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Targeted synthesis of a polypyridyl polyoxometalate coordination complex using microwave-assisted reaction conditions

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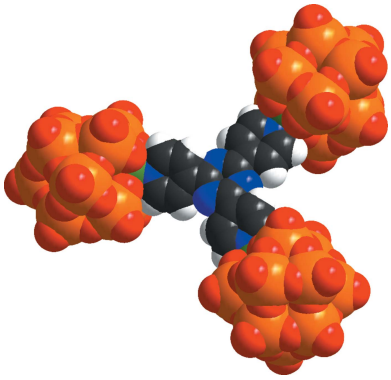
In this article, we build upon our recent efforts that have focused on demonstrating the value of microwave-assisted synthesis in polyoxometalate (POM) chemistry. Herein, we report for the first time a microwave-assisted approach that enabled the facile preparation and crystallization of a large POM-containing coordination complex. The judicious selection and reaction of a sparingly water-soluble transition-metal-substituted polyanion (TMSP) salt with the tritopic ligand 2,4,6-tris(4-pyridyl)-1,3,5-triazine (TPT) in a mixed solvent system under moderately forcing conditions yields $Ba_9[(B^{III}W^{VI}_{11}O_{39}Co^{III})_3(C_{18}H_{12}N_6)]\cdot 38H_2O$ in moderate yield. Crystallographic analysis reveals significant intermolecular interactions between the organic ligand and neighbouring polyanions, predominantly C—H···O(water) in nature; meanwhile, the solvated regions of the crystal show significant disorder. To supplement the crystallographic study, combustion analysis, and IR and ^{1}H NMR spectroscopic analyses were conducted, revealing good bulk purity and the stability of the complex in aqueous media.

1. Introduction

Polyoxometalates (POMs) are a class of molecular metal oxides with noteworthy diversity in terms of structure, composition and redox properties (Hill & Prosser-McCartha, 1995; Baker & Glick, 1998). Synthesized using controlled acid-driven condensation, POMs can, in some instances, be assembled with precise control regarding the placement of heteroatoms within their molecular frameworks (Weakley, 1973). One structural subclass of POMs is the Keggin anion, with the metal–oxo shell constructed from 12 WO_6 octahedra, in the form of four $\{W_3O_{13}\}$ triads connected *via* corner-shared oxo ligands in the α-isomer (Hill & Prosser-McCartha, 1995). The Keggin ion is also typically templated by a central tetrahedral template $\{XO_4\}$ (X = P, Si, B, Co, Ge *etc.*) that can have a notable impact on the properties of the anion, associated predominantly with the change in charge and polarization of the metal–oxo shell. Furthermore, one or more of the W atoms can be replaced by heteroatoms that include 3*d* transition metals, such as Co, Mn, Ni and Zn, to yield transition-metal-substituted polyoxometalates (TMSPs). This compositional modification tunes the reactivity and electronic structure of the POM, impacting processes such as electron transfer and stability (Shringarpure & Patel, 2015; Song *et al.*, 2014; Patel & Patel, 2012). Furthermore, a range of TMSPs contain coordination sites that can be accessed on the removal of weakly bound solvent molecules, such as those first studied by Baker & Figgis (1970). Since then, numerous TMSPs with coordinated organic ligands have been synthesized, crystallized and



reported (Han *et al.*, 2005*a*,*b*; Wang *et al.*, 2010). Surprisingly, no reliable general synthetic approach for the preparation of polypyridyl-coordinated TMSPs could be located in the literature, with the commonly adopted method being the reaction of an organic ligand(s) with a source of tungstate, heteroatom and transition metal salt under harsh hydrothermal reaction conditions over several days (Stein *et al.*, 1993; Liu *et al.*, 2009; Wang *et al.*, 2010). An additional complication to this approach is the limited control over the formation of TMSPs or POMs decorated with transition metals or complexes thereof on their surfaces (Stein *et al.*, 1993; Liu *et al.*, 2009; Wang *et al.*, 2010). Nonetheless, properties such as catalysis, electron transfer and photochromism validate efforts to develop new approaches for the reliable preparation of such compounds (Sha *et al.*, 2017; Zhu *et al.*, 2017; Parrot *et al.*, 2017).

Our group has focused on the microwave-assisted synthesis of polyoxometalates since 2016 and with this article expand our contribution into the domain of coordination chemistry (Spillane *et al.*, 2017; Karoui & Ritchie, 2018). This current study revisits the seminal work of Pope, Katsoulis, Weakley, Baker and Figgis, more than three decades ago, where the influence of the central heteroatom on the chemistry of the Keggin polyanions $[XW_{11}CoO_{39}(H_2O)]^{n-}$ (X = Si, B and P) was first examined (Baker *et al.*, 1966; Weakley & Malik, 1967; Baker & Figgis, 1970; Katsoulis & Pope, 1984). Of particular importance for this study was the identification of a TMSP with excellent stability, insensitivity to reduction and a tendency to form stable coordination compounds with pyridyl-containing ligands. Of all the TMSPs based on the monolacunary Keggin polyanion, $[B^{III}W^{VI}{}_{11}O_{39}Co^{III}]^{6-}$ was identified as the most suitable.

