.7108 (4)	0.2436 (6)	0.037 (3)
O123	0.2672 (3)	0.7345 (4)	0.2461 (6)	0.040 (5)
O124	0.2001 (3)	0.7036 (4)	0.1485 (6)	0.039 (5)
O125	0.2454 (3)	0.7405 (4)	0.1479 (6)	0.041 (5)
O126	0.3088 (6)	0.7140 (5)	0.0767 (10)	0.101 (10)
O127	0.3008 (5)	0.6618 (6)	0.0133 (8)	0.084 (7)
O128	0.3480 (5)	0.6940 (5)	0.0461 (9)	0.080 (8)
O129	0.3030 (3)	0.6494 (4)	0.1003 (7)	0.042 (5)
O130	0.3541 (6)	0.6792 (9)	0.1346 (9)	0.125 (12)
O131	0.2527 (3)	0.6811 (4)	0.1999 (7)	0.046 (5)
O132	0.3052 (4)	0.7040 (5)	0.2102 (7)	0.053 (5)
O133	0.3148 (3)	0.7039 (4)	0.3014 (6)	0.039 (5)
O134	0.2703 (3)	0.6811 (4)	0.3067 (6)	0.042 (5)
O135	0.3428 (4)	0.6793 (5)	0.3908 (7)	0.057 (6)
O136	0.2942 (4)	0.6837 (5)	0.4065 (8)	0.070 (7)
O137	0.3956 (4)	0.6955 (5)	0.4326 (9)	0.075 (7)
O138	0.4179 (6)	0.6451 (9)	0.4944 (10)	0.131 (11)
O139	0.4481 (4)	0.6779 (6)	0.4576 (12)	0.128 (13)
O140	0.3376 (4)	0.6189 (6)	0.4343 (8)	0.082 (7)
O141	0.3811 (4)	0.6297 (4)	0.4079 (7)	0.057 (6)
O142	0.4123 (6)	0.6642 (8)	0.3703 (8)	0.106 (9)
O143	0.3494 (3)	0.6411 (4)	0.3204 (8)	0.056 (6)
O144	0.3063 (3)	0.6439 (4)	0.3469 (6)	0.042 (5)
O145	0.2535 (3)	0.6228 (4)	0.3427 (7)	0.047 (5)
O146	0.2444 (3)	0.6267 (4)	0.2496 (6)	0.043 (5)
O147	0.2901 (3)	0.6452 (4)	0.2504 (6)	0.037 (5)
O148	0.2191 (3)	0.6255 (5)	0.1547 (7)	0.051 (5)
O149	0.2716 (3)	0.6337 (4)	0.1548 (6)	0.040 (3)
O150	0.3442 (4)	0.6307 (6)	0.0753 (8)	0.071 (7)
O151	0.2664 (4)	0.5962 (5)	0.0797 (7)	0.060 (6)

O152	0.3260 (4)	0.6333 (5)	0.1896 (8)	0.064 (6)
O153	0.2623 (3)	0.5827 (4)	0.2033 (7)	0.042 (5)
O154	0.2850 (3)	0.5848 (4)	0.3091 (7)	0.040 (5)
O155	0.3377 (3)	0.5850 (5)	0.3584 (7)	0.051 (5)
O156	0.4319 (4)	0.6128 (5)	0.4350 (8)	0.073 (6)
O157	0.3079 (3)	0.5236 (5)	0.3563 (8)	0.062 (4)
O158	0.2889 (3)	0.5285 (4)	0.2641 (8)	0.056 (6)
O159	0.3217 (3)	0.5764 (4)	0.2606 (7)	0.045 (5)
O160	0.2623 (3)	0.5164 (4)	0.1695 (7)	0.051 (5)
O161	0.2974 (3)	0.5714 (4)	0.1644 (6)	0.040 (3)
O162	0.3224 (3)	0.5861 (4)	0.1188 (7)	0.048 (5)
O163	0.3269 (5)	0.5675 (8)	0.0356 (9)	0.105 (9)
O164	0.3796 (4)	0.5775 (5)	0.0806 (8)	0.069 (6)
O165	0.3763 (4)	0.6030 (5)	0.1594 (7)	0.057 (6)
O166	0.3502 (4)	0.5399 (5)	0.1213 (7)	0.059 (6)
O167	0.2976 (4)	0.5206 (4)	0.1069 (7)	0.056 (6)
O168	0.3544 (3)	0.5639 (4)	0.2102 (6)	0.037 (4)
O169	0.3176 (3)	0.5202 (4)	0.2055 (7)	0.041 (3)
O170	0.3786 (3)	0.5772 (4)	0.3008 (6)	0.048 (5)
O171	0.3441 (3)	0.5259 (4)	0.3127 (7)	0.041 (3)
O172	0.4620 (5)	0.6020 (7)	0.3819 (13)	0.133 (13)
O173	0.4852 (4)	0.6209 (6)	0.4743 (11)	0.109 (11)
O174	0.4637 (4)	0.5683 (6)	0.4976 (7)	0.075 (7)
O175	0.4387 (3)	0.5481 (6)	0.4078 (7)	0.065 (7)
O176	0.3509 (4)	0.4663 (5)	0.3649 (8)	0.065 (6)
O177	0.3948 (3)	0.5038 (5)	0.3628 (6)	0.044 (5)
O178	0.3335 (3)	0.4636 (4)	0.2704 (7)	0.049 (3)
O179	0.3686 (3)	0.5070 (4)	0.2653 (7)	0.044 (5)
O180	0.3036 (3)	0.4511 (5)	0.1782 (8)	0.062 (4)
O181	0.3437 (3)	0.4971 (4)	0.1678 (7)	0.044 (5)
O182	0.3953 (3)	0.5219 (4)	0.1948 (8)	0.057 (6)
O183	0.3442 (4)	0.4723 (6)	0.0840 (8)	0.077 (7)
O184	0.3915 (4)	0.5079 (6)	0.1080 (7)	0.069 (6)
O185	0.3842 (3)	0.4557 (5)	0.1626 (7)	0.047 (5)
O186	0.3575 (5)	0.4373 (6)	0.2151 (12)	0.114 (4)
O187	0.4268 (3)	0.5281 (4)	0.3211 (6)	0.040 (3)
O188	0.3839 (4)	0.4427 (5)	0.3209 (6)	0.048 (5)
O189	0.4353 (4)	0.4833 (7)	0.4406 (8)	0.089 (8)
O190	0.4915 (3)	0.5596 (4)	0.4418 (7)	0.053 (5)
O191	0.4706 (3)	0.4990 (4)	0.3969 (6)	0.037 (4)
O192	0.4356 (3)	0.4610 (4)	0.3587 (6)	0.040 (3)
O193	0.3987 (3)	0.3962 (4)	0.2672 (7)	0.049 (3)
O194	0.4130 (3)	0.4591 (4)	0.2637 (7)	0.046 (5)
O195	0.3771 (3)	0.3838 (4)	0.1753 (7)	0.045 (5)
O196	0.4422 (3)	0.4904 (4)	0.2148 (7)	0.042 (5)
O197	0.4272 (3)	0.4190 (4)	0.2162 (7)	0.043 (5)
O198	0.4653 (3)	0.4822 (4)	0.3076 (6)	0.037 (5)
O199	0.4917 (5)	0.5462 (5)	0.3545 (8)	0.079 (7)

O200	0.4203 (3)	0.3911 (5)	0.3605 (8)	0.062 (4)	
O201	0.5174 (4)	0.5021 (6)	0.4799 (7)	0.066 (6)	
O202	0.5391 (4)	0.5398 (5)	0.4289 (7)	0.055 (5)	
O203	0.4800 (3)	0.4286 (5)	0.4161 (7)	0.055 (6)	
O204	0.5099 (3)	0.4793 (5)	0.3930 (6)	0.046 (5)	
O205	0.4536 (3)	0.4202 (5)	0.3200 (7)	0.055 (3)	
O206	0.4391 (3)	0.4873 (5)	0.1050 (7)	0.055 (3)	
O207	0.4509 (3)	0.4247 (5)	0.0715 (7)	0.055 (3)	
O208	0.4495 (3)	0.4267 (4)	0.1574 (6)	0.035 (4)	
O209	0.4813 (4)	0.4848 (5)	0.1877 (7)	0.051 (5)	
O210	0.4305 (3)	0.3600 (5)	0.1662 (8)	0.063 (6)	
O211	0.4750 (3)	0.4297 (4)	0.2562 (7)	0.047 (5)	
O212	0.4612 (3)	0.3684 (4)	0.2594 (7)	0.049 (3)	
O213	0.5008 (3)	0.4294 (4)	0.3502 (7)	0.045 (5)	
O214	0.4836 (3)	0.3595 (4)	0.3512 (7)	0.054 (6)	
O215	0.5142 (3)	0.3782 (5)	0.3039 (7)	0.055 (3)	
O216	0.5715 (6)	0.6001 (7)	0.4262 (14)	0.144 (14)	
O217	0.5616 (7)	0.5507 (7)	0.3496 (11)	0.127 (11)	
O218	0.6318 (6)	0.5282 (13)	0.4947 (14)	0.21 (2)	
O219	0.5915 (12)	0.5621 (14)	0.5122 (14)	0.25 (3)	
O220	0.5170 (3)	1.1429 (5)	0.1445 (7)	0.053 (5)	
O221	0.4868 (3)	1.1258 (4)	0.1972 (6)	0.038 (5)	
O222	0.4616 (3)	1.1386 (4)	0.2607 (7)	0.044 (5)	
Mo61	0.38631 (8)	0.22527 (8)	0.2538 (3)	0.152 (2)	
Mo62	0.38730 (8)	0.29085 (8)	0.2571 (3)	0.162 (3)	
Na1	0.4000 (3)	0.2022 (4)	0.4497 (6)	0.091 (4)	
Na2	0.4291 (7)	0.2918 (9)	0.4432 (13)	0.091 (4)	0.5
O223	0.3838 (8)	0.1837 (11)	0.3731 (15)	0.170 (15)	
O224	0.3947 (5)	0.2152 (6)	0.3159 (13)	0.114 (4)	
O225	0.3961 (7)	0.2958 (9)	0.3259 (12)	0.138 (12)	
O226	0.4204 (10)	0.3277 (11)	0.274 (2)	0.114 (4)	0.5
O227	0.3722 (10)	0.3041 (11)	0.187 (2)	0.114 (4)	0.5
O228	0.3608 (5)	0.2572 (6)	0.2602 (12)	0.114 (4)	
O229	0.4159 (5)	0.2588 (6)	0.2743 (12)	0.114 (4)	
O230	0.3738 (5)	0.2169 (6)	0.1842 (13)	0.114 (4)	
O231	0.4172 (5)	0.1884 (6)	0.2709 (12)	0.114 (4)	
O232	0.4511 (9)	0.2603 (8)	0.4995 (14)	0.20 (2)	
O233	0.3869 (7)	0.3293 (9)	0.3785 (13)	0.145 (12)	
O234	0.4179 (13)	0.2485 (16)	0.507 (2)	0.116 (19)	0.5
N1	0.3601 (6)	0.3329 (8)	0.2641 (11)	0.079 (8)	
N2	0.3555 (6)	0.1856 (8)	0.2575 (10)	0.088 (9)	
C1	0.3639 (7)	0.3402 (10)	0.3031 (13)	0.088 (5)	
C2	0.3471 (8)	0.3690 (10)	0.3115 (14)	0.088 (5)	
H2	0.349208	0.376200	0.341253	0.105*	
C3	0.3300 (8)	0.3829 (10)	0.2757 (14)	0.088 (5)	
H3	0.319479	0.401285	0.279427	0.105*	
C4	0.3262 (7)	0.3727 (9)	0.2337 (13)	0.073 (7)	
H4	0.312522	0.382686	0.208237	0.088*	

C5	0.3427 (7)	0.3469 (9)	0.2276 (13)	0.073 (7)	
H5	0.341275	0.340028	0.198023	0.088*	
C6	0.3830 (7)	0.3214 (10)	0.3404 (13)	0.088 (5)	
C7	0.3353 (7)	0.1751 (11)	0.2173 (14)	0.110 (5)	
H7	0.336530	0.181325	0.189203	0.132*	
C8	0.3134 (9)	0.1558 (11)	0.2162 (14)	0.110 (5)	
H8	0.298561	0.147768	0.191047	0.132*	
C9	0.3197 (9)	0.1519 (11)	0.2625 (12)	0.110 (5)	
H9	0.305816	0.138869	0.266191	0.132*	
C10	0.3382 (7)	0.1594 (11)	0.3058 (14)	0.110 (5)	
H10	0.336582	0.153000	0.333529	0.132*	
C11	0.3594 (9)	0.1779 (11)	0.3021 (13)	0.110 (5)	
C12	0.3827 (9)	0.1935 (12)	0.3381 (17)	0.110 (5)	
O249	0.2782 (7)	1.0186 (8)	0.0814 (12)	0.151 (14)	
O250	0.2514 (7)	0.8107 (8)	−0.0549 (17)	0.22 (3)	
O251	0.2884 (5)	0.8558 (7)	0.4289 (10)	0.108 (10)	
O252	0.3523 (8)	0.7215 (11)	0.2003 (17)	0.194 (19)	
O3	0.3618 (5)	0.9279 (7)	0.5149 (8)	0.084 (7)	
O240	0.2746 (5)	0.5912 (6)	−0.0028 (8)	0.081 (7)	
O241	0.5399 (7)	0.3549 (9)	0.4160 (11)	0.135 (11)	
O242	0.5244 (9)	0.6281 (11)	0.418 (2)	0.26 (3)	
O243	0.4115 (8)	0.9093 (10)	0.1884 (15)	0.21 (2)	
O244	0.4478 (7)	1.1426 (9)	0.0718 (12)	0.150 (12)	
O245	0.4846 (4)	1.0667 (6)	0.4255 (7)	0.075 (7)	
O246	0.3883 (6)	0.5507 (7)	0.4363 (11)	0.124 (11)	
O247	0.2023 (7)	0.9739 (9)	0.0842 (9)	0.143 (14)	
O248	0.5426 (7)	0.5981 (10)	0.5117 (14)	0.166 (17)	
O235	0.3529 (5)	0.8813 (7)	0.2540 (10)	0.103 (9)	
O236	0.3414 (6)	0.2559 (8)	0.3251 (12)	0.128 (11)	
O237	0.500000	0.6899 (9)	0.750000	0.15 (2)	
O238	0.3912 (7)	0.5758 (11)	0.5781 (15)	0.19 (2)	
Na3	0.4146 (5)	0.2909 (5)	0.4437 (8)	0.057 (7)	0.5
O239	0.4234 (13)	0.2351 (16)	0.551 (2)	0.13 (2)	0.5

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ce1	0.0402 (10)	0.0493 (11)	0.0918 (15)	−0.0153 (9)	0.0388 (11)	−0.0016 (10)
Ce2	0.0459 (11)	0.0328 (10)	0.0668 (13)	0.0113 (8)	0.0056 (10)	−0.0009 (9)
Ce3	0.0478 (11)	0.0421 (10)	0.0752 (14)	−0.0201 (8)	0.0349 (10)	−0.0183 (9)
Mo1	0.0224 (13)	0.0193 (12)	0.099 (2)	−0.0004 (10)	0.0299 (14)	0.0075 (13)
Mo2	0.0290 (14)	0.0400 (15)	0.0723 (19)	0.0085 (11)	0.0272 (14)	0.0013 (13)
Mo3	0.0320 (16)	0.073 (2)	0.117 (3)	−0.0189 (14)	0.0417 (18)	−0.0372 (19)
Mo4	0.0222 (13)	0.0318 (14)	0.0720 (19)	−0.0002 (10)	0.0242 (13)	0.0106 (13)
Mo5	0.0309 (14)	0.0190 (12)	0.0678 (18)	−0.0059 (10)	0.0229 (13)	−0.0038 (12)
Mo6	0.0371 (16)	0.0334 (15)	0.113 (3)	0.0076 (12)	0.0236 (17)	−0.0087 (16)
Mo7	0.0263 (14)	0.0411 (15)	0.093 (2)	0.0005 (12)	0.0245 (15)	−0.0103 (15)
Mo8	0.0230 (13)	0.0178 (12)	0.097 (2)	0.0005 (10)	0.0316 (14)	0.0086 (13)

Mo9	0.0201 (13)	0.0192 (12)	0.098 (2)	−0.0009 (10)	0.0283 (14)	−0.0064 (13)
Mo10	0.0312 (14)	0.0304 (14)	0.111 (2)	0.0077 (11)	0.0408 (16)	0.0022 (15)
Mo11	0.0207 (13)	0.0228 (13)	0.100 (2)	−0.0018 (10)	0.0305 (14)	−0.0044 (13)
Mo12	0.0258 (13)	0.0243 (13)	0.092 (2)	0.0005 (10)	0.0339 (14)	0.0094 (13)
Mo13	0.0258 (13)	0.0352 (14)	0.075 (2)	−0.0103 (11)	0.0223 (13)	0.0020 (13)
Mo14	0.0263 (13)	0.0273 (13)	0.080 (2)	0.0035 (11)	0.0291 (14)	0.0069 (13)
Mo15	0.0305 (14)	0.0302 (14)	0.092 (2)	0.0056 (11)	0.0208 (15)	0.0004 (14)
Mo16	0.0401 (19)	0.0401 (19)	0.229 (5)	0.0083 (15)	0.018 (2)	−0.040 (2)
Mo17	0.0393 (16)	0.0485 (16)	0.084 (2)	0.0200 (13)	0.0360 (16)	0.0037 (15)
Mo18	0.0228 (13)	0.0294 (13)	0.0758 (19)	0.0057 (11)	0.0213 (13)	−0.0049 (13)
Mo19	0.0604 (19)	0.0388 (16)	0.112 (3)	0.0157 (14)	0.0618 (19)	0.0108 (16)
Mo20	0.0326 (14)	0.0321 (14)	0.082 (2)	0.0068 (11)	0.0338 (14)	−0.0005 (13)
Mo21	0.0184 (12)	0.0235 (13)	0.087 (2)	−0.0004 (10)	0.0285 (13)	−0.0048 (13)
Mo22	0.0442 (17)	0.0339 (15)	0.101 (3)	0.0153 (13)	0.0072 (17)	−0.0100 (16)
Mo23	0.0366 (15)	0.0279 (14)	0.0722 (19)	0.0087 (11)	0.0232 (14)	0.0043 (13)
Mo24	0.0261 (13)	0.0270 (13)	0.079 (2)	0.0044 (11)	0.0284 (13)	0.0049 (13)
Mo25	0.0254 (14)	0.0477 (16)	0.0674 (19)	−0.0065 (12)	0.0195 (13)	−0.0029 (14)
Mo26	0.0220 (13)	0.0250 (13)	0.078 (2)	0.0007 (10)	0.0249 (13)	−0.0060 (12)
Mo27	0.090 (3)	0.0351 (17)	0.185 (4)	0.0135 (16)	0.106 (3)	0.013 (2)
Mo28	0.0256 (13)	0.0235 (13)	0.0746 (19)	−0.0011 (10)	0.0247 (13)	−0.0059 (12)
Mo29	0.0317 (14)	0.0281 (13)	0.0703 (19)	0.0053 (11)	0.0283 (13)	0.0016 (12)
Mo30	0.0328 (15)	0.0310 (14)	0.079 (2)	0.0109 (11)	0.0145 (14)	−0.0019 (13)
Mo31	0.0454 (16)	0.0254 (13)	0.074 (2)	0.0006 (11)	0.0369 (15)	−0.0056 (13)
Mo32	0.082 (2)	0.0324 (15)	0.102 (3)	−0.0162 (14)	0.067 (2)	−0.0164 (15)
Mo33	0.0318 (13)	0.0286 (13)	0.0496 (16)	−0.0005 (10)	0.0197 (12)	−0.0036 (11)
Mo34	0.0216 (12)	0.0262 (13)	0.0579 (17)	0.0028 (10)	0.0187 (12)	−0.0022 (11)
Mo35	0.0228 (13)	0.0405 (14)	0.0488 (16)	0.0084 (11)	0.0160 (12)	−0.0002 (12)
Mo36	0.0276 (13)	0.0290 (13)	0.0591 (17)	0.0088 (10)	0.0234 (13)	0.0004 (12)
Mo37	0.0343 (14)	0.0331 (14)	0.0566 (17)	−0.0062 (11)	0.0218 (13)	−0.0093 (12)
Mo38	0.0255 (13)	0.0265 (13)	0.0476 (16)	0.0042 (10)	0.0138 (12)	−0.0018 (11)
Mo39	0.0245 (13)	0.0308 (13)	0.0475 (16)	0.0102 (10)	0.0156 (12)	−0.0024 (11)
Mo40	0.0296 (14)	0.0341 (14)	0.0622 (18)	0.0091 (11)	0.0119 (13)	0.0023 (13)
Mo41	0.0298 (15)	0.0491 (17)	0.087 (2)	0.0121 (12)	0.0195 (15)	0.0317 (16)
Mo42	0.0300 (13)	0.0316 (13)	0.0446 (16)	0.0117 (11)	0.0112 (12)	0.0004 (11)
Mo43	0.0263 (13)	0.0297 (13)	0.0508 (16)	0.0091 (10)	0.0135 (12)	−0.0041 (12)
Mo44	0.0329 (14)	0.0292 (13)	0.0444 (16)	0.0125 (11)	0.0108 (12)	−0.0018 (11)
Mo45	0.0212 (12)	0.0261 (13)	0.0523 (16)	0.0055 (10)	0.0102 (12)	−0.0008 (11)
Mo46	0.0294 (15)	0.0441 (16)	0.099 (2)	−0.0165 (12)	0.0238 (15)	−0.0264 (16)
Mo47	0.0286 (14)	0.0329 (14)	0.0682 (19)	−0.0067 (11)	0.0178 (13)	−0.0086 (13)
Mo48	0.0235 (13)	0.0235 (12)	0.0542 (17)	0.0067 (10)	0.0062 (12)	0.0031 (11)
Mo49	0.0277 (13)	0.0254 (13)	0.0508 (16)	0.0095 (10)	0.0115 (12)	−0.0040 (11)
Mo50	0.0289 (13)	0.0288 (13)	0.0528 (17)	0.0096 (11)	0.0122 (12)	0.0042 (12)
Mo51	0.0441 (16)	0.0419 (16)	0.096 (2)	0.0215 (13)	0.0393 (17)	0.0217 (16)
Mo52	0.0369 (16)	0.0355 (15)	0.101 (2)	0.0143 (12)	0.0264 (16)	0.0130 (15)
Mo53	0.0270 (13)	0.0215 (12)	0.0553 (17)	0.0040 (10)	0.0055 (12)	−0.0029 (11)
Mo54	0.0432 (15)	0.0201 (13)	0.0548 (17)	0.0061 (11)	0.0069 (13)	−0.0008 (12)
Mo55	0.0256 (13)	0.0243 (13)	0.0551 (17)	0.0012 (10)	0.0061 (12)	0.0035 (12)
Mo56	0.0222 (13)	0.0310 (13)	0.0536 (17)	−0.0048 (10)	0.0056 (12)	0.0007 (12)