2. Experimental

2.1. Materials and methods

$K_8[BW_{11}O_{39}H]\cdot 13H_2O$ and 2,4,6-tris(pyridin-4-yl)-1,3,5-triazine were prepared as described in the literature (Tézé *et al.*, 1997; Aakeröy *et al.*, 2013). $K_7[B^{III}W^{VI}{}_{11}O_{39}Co^{II}(H_2O)]$ and $Ba_3[B^{III}W^{VI}{}_{11}O_{39}Co^{III}(H_2O)]$ were prepared using a modified synthetic procedure based on previous literature for the synthesis of $[XW_{11}O_{39}Co(H_2O)]^{n-}$ anions with X = Si and Ge (Weakley & Malik, 1967). All other chemicals and solvents were purchased from commercial sources and used as received.

^{1}H NMR spectroscopy was performed on a Varian 400 MHz NMR spectrometer using a pulse width of $\pi/2$ (11.25 µs), carbon decoupled and referenced against D_2O. FT–IR measurements were made using a Bruker Tensor 27 FT–IR spectrometer in the wavenumber range 4000–400 cm^{-1}, with an average of 32 scans. Samples were prepared as KBr pellets. Signals are listed as wavenumbers (cm^{-1}) with the following abbreviations: *s* = strong, *m* = medium and *w* = weak. UV–Vis spectroscopy was performed on an Agilent Technologies Cary 60 UV–Vis using Agilent Technologies standard quartz cuvettes (d = 1 cm) in the wavelength range 200–800 nm^{-1}. $Ba_9[(B^{III}W^{VI}{}_{11}O_{39}Co^{III})_3(C_{18}H_{12}N_6)]\cdot 38H_2O$, **1**, was measured in water at two concentrations: 0.5 m*M* and 10 µ*M*. Combustion analysis was conducted by the Campbell Microanalytical Laboratory and the Centre for Trace Element Analysis at the University of Otago, New Zealand. Thermogravimetric analysis (TGA) data were collected using a Mettler Toledo TGA/SDTA851e thermogravimetric analyser, heating from 25 to 800 °C at a ramp of 10 °C min^{-1} under a flow of nitrogen (30 ml min^{-1}). Single-crystal X-ray diffraction data were collected using an Agilent Technologies SuperNova Dual Wavelength single-crystal X-ray diffractometer at 130 K using Cu $K\alpha$ radiation (λ = 1.54184 Å) fitted with a mirror monochromator. Ba, Co and W atoms were refined anisotropically, with B, C, H, N and O atoms refined isotropically.

2.2. Synthesis and crystallization

2.2.1. Synthesis of $K_7[B^{III}W^{VI}{}_{11}O_{39}Co^{II}(H_2O)]$. $CoCl_2$ (130 mg, 1 mmol) was dissolved in water (5 ml) and added dropwise over a period of 5 min to a solution of $K_8[BW_{11}O_{39}H]$ (3.2 g, 1 mmol) in 90 °C water (20 ml). The resulting mixture was heated for a further 2 h at 90 °C, hot filtered and cooled to room temperature. The solution was cooled to 3 °C, with crystallization of the desired product as dark-red crystals occurring over a period of several hours. Yield: 2.5 g (83% based on W). Selected IR (KBr, cm^{-1}): 3082 (*m*), 3053 (*w*), 2959 (*w*), 2922 (*w*), 2851 (*w*), 2361 (*w*), 1630 (*s*), 1472 (*s*), 1316 (*m*), 1217 (*m*), 1119 (*m*), 1066 (*m*), 1014 (*m*), 848 (*w*), 770 (*w*), 670 (*w*), 614 (*w*), 536 (*w*).

2.2.2. Synthesis of $Ba_3[B^{III}W^{VI}{}_{11}O_{39}Co^{III}(H_2O)]$. $K_7[B^{III}W^{VI}{}_{11}O_{39}Co^{II}(H_2O)]$ (1.2 g. 0.40 mmol) was added to water (20 ml) and heated to 90 °C. On complete dissolution, sodium