Mo57	0.0241 (13)	0.0348 (14)	0.075 (2)	−0.0077 (11)	0.0139 (13)	−0.0114 (14)
Mo58	0.0247 (13)	0.0230 (13)	0.0592 (17)	−0.0017 (10)	0.0075 (12)	0.0016 (12)
Mo59	0.0226 (13)	0.0212 (12)	0.0557 (17)	−0.0005 (10)	0.0047 (12)	0.0023 (11)
Mo60	0.0230 (13)	0.0176 (12)	0.096 (2)	−0.0027 (10)	0.0287 (14)	−0.0092 (13)
O1	0.034 (11)	0.032 (10)	0.072 (14)	−0.013 (8)	0.014 (10)	−0.004 (10)
O2	0.026 (10)	0.033 (11)	0.063 (13)	0.010 (8)	−0.007 (9)	0.011 (9)
O253	0.034 (11)	0.045 (12)	0.058 (13)	−0.003 (9)	0.005 (10)	−0.007 (10)
O4	0.041 (12)	0.082 (15)	0.038 (12)	−0.014 (10)	0.017 (10)	−0.006 (11)
O5	0.049 (5)	0.049 (5)	0.049 (5)	−0.0001 (10)	0.018 (2)	0.0001 (10)
O6	0.026 (10)	0.010 (8)	0.053 (12)	0.007 (7)	0.004 (9)	0.010 (8)
O7	0.034 (11)	0.034 (11)	0.104 (18)	−0.002 (9)	0.013 (12)	0.012 (11)
O8	0.019 (9)	0.011 (8)	0.079 (14)	0.004 (7)	0.022 (9)	0.001 (8)
O9	0.029 (10)	0.051 (12)	0.051 (13)	−0.010 (9)	0.000 (9)	−0.010 (10)
O10	0.028 (10)	0.038 (11)	0.064 (14)	−0.021 (9)	0.003 (10)	−0.007 (10)
O11	0.022 (10)	0.037 (11)	0.101 (17)	0.015 (8)	0.027 (11)	0.017 (11)
O12	0.024 (10)	0.025 (10)	0.070 (14)	−0.011 (8)	−0.002 (9)	−0.004 (9)
O13	0.029 (4)	0.029 (4)	0.029 (4)	0.0001 (10)	0.0109 (17)	−0.0001 (10)
O14	0.035 (11)	0.020 (9)	0.071 (14)	0.002 (8)	0.012 (10)	−0.003 (9)
O15	0.027 (10)	0.031 (10)	0.057 (13)	0.022 (8)	−0.001 (9)	−0.003 (9)
O16	0.061 (13)	0.022 (10)	0.062 (14)	0.007 (9)	0.015 (11)	0.009 (9)
O17	0.020 (9)	0.009 (8)	0.069 (13)	0.001 (7)	0.014 (9)	−0.008 (8)
O18	0.037 (11)	0.017 (9)	0.069 (14)	0.004 (8)	0.004 (10)	−0.008 (9)
O19	0.020 (9)	0.014 (9)	0.056 (12)	−0.007 (7)	0.001 (8)	0.010 (8)
O20	0.034 (11)	0.023 (10)	0.065 (13)	−0.013 (8)	0.005 (10)	−0.009 (9)
O21	0.057 (13)	0.041 (12)	0.052 (13)	0.010 (10)	−0.011 (11)	0.002 (10)
O22	0.045 (12)	0.081 (15)	0.021 (10)	−0.024 (11)	0.003 (9)	0.002 (10)
O23	0.051 (12)	0.040 (11)	0.043 (12)	−0.020 (9)	0.011 (10)	0.001 (9)
O24	0.059 (14)	0.078 (15)	0.050 (13)	0.021 (12)	0.012 (11)	0.013 (11)
O25	0.027 (11)	0.036 (11)	0.122 (19)	0.002 (9)	0.021 (12)	0.010 (12)
O26	0.016 (9)	0.026 (10)	0.057 (12)	−0.012 (7)	−0.003 (8)	−0.006 (9)
O27	0.030 (10)	0.022 (9)	0.041 (11)	0.013 (8)	0.007 (8)	−0.005 (8)
O28	0.033 (10)	0.015 (9)	0.075 (14)	0.004 (8)	0.008 (10)	0.003 (9)
O29	0.09 (2)	0.14 (3)	0.047 (15)	0.022 (18)	−0.001 (14)	−0.011 (15)
O30	0.058 (14)	0.069 (15)	0.103 (19)	0.012 (12)	0.037 (14)	0.043 (14)
O31	0.17 (3)	0.09 (2)	0.09 (2)	0.08 (2)	−0.02 (2)	−0.006 (17)
O32	0.051 (13)	0.070 (14)	0.094 (17)	0.013 (11)	0.051 (13)	0.017 (13)
O33	0.039 (12)	0.063 (14)	0.13 (2)	0.024 (11)	0.047 (14)	0.036 (14)
O34	0.072 (16)	0.082 (17)	0.066 (16)	−0.001 (13)	0.008 (13)	−0.028 (13)
O35	0.017 (9)	0.058 (12)	0.064 (13)	0.010 (8)	0.025 (9)	0.016 (10)
O36	0.036 (12)	0.051 (13)	0.13 (2)	0.000 (10)	0.036 (13)	0.025 (13)
O37	0.047 (13)	0.073 (16)	0.14 (2)	0.026 (12)	0.062 (15)	0.042 (15)
O38	0.036 (11)	0.067 (14)	0.069 (14)	0.018 (10)	0.028 (11)	0.006 (11)
O39	0.029 (6)	0.025 (6)	0.060 (7)	0.011 (4)	0.012 (5)	−0.003 (5)
O40	0.031 (7)	0.033 (7)	0.050 (9)	0.011 (6)	0.011 (6)	0.003 (6)
O41	0.12 (3)	0.10 (2)	0.13 (3)	−0.029 (19)	0.02 (2)	0.04 (2)
O42	0.032 (3)	0.032 (3)	0.033 (3)	0.0004 (10)	0.0124 (14)	−0.0001 (10)
O43	0.027 (10)	0.025 (9)	0.039 (11)	−0.014 (8)	0.000 (8)	−0.004 (8)
O44	0.009 (9)	0.033 (11)	0.094 (16)	0.004 (8)	0.006 (10)	0.013 (10)

O45	0.040 (12)	0.082 (15)	0.056 (13)	−0.008 (10)	0.036 (10)	−0.026 (11)
O46	0.10 (2)	0.14 (3)	0.10 (2)	−0.07 (2)	−0.031 (17)	0.041 (19)
O47	0.40 (7)	0.12 (3)	0.20 (4)	0.06 (4)	0.21 (5)	0.01 (3)
O48	0.07 (2)	0.47 (7)	0.08 (2)	−0.05 (3)	0.038 (18)	0.06 (3)
O49	0.12 (2)	0.080 (19)	0.21 (4)	−0.008 (17)	0.10 (3)	−0.04 (2)
O50	0.083 (18)	0.077 (17)	0.11 (2)	0.024 (14)	0.032 (16)	0.054 (15)
O51	0.009 (8)	0.028 (10)	0.061 (12)	0.004 (7)	0.002 (8)	−0.004 (9)
O52	0.039 (11)	0.030 (10)	0.061 (13)	−0.022 (8)	0.021 (10)	−0.002 (9)
O53	0.014 (8)	0.028 (9)	0.042 (11)	−0.007 (7)	0.015 (8)	0.003 (8)
O54	0.038 (4)	0.038 (4)	0.038 (4)	0.0005 (10)	0.0141 (19)	−0.0002 (10)
O55	0.13 (2)	0.038 (13)	0.11 (2)	0.042 (13)	0.075 (18)	0.030 (13)
O56	0.068 (15)	0.040 (12)	0.096 (17)	0.023 (11)	0.043 (13)	0.009 (11)
O57	0.040 (11)	0.026 (10)	0.058 (13)	0.017 (8)	0.004 (10)	0.004 (9)
O58	0.031 (7)	0.033 (7)	0.050 (9)	0.011 (6)	0.011 (6)	0.003 (6)
O59	0.050 (12)	0.069 (14)	0.047 (13)	−0.006 (10)	0.019 (10)	−0.027 (11)
O60	0.055 (13)	0.066 (14)	0.067 (15)	0.019 (11)	0.029 (12)	−0.003 (11)
O61	0.012 (9)	0.072 (14)	0.081 (15)	−0.002 (9)	0.013 (10)	−0.047 (12)
O62	0.035 (10)	0.026 (10)	0.048 (12)	0.006 (8)	0.011 (9)	0.003 (8)
O63	0.029 (6)	0.025 (6)	0.060 (7)	0.011 (4)	0.012 (5)	−0.003 (5)
O64	0.026 (9)	0.020 (9)	0.052 (12)	0.002 (7)	0.017 (9)	−0.003 (8)
O65	0.024 (5)	0.022 (5)	0.075 (8)	0.004 (4)	0.030 (5)	0.006 (5)
O66	0.032 (3)	0.032 (3)	0.033 (3)	0.0004 (10)	0.0124 (14)	−0.0001 (10)
O67	0.029 (6)	0.025 (6)	0.060 (7)	0.011 (4)	0.012 (5)	−0.003 (5)
O68	0.028 (10)	0.026 (10)	0.054 (12)	0.017 (8)	0.009 (9)	0.008 (9)
O69	0.045 (12)	0.046 (12)	0.069 (14)	−0.020 (9)	0.028 (11)	−0.003 (10)
O70	0.104 (19)	0.068 (15)	0.13 (2)	−0.014 (13)	0.101 (18)	−0.039 (15)
O71	0.064 (14)	0.045 (12)	0.053 (13)	−0.005 (10)	0.028 (11)	−0.004 (10)
O72	0.027 (10)	0.034 (11)	0.055 (13)	−0.001 (8)	−0.013 (9)	0.008 (9)
O73	0.058 (13)	0.049 (12)	0.068 (14)	0.016 (10)	0.033 (11)	−0.009 (11)
O74	0.040 (11)	0.070 (13)	0.024 (11)	0.014 (10)	0.009 (9)	−0.005 (9)
O75	0.063 (13)	0.038 (11)	0.046 (12)	0.033 (10)	0.030 (10)	0.005 (9)
O76	0.042 (11)	0.025 (10)	0.049 (12)	0.005 (8)	0.027 (9)	−0.012 (8)
O77	0.12 (3)	0.38 (7)	0.14 (3)	−0.12 (4)	0.07 (3)	0.03 (4)
O78	0.42 (7)	0.07 (2)	0.07 (2)	0.06 (3)	0.02 (3)	−0.006 (17)
O79	0.19 (3)	0.040 (13)	0.091 (19)	−0.007 (15)	0.08 (2)	−0.004 (13)
O80	0.055 (18)	0.044 (17)	0.47 (7)	0.004 (14)	0.02 (3)	−0.05 (3)
O81	0.049 (12)	0.042 (11)	0.068 (14)	−0.003 (9)	0.031 (11)	0.001 (10)
O82	0.17 (3)	0.083 (18)	0.10 (2)	0.045 (18)	0.09 (2)	0.025 (16)
O83	0.033 (10)	0.041 (11)	0.038 (11)	0.001 (8)	0.020 (9)	0.010 (9)
O84	0.048 (12)	0.031 (10)	0.060 (13)	0.014 (9)	0.031 (10)	−0.010 (9)
O85	0.025 (9)	0.020 (9)	0.060 (12)	0.013 (7)	0.023 (9)	0.001 (8)
O86	0.024 (5)	0.022 (5)	0.075 (8)	0.004 (4)	0.030 (5)	0.006 (5)
O87	0.031 (10)	0.012 (9)	0.071 (14)	0.009 (7)	0.008 (10)	0.007 (9)
O88	0.035 (10)	0.031 (10)	0.042 (12)	0.001 (8)	0.001 (9)	0.007 (9)
O89	0.035 (10)	0.034 (10)	0.042 (11)	−0.001 (8)	0.022 (9)	0.009 (8)
O90	0.053 (14)	0.096 (18)	0.099 (19)	0.009 (13)	0.027 (14)	−0.028 (15)
O91	0.085 (17)	0.079 (16)	0.039 (13)	0.031 (13)	0.003 (12)	0.015 (12)
O92	0.058 (13)	0.026 (10)	0.097 (16)	0.005 (9)	0.056 (12)	0.003 (10)

O93	0.054 (12)	0.039 (11)	0.047 (12)	−0.008 (9)	0.019 (10)	−0.007 (9)
O94	0.055 (12)	0.019 (9)	0.067 (14)	−0.005 (8)	0.033 (11)	−0.013 (9)
O95	0.028 (10)	0.039 (10)	0.052 (12)	0.004 (8)	0.030 (9)	−0.012 (9)
O96	0.018 (9)	0.031 (10)	0.050 (12)	0.007 (7)	0.009 (8)	−0.011 (8)
O97	0.034 (11)	0.055 (12)	0.047 (12)	−0.004 (9)	0.021 (9)	−0.023 (10)
O98	0.024 (10)	0.038 (11)	0.061 (13)	0.011 (8)	0.010 (9)	−0.009 (9)
O99	0.036 (12)	0.055 (13)	0.088 (16)	0.024 (10)	0.015 (11)	−0.019 (12)
O100	0.094 (18)	0.107 (19)	0.041 (13)	0.035 (15)	0.038 (13)	0.022 (13)
O101	0.063 (15)	0.029 (12)	0.13 (2)	−0.003 (10)	0.012 (14)	−0.011 (13)
O102	0.035 (11)	0.051 (12)	0.042 (12)	0.023 (9)	0.016 (9)	0.007 (9)
O103	0.052 (12)	0.030 (10)	0.060 (13)	0.023 (9)	0.034 (10)	0.001 (9)
O104	0.091 (16)	0.010 (9)	0.068 (14)	−0.004 (9)	0.029 (12)	−0.003 (9)
O105	0.044 (11)	0.034 (11)	0.070 (14)	0.012 (9)	0.035 (11)	−0.003 (10)
O106	0.058 (12)	0.019 (9)	0.068 (14)	0.001 (8)	0.041 (11)	0.000 (9)
O107	0.025 (10)	0.043 (11)	0.049 (12)	0.013 (8)	−0.012 (9)	−0.009 (9)
O108	0.021 (9)	0.025 (9)	0.055 (12)	0.010 (7)	0.016 (9)	0.006 (8)
O109	0.13 (2)	0.16 (3)	0.050 (15)	−0.07 (2)	0.054 (16)	−0.069 (17)
O110	0.12 (2)	0.024 (11)	0.20 (3)	−0.011 (12)	0.13 (2)	−0.008 (14)
O111	0.049 (13)	0.055 (13)	0.097 (17)	−0.003 (10)	0.053 (12)	−0.022 (12)
O112	0.057 (14)	0.078 (15)	0.058 (14)	−0.007 (12)	0.018 (11)	−0.021 (12)
O113	0.052 (15)	0.073 (17)	0.15 (3)	0.001 (13)	0.026 (16)	0.019 (17)
O114	0.035 (11)	0.024 (10)	0.063 (14)	0.006 (8)	−0.007 (10)	−0.006 (9)
O115	0.023 (10)	0.062 (13)	0.067 (14)	−0.017 (9)	0.025 (10)	−0.016 (11)
O116	0.021 (10)	0.063 (13)	0.054 (13)	0.011 (9)	0.018 (9)	0.006 (10)
O117	0.106 (19)	0.063 (14)	0.042 (13)	0.020 (13)	0.018 (13)	0.010 (11)
O118	0.038 (11)	0.020 (10)	0.068 (14)	0.013 (8)	0.004 (10)	0.001 (9)
O119	0.028 (11)	0.073 (15)	0.095 (17)	0.010 (10)	0.030 (11)	0.004 (13)
O120	0.042 (5)	0.042 (5)	0.042 (5)	0.0004 (10)	0.0159 (19)	−0.0001 (10)
O121	0.037 (11)	0.024 (10)	0.116 (18)	−0.014 (9)	0.024 (12)	−0.008 (11)
O122	0.024 (5)	0.022 (5)	0.075 (8)	0.004 (4)	0.030 (5)	0.006 (5)
O123	0.028 (10)	0.036 (10)	0.066 (13)	−0.005 (8)	0.028 (10)	−0.002 (9)
O124	0.017 (9)	0.014 (9)	0.084 (14)	−0.003 (7)	0.016 (9)	0.003 (9)
O125	0.043 (11)	0.029 (10)	0.061 (13)	0.011 (8)	0.031 (10)	−0.013 (9)
O126	0.15 (2)	0.037 (13)	0.19 (3)	−0.019 (14)	0.15 (2)	−0.020 (15)
O127	0.073 (16)	0.096 (18)	0.068 (16)	−0.027 (14)	0.011 (13)	−0.005 (14)
O128	0.089 (17)	0.048 (13)	0.14 (2)	−0.001 (12)	0.091 (17)	0.017 (14)
O129	0.031 (10)	0.025 (10)	0.082 (14)	0.003 (8)	0.036 (10)	−0.010 (9)
O130	0.10 (2)	0.20 (3)	0.09 (2)	−0.08 (2)	0.044 (17)	−0.05 (2)
O131	0.027 (10)	0.032 (10)	0.082 (15)	−0.007 (8)	0.025 (10)	−0.009 (10)
O132	0.043 (12)	0.048 (12)	0.082 (15)	0.001 (9)	0.040 (11)	0.013 (11)
O133	0.037 (11)	0.019 (9)	0.072 (14)	0.006 (8)	0.032 (10)	0.003 (9)
O134	0.021 (10)	0.031 (10)	0.078 (14)	−0.004 (8)	0.024 (10)	−0.005 (9)
O135	0.035 (11)	0.038 (11)	0.084 (16)	0.025 (9)	0.007 (11)	0.000 (10)
O136	0.054 (13)	0.067 (15)	0.096 (18)	0.027 (11)	0.036 (13)	0.035 (13)
O137	0.041 (13)	0.038 (12)	0.14 (2)	0.004 (10)	0.020 (13)	−0.011 (13)
O138	0.11 (2)	0.17 (3)	0.10 (2)	−0.01 (2)	0.013 (19)	0.00 (2)
O139	0.035 (13)	0.044 (14)	0.26 (4)	−0.003 (11)	0.004 (18)	−0.027 (18)
O140	0.064 (15)	0.099 (19)	0.086 (18)	0.026 (14)	0.032 (14)	0.025 (15)

O141	0.045 (12)	0.031 (11)	0.100 (17)	0.021 (9)	0.034 (12)	−0.003 (11)
O142	0.11 (2)	0.16 (3)	0.057 (17)	−0.004 (19)	0.037 (16)	0.010 (17)
O143	0.021 (10)	0.027 (10)	0.124 (19)	0.001 (8)	0.033 (11)	0.010 (11)
O144	0.027 (10)	0.023 (10)	0.079 (14)	0.012 (8)	0.021 (10)	0.006 (9)
O145	0.045 (11)	0.027 (10)	0.091 (15)	0.017 (8)	0.053 (11)	0.014 (10)
O146	0.043 (5)	0.043 (5)	0.044 (5)	0.0004 (10)	0.017 (2)	−0.0002 (10)
O147	0.027 (10)	0.023 (9)	0.076 (14)	0.003 (7)	0.037 (10)	0.001 (9)
O148	0.016 (10)	0.053 (12)	0.078 (15)	0.009 (9)	0.011 (10)	−0.013 (11)
O149	0.024 (7)	0.024 (7)	0.078 (10)	0.007 (5)	0.024 (7)	−0.015 (6)
O150	0.057 (14)	0.093 (17)	0.093 (17)	0.036 (12)	0.063 (13)	0.045 (14)
O151	0.036 (12)	0.083 (15)	0.059 (14)	0.004 (11)	0.015 (10)	−0.006 (12)
O152	0.027 (11)	0.070 (14)	0.096 (17)	0.007 (10)	0.026 (11)	−0.005 (13)
O153	0.023 (10)	0.018 (9)	0.090 (15)	−0.003 (7)	0.027 (10)	−0.026 (9)
O154	0.020 (9)	0.017 (9)	0.089 (15)	0.005 (7)	0.026 (10)	0.002 (9)
O155	0.024 (10)	0.051 (12)	0.084 (15)	0.020 (9)	0.028 (10)	0.023 (11)
O156	0.063 (9)	0.051 (9)	0.093 (10)	0.003 (8)	0.017 (8)	−0.008 (8)
O157	0.023 (6)	0.043 (7)	0.129 (11)	0.000 (5)	0.039 (7)	0.019 (7)
O158	0.026 (10)	0.029 (10)	0.120 (18)	−0.002 (8)	0.035 (11)	−0.008 (11)
O159	0.030 (10)	0.024 (10)	0.092 (15)	−0.013 (8)	0.035 (11)	−0.005 (10)
O160	0.037 (11)	0.027 (10)	0.096 (16)	−0.009 (8)	0.033 (11)	−0.022 (10)
O161	0.024 (7)	0.024 (7)	0.078 (10)	0.007 (5)	0.024 (7)	−0.015 (6)
O162	0.036 (11)	0.028 (10)	0.080 (15)	0.003 (8)	0.023 (10)	−0.005 (10)
O163	0.071 (18)	0.17 (3)	0.072 (18)	0.023 (18)	0.022 (15)	0.005 (18)
O164	0.046 (13)	0.069 (15)	0.107 (19)	0.011 (11)	0.046 (13)	−0.004 (13)
O165	0.070 (14)	0.056 (13)	0.059 (14)	−0.021 (11)	0.042 (12)	0.006 (11)
O166	0.047 (12)	0.037 (11)	0.098 (17)	0.006 (9)	0.033 (12)	−0.017 (11)
O167	0.052 (13)	0.031 (11)	0.101 (17)	0.019 (9)	0.049 (12)	0.000 (11)
O168	0.026 (10)	0.018 (9)	0.072 (13)	0.002 (7)	0.024 (9)	−0.006 (9)
O169	0.021 (7)	0.019 (7)	0.088 (10)	0.002 (5)	0.025 (7)	0.011 (6)
O170	0.038 (11)	0.041 (11)	0.067 (14)	−0.020 (9)	0.021 (10)	−0.024 (10)
O171	0.021 (7)	0.019 (7)	0.088 (10)	0.002 (5)	0.025 (7)	0.011 (6)
O172	0.058 (17)	0.10 (2)	0.25 (4)	0.013 (15)	0.07 (2)	0.06 (2)
O173	0.039 (13)	0.045 (14)	0.22 (3)	−0.011 (11)	0.018 (17)	−0.042 (17)
O174	0.083 (16)	0.104 (18)	0.054 (14)	0.047 (14)	0.045 (13)	0.044 (13)
O175	0.029 (11)	0.093 (16)	0.068 (15)	0.019 (11)	0.010 (10)	−0.047 (13)
O176	0.047 (13)	0.032 (11)	0.13 (2)	0.008 (9)	0.052 (14)	0.009 (12)
O177	0.018 (10)	0.058 (12)	0.061 (13)	0.008 (9)	0.020 (9)	0.009 (10)
O178	0.017 (5)	0.015 (5)	0.117 (10)	−0.006 (4)	0.026 (6)	−0.008 (6)
O179	0.023 (10)	0.037 (11)	0.085 (15)	−0.004 (8)	0.035 (10)	0.013 (10)
O180	0.023 (6)	0.043 (7)	0.129 (11)	0.000 (5)	0.039 (7)	0.019 (7)
O181	0.025 (10)	0.032 (10)	0.077 (14)	−0.001 (8)	0.022 (10)	0.001 (10)
O182	0.025 (10)	0.035 (11)	0.121 (19)	0.015 (9)	0.038 (12)	0.010 (12)
O183	0.045 (13)	0.093 (18)	0.087 (17)	0.010 (12)	0.019 (12)	−0.015 (14)
O184	0.069 (6)	0.069 (6)	0.070 (6)	0.0003 (10)	0.026 (2)	0.0000 (10)
O185	0.032 (11)	0.046 (12)	0.074 (14)	−0.005 (9)	0.034 (10)	−0.009 (10)
O186	0.092 (7)	0.037 (5)	0.242 (12)	0.003 (5)	0.096 (8)	−0.012 (6)
O187	0.021 (7)	0.036 (7)	0.065 (9)	0.013 (6)	0.020 (6)	0.028 (7)
O188	0.048 (5)	0.048 (5)	0.049 (5)	−0.0002 (10)	0.018 (2)	0.0003 (10)

O189	0.047 (14)	0.17 (3)	0.066 (16)	0.012 (15)	0.038 (13)	0.030 (16)
O190	0.039 (11)	0.031 (11)	0.095 (16)	−0.005 (9)	0.030 (11)	−0.018 (10)
O191	0.020 (9)	0.047 (11)	0.055 (12)	0.006 (8)	0.025 (9)	0.003 (9)
O192	0.021 (7)	0.036 (7)	0.065 (9)	0.013 (6)	0.020 (6)	0.028 (7)
O193	0.017 (5)	0.015 (5)	0.117 (10)	−0.006 (4)	0.026 (6)	−0.008 (6)
O194	0.026 (10)	0.033 (10)	0.076 (14)	−0.005 (8)	0.015 (10)	−0.004 (10)
O195	0.043 (10)	0.019 (9)	0.081 (12)	−0.004 (7)	0.033 (9)	−0.013 (8)
O196	0.021 (9)	0.025 (10)	0.086 (15)	0.001 (8)	0.026 (10)	−0.002 (9)
O197	0.031 (10)	0.014 (9)	0.098 (16)	0.001 (8)	0.040 (11)	−0.003 (9)
O198	0.022 (9)	0.021 (9)	0.070 (13)	−0.004 (7)	0.019 (9)	0.013 (9)
O199	0.098 (18)	0.040 (13)	0.11 (2)	0.018 (12)	0.054 (16)	0.026 (13)
O200	0.023 (6)	0.043 (7)	0.129 (11)	0.000 (5)	0.039 (7)	0.019 (7)
O201	0.031 (11)	0.087 (16)	0.073 (16)	0.004 (11)	0.011 (11)	0.003 (13)
O202	0.055 (5)	0.054 (5)	0.055 (5)	−0.0001 (10)	0.021 (2)	−0.0002 (10)
O203	0.014 (10)	0.065 (13)	0.088 (16)	0.005 (9)	0.022 (10)	0.010 (12)
O204	0.018 (10)	0.061 (13)	0.058 (13)	−0.016 (9)	0.012 (9)	0.008 (10)
O205	0.032 (6)	0.045 (6)	0.102 (9)	0.011 (4)	0.041 (6)	0.004 (6)
O206	0.032 (6)	0.045 (6)	0.102 (9)	0.011 (4)	0.041 (6)	0.004 (6)
O207	0.032 (6)	0.045 (6)	0.102 (9)	0.011 (4)	0.041 (6)	0.004 (6)
O208	0.011 (9)	0.025 (9)	0.067 (13)	0.003 (7)	0.011 (9)	0.000 (9)
O209	0.048 (12)	0.040 (11)	0.074 (15)	−0.006 (9)	0.034 (11)	−0.011 (10)
O210	0.025 (11)	0.062 (13)	0.116 (19)	−0.010 (10)	0.042 (12)	−0.026 (13)
O211	0.031 (10)	0.016 (9)	0.100 (16)	0.004 (8)	0.031 (11)	−0.015 (10)
O212	0.017 (5)	0.015 (5)	0.117 (10)	−0.006 (4)	0.026 (6)	−0.008 (6)
O213	0.015 (9)	0.048 (12)	0.076 (14)	−0.002 (8)	0.022 (10)	0.001 (10)
O214	0.038 (11)	0.027 (10)	0.107 (17)	0.016 (9)	0.037 (12)	0.019 (11)
O215	0.032 (6)	0.045 (6)	0.102 (9)	0.011 (4)	0.041 (6)	0.004 (6)
O216	0.13 (3)	0.068 (19)	0.28 (5)	−0.006 (17)	0.13 (3)	−0.03 (2)
O217	0.16 (3)	0.09 (2)	0.13 (3)	0.05 (2)	0.05 (2)	0.041 (19)
O218	0.044 (18)	0.35 (6)	0.21 (4)	−0.06 (3)	0.00 (2)	0.14 (4)
O219	0.33 (7)	0.25 (6)	0.12 (3)	0.02 (5)	0.02 (4)	−0.07 (4)
O220	0.022 (10)	0.058 (13)	0.068 (14)	−0.009 (9)	0.004 (10)	0.009 (11)
O221	0.026 (10)	0.013 (9)	0.062 (13)	−0.009 (7)	0.001 (9)	0.007 (8)
O222	0.025 (10)	0.018 (9)	0.079 (14)	−0.001 (7)	0.010 (10)	0.012 (9)
Mo61	0.087 (3)	0.0262 (17)	0.380 (7)	−0.0019 (17)	0.129 (4)	0.009 (3)
Mo62	0.097 (3)	0.0207 (17)	0.430 (10)	0.0005 (18)	0.170 (5)	0.002 (3)
Na1	0.090 (7)	0.079 (7)	0.113 (8)	−0.002 (6)	0.049 (7)	−0.003 (6)
Na2	0.090 (7)	0.079 (7)	0.113 (8)	−0.002 (6)	0.049 (7)	−0.003 (6)
O223	0.170 (17)	0.168 (18)	0.175 (17)	0.007 (10)	0.067 (11)	−0.007 (10)
O224	0.092 (7)	0.037 (5)	0.242 (12)	0.003 (5)	0.096 (8)	−0.012 (6)
O225	0.129 (14)	0.136 (15)	0.151 (15)	0.001 (9)	0.055 (10)	0.008 (9)
O226	0.092 (7)	0.037 (5)	0.242 (12)	0.003 (5)	0.096 (8)	−0.012 (6)
O227	0.092 (7)	0.037 (5)	0.242 (12)	0.003 (5)	0.096 (8)	−0.012 (6)
O228	0.092 (7)	0.037 (5)	0.242 (12)	0.003 (5)	0.096 (8)	−0.012 (6)
O229	0.092 (7)	0.037 (5)	0.242 (12)	0.003 (5)	0.096 (8)	−0.012 (6)
O230	0.092 (7)	0.037 (5)	0.242 (12)	0.003 (5)	0.096 (8)	−0.012 (6)
O231	0.092 (7)	0.037 (5)	0.242 (12)	0.003 (5)	0.096 (8)	−0.012 (6)
O232	0.21 (4)	0.07 (2)	0.20 (4)	0.00 (2)	−0.05 (3)	0.07 (2)

O233	0.141 (15)	0.148 (15)	0.142 (15)	−0.008 (9)	0.048 (10)	0.011 (10)
O234	0.12 (2)	0.12 (2)	0.11 (2)	0.008 (10)	0.043 (12)	−0.005 (10)
N1	0.079 (8)	0.079 (8)	0.079 (8)	−0.0001 (10)	0.030 (3)	0.0001 (10)
N2	0.088 (9)	0.087 (9)	0.088 (9)	0.0001 (10)	0.033 (3)	−0.0001 (10)
C1	0.088 (5)	0.088 (5)	0.088 (5)	−0.0001 (5)	0.033 (2)	0.0001 (5)
C2	0.088 (5)	0.088 (5)	0.088 (5)	−0.0001 (5)	0.033 (2)	0.0001 (5)
C3	0.088 (5)	0.088 (5)	0.088 (5)	−0.0001 (5)	0.033 (2)	0.0001 (5)
C4	0.073 (7)	0.073 (7)	0.073 (7)	−0.0002 (7)	0.028 (3)	0.0001 (7)
C5	0.073 (7)	0.073 (7)	0.073 (7)	−0.0002 (7)	0.028 (3)	0.0001 (7)
C6	0.088 (5)	0.088 (5)	0.088 (5)	−0.0001 (5)	0.033 (2)	0.0001 (5)
C7	0.110 (5)	0.110 (5)	0.110 (5)	0.0001 (4)	0.041 (2)	0.0000 (4)
C8	0.110 (5)	0.110 (5)	0.110 (5)	0.0001 (4)	0.041 (2)	0.0000 (4)
C9	0.110 (5)	0.110 (5)	0.110 (5)	0.0001 (4)	0.041 (2)	0.0000 (4)
C10	0.110 (5)	0.110 (5)	0.110 (5)	0.0001 (4)	0.041 (2)	0.0000 (4)
C11	0.110 (5)	0.110 (5)	0.110 (5)	0.0001 (4)	0.041 (2)	0.0000 (4)
C12	0.110 (5)	0.110 (5)	0.110 (5)	0.0001 (4)	0.041 (2)	0.0000 (4)
O249	0.17 (3)	0.11 (2)	0.17 (3)	0.05 (2)	0.06 (3)	−0.03 (2)
O250	0.13 (3)	0.08 (2)	0.33 (6)	0.04 (2)	−0.05 (3)	−0.12 (3)
O251	0.09 (2)	0.080 (18)	0.13 (2)	0.026 (15)	0.008 (17)	−0.033 (17)
O252	0.15 (4)	0.19 (4)	0.28 (5)	−0.03 (3)	0.13 (4)	−0.04 (4)
O3	0.076 (17)	0.11 (2)	0.057 (15)	−0.018 (15)	0.017 (13)	0.011 (14)
O240	0.099 (19)	0.072 (16)	0.072 (17)	0.003 (14)	0.030 (15)	−0.017 (13)
O241	0.135 (11)	0.135 (11)	0.136 (11)	0.000 (2)	0.051 (5)	0.001 (2)
O242	0.18 (4)	0.14 (3)	0.55 (10)	0.00 (3)	0.22 (6)	−0.01 (5)
O243	0.17 (4)	0.13 (3)	0.24 (5)	−0.07 (3)	−0.02 (3)	0.08 (3)
O244	0.150 (13)	0.149 (13)	0.150 (13)	0.000 (2)	0.056 (5)	0.000 (2)
O245	0.053 (14)	0.091 (17)	0.064 (15)	0.039 (12)	0.003 (12)	0.008 (13)
O246	0.15 (3)	0.10 (2)	0.15 (3)	0.06 (2)	0.09 (2)	0.05 (2)
O247	0.16 (3)	0.19 (3)	0.08 (2)	0.12 (3)	0.04 (2)	0.02 (2)
O248	0.13 (3)	0.17 (3)	0.24 (4)	−0.05 (2)	0.12 (3)	−0.11 (3)
O235	0.071 (17)	0.10 (2)	0.16 (3)	0.017 (15)	0.064 (18)	0.012 (19)
O236	0.103 (16)	0.124 (18)	0.169 (19)	0.000 (14)	0.063 (15)	0.009 (15)
O237	0.11 (3)	0.05 (2)	0.32 (7)	0.000	0.11 (4)	0.000
O238	0.09 (2)	0.20 (4)	0.25 (5)	0.00 (2)	0.04 (3)	0.13 (4)
Na3	0.081 (11)	0.017 (8)	0.045 (10)	0.007 (8)	−0.008 (8)	−0.003 (7)
O239	0.13 (3)	0.11 (3)	0.15 (3)	0.019 (18)	0.056 (19)	0.006 (19)

Geometric parameters (Å, º)

Ce1—O41	2.47 (3)	Mo32—O94	2.131 (17)
Ce1—O164^{i}	2.593 (19)	Mo33—O88	2.010 (16)
Ce1—O184^{i}	2.43 (2)	Mo33—O89	2.010 (15)
Ce1—O202	2.499 (19)	Mo33—O93	1.700 (18)
Ce1—O206^{i}	2.465 (18)	Mo33—O94	1.948 (16)
Ce1—O216	2.53 (3)	Mo33—O95	2.114 (15)
Ce1—O217	2.58 (3)	Mo33—O96	2.224 (16)
Ce1—O218	2.51 (3)	Mo33—O108	2.030 (15)
Ce1—O219	2.53 (4)	Mo34—O95	2.131 (16)

Ce2—O61	2.65 (2)	Mo34—O105	2.386 (19)
Ce2—O77	2.61 (3)	Mo34—O106	1.868 (18)
Ce2—O78	2.59 (3)	Mo34—O107	1.685 (16)
Ce2—O79	2.52 (2)	Mo34—O108	1.994 (16)
Ce2—O80	2.42 (3)	Mo34—O115	1.832 (19)
Ce2—O81	2.496 (18)	Mo35—O85	1.964 (15)
Ce2—O82	2.57 (2)	Mo35—O95	2.450 (17)
Ce2—O99	2.576 (18)	Mo35—O96	1.769 (17)
Ce2—O101	2.43 (2)	Mo35—O97	2.102 (16)
Ce3—O23	2.620 (17)	Mo35—O98	1.683 (17)
Ce3—O45	2.420 (19)	Mo35—O105	1.950 (17)
Ce3—O46	2.52 (3)	Mo36—O97	2.024 (18)
Ce3—O47	2.54 (4)	Mo36—O102	1.970 (16)
Ce3—O48	2.51 (3)	Mo36—O103	1.710 (16)
Ce3—O49	2.51 (3)	Mo36—O105	2.382 (17)
Ce3—O50	2.58 (2)	Mo36—O106	1.915 (19)
Ce3—O69	2.489 (18)	Mo36—O116	1.870 (19)
Ce3—O70	2.46 (2)	Mo37—O68	1.804 (16)
Mo1—O205	2.089 (16)	Mo37—O69	1.748 (18)
Mo1—O211	2.319 (19)	Mo37—O71	2.35 (2)
Mo1—O212	1.842 (19)	Mo37—O72	1.691 (16)
Mo1—O213	1.995 (18)	Mo37—O88	2.182 (17)
Mo1—O214	1.654 (18)	Mo37—O89	2.082 (16)
Mo1—O215	1.867 (16)	Mo38—O76	1.877 (16)
Mo2—O204^{i}	2.041 (18)	Mo38—O85	2.429 (16)
Mo2—O206	1.755 (18)	Mo38—O86	1.886 (17)
Mo2—O207	2.43 (2)	Mo38—O87	1.688 (16)
Mo2—O208	1.843 (16)	Mo38—O88	1.963 (18)
Mo2—O209	1.732 (19)	Mo38—O95	2.117 (16)
Mo2—O213^{i}	2.112 (16)	Mo39—O75	1.928 (18)
Mo3—O190	1.801 (17)	Mo39—O83	1.947 (16)
Mo3—O191	2.126 (16)	Mo39—O84	1.693 (17)
Mo3—O199	2.06 (2)	Mo39—O85	2.367 (16)
Mo3—O201	2.02 (2)	Mo39—O86	1.899 (18)
Mo3—O202	1.729 (19)	Mo39—O97	2.000 (17)
Mo3—O204	2.072 (19)	Mo40—O62	2.090 (17)
Mo4—O191	1.947 (17)	Mo40—O64	2.122 (15)
Mo4—O192	2.032 (15)	Mo40—O73	2.305 (18)
Mo4—O198	2.187 (17)	Mo40—O74	1.724 (17)
Mo4—O203	1.67 (2)	Mo40—O81	1.710 (19)
Mo4—O204	1.997 (15)	Mo40—O83	1.862 (16)
Mo4—O205	2.11 (2)	Mo41—O56	1.77 (2)
Mo4—O213	2.032 (16)	Mo41—O57	2.136 (17)
Mo5—O194	1.899 (17)	Mo41—O59	1.767 (18)
Mo5—O196	1.718 (18)	Mo41—O60	2.33 (2)
Mo5—O197	2.096 (17)	Mo41—O61	1.65 (2)
Mo5—O198	1.753 (18)	Mo41—O62	2.015 (16)
Mo5—O205	2.46 (2)	Mo42—O40	2.015 (17)

Mo5—O211	1.979 (15)	Mo42—O53	2.213 (16)
Mo6—O156	1.87 (2)	Mo42—O54	2.126 (17)
Mo6—O172	2.20 (4)	Mo42—O57	1.974 (17)
Mo6—O173	1.67 (2)	Mo42—O58	1.687 (17)
Mo6—O174	1.699 (19)	Mo42—O62	2.021 (16)
Mo6—O175	2.198 (19)	Mo42—O64	2.021 (15)
Mo6—O190	1.981 (17)	Mo43—O54	2.130 (17)
Mo7—O175	1.709 (19)	Mo43—O63	1.701 (17)
Mo7—O177	1.858 (16)	Mo43—O64	1.993 (15)
Mo7—O187	1.734 (17)	Mo43—O65	1.864 (17)
Mo7—O189	2.31 (2)	Mo43—O66	2.402 (16)
Mo7—O191	2.089 (15)	Mo43—O75	1.82 (2)
Mo7—O192	2.098 (17)	Mo44—O42	1.964 (16)
Mo8—O188	1.849 (18)	Mo44—O51	2.131 (15)
Mo8—O192	1.992 (18)	Mo44—O52	1.686 (18)
Mo8—O193	1.910 (19)	Mo44—O53	1.765 (16)
Mo8—O194	2.331 (19)	Mo44—O54	2.433 (17)
Mo8—O200	1.64 (2)	Mo44—O66	1.990 (16)
Mo8—O205	2.135 (16)	Mo45—O51	2.004 (15)
Mo9—O185	2.013 (19)	Mo45—O65	1.907 (18)
Mo9—O186	1.91 (2)	Mo45—O66	2.402 (16)
Mo9—O193	1.92 (2)	Mo45—O67	1.678 (16)
Mo9—O194	2.343 (18)	Mo45—O68	2.002 (17)
Mo9—O195	1.697 (16)	Mo45—O76	1.895 (16)
Mo9—O197	2.022 (15)	Mo46—O10	2.130 (16)
Mo10—O166	2.055 (18)	Mo46—O20	2.079 (18)
Mo10—O181	2.124 (16)	Mo46—O21	2.361 (19)
Mo10—O182	1.70 (2)	Mo46—O22	1.735 (18)
Mo10—O183	2.36 (2)	Mo46—O23	1.717 (16)
Mo10—O184	1.74 (2)	Mo46—O30^{i}	1.81 (2)
Mo10—O185	1.802 (18)	Mo47—O19	2.119 (14)
Mo11—O169	2.071 (15)	Mo47—O20	2.045 (18)
Mo11—O178	1.85 (2)	Mo47—O24	2.35 (2)
Mo11—O179	2.490 (18)	Mo47—O25	1.71 (2)
Mo11—O180	1.708 (19)	Mo47—O43	1.814 (17)
Mo11—O181	2.010 (18)	Mo47—O45	1.743 (18)
Mo11—O186	1.86 (2)	Mo48—O1	1.92 (2)
Mo12—O171	1.991 (15)	Mo48—O26	1.918 (15)
Mo12—O176	1.66 (2)	Mo48—O42	2.383 (16)
Mo12—O177	1.969 (17)	Mo48—O43	1.992 (17)
Mo12—O178	1.946 (19)	Mo48—O44	1.678 (16)
Mo12—O179	2.328 (17)	Mo48—O51	1.998 (16)
Mo12—O188	1.927 (18)	Mo49—O1	1.871 (19)
Mo13—O159	1.921 (16)	Mo49—O27	1.830 (16)
Mo13—O168	1.760 (18)	Mo49—O39	1.677 (17)
Mo13—O169	2.503 (17)	Mo49—O40	1.973 (16)
Mo13—O170	1.678 (17)	Mo49—O42	2.382 (16)
Mo13—O171	2.116 (17)	Mo49—O54	2.091 (17)

Mo13—O179	1.986 (17)	Mo50—O28	1.830 (16)
Mo14—O154	1.930 (15)	Mo50—O34	2.33 (2)
Mo14—O155	2.00 (2)	Mo50—O35	1.747 (16)
Mo14—O157	1.66 (2)	Mo50—O38	1.67 (2)
Mo14—O158	1.92 (2)	Mo50—O40	2.142 (16)
Mo14—O159	2.332 (18)	Mo50—O57	2.062 (19)
Mo14—O171	2.050 (15)	Mo51—O33	1.90 (2)
Mo15—O135	2.082 (18)	Mo51—O35	2.226 (17)
Mo15—O140	2.31 (2)	Mo51—O36	2.31 (3)
Mo15—O141	1.780 (19)	Mo51—O37	1.73 (2)
Mo15—O143	1.69 (2)	Mo51—O55	1.68 (3)
Mo15—O144	2.131 (16)	Mo51—O56	2.01 (2)
Mo15—O155	1.807 (19)	Mo52—O5^{i}	2.197 (18)
Mo16—O137	1.957 (19)	Mo52—O29	2.17 (2)
Mo16—O138	2.00 (3)	Mo52—O30	1.99 (2)
Mo16—O139	1.72 (2)	Mo52—O31	1.80 (3)
Mo16—O141	2.142 (19)	Mo52—O32	1.74 (2)
Mo16—O142	1.92 (2)	Mo52—O33	1.822 (18)
Mo16—O156	1.84 (2)	Mo53—O13	1.945 (15)
Mo17—O150	1.84 (2)	Mo53—O14	2.025 (17)
Mo17—O162	2.092 (18)	Mo53—O15	1.703 (17)
Mo17—O163	1.70 (3)	Mo53—O17	2.285 (16)
Mo17—O164	1.746 (18)	Mo53—O27	1.932 (16)
Mo17—O165	2.38 (2)	Mo53—O28	1.981 (16)
Mo17—O166	2.05 (2)	Mo54—O8	1.966 (15)
Mo18—O161	2.032 (15)	Mo54—O12	2.516 (17)
Mo18—O162	2.032 (18)	Mo54—O14	2.079 (17)
Mo18—O166	1.998 (19)	Mo54—O16	1.699 (17)
Mo18—O167	1.68 (2)	Mo54—O17	1.988 (15)
Mo18—O168	2.262 (17)	Mo54—O18	1.733 (18)
Mo18—O169	2.066 (18)	Mo55—O11	1.676 (18)
Mo18—O181	1.982 (16)	Mo55—O12	2.082 (18)
Mo19—O126	1.90 (2)	Mo55—O13	1.851 (16)
Mo19—O127	1.72 (2)	Mo55—O17	2.459 (16)
Mo19—O128	1.722 (19)	Mo55—O19	2.007 (17)
Mo19—O129	2.182 (17)	Mo55—O26	1.849 (16)
Mo19—O130	2.21 (3)	Mo56—O6	2.010 (15)
Mo19—O150	1.94 (2)	Mo56—O9	1.670 (19)
Mo20—O129	1.762 (18)	Mo56—O10	1.976 (19)
Mo20—O149	1.854 (15)	Mo56—O12	2.099 (18)
Mo20—O151	2.34 (2)	Mo56—O18	2.235 (18)
Mo20—O152	1.70 (2)	Mo56—O19	2.001 (16)
Mo20—O161	2.078 (17)	Mo56—O20	1.991 (15)
Mo20—O162	2.084 (17)	Mo57—O253	1.885 (18)
Mo21—O153	1.851 (15)	Mo57—O4	2.330 (19)
Mo21—O158	1.88 (2)	Mo57—O5	1.703 (18)
Mo21—O159	2.473 (17)	Mo57—O6	2.090 (16)
Mo21—O160	1.696 (17)	Mo57—O7	1.69 (2)

Mo21—O161	2.021 (18)	Mo57—O10	2.080 (16)
Mo21—O169	2.086 (15)	Mo58—O253	1.946 (17)
Mo22—O99	1.72 (2)	Mo58—O8^{i}	2.282 (17)
Mo22—O117	1.76 (2)	Mo58—O14^{i}	2.028 (17)
Mo22—O118	2.035 (17)	Mo58—O220	1.710 (19)
Mo22—O119	2.33 (2)	Mo58—O221	1.909 (17)
Mo22—O135	2.112 (19)	Mo58—O222^{i}	1.921 (17)
Mo22—O137	1.798 (19)	Mo59—O2	1.699 (16)
Mo23—O118	1.987 (17)	Mo59—O6	2.012 (16)
Mo23—O120	1.976 (17)	Mo59—O8	2.450 (16)
Mo23—O133	2.245 (17)	Mo59—O12	2.057 (16)
Mo23—O134	2.114 (17)	Mo59—O221	1.861 (16)
Mo23—O135	1.977 (17)	Mo59—O222	1.88 (2)
Mo23—O136	1.74 (2)	Mo60—O197	1.990 (15)
Mo23—O144	2.009 (16)	Mo60—O208	1.950 (17)
Mo24—O134	2.074 (16)	Mo60—O210	1.695 (19)
Mo24—O144	1.978 (17)	Mo60—O211	2.352 (18)
Mo24—O145	1.723 (16)	Mo60—O212	1.94 (2)
Mo24—O146	1.835 (18)	Mo60—O215^{i}	1.928 (17)
Mo24—O147	2.495 (16)	Mo61—Mo62	2.553 (5)
Mo24—O154	1.835 (15)	Mo61—O224	1.89 (4)
Mo25—O123	1.956 (16)	Mo61—O228	1.93 (2)
Mo25—O131	2.084 (17)	Mo61—O229	1.98 (2)
Mo25—O132	1.707 (18)	Mo61—O230	2.08 (4)
Mo25—O133	1.773 (19)	Mo61—O231	2.12 (2)
Mo25—O147	1.952 (15)	Mo61—N2	2.31 (3)
Mo26—O131	2.015 (16)	Mo62—O225	2.06 (4)
Mo26—O146	1.941 (18)	Mo62—O226	2.20 (5)
Mo26—O147	2.304 (17)	Mo62—O227	2.12 (7)
Mo26—O148	1.696 (17)	Mo62—O228	1.98 (2)
Mo26—O149	1.968 (17)	Mo62—O229	1.90 (2)
Mo26—O153	1.915 (15)	Mo62—N1	2.27 (3)
Mo27—O92	1.960 (17)	Na1—Na2	3.87 (4)
Mo27—O109	2.16 (2)	Na1—O223	2.36 (5)
Mo27—O110	1.70 (2)	Na1—O234	2.48 (6)
Mo27—O111	2.202 (17)	Na1—Na3	3.56 (3)
Mo27—O113	1.85 (3)	Na2—O232	2.12 (5)
Mo27—O126	1.83 (2)	Na2—O233	2.84 (5)
Mo28—O115	1.961 (19)	Na2—O234	2.87 (8)
Mo28—O122	1.955 (17)	O223—C12	1.16 (5)
Mo28—O123	2.310 (17)	O224—C12	1.40 (4)
Mo28—O124	1.689 (16)	O225—C6	1.40 (4)
Mo28—O125	1.984 (17)	O232—Na3	2.42 (4)
Mo28—O131	2.034 (17)	O233—C6	1.19 (4)
Mo29—O116	1.914 (18)	O233—Na3	2.53 (4)
Mo29—O120	1.995 (17)	N1—C1	1.21 (4)
Mo29—O121	1.67 (2)	N1—C5	1.31 (4)
Mo29—O122	1.834 (18)	N2—C7	1.39 (2)

Mo29—O123	2.481 (17)	N2—C11	1.38 (2)
Mo29—O134	2.062 (16)	C1—C2	1.53 (5)
Mo30—O100	2.35 (2)	C1—C6	1.44 (2)
Mo30—O101	1.75 (2)	C2—H2	0.9500
Mo30—O102	1.838 (15)	C2—C3	1.28 (5)
Mo30—O104	1.73 (2)	C3—H3	0.9500
Mo30—O118	2.076 (16)	C3—C4	1.33 (5)
Mo30—O120	2.149 (17)	C4—H4	0.9500
Mo31—O94	2.077 (16)	C4—C5	1.41 (5)
Mo31—O108	2.104 (15)	C5—H5	0.9500
Mo31—O111	1.761 (18)	C7—H7	0.9500
Mo31—O112	2.36 (2)	C7—C8	1.39 (2)
Mo31—O114	1.696 (17)	C8—H8	0.9500
Mo31—O125	1.834 (17)	C8—C9	1.39 (2)
Mo32—O70	1.74 (2)	C9—H9	0.9500
Mo32—O89	2.014 (16)	C9—C10	1.39 (2)
Mo32—O90	2.33 (2)	C10—H10	0.9500
Mo32—O91	1.74 (2)	C10—C11	1.40 (2)
Mo32—O92	1.776 (17)	C11—C12	1.48 (6)

O41—Ce1—O164^{i}	141.0 (9)	O86—Mo38—O85	72.8 (6)
O41—Ce1—O202	77.5 (9)	O86—Mo38—O88	152.2 (7)
O41—Ce1—O216	134.6 (12)	O86—Mo38—O95	95.1 (6)
O41—Ce1—O217	133.6 (10)	O87—Mo38—O76	104.1 (7)
O41—Ce1—O218	70.9 (11)	O87—Mo38—O85	169.5 (6)
O41—Ce1—O219	71.1 (16)	O87—Mo38—O86	103.1 (8)
O184^{i}—Ce1—O41	98.7 (10)	O87—Mo38—O88	102.1 (8)
O184^{i}—Ce1—O164^{i}	68.8 (7)	O87—Mo38—O95	95.5 (7)
O184^{i}—Ce1—O202	132.7 (7)	O88—Mo38—O85	80.3 (6)
O184^{i}—Ce1—O206^{i}	68.0 (7)	O88—Mo38—O95	70.9 (6)
O184^{i}—Ce1—O216	126.7 (9)	O95—Mo38—O85	75.5 (6)
O184^{i}—Ce1—O217	70.9 (8)	O75—Mo39—O83	85.5 (7)
O184^{i}—Ce1—O218	78.4 (14)	O75—Mo39—O85	87.0 (6)
O184^{i}—Ce1—O219	145.4 (15)	O75—Mo39—O97	153.7 (7)
O202—Ce1—O164^{i}	138.6 (6)	O83—Mo39—O85	83.1 (6)
O202—Ce1—O216	71.9 (8)	O83—Mo39—O97	82.5 (7)
O202—Ce1—O217	78.4 (9)	O84—Mo39—O75	104.8 (7)
O202—Ce1—O218	139.0 (10)	O84—Mo39—O83	100.2 (8)
O202—Ce1—O219	78.7 (15)	O84—Mo39—O85	167.9 (7)
O206^{i}—Ce1—O41	65.3 (9)	O84—Mo39—O86	101.4 (8)
O206^{i}—Ce1—O164^{i}	132.4 (7)	O84—Mo39—O97	100.3 (7)
O206^{i}—Ce1—O202	67.9 (6)	O86—Mo39—O75	96.3 (7)
O206^{i}—Ce1—O216	127.7 (9)	O86—Mo39—O83	157.1 (7)
O206^{i}—Ce1—O217	69.1 (9)	O86—Mo39—O85	74.2 (6)
O206^{i}—Ce1—O218	118.1 (13)	O86—Mo39—O97	86.2 (7)
O206^{i}—Ce1—O219	129.2 (15)	O97—Mo39—O85	68.4 (6)
O216—Ce1—O164^{i}	68.3 (8)	O62—Mo40—O64	69.0 (6)
O216—Ce1—O217	71.3 (11)	O62—Mo40—O73	81.7 (7)

O216—Ce1—O219	70.7 (15)	O64—Mo40—O73	77.7 (7)
O217—Ce1—O164[i]	78.9 (9)	O74—Mo40—O62	91.1 (8)
O218—Ce1—O164[i]	70.4 (9)	O74—Mo40—O64	93.7 (8)
O218—Ce1—O216	114.2 (15)	O74—Mo40—O73	170.3 (8)
O218—Ce1—O217	142.6 (12)	O74—Mo40—O83	101.0 (8)
O218—Ce1—O219	67.0 (18)	O81—Mo40—O62	90.7 (8)
O219—Ce1—O164[i]	97.9 (16)	O81—Mo40—O64	152.8 (8)
O219—Ce1—O217	140.0 (14)	O81—Mo40—O73	81.7 (8)
O77—Ce2—O61	120.4 (12)	O81—Mo40—O74	105.0 (9)
O78—Ce2—O61	129.0 (11)	O81—Mo40—O83	105.1 (8)
O78—Ce2—O77	64.3 (16)	O83—Mo40—O62	156.6 (7)
O79—Ce2—O61	70.6 (7)	O83—Mo40—O64	90.2 (7)
O79—Ce2—O77	63.9 (11)	O83—Mo40—O73	83.6 (7)
O79—Ce2—O78	68.6 (8)	O56—Mo41—O57	89.1 (8)
O79—Ce2—O82	140.7 (8)	O56—Mo41—O60	83.2 (9)
O79—Ce2—O99	136.1 (7)	O56—Mo41—O62	154.2 (8)
O80—Ce2—O61	72.6 (8)	O57—Mo41—O60	78.5 (7)
O80—Ce2—O77	140.7 (16)	O59—Mo41—O56	96.9 (9)
O80—Ce2—O78	78.9 (17)	O59—Mo41—O57	94.9 (8)
O80—Ce2—O79	91.0 (13)	O59—Mo41—O60	173.4 (9)
O80—Ce2—O81	136.0 (10)	O59—Mo41—O62	96.1 (8)
O80—Ce2—O82	80.3 (15)	O61—Mo41—O56	105.8 (8)
O80—Ce2—O99	73.4 (8)	O61—Mo41—O57	154.1 (8)
O80—Ce2—O101	135.5 (10)	O61—Mo41—O59	104.0 (10)
O81—Ce2—O61	64.9 (5)	O61—Mo41—O60	82.3 (9)
O81—Ce2—O77	75.1 (12)	O61—Mo41—O62	92.5 (7)
O81—Ce2—O78	138.3 (11)	O62—Mo41—O57	67.6 (7)
O81—Ce2—O79	85.9 (7)	O62—Mo41—O60	81.4 (7)
O81—Ce2—O82	75.0 (7)	O40—Mo42—O53	82.9 (6)
O81—Ce2—O99	133.6 (6)	O40—Mo42—O54	69.7 (6)
O82—Ce2—O61	70.2 (8)	O40—Mo42—O62	143.0 (7)
O82—Ce2—O77	138.4 (11)	O40—Mo42—O64	140.7 (7)
O82—Ce2—O78	144.1 (9)	O54—Mo42—O53	72.7 (6)
O82—Ce2—O99	78.0 (8)	O57—Mo42—O40	72.7 (7)
O99—Ce2—O61	136.5 (6)	O57—Mo42—O53	84.7 (7)
O99—Ce2—O77	103.1 (13)	O57—Mo42—O54	138.0 (7)
O99—Ce2—O78	68.2 (8)	O57—Mo42—O62	70.6 (7)
O101—Ce2—O61	128.6 (7)	O57—Mo42—O64	140.3 (6)
O101—Ce2—O77	68.7 (11)	O58—Mo42—O40	93.7 (8)
O101—Ce2—O78	101.3 (13)	O58—Mo42—O53	170.0 (7)
O101—Ce2—O79	131.1 (9)	O58—Mo42—O54	97.3 (7)
O101—Ce2—O81	70.7 (6)	O58—Mo42—O57	103.3 (8)
O101—Ce2—O82	74.4 (10)	O58—Mo42—O62	99.1 (7)
O101—Ce2—O99	66.0 (6)	O58—Mo42—O64	96.1 (7)
O45—Ce3—O23	68.1 (6)	O62—Mo42—O53	89.2 (6)
O45—Ce3—O46	79.7 (9)	O62—Mo42—O54	141.3 (7)
O45—Ce3—O47	146.5 (10)	O64—Mo42—O53	81.0 (6)
O45—Ce3—O48	97.5 (13)	O64—Mo42—O54	71.3 (6)

O45—Ce3—O49	127.3 (9)	O64—Mo42—O62	72.3 (6)
O45—Ce3—O50	74.3 (8)	O54—Mo43—O66	76.4 (6)
O45—Ce3—O69	69.6 (6)	O63—Mo43—O54	96.2 (7)
O45—Ce3—O70	134.8 (6)	O63—Mo43—O64	102.4 (7)
O46—Ce3—O23	68.7 (7)	O63—Mo43—O65	103.3 (7)
O46—Ce3—O47	66.8 (12)	O63—Mo43—O66	171.5 (7)
O46—Ce3—O50	143.9 (8)	O63—Mo43—O75	103.3 (8)
O47—Ce3—O23	98.0 (13)	O64—Mo43—O54	71.7 (6)
O47—Ce3—O50	134.8 (11)	O64—Mo43—O66	79.6 (6)
O48—Ce3—O23	136.7 (9)	O65—Mo43—O54	95.2 (6)
O48—Ce3—O46	68.5 (10)	O65—Mo43—O64	152.2 (7)
O48—Ce3—O47	71.3 (16)	O65—Mo43—O66	73.5 (6)
O48—Ce3—O50	138.8 (8)	O75—Mo43—O54	155.1 (7)
O49—Ce3—O23	69.3 (8)	O75—Mo43—O64	88.8 (7)
O49—Ce3—O46	111.6 (12)	O75—Mo43—O65	95.3 (7)
O49—Ce3—O47	68.5 (13)	O75—Mo43—O66	85.0 (6)
O49—Ce3—O48	135.0 (15)	O42—Mo44—O51	76.3 (6)
O49—Ce3—O50	68.2 (10)	O42—Mo44—O54	75.6 (6)
O50—Ce3—O23	78.5 (7)	O42—Mo44—O66	142.7 (6)
O69—Ce3—O23	132.7 (6)	O51—Mo44—O54	82.9 (6)
O69—Ce3—O46	122.4 (10)	O52—Mo44—O42	102.8 (7)
O69—Ce3—O47	129.2 (13)	O52—Mo44—O51	98.8 (8)
O69—Ce3—O48	68.8 (8)	O52—Mo44—O53	104.7 (8)
O69—Ce3—O49	125.9 (9)	O52—Mo44—O54	177.4 (7)
O69—Ce3—O50	70.5 (7)	O52—Mo44—O66	104.1 (7)
O70—Ce3—O23	141.0 (7)	O53—Mo44—O42	99.7 (7)
O70—Ce3—O46	135.7 (9)	O53—Mo44—O51	156.5 (7)
O70—Ce3—O47	75.3 (11)	O53—Mo44—O54	73.7 (6)
O70—Ce3—O48	78.4 (13)	O53—Mo44—O66	97.9 (6)
O70—Ce3—O49	72.6 (8)	O66—Mo44—O51	74.5 (6)
O70—Ce3—O50	79.9 (8)	O66—Mo44—O54	78.2 (6)
O70—Ce3—O69	67.0 (6)	O51—Mo45—O66	68.3 (6)
O205—Mo1—O211	75.7 (7)	O65—Mo45—O51	87.5 (7)
O212—Mo1—O205	95.8 (8)	O65—Mo45—O66	72.8 (6)
O212—Mo1—O211	73.3 (7)	O65—Mo45—O68	156.7 (7)
O212—Mo1—O213	152.4 (8)	O67—Mo45—O51	102.6 (7)
O212—Mo1—O215	93.9 (8)	O67—Mo45—O65	100.8 (8)
O213—Mo1—O205	72.0 (7)	O67—Mo45—O66	168.7 (7)
O213—Mo1—O211	79.7 (7)	O67—Mo45—O68	101.8 (7)
O214—Mo1—O205	97.5 (8)	O67—Mo45—O76	103.7 (8)
O214—Mo1—O211	171.2 (7)	O68—Mo45—O51	81.8 (7)
O214—Mo1—O212	102.2 (9)	O68—Mo45—O66	84.0 (6)
O214—Mo1—O213	103.9 (9)	O76—Mo45—O51	152.7 (7)
O214—Mo1—O215	101.1 (8)	O76—Mo45—O65	94.5 (7)
O215—Mo1—O205	156.7 (8)	O76—Mo45—O66	86.3 (6)
O215—Mo1—O211	86.9 (7)	O76—Mo45—O68	85.9 (7)
O215—Mo1—O213	89.9 (8)	O10—Mo46—O21	76.1 (7)
O204^{i}—Mo2—O207	80.9 (7)	O20—Mo46—O10	67.0 (7)

O204^{i}—Mo2—O213^{i}	67.6 (7)	O20—Mo46—O21	81.9 (7)
O206—Mo2—O204^{i}	93.1 (8)	O22—Mo46—O10	98.5 (8)
O206—Mo2—O207	83.4 (8)	O22—Mo46—O20	94.3 (8)
O206—Mo2—O208	103.1 (7)	O22—Mo46—O21	174.3 (8)
O206—Mo2—O213^{i}	154.7 (8)	O22—Mo46—O30^{i}	101.4 (11)
O208—Mo2—O204^{i}	152.6 (7)	O23—Mo46—O10	152.8 (8)
O208—Mo2—O207	79.1 (7)	O23—Mo46—O20	92.6 (8)
O208—Mo2—O213^{i}	89.8 (6)	O23—Mo46—O21	83.6 (8)
O209—Mo2—O204^{i}	94.7 (8)	O23—Mo46—O22	100.9 (8)
O209—Mo2—O206	104.5 (9)	O23—Mo46—O30^{i}	104.9 (9)
O209—Mo2—O207	171.2 (7)	O30^{i}—Mo46—O10	89.6 (8)
O209—Mo2—O208	102.3 (8)	O30^{i}—Mo46—O20	153.6 (8)
O209—Mo2—O213^{i}	93.5 (8)	O30^{i}—Mo46—O21	80.7 (9)
O213^{i}—Mo2—O207	77.7 (6)	O19—Mo47—O24	76.4 (7)
O190—Mo3—O191	89.0 (7)	O20—Mo47—O19	68.0 (6)
O190—Mo3—O199	93.6 (9)	O20—Mo47—O24	78.2 (7)
O190—Mo3—O201	88.7 (9)	O25—Mo47—O19	95.2 (8)
O190—Mo3—O204	155.3 (7)	O25—Mo47—O20	93.4 (8)
O199—Mo3—O191	82.5 (8)	O25—Mo47—O24	169.9 (8)
O199—Mo3—O204	88.6 (8)	O25—Mo47—O43	102.3 (9)
O201—Mo3—O191	88.4 (7)	O25—Mo47—O45	104.2 (10)
O201—Mo3—O199	170.6 (9)	O43—Mo47—O19	89.8 (6)
O201—Mo3—O204	85.5 (8)	O43—Mo47—O20	154.0 (7)
O202—Mo3—O190	108.8 (8)	O43—Mo47—O24	83.6 (7)
O202—Mo3—O191	162.0 (8)	O45—Mo47—O19	153.0 (8)
O202—Mo3—O199	93.5 (9)	O45—Mo47—O20	92.0 (7)
O202—Mo3—O201	94.4 (8)	O45—Mo47—O24	82.0 (9)
O202—Mo3—O204	95.6 (8)	O45—Mo47—O43	103.9 (7)
O204—Mo3—O191	66.9 (6)	O1—Mo48—O26	90.4 (7)
O191—Mo4—O192	72.4 (7)	O1—Mo48—O42	73.2 (7)
O191—Mo4—O198	85.6 (7)	O1—Mo48—O43	158.4 (7)
O191—Mo4—O204	71.8 (7)	O1—Mo48—O51	89.1 (7)
O191—Mo4—O205	140.0 (7)	O26—Mo48—O42	84.8 (6)
O191—Mo4—O213	140.5 (6)	O26—Mo48—O43	85.8 (7)
O192—Mo4—O198	83.2 (6)	O26—Mo48—O51	153.8 (6)
O192—Mo4—O205	71.7 (7)	O43—Mo48—O42	85.3 (6)
O192—Mo4—O213	142.4 (7)	O43—Mo48—O51	85.1 (7)
O203—Mo4—O191	101.9 (9)	O44—Mo48—O1	100.4 (9)
O203—Mo4—O192	94.2 (7)	O44—Mo48—O26	104.6 (7)
O203—Mo4—O198	171.0 (8)	O44—Mo48—O42	168.8 (7)
O203—Mo4—O204	100.3 (8)	O44—Mo48—O43	101.1 (8)
O203—Mo4—O205	97.7 (9)	O44—Mo48—O51	101.3 (7)
O203—Mo4—O213	94.4 (8)	O51—Mo48—O42	70.0 (6)
O204—Mo4—O192	143.4 (7)	O1—Mo49—O40	151.3 (7)
O204—Mo4—O198	86.7 (6)	O1—Mo49—O42	74.0 (7)
O204—Mo4—O205	137.8 (7)	O1—Mo49—O54	93.2 (7)
O204—Mo4—O213	70.0 (7)	O27—Mo49—O1	97.8 (7)
O205—Mo4—O198	73.3 (7)	O27—Mo49—O40	88.1 (7)

O213—Mo4—O198	82.7 (7)	O27—Mo49—O42	85.4 (6)
O213—Mo4—O205	70.9 (7)	O27—Mo49—O54	153.5 (6)
O194—Mo5—O197	76.7 (7)	O39—Mo49—O1	102.5 (8)
O194—Mo5—O205	75.9 (7)	O39—Mo49—O27	102.8 (8)
O194—Mo5—O211	140.0 (7)	O39—Mo49—O40	103.5 (8)
O196—Mo5—O194	105.2 (8)	O39—Mo49—O42	171.5 (7)
O196—Mo5—O197	98.4 (8)	O39—Mo49—O54	98.2 (7)
O196—Mo5—O198	104.7 (8)	O40—Mo49—O42	78.6 (6)
O196—Mo5—O205	177.6 (8)	O40—Mo49—O54	71.2 (7)
O196—Mo5—O211	105.5 (8)	O54—Mo49—O42	74.6 (6)
O197—Mo5—O205	84.0 (7)	O28—Mo50—O34	80.2 (9)
O198—Mo5—O194	100.0 (8)	O28—Mo50—O40	89.3 (7)
O198—Mo5—O197	156.7 (7)	O28—Mo50—O57	153.1 (7)
O198—Mo5—O205	72.9 (7)	O35—Mo50—O28	106.6 (8)
O198—Mo5—O211	96.3 (7)	O35—Mo50—O34	84.6 (8)
O211—Mo5—O197	74.1 (7)	O35—Mo50—O40	153.3 (7)
O211—Mo5—O205	74.5 (7)	O35—Mo50—O57	89.7 (7)
O156—Mo6—O172	86.1 (10)	O38—Mo50—O28	100.3 (9)
O156—Mo6—O175	84.0 (8)	O38—Mo50—O34	170.7 (8)
O156—Mo6—O190	157.9 (9)	O38—Mo50—O35	104.0 (9)
O173—Mo6—O156	99.4 (10)	O38—Mo50—O40	93.7 (7)
O173—Mo6—O172	92.3 (14)	O38—Mo50—O57	96.1 (8)
O173—Mo6—O174	101.0 (15)	O40—Mo50—O34	77.0 (7)
O173—Mo6—O175	168.3 (13)	O57—Mo50—O34	80.3 (8)
O173—Mo6—O190	93.7 (9)	O57—Mo50—O40	68.4 (6)
O174—Mo6—O156	98.7 (10)	O33—Mo51—O35	83.6 (7)
O174—Mo6—O172	164.9 (12)	O33—Mo51—O36	82.8 (9)
O174—Mo6—O175	89.5 (11)	O33—Mo51—O56	158.5 (9)
O174—Mo6—O190	96.2 (9)	O35—Mo51—O36	76.2 (7)
O175—Mo6—O172	76.7 (10)	O37—Mo51—O33	97.7 (9)
O190—Mo6—O172	75.6 (9)	O37—Mo51—O35	162.8 (10)
O190—Mo6—O175	79.9 (7)	O37—Mo51—O36	86.9 (10)
O175—Mo7—O177	106.1 (8)	O37—Mo51—O56	94.2 (8)
O175—Mo7—O187	102.9 (10)	O55—Mo51—O33	98.8 (11)
O175—Mo7—O189	85.2 (11)	O55—Mo51—O35	93.2 (8)
O175—Mo7—O191	89.4 (8)	O55—Mo51—O36	169.1 (8)
O175—Mo7—O192	153.4 (8)	O55—Mo51—O37	103.5 (11)
O177—Mo7—O189	81.0 (8)	O55—Mo51—O56	95.8 (11)
O177—Mo7—O191	154.0 (7)	O56—Mo51—O35	79.8 (7)
O177—Mo7—O192	90.4 (7)	O56—Mo51—O36	80.0 (8)
O187—Mo7—O177	98.4 (8)	O29—Mo52—O5^{i}	83.2 (9)
O187—Mo7—O189	171.7 (9)	O30—Mo52—O5^{i}	82.0 (7)
O187—Mo7—O191	98.2 (7)	O30—Mo52—O29	81.8 (11)
O187—Mo7—O192	94.9 (7)	O31—Mo52—O5^{i}	85.3 (10)
O191—Mo7—O189	79.7 (7)	O31—Mo52—O29	167.7 (14)
O191—Mo7—O192	68.3 (6)	O31—Mo52—O30	92.1 (15)
O192—Mo7—O189	76.8 (8)	O31—Mo52—O33	97.8 (14)
O188—Mo8—O192	89.2 (7)	O32—Mo52—O5^{i}	172.7 (8)

O188—Mo8—O193	96.3 (7)	O32—Mo52—O29	90.6 (11)
O188—Mo8—O194	86.6 (7)	O32—Mo52—O30	93.2 (8)
O188—Mo8—O205	155.2 (7)	O32—Mo52—O31	100.5 (12)
O192—Mo8—O194	80.1 (6)	O32—Mo52—O33	101.9 (9)
O192—Mo8—O205	71.9 (7)	O33—Mo52—O5^{i}	81.6 (8)
O193—Mo8—O192	153.3 (7)	O33—Mo52—O29	84.9 (11)
O193—Mo8—O194	74.2 (7)	O33—Mo52—O30	160.0 (10)
O193—Mo8—O205	94.1 (7)	O13—Mo53—O14	87.8 (7)
O200—Mo8—O188	104.4 (8)	O13—Mo53—O17	73.6 (6)
O200—Mo8—O192	102.9 (9)	O13—Mo53—O28	157.0 (7)
O200—Mo8—O193	101.1 (9)	O14—Mo53—O17	70.8 (6)
O200—Mo8—O194	168.6 (8)	O15—Mo53—O13	99.6 (7)
O200—Mo8—O205	95.7 (8)	O15—Mo53—O14	99.0 (8)
O205—Mo8—O194	74.7 (7)	O15—Mo53—O17	167.7 (8)
O185—Mo9—O194	86.6 (7)	O15—Mo53—O27	103.4 (7)
O185—Mo9—O197	84.6 (7)	O15—Mo53—O28	103.3 (8)
O186—Mo9—O185	86.5 (10)	O27—Mo53—O13	91.1 (7)
O186—Mo9—O193	91.2 (11)	O27—Mo53—O14	157.4 (7)
O186—Mo9—O194	87.0 (10)	O27—Mo53—O17	87.2 (6)
O186—Mo9—O197	154.7 (9)	O27—Mo53—O28	85.1 (7)
O193—Mo9—O185	160.3 (7)	O28—Mo53—O14	87.1 (7)
O193—Mo9—O194	73.7 (7)	O28—Mo53—O17	83.5 (7)
O193—Mo9—O197	89.3 (7)	O8—Mo54—O12	74.0 (6)
O195—Mo9—O185	101.1 (8)	O8—Mo54—O14	76.5 (7)
O195—Mo9—O186	103.8 (10)	O8—Mo54—O17	140.0 (6)
O195—Mo9—O193	98.5 (8)	O14—Mo54—O12	86.3 (6)
O195—Mo9—O194	167.0 (7)	O16—Mo54—O8	105.0 (8)
O195—Mo9—O197	101.1 (7)	O16—Mo54—O12	175.4 (8)
O197—Mo9—O194	68.9 (6)	O16—Mo54—O14	97.9 (8)
O166—Mo10—O181	67.9 (7)	O16—Mo54—O17	107.2 (8)
O166—Mo10—O183	80.0 (8)	O16—Mo54—O18	103.9 (8)
O181—Mo10—O183	78.3 (7)	O17—Mo54—O12	75.7 (6)
O182—Mo10—O166	94.0 (8)	O17—Mo54—O14	76.1 (6)
O182—Mo10—O181	92.1 (8)	O18—Mo54—O8	97.6 (8)
O182—Mo10—O183	170.1 (8)	O18—Mo54—O12	72.0 (7)
O182—Mo10—O184	105.2 (10)	O18—Mo54—O14	158.2 (7)
O182—Mo10—O185	103.5 (9)	O18—Mo54—O17	97.2 (8)
O184—Mo10—O166	91.7 (9)	O11—Mo55—O12	95.0 (7)
O184—Mo10—O181	154.3 (9)	O11—Mo55—O13	103.1 (9)
O184—Mo10—O183	82.9 (9)	O11—Mo55—O17	168.1 (7)
O184—Mo10—O185	103.9 (9)	O11—Mo55—O19	104.0 (8)
O185—Mo10—O166	152.4 (8)	O11—Mo55—O26	103.3 (8)
O185—Mo10—O181	89.9 (7)	O12—Mo55—O17	75.5 (6)
O185—Mo10—O183	79.5 (8)	O13—Mo55—O12	93.7 (7)
O169—Mo11—O179	73.6 (6)	O13—Mo55—O17	70.9 (6)
O178—Mo11—O169	95.8 (7)	O13—Mo55—O19	149.9 (6)
O178—Mo11—O179	71.6 (6)	O19—Mo55—O12	71.3 (6)
O178—Mo11—O181	150.5 (7)	O19—Mo55—O17	80.0 (6)

O178—Mo11—O186	95.5 (12)	O26—Mo55—O12	156.0 (7)
O180—Mo11—O169	97.0 (8)	O26—Mo55—O13	97.1 (7)
O180—Mo11—O178	103.7 (9)	O26—Mo55—O17	87.9 (6)
O180—Mo11—O179	168.7 (7)	O26—Mo55—O19	89.1 (7)
O180—Mo11—O181	103.7 (9)	O6—Mo56—O12	71.3 (7)
O180—Mo11—O186	101.6 (11)	O6—Mo56—O18	84.0 (6)
O181—Mo11—O169	70.4 (7)	O9—Mo56—O6	93.2 (7)
O181—Mo11—O179	79.4 (6)	O9—Mo56—O10	102.5 (9)
O186—Mo11—O169	155.2 (8)	O9—Mo56—O12	99.6 (8)
O186—Mo11—O179	89.3 (10)	O9—Mo56—O18	172.5 (7)
O186—Mo11—O181	89.2 (10)	O9—Mo56—O19	92.8 (8)
O171—Mo12—O179	69.1 (7)	O9—Mo56—O20	99.3 (8)
O176—Mo12—O171	99.4 (8)	O10—Mo56—O6	72.2 (6)
O176—Mo12—O177	101.5 (9)	O10—Mo56—O12	137.9 (7)
O176—Mo12—O178	101.0 (9)	O10—Mo56—O18	83.3 (7)
O176—Mo12—O179	167.4 (8)	O10—Mo56—O19	141.8 (6)
O176—Mo12—O188	102.9 (8)	O10—Mo56—O20	71.7 (7)
O177—Mo12—O171	87.8 (7)	O12—Mo56—O18	72.8 (6)
O177—Mo12—O179	83.7 (7)	O19—Mo56—O6	142.3 (7)
O178—Mo12—O171	87.6 (7)	O19—Mo56—O12	71.0 (7)
O178—Mo12—O177	157.5 (8)	O19—Mo56—O18	85.3 (6)
O178—Mo12—O179	74.1 (7)	O20—Mo56—O6	143.5 (7)
O188—Mo12—O171	157.7 (7)	O20—Mo56—O12	138.5 (7)
O188—Mo12—O177	86.8 (7)	O20—Mo56—O18	87.0 (7)
O188—Mo12—O178	89.2 (7)	O20—Mo56—O19	71.4 (7)
O188—Mo12—O179	88.7 (7)	O253—Mo57—O4	78.6 (7)
O159—Mo13—O169	75.7 (6)	O253—Mo57—O6	89.4 (7)
O159—Mo13—O171	78.7 (7)	O253—Mo57—O10	150.7 (7)
O159—Mo13—O179	140.5 (6)	O5—Mo57—O253	106.5 (8)
O168—Mo13—O159	101.0 (8)	O5—Mo57—O4	83.7 (8)
O168—Mo13—O169	72.2 (7)	O5—Mo57—O6	155.1 (8)
O168—Mo13—O171	157.3 (7)	O5—Mo57—O10	89.4 (8)
O168—Mo13—O179	94.1 (7)	O6—Mo57—O4	80.8 (7)
O170—Mo13—O159	105.2 (8)	O7—Mo57—O253	100.8 (8)
O170—Mo13—O168	104.7 (8)	O7—Mo57—O4	173.3 (9)
O170—Mo13—O169	176.9 (8)	O7—Mo57—O5	102.9 (9)
O170—Mo13—O171	97.1 (8)	O7—Mo57—O6	92.5 (8)
O170—Mo13—O179	105.8 (8)	O7—Mo57—O10	99.4 (8)
O171—Mo13—O169	85.9 (6)	O10—Mo57—O4	78.9 (7)
O179—Mo13—O169	74.6 (6)	O10—Mo57—O6	68.6 (7)
O179—Mo13—O171	73.8 (6)	O253—Mo58—O8^{i}	83.3 (7)
O154—Mo14—O155	86.4 (7)	O253—Mo58—O14^{i}	87.3 (7)
O154—Mo14—O159	87.5 (7)	O14^{i}—Mo58—O8^{i}	70.8 (6)
O154—Mo14—O171	158.4 (7)	O220—Mo58—O253	101.8 (9)
O155—Mo14—O159	84.0 (7)	O220—Mo58—O8^{i}	168.3 (7)
O155—Mo14—O171	87.9 (7)	O220—Mo58—O14^{i}	98.8 (8)
O157—Mo14—O154	104.2 (8)	O220—Mo58—O221	102.5 (8)
O157—Mo14—O155	102.9 (9)	O220—Mo58—O222^{i}	100.4 (8)

O157—Mo14—O158	98.7 (9)	O221—Mo58—O253	86.9 (7)
O157—Mo14—O159	166.7 (8)	O221—Mo58—O8^{i}	88.1 (6)
O157—Mo14—O171	97.3 (8)	O221—Mo58—O14^{i}	158.7 (7)
O158—Mo14—O154	87.8 (7)	O221—Mo58—O222^{i}	87.9 (7)
O158—Mo14—O155	158.4 (8)	O222^{i}—Mo58—O253	157.8 (8)
O158—Mo14—O159	75.0 (7)	O222^{i}—Mo58—O8^{i}	74.9 (7)
O158—Mo14—O171	89.9 (7)	O222^{i}—Mo58—O14^{i}	89.7 (7)
O171—Mo14—O159	71.2 (6)	O2—Mo59—O6	104.4 (8)
O135—Mo15—O140	78.7 (9)	O2—Mo59—O8	168.6 (7)
O135—Mo15—O144	69.0 (7)	O2—Mo59—O12	95.7 (8)
O141—Mo15—O135	90.0 (7)	O2—Mo59—O221	102.1 (8)
O141—Mo15—O140	85.9 (9)	O2—Mo59—O222	104.3 (8)
O141—Mo15—O144	155.9 (8)	O6—Mo59—O8	77.7 (6)
O141—Mo15—O155	106.4 (8)	O6—Mo59—O12	72.1 (7)
O143—Mo15—O135	96.0 (8)	O12—Mo59—O8	74.1 (6)
O143—Mo15—O140	170.7 (8)	O221—Mo59—O6	86.3 (7)
O143—Mo15—O141	101.9 (9)	O221—Mo59—O8	89.2 (6)
O143—Mo15—O144	92.2 (8)	O221—Mo59—O12	154.9 (7)
O143—Mo15—O155	99.9 (9)	O221—Mo59—O222	100.6 (7)
O144—Mo15—O140	78.8 (7)	O222—Mo59—O6	148.3 (7)
O155—Mo15—O135	154.1 (8)	O222—Mo59—O8	71.6 (6)
O155—Mo15—O140	82.5 (9)	O222—Mo59—O12	91.8 (7)
O155—Mo15—O144	90.0 (7)	O197—Mo60—O211	68.3 (6)
O137—Mo16—O138	86.7 (13)	O208—Mo60—O197	82.5 (7)
O137—Mo16—O141	82.4 (7)	O208—Mo60—O211	84.7 (7)
O138—Mo16—O141	84.4 (11)	O210—Mo60—O197	100.3 (8)
O139—Mo16—O137	96.2 (10)	O210—Mo60—O208	102.3 (9)
O139—Mo16—O138	91.5 (16)	O210—Mo60—O211	166.0 (8)
O139—Mo16—O141	175.8 (14)	O210—Mo60—O212	101.1 (9)
O139—Mo16—O142	98.7 (16)	O210—Mo60—O215^{i}	104.9 (8)
O139—Mo16—O156	98.0 (10)	O212—Mo60—O197	86.5 (7)
O142—Mo16—O137	90.2 (12)	O212—Mo60—O208	155.5 (7)
O142—Mo16—O138	169.6 (12)	O212—Mo60—O211	70.9 (7)
O142—Mo16—O141	85.3 (10)	O215^{i}—Mo60—O197	154.2 (7)
O156—Mo16—O137	163.9 (10)	O215^{i}—Mo60—O208	86.9 (7)
O156—Mo16—O138	85.5 (13)	O215^{i}—Mo60—O211	87.4 (7)
O156—Mo16—O141	82.8 (8)	O215^{i}—Mo60—O212	93.8 (8)
O156—Mo16—O142	95.0 (12)	Mo49—O1—Mo48	123.4 (10)
O150—Mo17—O162	88.3 (7)	Mo57—O253—Mo58	146.6 (11)
O150—Mo17—O165	81.8 (9)	Mo57—O5—Mo52^{i}	155.6 (11)
O150—Mo17—O166	153.1 (8)	Mo56—O6—Mo57	108.2 (7)
O162—Mo17—O165	77.1 (7)	Mo56—O6—Mo59	108.5 (7)
O163—Mo17—O150	102.3 (13)	Mo59—O6—Mo57	141.3 (8)
O163—Mo17—O162	96.1 (10)	Mo54—O8—Mo58^{i}	103.4 (7)
O163—Mo17—O164	103.2 (11)	Mo54—O8—Mo59	108.6 (7)
O163—Mo17—O165	172.0 (10)	Mo58^{i}—O8—Mo59	89.3 (5)
O163—Mo17—O166	93.6 (12)	Mo56—O10—Mo46	109.8 (8)
O164—Mo17—O150	101.9 (9)	Mo56—O10—Mo57	110.0 (8)

O164—Mo17—O162	155.5 (9)	Mo57—O10—Mo46	139.2 (10)
O164—Mo17—O165	82.4 (9)	Mo55—O12—Mo54	101.9 (7)
O164—Mo17—O166	95.3 (9)	Mo55—O12—Mo56	104.1 (7)
O166—Mo17—O162	68.4 (7)	Mo56—O12—Mo54	95.8 (6)
O166—Mo17—O165	80.1 (7)	Mo59—O12—Mo54	103.3 (6)
O161—Mo18—O162	72.3 (7)	Mo59—O12—Mo55	140.1 (8)
O161—Mo18—O168	84.6 (6)	Mo59—O12—Mo56	103.5 (9)
O161—Mo18—O169	71.9 (7)	Mo55—O13—Mo53	124.3 (8)
O162—Mo18—O168	84.6 (7)	Mo53—O14—Mo54	109.3 (8)
O162—Mo18—O169	139.1 (7)	Mo53—O14—Mo58^{i}	139.0 (8)
O166—Mo18—O161	142.3 (7)	Mo58^{i}—O14—Mo54	108.8 (8)
O166—Mo18—O162	70.6 (7)	Mo53—O17—Mo55	90.0 (5)
O166—Mo18—O168	85.5 (7)	Mo54—O17—Mo53	102.9 (6)
O166—Mo18—O169	138.3 (7)	Mo54—O17—Mo55	106.8 (7)
O167—Mo18—O161	92.6 (7)	Mo54—O18—Mo56	119.4 (8)
O167—Mo18—O162	99.4 (8)	Mo55—O19—Mo47	139.7 (9)
O167—Mo18—O166	99.8 (8)	Mo56—O19—Mo47	108.2 (8)
O167—Mo18—O168	174.2 (8)	Mo56—O19—Mo55	110.7 (7)
O167—Mo18—O169	101.2 (8)	Mo47—O20—Mo46	135.2 (8)
O167—Mo18—O181	94.0 (8)	Mo56—O20—Mo46	111.3 (8)
O169—Mo18—O168	73.1 (6)	Mo56—O20—Mo47	111.6 (8)
O181—Mo18—O161	142.9 (8)	Mo46—O23—Ce3	150.8 (10)
O181—Mo18—O162	141.8 (7)	Mo55—O26—Mo48	157.1 (10)
O181—Mo18—O166	71.9 (7)	Mo49—O27—Mo53	158.7 (9)
O181—Mo18—O168	85.3 (6)	Mo50—O28—Mo53	150.1 (10)
O181—Mo18—O169	71.0 (7)	Mo46^{i}—O30—Mo52	157.6 (13)
O126—Mo19—O129	81.4 (7)	Mo52—O33—Mo51	140.4 (11)
O126—Mo19—O130	85.6 (14)	Mo50—O35—Mo51	139.9 (10)
O126—Mo19—O150	157.8 (11)	Mo42—O40—Mo50	106.4 (7)
O127—Mo19—O126	99.8 (13)	Mo49—O40—Mo42	111.5 (8)
O127—Mo19—O129	89.2 (9)	Mo49—O40—Mo50	140.8 (9)
O127—Mo19—O130	166.9 (11)	Mo44—O42—Mo48	102.2 (7)
O127—Mo19—O150	95.5 (11)	Mo44—O42—Mo49	107.9 (7)
O128—Mo19—O126	99.3 (9)	Mo49—O42—Mo48	88.8 (5)
O128—Mo19—O127	102.4 (12)	Mo47—O43—Mo48	148.8 (9)
O128—Mo19—O129	168.1 (11)	Mo47—O45—Ce3	156.8 (11)
O128—Mo19—O130	88.4 (11)	Mo45—O51—Mo44	113.1 (8)
O128—Mo19—O150	93.1 (9)	Mo48—O51—Mo44	110.5 (7)
O129—Mo19—O130	79.8 (8)	Mo48—O51—Mo45	135.9 (8)
O150—Mo19—O129	82.8 (7)	Mo44—O53—Mo42	117.2 (7)
O150—Mo19—O130	76.3 (12)	Mo42—O54—Mo43	101.9 (7)
O129—Mo20—O149	107.4 (7)	Mo42—O54—Mo44	96.4 (6)
O129—Mo20—O151	83.9 (8)	Mo43—O54—Mo44	100.0 (6)
O129—Mo20—O161	152.3 (7)	Mo49—O54—Mo42	102.8 (7)
O129—Mo20—O162	86.9 (7)	Mo49—O54—Mo43	144.7 (8)
O149—Mo20—O151	79.9 (7)	Mo49—O54—Mo44	101.9 (7)
O149—Mo20—O161	88.8 (7)	Mo41—O56—Mo51	155.7 (13)
O149—Mo20—O162	153.7 (7)	Mo42—O57—Mo41	109.1 (8)

O152—Mo20—O129	102.8 (9)	Mo42—O57—Mo50	111.2 (8)
O152—Mo20—O149	100.6 (8)	Mo50—O57—Mo41	138.9 (9)
O152—Mo20—O151	172.6 (9)	Mo41—O61—Ce2	162.4 (9)
O152—Mo20—O161	95.7 (9)	Mo41—O62—Mo40	134.8 (8)
O152—Mo20—O162	97.3 (8)	Mo41—O62—Mo42	112.1 (8)
O161—Mo20—O151	76.9 (7)	Mo42—O62—Mo40	109.1 (7)
O161—Mo20—O162	70.3 (7)	Mo42—O64—Mo40	107.8 (7)
O162—Mo20—O151	79.9 (7)	Mo43—O64—Mo40	140.7 (8)
O153—Mo21—O158	100.0 (8)	Mo43—O64—Mo42	110.9 (7)
O153—Mo21—O159	88.7 (6)	Mo43—O65—Mo45	125.1 (8)
O153—Mo21—O161	86.9 (7)	Mo44—O66—Mo43	105.3 (7)
O153—Mo21—O169	154.7 (6)	Mo44—O66—Mo45	103.2 (6)
O158—Mo21—O159	72.2 (7)	Mo45—O66—Mo43	88.3 (5)
O158—Mo21—O161	148.7 (7)	Mo37—O68—Mo45	150.2 (10)
O158—Mo21—O169	92.0 (7)	Mo37—O69—Ce3	155.8 (11)
O160—Mo21—O153	103.9 (8)	Mo32—O70—Ce3	162.7 (10)
O160—Mo21—O158	105.0 (9)	Mo43—O75—Mo39	156.9 (9)
O160—Mo21—O159	167.4 (7)	Mo38—O76—Mo45	155.0 (9)
O160—Mo21—O161	102.7 (8)	Mo40—O81—Ce2	156.1 (10)
O160—Mo21—O169	94.2 (7)	Mo40—O83—Mo39	151.8 (9)
O161—Mo21—O159	77.6 (6)	Mo35—O85—Mo38	106.1 (7)
O161—Mo21—O169	71.7 (6)	Mo35—O85—Mo39	103.2 (7)
O169—Mo21—O159	73.8 (6)	Mo39—O85—Mo38	88.3 (5)
O99—Mo22—O117	101.6 (10)	Mo38—O86—Mo39	124.0 (8)
O99—Mo22—O118	94.1 (8)	Mo33—O88—Mo37	106.0 (8)
O99—Mo22—O119	84.7 (9)	Mo38—O88—Mo33	113.0 (8)
O99—Mo22—O135	156.4 (9)	Mo38—O88—Mo37	139.0 (9)
O99—Mo22—O137	106.3 (9)	Mo32—O89—Mo37	133.7 (8)
O117—Mo22—O118	95.7 (10)	Mo33—O89—Mo32	112.2 (8)
O117—Mo22—O119	173.0 (9)	Mo33—O89—Mo37	109.8 (7)
O117—Mo22—O135	94.2 (10)	Mo32—O92—Mo27	162.6 (11)
O117—Mo22—O137	98.0 (11)	Mo31—O94—Mo32	137.4 (8)
O118—Mo22—O119	80.7 (7)	Mo33—O94—Mo31	112.2 (8)
O118—Mo22—O135	66.7 (6)	Mo33—O94—Mo32	109.9 (7)
O135—Mo22—O119	78.9 (8)	Mo33—O95—Mo34	101.4 (7)
O137—Mo22—O118	152.4 (9)	Mo33—O95—Mo35	95.8 (5)
O137—Mo22—O119	82.9 (10)	Mo33—O95—Mo38	103.1 (7)
O137—Mo22—O135	88.5 (8)	Mo34—O95—Mo35	100.3 (7)
O118—Mo23—O133	84.9 (7)	Mo38—O95—Mo34	145.7 (7)
O118—Mo23—O134	139.1 (7)	Mo38—O95—Mo35	100.7 (6)
O118—Mo23—O144	143.2 (7)	Mo35—O96—Mo33	115.9 (7)
O120—Mo23—O118	72.9 (7)	Mo36—O97—Mo35	110.3 (8)
O120—Mo23—O133	84.7 (6)	Mo39—O97—Mo35	112.1 (8)
O120—Mo23—O134	70.4 (7)	Mo39—O97—Mo36	137.4 (9)
O120—Mo23—O135	142.3 (7)	Mo22—O99—Ce2	154.0 (10)
O120—Mo23—O144	140.7 (7)	Mo30—O101—Ce2	166.4 (12)
O134—Mo23—O133	74.5 (6)	Mo30—O102—Mo36	147.3 (10)
O135—Mo23—O118	70.3 (7)	Mo35—O105—Mo34	108.2 (8)

O135—Mo23—O133	84.0 (8)	Mo35—O105—Mo36	102.4 (7)
O135—Mo23—O134	139.2 (7)	Mo36—O105—Mo34	88.6 (5)
O135—Mo23—O144	73.5 (7)	Mo34—O106—Mo36	123.3 (9)
O136—Mo23—O118	100.9 (10)	Mo33—O108—Mo31	107.8 (7)
O136—Mo23—O120	94.0 (8)	Mo34—O108—Mo31	141.3 (8)
O136—Mo23—O133	173.3 (9)	Mo34—O108—Mo33	109.4 (7)
O136—Mo23—O134	99.0 (9)	Mo31—O111—Mo27	144.5 (11)
O136—Mo23—O135	100.8 (9)	Mo34—O115—Mo28	155.8 (9)
O136—Mo23—O144	92.3 (9)	Mo36—O116—Mo29	154.8 (9)
O144—Mo23—O133	84.7 (7)	Mo22—O118—Mo30	135.4 (9)
O144—Mo23—O134	70.4 (7)	Mo23—O118—Mo22	112.7 (7)
O134—Mo24—O147	74.4 (6)	Mo23—O118—Mo30	110.5 (8)
O144—Mo24—O134	71.8 (6)	Mo23—O120—Mo29	111.7 (8)
O144—Mo24—O147	78.1 (7)	Mo23—O120—Mo30	108.0 (8)
O145—Mo24—O134	96.2 (7)	Mo29—O120—Mo30	138.7 (9)
O145—Mo24—O144	104.5 (9)	Mo29—O122—Mo28	125.1 (8)
O145—Mo24—O146	104.1 (9)	Mo25—O123—Mo28	103.8 (7)
O145—Mo24—O147	169.1 (6)	Mo25—O123—Mo29	107.7 (7)
O145—Mo24—O154	101.5 (7)	Mo28—O123—Mo29	89.1 (5)
O146—Mo24—O134	91.1 (7)	Mo31—O125—Mo28	149.4 (9)
O146—Mo24—O144	147.9 (8)	Mo27—O126—Mo19	139.3 (12)
O146—Mo24—O147	71.1 (7)	Mo20—O129—Mo19	151.9 (9)
O146—Mo24—O154	100.2 (8)	Mo26—O131—Mo25	109.8 (8)
O154—Mo24—O134	155.9 (6)	Mo26—O131—Mo28	138.4 (9)
O154—Mo24—O144	87.9 (7)	Mo28—O131—Mo25	109.5 (8)
O154—Mo24—O147	89.1 (6)	Mo25—O133—Mo23	118.0 (8)
O123—Mo25—O131	76.1 (7)	Mo24—O134—Mo23	103.1 (7)
O132—Mo25—O123	107.5 (8)	Mo29—O134—Mo23	103.8 (7)
O132—Mo25—O131	98.5 (9)	Mo29—O134—Mo24	141.8 (8)
O132—Mo25—O133	103.9 (9)	Mo15—O135—Mo22	139.2 (9)
O132—Mo25—O147	104.0 (8)	Mo23—O135—Mo15	110.0 (9)
O133—Mo25—O123	96.6 (7)	Mo23—O135—Mo22	109.9 (8)
O133—Mo25—O131	157.6 (7)	Mo22—O137—Mo16	162.1 (12)
O133—Mo25—O147	98.6 (7)	Mo15—O141—Mo16	147.8 (11)
O147—Mo25—O123	140.4 (6)	Mo23—O144—Mo15	106.9 (8)
O147—Mo25—O131	76.0 (7)	Mo24—O144—Mo15	141.4 (9)
O131—Mo26—O147	70.0 (6)	Mo24—O144—Mo23	110.7 (7)
O146—Mo26—O131	89.3 (7)	Mo24—O146—Mo26	124.8 (9)
O146—Mo26—O147	74.1 (7)	Mo25—O147—Mo24	108.4 (7)
O146—Mo26—O149	156.8 (7)	Mo25—O147—Mo26	103.7 (7)
O148—Mo26—O131	99.8 (8)	Mo26—O147—Mo24	88.4 (5)
O148—Mo26—O146	100.5 (8)	Mo20—O149—Mo26	149.6 (10)
O148—Mo26—O147	168.2 (7)	Mo17—O150—Mo19	156.9 (11)
O148—Mo26—O149	102.6 (8)	Mo21—O153—Mo26	157.6 (10)
O148—Mo26—O153	102.2 (8)	Mo24—O154—Mo14	158.1 (9)
O149—Mo26—O131	87.6 (7)	Mo15—O155—Mo14	148.6 (10)
O149—Mo26—O147	83.3 (6)	Mo16—O156—Mo6	142.1 (12)
O153—Mo26—O131	158.0 (7)	Mo21—O158—Mo14	123.4 (9)

O153—Mo26—O146	87.5 (8)	Mo13—O159—Mo14	103.0 (8)
O153—Mo26—O147	88.3 (6)	Mo13—O159—Mo21	108.4 (7)
O153—Mo26—O149	86.9 (7)	Mo14—O159—Mo21	88.0 (5)
O92—Mo27—O109	84.7 (10)	Mo18—O161—Mo20	108.4 (8)
O92—Mo27—O111	79.7 (7)	Mo21—O161—Mo18	107.4 (7)
O109—Mo27—O111	79.7 (9)	Mo21—O161—Mo20	143.0 (8)
O110—Mo27—O92	95.8 (8)	Mo18—O162—Mo17	108.8 (7)
O110—Mo27—O109	91.4 (12)	Mo18—O162—Mo20	108.2 (8)
O110—Mo27—O111	170.3 (12)	Mo20—O162—Mo17	142.0 (9)
O110—Mo27—O113	100.7 (13)	Mo17—O164—Ce1^{i}	150.9 (11)
O110—Mo27—O126	100.3 (9)	Mo17—O166—Mo10	136.4 (10)
O113—Mo27—O92	90.7 (10)	Mo18—O166—Mo10	110.6 (10)
O113—Mo27—O109	167.5 (10)	Mo18—O166—Mo17	111.8 (8)
O113—Mo27—O111	88.0 (10)	Mo13—O168—Mo18	117.2 (8)
O126—Mo27—O92	161.5 (9)	Mo11—O169—Mo13	104.2 (7)
O126—Mo27—O109	85.9 (13)	Mo11—O169—Mo21	137.9 (8)
O126—Mo27—O111	83.0 (8)	Mo18—O169—Mo11	104.8 (8)
O126—Mo27—O113	95.2 (13)	Mo18—O169—Mo13	97.3 (6)
O115—Mo28—O123	89.5 (7)	Mo18—O169—Mo21	103.8 (7)
O115—Mo28—O125	85.9 (7)	Mo21—O169—Mo13	102.0 (7)
O115—Mo28—O131	158.7 (7)	Mo12—O171—Mo13	112.1 (8)
O122—Mo28—O115	90.8 (7)	Mo12—O171—Mo14	139.0 (8)
O122—Mo28—O123	73.4 (6)	Mo14—O171—Mo13	106.5 (7)
O122—Mo28—O125	157.6 (7)	Mo7—O175—Mo6	158.5 (10)
O122—Mo28—O131	87.7 (7)	Mo7—O177—Mo12	147.9 (10)
O124—Mo28—O115	102.0 (7)	Mo11—O178—Mo12	124.5 (8)
O124—Mo28—O122	100.6 (8)	Mo12—O179—Mo11	88.5 (5)
O124—Mo28—O123	167.2 (7)	Mo13—O179—Mo11	107.3 (7)
O124—Mo28—O125	101.7 (8)	Mo13—O179—Mo12	104.0 (7)
O124—Mo28—O131	99.1 (7)	Mo11—O181—Mo10	139.1 (9)
O125—Mo28—O123	84.5 (7)	Mo18—O181—Mo10	108.5 (8)
O125—Mo28—O131	87.5 (7)	Mo18—O181—Mo11	110.4 (8)
O131—Mo28—O123	69.7 (6)	Mo10—O184—Ce1^{i}	160.8 (12)
O116—Mo29—O120	90.2 (7)	Mo10—O185—Mo9	146.9 (10)
O116—Mo29—O123	88.2 (6)	Mo11—O186—Mo9	156.5 (15)
O116—Mo29—O134	156.9 (7)	Mo8—O188—Mo12	156.6 (11)
O120—Mo29—O123	79.3 (6)	Mo3—O190—Mo6	161.3 (11)
O120—Mo29—O134	71.1 (7)	Mo4—O191—Mo3	110.5 (7)
O121—Mo29—O116	103.5 (8)	Mo4—O191—Mo7	110.5 (8)
O121—Mo29—O120	105.0 (9)	Mo7—O191—Mo3	135.0 (8)
O121—Mo29—O122	102.6 (8)	Mo4—O192—Mo7	106.9 (8)
O121—Mo29—O123	167.4 (7)	Mo8—O192—Mo4	110.6 (8)
O121—Mo29—O134	94.8 (8)	Mo8—O192—Mo7	140.2 (8)
O122—Mo29—O116	95.9 (7)	Mo8—O193—Mo9	120.4 (8)
O122—Mo29—O120	149.5 (7)	Mo5—O194—Mo8	110.7 (8)
O122—Mo29—O123	71.1 (6)	Mo5—O194—Mo9	103.9 (8)
O122—Mo29—O134	93.9 (7)	Mo8—O194—Mo9	90.8 (6)
O134—Mo29—O123	75.3 (6)	Mo9—O197—Mo5	108.9 (7)

O101—Mo30—O100	86.0 (11)	Mo60—O197—Mo5	112.6 (7)
O101—Mo30—O102	105.8 (9)	Mo60—O197—Mo9	138.2 (9)
O101—Mo30—O118	91.3 (8)	Mo5—O198—Mo4	118.2 (7)
O101—Mo30—O120	155.1 (9)	Mo3—O202—Ce1	160.9 (11)
O102—Mo30—O100	79.8 (8)	Mo2^{i}—O204—Mo3	131.8 (8)
O102—Mo30—O118	152.2 (8)	Mo4—O204—Mo2^{i}	112.3 (9)
O102—Mo30—O120	89.6 (7)	Mo4—O204—Mo3	110.8 (8)
O104—Mo30—O100	168.2 (9)	Mo1—O205—Mo4	103.8 (8)
O104—Mo30—O101	104.6 (11)	Mo1—O205—Mo5	100.7 (7)
O104—Mo30—O102	102.0 (9)	Mo1—O205—Mo8	145.4 (10)
O104—Mo30—O118	94.4 (8)	Mo4—O205—Mo5	95.6 (7)
O104—Mo30—O120	90.8 (7)	Mo4—O205—Mo8	102.5 (8)
O118—Mo30—O100	79.8 (8)	Mo8—O205—Mo5	98.7 (7)
O118—Mo30—O120	67.7 (7)	Mo2—O206—Ce1^{i}	160.7 (10)
O120—Mo30—O100	77.4 (8)	Mo2—O208—Mo60	149.0 (9)
O94—Mo31—O108	67.4 (6)	Mo1—O211—Mo60	91.2 (6)
O94—Mo31—O112	79.2 (7)	Mo5—O211—Mo1	109.0 (8)
O108—Mo31—O112	75.7 (7)	Mo5—O211—Mo60	103.1 (7)
O111—Mo31—O94	90.5 (8)	Mo1—O212—Mo60	123.9 (8)
O111—Mo31—O108	152.2 (9)	Mo1—O213—Mo2^{i}	139.8 (9)
O111—Mo31—O112	84.0 (9)	Mo1—O213—Mo4	110.1 (7)
O111—Mo31—O125	106.1 (8)	Mo4—O213—Mo2^{i}	108.0 (8)
O114—Mo31—O94	96.6 (8)	Mo1—O215—Mo60^{i}	154.0 (11)
O114—Mo31—O108	96.5 (8)	Mo59—O221—Mo58	159.1 (9)
O114—Mo31—O111	102.9 (10)	Mo59—O222—Mo58^{i}	122.5 (9)
O114—Mo31—O112	172.0 (8)	O224—Mo61—Mo62	99.8 (8)
O114—Mo31—O125	98.6 (9)	O224—Mo61—O228	85.6 (13)
O125—Mo31—O94	154.3 (7)	O224—Mo61—O229	87.0 (13)
O125—Mo31—O108	90.2 (6)	O224—Mo61—O230	158.5 (10)
O125—Mo31—O112	83.1 (8)	O224—Mo61—O231	74.7 (12)
O70—Mo32—O89	95.3 (8)	O224—Mo61—N2	72.7 (11)
O70—Mo32—O90	83.8 (11)	O228—Mo61—Mo62	50.0 (7)
O70—Mo32—O92	104.5 (9)	O228—Mo61—O229	93.9 (10)
O70—Mo32—O94	154.9 (9)	O228—Mo61—O230	104.6 (13)
O89—Mo32—O90	81.6 (7)	O228—Mo61—O231	160.3 (15)
O89—Mo32—O94	66.8 (6)	O228—Mo61—N2	82.1 (10)
O91—Mo32—O70	102.8 (12)	O229—Mo61—Mo62	47.6 (7)
O91—Mo32—O89	94.9 (9)	O229—Mo61—O230	110.6 (12)
O91—Mo32—O90	172.8 (10)	O229—Mo61—O231	84.0 (9)
O91—Mo32—O92	97.6 (10)	O229—Mo61—N2	159.5 (13)
O91—Mo32—O94	96.4 (10)	O230—Mo61—Mo62	101.1 (7)
O92—Mo32—O89	153.5 (8)	O230—Mo61—O231	94.4 (11)
O92—Mo32—O90	83.3 (9)	O230—Mo61—N2	89.8 (10)
O92—Mo32—O94	88.6 (7)	O231—Mo61—Mo62	131.6 (7)
O94—Mo32—O90	76.4 (8)	O231—Mo61—N2	93.0 (10)
O88—Mo33—O89	73.1 (7)	N2—Mo61—Mo62	132.1 (8)
O88—Mo33—O95	70.1 (7)	O225—Mo62—Mo61	97.5 (10)
O88—Mo33—O96	83.5 (6)	O225—Mo62—O226	81 (2)

O88—Mo33—O108	142.1 (7)	O225—Mo62—O227	158.5 (16)
O89—Mo33—O95	140.7 (7)	O225—Mo62—N1	74.3 (13)
O89—Mo33—O96	88.8 (6)	O226—Mo62—Mo61	131.6 (12)
O89—Mo33—O108	141.5 (6)	O226—Mo62—N1	90.4 (14)
O93—Mo33—O88	95.4 (7)	O227—Mo62—Mo61	101.9 (13)
O93—Mo33—O89	98.4 (8)	O227—Mo62—O226	93 (2)
O93—Mo33—O94	102.1 (8)	O227—Mo62—N1	85.2 (15)
O93—Mo33—O95	98.3 (8)	O228—Mo62—Mo61	48.3 (6)
O93—Mo33—O96	172.0 (7)	O228—Mo62—O225	83.9 (14)
O93—Mo33—O108	93.4 (7)	O228—Mo62—O226	164 (2)
O94—Mo33—O88	141.3 (7)	O228—Mo62—O227	102.2 (17)
O94—Mo33—O89	70.4 (7)	O228—Mo62—N1	87.8 (10)
O94—Mo33—O95	138.8 (7)	O229—Mo62—Mo61	50.2 (7)
O94—Mo33—O96	83.4 (7)	O229—Mo62—O225	85.4 (14)
O94—Mo33—O108	71.4 (7)	O229—Mo62—O226	81.6 (14)
O95—Mo33—O96	73.8 (6)	O229—Mo62—O227	114.3 (16)
O108—Mo33—O95	72.1 (6)	O229—Mo62—O228	94.7 (10)
O108—Mo33—O96	82.9 (6)	O229—Mo62—N1	159.2 (14)
O95—Mo34—O105	74.9 (6)	N1—Mo62—Mo61	136.1 (8)
O106—Mo34—O95	93.3 (7)	O223—Na1—Na2	102.7 (13)
O106—Mo34—O105	74.2 (7)	O223—Na1—O234	150 (2)
O106—Mo34—O108	151.9 (7)	O223—Na1—Na3	104.1 (12)
O107—Mo34—O95	97.2 (8)	O234—Na1—Na2	47.9 (17)
O107—Mo34—O105	171.7 (7)	O232—Na2—Na1	63.0 (13)
O107—Mo34—O106	104.1 (9)	O232—Na2—O233	162 (2)
O107—Mo34—O108	101.8 (8)	O232—Na2—O234	43.1 (19)
O107—Mo34—O115	101.9 (8)	O233—Na2—Na1	105.5 (13)
O108—Mo34—O95	72.5 (6)	O233—Na2—O234	118.8 (19)
O108—Mo34—O105	78.7 (6)	O234—Na2—Na1	39.9 (13)
O115—Mo34—O95	155.5 (6)	C12—O223—Na1	139 (4)
O115—Mo34—O105	86.4 (7)	C12—O224—Mo61	132 (3)
O115—Mo34—O106	96.7 (8)	C6—O225—Mo62	118 (3)
O115—Mo34—O108	88.6 (7)	Mo61—O228—Mo62	81.7 (9)
O85—Mo35—O95	77.7 (6)	Mo62—O229—Mo61	82.1 (10)
O85—Mo35—O97	74.9 (7)	C6—O233—Na2	113 (3)
O96—Mo35—O85	97.0 (7)	C6—O233—Na3	120 (3)
O96—Mo35—O95	74.4 (6)	Na1—O234—Na2	92 (2)
O96—Mo35—O97	156.9 (7)	C1—N1—Mo62	114 (3)
O96—Mo35—O105	100.1 (7)	C1—N1—C5	126 (4)
O97—Mo35—O95	82.7 (6)	C5—N1—Mo62	120 (3)
O98—Mo35—O85	103.4 (7)	C7—N2—Mo61	119 (2)
O98—Mo35—O95	177.1 (7)	C11—N2—Mo61	111 (2)
O98—Mo35—O96	102.8 (8)	C11—N2—C7	130 (4)
O98—Mo35—O97	100.2 (8)	N1—C1—C2	118 (3)
O98—Mo35—O105	103.5 (8)	N1—C1—C6	121 (4)
O105—Mo35—O85	143.9 (6)	C6—C1—C2	121 (4)
O105—Mo35—O95	76.6 (7)	C1—C2—H2	122.1
O105—Mo35—O97	77.0 (7)	C3—C2—C1	116 (4)

O97—Mo36—O105	69.4 (6)	C3—C2—H2	122.1
O102—Mo36—O97	84.3 (7)	C2—C3—H3	118.4
O102—Mo36—O105	86.3 (7)	C2—C3—C4	123 (4)
O103—Mo36—O97	100.5 (7)	C4—C3—H3	118.4
O103—Mo36—O102	100.2 (8)	C3—C4—H4	120.5
O103—Mo36—O105	167.6 (7)	C3—C4—C5	119 (4)
O103—Mo36—O106	99.9 (8)	C5—C4—H4	120.5
O103—Mo36—O116	104.8 (8)	N1—C5—C4	117 (4)
O106—Mo36—O97	90.1 (7)	N1—C5—H5	121.3
O106—Mo36—O102	159.8 (7)	C4—C5—H5	121.3
O106—Mo36—O105	73.5 (7)	O225—C6—C1	113 (4)
O116—Mo36—O97	154.4 (7)	O233—C6—O225	127 (4)
O116—Mo36—O102	87.4 (7)	O233—C6—C1	120 (4)
O116—Mo36—O105	85.9 (7)	N2—C7—H7	118.3
O116—Mo36—O106	89.4 (7)	C8—C7—N2	123 (4)
O68—Mo37—O71	80.5 (7)	C8—C7—H7	118.3
O68—Mo37—O88	89.4 (7)	C7—C8—H8	130.2
O68—Mo37—O89	153.2 (7)	C9—C8—C7	100 (4)
O69—Mo37—O68	104.8 (8)	C9—C8—H8	130.2
O69—Mo37—O71	83.4 (8)	C8—C9—H9	107.5
O69—Mo37—O88	154.1 (8)	C8—C9—C10	145 (5)
O69—Mo37—O89	91.4 (7)	C10—C9—H9	107.5
O72—Mo37—O68	103.3 (8)	C9—C10—H10	125.2
O72—Mo37—O69	104.1 (9)	C9—C10—C11	110 (4)
O72—Mo37—O71	170.1 (7)	C11—C10—H10	125.2
O72—Mo37—O88	93.2 (8)	N2—C11—C10	112 (4)
O72—Mo37—O89	92.9 (7)	N2—C11—C12	117 (3)
O88—Mo37—O71	77.6 (6)	C10—C11—C12	130 (3)
O89—Mo37—O71	80.4 (6)	O223—C12—O224	145 (6)
O89—Mo37—O88	68.3 (6)	O223—C12—C11	109 (4)
O76—Mo38—O85	86.0 (6)	O224—C12—C11	107 (4)
O76—Mo38—O86	94.8 (7)	O232—Na3—Na1	67.7 (10)
O76—Mo38—O88	90.2 (7)	O232—Na3—O233	164 (2)
O76—Mo38—O95	155.3 (6)	O233—Na3—Na1	122.6 (12)

O1—Mo49—O27—Mo53	−129 (3)	O123—Mo29—O122—Mo28	−10.5 (8)
O2—Mo59—O221—Mo58	−122 (3)	O125—Mo31—O111—Mo27	−146.5 (19)
O2—Mo59—O222—Mo58^{i}	−179.2 (10)	O129—Mo20—O149—Mo26	−169.1 (17)
O253—Mo57—O5—Mo52^{i}	174 (2)	O131—Mo25—O133—Mo23	4 (2)
O4—Mo57—O253—Mo58	120.6 (19)	O132—Mo25—O133—Mo23	−177.0 (8)
O4—Mo57—O5—Mo52^{i}	−110 (3)	O134—Mo24—O146—Mo26	85.3 (11)
O5^{i}—Mo52—O33—Mo51	173 (2)	O134—Mo24—O154—Mo14	13 (5)
O5—Mo57—O253—Mo58	−159.6 (17)	O134—Mo29—O122—Mo28	−83.5 (10)
O6—Mo57—O253—Mo58	39.8 (18)	O135—Mo15—O141—Mo16	−47 (2)
O6—Mo57—O5—Mo52^{i}	−59 (4)	O135—Mo15—O155—Mo14	70 (3)
O6—Mo59—O221—Mo58	−18 (3)	O135—Mo22—O99—Ce2	83 (4)
O6—Mo59—O222—Mo58^{i}	26.6 (18)	O135—Mo22—O137—Mo16	−3 (5)
O7—Mo57—O253—Mo58	−53 (2)	O137—Mo16—O156—Mo6	−156 (3)

O7—Mo57—O5—Mo52^{i}	68 (3)	O137—Mo22—O99—Ce2	−150 (2)
O8—Mo54—O18—Mo56	−70.0 (10)	O138—Mo16—O156—Mo6	−95 (2)
O8—Mo59—O221—Mo58	60 (3)	O139—Mo16—O156—Mo6	−4 (3)
O8—Mo59—O222—Mo58^{i}	11.9 (8)	O140—Mo15—O141—Mo16	−126 (2)
O10—Mo46—O23—Ce3	93 (2)	O140—Mo15—O155—Mo14	114 (2)
O10—Mo57—O253—Mo58	80 (3)	O141—Mo15—O155—Mo14	−162.7 (19)
O10—Mo57—O5—Mo52^{i}	−31 (3)	O141—Mo16—O156—Mo6	−180 (2)
O11—Mo55—O13—Mo53	−179.6 (9)	O142—Mo16—O156—Mo6	96 (2)
O11—Mo55—O26—Mo48	124 (3)	O143—Mo15—O141—Mo16	49 (2)
O12—Mo54—O18—Mo56	0.3 (8)	O143—Mo15—O155—Mo14	−57 (2)
O12—Mo55—O13—Mo53	−83.5 (10)	O144—Mo15—O141—Mo16	−75 (3)
O12—Mo55—O26—Mo48	−15 (4)	O144—Mo15—O155—Mo14	35 (2)
O12—Mo59—O221—Mo58	12 (4)	O144—Mo24—O146—Mo26	29 (2)
O12—Mo59—O222—Mo58^{i}	84.4 (10)	O144—Mo24—O154—Mo14	−19 (3)
O13—Mo55—O26—Mo48	−131 (3)	O145—Mo24—O146—Mo26	−178.0 (10)
O14—Mo54—O18—Mo56	2 (3)	O145—Mo24—O154—Mo14	−123 (3)
O16—Mo54—O18—Mo56	−177.6 (10)	O146—Mo24—O154—Mo14	130 (3)
O17—Mo54—O18—Mo56	72.6 (10)	O147—Mo24—O146—Mo26	12.2 (9)
O17—Mo55—O13—Mo53	−10.3 (8)	O147—Mo24—O154—Mo14	59 (3)
O17—Mo55—O26—Mo48	−61 (3)	O147—Mo25—O133—Mo23	−70.2 (8)
O19—Mo47—O43—Mo48	−41.6 (17)	O149—Mo20—O129—Mo19	159.9 (19)
O19—Mo47—O45—Ce3	103 (3)	O150—Mo17—O164—Ce1^{i}	−157 (2)
O19—Mo55—O13—Mo53	−25.6 (19)	O151—Mo20—O129—Mo19	−123 (2)
O19—Mo55—O26—Mo48	19 (3)	O151—Mo20—O149—Mo26	110.6 (19)
O20—Mo46—O23—Ce3	53 (2)	O152—Mo20—O129—Mo19	54 (2)
O20—Mo47—O43—Mo48	−72 (3)	O152—Mo20—O149—Mo26	−62 (2)
O20—Mo47—O45—Ce3	62 (3)	O153—Mo21—O158—Mo14	−74.2 (11)
O21—Mo46—O23—Ce3	135 (2)	O154—Mo24—O146—Mo26	−73.3 (12)
O22—Mo46—O23—Ce3	−41 (2)	O155—Mo15—O141—Mo16	153.5 (19)
O24—Mo47—O43—Mo48	−118.0 (18)	O158—Mo21—O153—Mo26	130 (3)
O24—Mo47—O45—Ce3	140 (3)	O159—Mo13—O168—Mo18	−67.9 (9)
O25—Mo47—O43—Mo48	53.7 (18)	O159—Mo21—O153—Mo26	59 (3)
O25—Mo47—O45—Ce3	−32 (3)	O159—Mo21—O158—Mo14	11.2 (9)
O26—Mo55—O13—Mo53	75.0 (10)	O160—Mo21—O153—Mo26	−121 (3)
O27—Mo49—O1—Mo48	75.5 (10)	O160—Mo21—O158—Mo14	178.4 (10)
O28—Mo50—O35—Mo51	−141.8 (13)	O161—Mo20—O129—Mo19	−77 (3)
O29—Mo52—O33—Mo51	89 (2)	O161—Mo20—O149—Mo26	33.7 (19)
O30^{i}—Mo46—O23—Ce3	−146.5 (19)	O161—Mo21—O153—Mo26	−19 (3)
O30—Mo52—O33—Mo51	138 (2)	O161—Mo21—O158—Mo14	26.6 (19)
O31—Mo52—O33—Mo51	−103 (2)	O162—Mo17—O150—Mo19	−33 (3)
O32—Mo52—O33—Mo51	0 (3)	O162—Mo17—O164—Ce1^{i}	91 (3)
O34—Mo50—O28—Mo53	−113 (2)	O162—Mo20—O129—Mo19	−43 (2)
O34—Mo50—O35—Mo51	140.1 (15)	O162—Mo20—O149—Mo26	70 (3)
O35—Mo50—O28—Mo53	166 (2)	O163—Mo17—O150—Mo19	63 (4)
O38—Mo50—O28—Mo53	58 (2)	O163—Mo17—O164—Ce1^{i}	−51 (3)
O38—Mo50—O35—Mo51	−36.4 (16)	O164—Mo17—O150—Mo19	169 (3)
O39—Mo49—O1—Mo48	−179.4 (10)	O165—Mo17—O150—Mo19	−110 (3)
O39—Mo49—O27—Mo53	126 (3)	O165—Mo17—O164—Ce1^{i}	124 (3)

O40—Mo49—O1—Mo48	−25 (2)	O166—Mo10—O184—Ce1[i]	54 (4)
O40—Mo49—O27—Mo53	23 (3)	O166—Mo10—O185—Mo9	−80 (3)
O40—Mo50—O28—Mo53	−36 (2)	O166—Mo17—O150—Mo19	−62 (5)
O40—Mo50—O35—Mo51	94 (2)	O166—Mo17—O164—Ce1[i]	44 (3)
O42—Mo44—O53—Mo42	70.8 (8)	O169—Mo11—O178—Mo12	−80.8 (10)
O42—Mo49—O1—Mo48	−7.4 (9)	O169—Mo11—O186—Mo9	−14 (7)
O42—Mo49—O27—Mo53	−56 (3)	O169—Mo13—O168—Mo18	3.1 (6)
O43—Mo47—O45—Ce3	−138 (2)	O169—Mo21—O153—Mo26	13 (4)
O45—Mo47—O43—Mo48	161.9 (17)	O169—Mo21—O158—Mo14	83.5 (10)
O51—Mo44—O53—Mo42	−7 (2)	O170—Mo13—O168—Mo18	−177.0 (8)
O51—Mo45—O76—Mo38	−31 (3)	O171—Mo13—O168—Mo18	19 (2)
O52—Mo44—O53—Mo42	176.9 (7)	O172—Mo6—O156—Mo16	−85 (2)
O54—Mo43—O65—Mo45	80.4 (10)	O173—Mo6—O156—Mo16	7 (3)
O54—Mo43—O75—Mo39	6 (4)	O174—Mo6—O156—Mo16	110 (2)
O54—Mo44—O53—Mo42	−1.0 (6)	O175—Mo6—O156—Mo16	−162 (2)
O54—Mo49—O1—Mo48	−80.3 (10)	O175—Mo7—O177—Mo12	163.4 (19)
O54—Mo49—O27—Mo53	−16 (4)	O177—Mo7—O175—Mo6	175 (4)
O56—Mo41—O61—Ce2	172 (4)	O178—Mo11—O186—Mo9	−131 (5)
O57—Mo41—O56—Mo51	−36 (3)	O179—Mo11—O178—Mo12	−10.3 (8)
O57—Mo41—O61—Ce2	−65 (5)	O179—Mo11—O186—Mo9	−59 (5)
O57—Mo50—O28—Mo53	−69 (3)	O179—Mo13—O168—Mo18	75.5 (8)
O57—Mo50—O35—Mo51	59.9 (14)	O180—Mo11—O178—Mo12	−179.6 (10)
O59—Mo41—O56—Mo51	−131 (3)	O180—Mo11—O186—Mo9	124 (5)
O59—Mo41—O61—Ce2	71 (4)	O181—Mo10—O184—Ce1[i]	90 (4)
O60—Mo41—O56—Mo51	43 (3)	O181—Mo10—O185—Mo9	−44.9 (18)
O60—Mo41—O61—Ce2	−107 (4)	O181—Mo11—O178—Mo12	−21 (2)
O61—Mo41—O56—Mo51	123 (3)	O181—Mo11—O186—Mo9	20 (5)
O62—Mo40—O81—Ce2	−69 (3)	O182—Mo10—O184—Ce1[i]	−41 (4)
O62—Mo40—O83—Mo39	50 (3)	O182—Mo10—O185—Mo9	47.3 (19)
O62—Mo41—O56—Mo51	−11 (4)	O183—Mo10—O184—Ce1[i]	133 (4)
O62—Mo41—O61—Ce2	−26 (4)	O183—Mo10—O185—Mo9	−123.0 (18)
O63—Mo43—O65—Mo45	178.0 (10)	O184—Mo10—O185—Mo9	157.1 (18)
O63—Mo43—O75—Mo39	−134 (3)	O185—Mo10—O184—Ce1[i]	−149 (4)
O64—Mo40—O81—Ce2	−110 (3)	O186—Mo11—O178—Mo12	77.0 (12)
O64—Mo40—O83—Mo39	24 (2)	O187—Mo7—O175—Mo6	−82 (4)
O64—Mo43—O65—Mo45	21 (2)	O187—Mo7—O177—Mo12	57 (2)
O64—Mo43—O75—Mo39	−32 (3)	O189—Mo7—O175—Mo6	96 (4)
O65—Mo43—O75—Mo39	121 (3)	O189—Mo7—O177—Mo12	−114 (2)
O65—Mo45—O76—Mo38	−124 (2)	O190—Mo3—O202—Ce1	167 (3)
O66—Mo43—O65—Mo45	6.2 (8)	O190—Mo6—O156—Mo16	−118 (2)
O66—Mo43—O75—Mo39	48 (3)	O191—Mo3—O190—Mo6	−24 (4)
O66—Mo44—O53—Mo42	−76.2 (8)	O191—Mo3—O202—Ce1	−22 (5)
O66—Mo45—O76—Mo38	−52 (2)	O191—Mo7—O175—Mo6	16 (4)
O67—Mo45—O76—Mo38	134 (2)	O191—Mo7—O177—Mo12	−72 (3)
O68—Mo37—O69—Ce3	139 (2)	O192—Mo7—O175—Mo6	49 (5)
O68—Mo45—O76—Mo38	33 (2)	O192—Mo7—O177—Mo12	−37.8 (19)
O69—Mo37—O68—Mo45	−163.5 (18)	O192—Mo8—O188—Mo12	19 (3)
O70—Mo32—O92—Mo27	133 (4)	O193—Mo8—O188—Mo12	−134 (3)

O71—Mo37—O68—Mo45	115.9 (19)	O194—Mo5—O198—Mo4	70.0 (9)
O71—Mo37—O69—Ce3	−142 (2)	O194—Mo8—O188—Mo12	−61 (3)
O72—Mo37—O68—Mo45	−55 (2)	O196—Mo5—O194—Mo8	−177.6 (8)
O72—Mo37—O69—Ce3	31 (3)	O196—Mo5—O194—Mo9	86.2 (9)
O73—Mo40—O81—Ce2	−151 (3)	O196—Mo5—O198—Mo4	178.8 (8)
O73—Mo40—O83—Mo39	101 (2)	O197—Mo5—O194—Mo8	87.1 (8)
O74—Mo40—O81—Ce2	22 (3)	O197—Mo5—O194—Mo9	−9.1 (7)
O74—Mo40—O83—Mo39	−70 (2)	O197—Mo5—O198—Mo4	−9 (2)
O75—Mo39—O86—Mo38	77.2 (10)	O198—Mo5—O194—Mo8	−69.3 (9)
O75—Mo43—O65—Mo45	−77.0 (10)	O198—Mo5—O194—Mo9	−165.5 (7)
O76—Mo38—O86—Mo39	−76.6 (10)	O199—Mo3—O190—Mo6	59 (4)
O81—Mo40—O83—Mo39	−179 (2)	O199—Mo3—O202—Ce1	−98 (3)
O83—Mo39—O86—Mo38	−16 (2)	O200—Mo8—O188—Mo12	122 (3)
O83—Mo40—O81—Ce2	128 (2)	O201—Mo3—O190—Mo6	−112 (4)
O84—Mo39—O86—Mo38	−176.2 (10)	O201—Mo3—O202—Ce1	77 (3)
O85—Mo35—O96—Mo33	−76.8 (8)	O202—Mo3—O190—Mo6	154 (4)
O85—Mo38—O76—Mo45	51 (2)	O204^{i}—Mo2—O206—Ce1^{i}	−45 (3)
O85—Mo38—O86—Mo39	7.7 (8)	O204^{i}—Mo2—O208—Mo60	74 (3)
O85—Mo39—O86—Mo38	−7.8 (8)	O204—Mo3—O190—Mo6	−36 (5)
O86—Mo38—O76—Mo45	123 (2)	O204—Mo3—O202—Ce1	−9 (3)
O87—Mo38—O76—Mo45	−132 (2)	O205—Mo1—O212—Mo60	81.4 (10)
O87—Mo38—O86—Mo39	177.6 (9)	O205—Mo1—O215—Mo60^{i}	14 (5)
O88—Mo37—O68—Mo45	38.4 (19)	O205—Mo5—O194—Mo8	0.1 (7)
O88—Mo37—O69—Ce3	−99 (3)	O205—Mo5—O194—Mo9	−96.1 (8)
O88—Mo38—O76—Mo45	−29 (2)	O205—Mo5—O198—Mo4	−1.7 (7)
O88—Mo38—O86—Mo39	23 (2)	O205—Mo8—O188—Mo12	−20 (4)
O89—Mo32—O70—Ce3	−12 (5)	O206—Mo2—O208—Mo60	−161.2 (18)
O89—Mo32—O92—Mo27	−4 (5)	O207—Mo2—O206—Ce1^{i}	−125 (3)
O89—Mo37—O68—Mo45	71 (3)	O207—Mo2—O208—Mo60	118.3 (19)
O89—Mo37—O69—Ce3	−62 (2)	O208—Mo2—O206—Ce1^{i}	158 (3)
O90—Mo32—O70—Ce3	−93 (5)	O209—Mo2—O206—Ce1^{i}	51 (3)
O90—Mo32—O92—Mo27	51 (4)	O209—Mo2—O208—Mo60	−52.9 (19)
O91—Mo32—O70—Ce3	84 (5)	O211—Mo1—O212—Mo60	8.2 (8)
O91—Mo32—O92—Mo27	−122 (4)	O211—Mo1—O215—Mo60^{i}	55 (3)
O92—Mo27—O126—Mo19	153 (2)	O211—Mo5—O194—Mo8	43.3 (16)
O92—Mo32—O70—Ce3	−174 (5)	O211—Mo5—O194—Mo9	−52.9 (15)
O94—Mo31—O111—Mo27	53 (2)	O211—Mo5—O198—Mo4	−73.3 (9)
O94—Mo31—O125—Mo28	−63 (3)	O212—Mo1—O215—Mo60^{i}	128 (3)
O94—Mo32—O70—Ce3	−55 (7)	O213—Mo1—O212—Mo60	20 (2)
O94—Mo32—O92—Mo27	−25 (4)	O213—Mo1—O215—Mo60^{i}	−24 (3)
O95—Mo34—O106—Mo36	−79.8 (10)	O213^{i}—Mo2—O206—Ce1^{i}	−83 (4)
O95—Mo34—O115—Mo28	−12 (4)	O213^{i}—Mo2—O208—Mo60	40.7 (19)
O95—Mo35—O96—Mo33	−1.7 (7)	O214—Mo1—O212—Mo60	−179.6 (10)
O95—Mo38—O76—Mo45	10 (4)	O214—Mo1—O215—Mo60^{i}	−129 (3)
O95—Mo38—O86—Mo39	80.8 (10)	O215—Mo1—O212—Mo60	−77.4 (11)
O97—Mo35—O96—Mo33	−9 (2)	O221—Mo59—O222—Mo58^{i}	−73.7 (10)
O97—Mo36—O116—Mo29	47 (4)	O222—Mo59—O221—Mo58	131 (3)
O97—Mo39—O86—Mo38	−76.5 (10)	Mo61—O224—C12—O223	−179 (7)

O98—Mo35—O96—Mo33	177.7 (8)	Mo61—O224—C12—C11	−1 (5)
O99—Mo22—O137—Mo16	−164 (5)	Mo61—N2—C7—C8	−169 (3)
O100—Mo30—O101—Ce2	108 (6)	Mo61—N2—C11—C10	168 (3)
O100—Mo30—O102—Mo36	−123 (2)	Mo61—N2—C11—C12	−4 (5)
O101—Mo30—O102—Mo36	153.9 (19)	Mo62—Mo61—O224—C12	130 (3)
O102—Mo30—O101—Ce2	−174 (6)	Mo62—O225—C6—O233	−175 (4)
O102—Mo36—O116—Mo29	−24 (2)	Mo62—O225—C6—C1	2 (5)
O103—Mo36—O116—Mo29	−124 (2)	Mo62—N1—C1—C2	178 (3)
O104—Mo30—O101—Ce2	−66 (6)	Mo62—N1—C1—C6	−4 (5)
O104—Mo30—O102—Mo36	45 (2)	Mo62—N1—C5—C4	179 (2)
O105—Mo34—O106—Mo36	−6.5 (9)	Na1—O223—C12—O224	26 (13)
O105—Mo34—O115—Mo28	−51 (3)	Na1—O223—C12—C11	−153 (4)
O105—Mo35—O96—Mo33	71.2 (9)	Na2—O233—C6—O225	2 (6)
O105—Mo36—O116—Mo29	63 (2)	Na2—O233—C6—C1	−174 (3)
O106—Mo34—O115—Mo28	−125 (3)	O228—Mo61—O224—C12	82 (3)
O106—Mo36—O116—Mo29	136 (2)	O229—Mo61—O224—C12	176 (3)
O107—Mo34—O106—Mo36	−178.1 (10)	O230—Mo61—O224—C12	−38 (5)
O107—Mo34—O115—Mo28	129 (3)	O231—Mo61—O224—C12	−99 (3)
O108—Mo31—O111—Mo27	90 (3)	N1—C1—C2—C3	1 (6)
O108—Mo31—O125—Mo28	−35 (2)	N1—C1—C6—O225	2 (6)
O108—Mo34—O106—Mo36	−22 (2)	N1—C1—C6—O233	179 (4)
O108—Mo34—O115—Mo28	27 (3)	N2—Mo61—O224—C12	−1 (3)
O109—Mo27—O126—Mo19	94 (3)	N2—C7—C8—C9	−1 (6)
O110—Mo27—O126—Mo19	3 (3)	N2—C11—C12—O223	−177 (4)
O111—Mo27—O126—Mo19	174 (3)	N2—C11—C12—O224	4 (6)
O111—Mo31—O125—Mo28	168.2 (19)	C1—N1—C5—C4	−2 (6)
O112—Mo31—O111—Mo27	132 (2)	C1—C2—C3—C4	2 (6)
O112—Mo31—O125—Mo28	−110 (2)	C2—C1—C6—O225	179 (3)
O113—Mo27—O126—Mo19	−99 (3)	C2—C1—C6—O233	−4 (6)
O114—Mo31—O111—Mo27	−43 (2)	C2—C3—C4—C5	−4 (6)
O114—Mo31—O125—Mo28	62 (2)	C3—C4—C5—N1	4 (5)
O115—Mo34—O106—Mo36	77.8 (10)	C5—N1—C1—C2	−1 (6)
O116—Mo29—O122—Mo28	75.5 (10)	C5—N1—C1—C6	177 (4)
O117—Mo22—O99—Ce2	−48 (3)	C6—C1—C2—C3	−177 (4)
O117—Mo22—O137—Mo16	91 (5)	C7—N2—C11—C10	−6 (7)
O118—Mo22—O99—Ce2	49 (3)	C7—N2—C11—C12	−179 (4)
O118—Mo22—O137—Mo16	−28 (7)	C7—C8—C9—C10	0 (9)
O118—Mo30—O101—Ce2	28 (6)	C8—C9—C10—C11	−2 (10)
O118—Mo30—O102—Mo36	−80 (2)	C9—C10—C11—N2	4 (6)
O119—Mo22—O99—Ce2	129 (3)	C9—C10—C11—C12	175 (5)
O119—Mo22—O137—Mo16	−82 (5)	C10—C11—C12—O223	12 (8)
O120—Mo29—O122—Mo28	−25.0 (19)	C10—C11—C12—O224	−167 (5)
O120—Mo30—O101—Ce2	60 (8)	C11—N2—C7—C8	5 (7)
O120—Mo30—O102—Mo36	−45.9 (19)	Na3—O233—C6—O225	−13 (6)
O121—Mo29—O122—Mo28	−179.2 (10)	Na3—O233—C6—C1	170 (3)
O123—Mo25—O133—Mo23	73.1 (9)		

Symmetry code: (i) −*x*+1, *y*, −*z*+1/2.