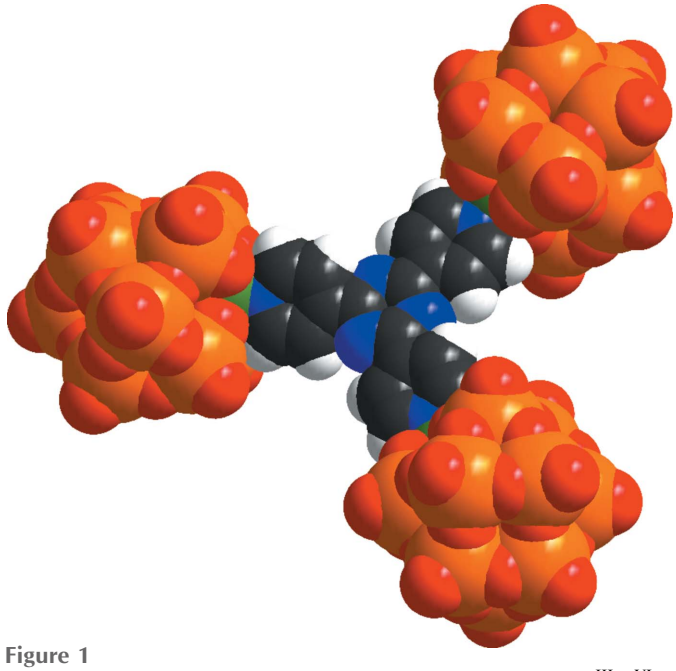


Figure 1
Space-filling representation of the coordination complex $[(B^{III}W^{VI}{}_{11}O_{39}Co^{III})_3(C_{18}H_{12}N_6)]^{18-}$ in **1**. Colour key: C atoms black, H white, N blue, Co green, O red and W orange.

Table 1
Experimental details.

Crystal data	
Chemical formula	$Ba_9[(BW_{11}O_{39}Co)_3(C_{18}H_{12}N_6)]\cdot 38H_2O$
M_r	10381.18
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	130
a, b, c (Å)	22.1764 (11), 38.1422 (19), 23.9668 (15)
β (°)	114.657 (7)
V (Å^3)	18424.1 (19)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	54.67
Crystal size (mm)	0.18 × 0.05 × 0.05
Data collection	
Diffractometer	Agilent SuperNova Dual Source diffractometer with an Atlas detector
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.029, 0.250
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	52897, 30384, 11689
R_{int}	0.147
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.631
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.120, 0.334, 0.88
No. of reflections	30384
No. of parameters	1134
No. of restraints	44
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	5.36, −4.51

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXL2018* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

persulfate (60 mg, 0.25 mmol) was added and the solution maintained at 90 °C for a further 3 h. During this time, the solution became dark green. The addition of $BaCl_2$ (250 mg, 1.20 mmol) yielded a beige precipitate that was removed by filtration. The filtrate was cooled to 3 °C with the formation of green crystals overnight. Yield: 800 mg (65% based on W). Selected IR (KBr, cm^{-1}): 2361 (*w*), 2335 (*w*), 1630 (*m*), 1385 (*w*), 948 (*m*), 896 (*m*), 818 (*s*), 689 (*w*), 506 (*w*).

2.2.3. Synthesis of $Ba_9[(B^{III}W^{VI}{}_{11}O_{39}Co^{III})_3(C_{18}H_{12}N_6)]\cdot 38H_2O$, 1. $Ba_3[B^{III}W^{VI}{}_{11}O_{39}Co^{III}(H_2O)]$ (75 mg, 0.02 mmol) and 2,4,6-tris(4-pyridyl)-1,3,5-triazine (2.5 mg, 0.008 mmol) were suspended in 3 ml water (1% CH_3CN) in a 2–5 ml Biotage microwave reaction vessel. The reaction mixture was heated to 105 °C, under a pressure of 4 bar (1 bar = 10^5 Pa), for 10 min. After cooling to room temperature, the reaction mixture was centrifuged to remove fine particulates. The dark-green filtrate was cooled to 3 °C with the formation of green crystals overnight. Yield: 35 mg (51% based on W). Selected IR (KBr, cm^{-1}): 3433 (*s*), 2920 (*m*), 2848 (*w*), 1620 (*m*), 1524 (*w*), 1467 (*w*), 1380 (*w*), 988 (*w*), 947 (*m*), 902 (*m*), 810 (*s*), 674 (*w*), 510 (*w*). ^{1}H NMR (400 MHz, D_2O): δ 8.81 (*s*, 6H), 8.60 (*s*, 6H). See the supporting information for the ^{1}H NMR spectra (Figs. S1 and S2). Elemental analysis (%) calculated (found): C 2.08 (2.22), H 0.85 (0.76), N 0.81 (0.75). Thermogravimetric analysis (TGA) was also conducted to assist with the formulation of a bulk sample of **1**. The mass loss associated with dehydration (T = 100–300 °C) was measured as 4.00 weight%, which corresponds to the loss of 38 water molecules per trimeric complex (calculated 4.40%). The second mass loss (T = 600–750 °C) was measured as 2.7% and corresponds to the combustion of one TPT ligand (calculated 3.0%).

2.3. IR spectroscopy

The IR spectra of 2,4,6-tris(pyridin-4-yl)-1,3,5-triazine (TPT) and compound **1** are included in the supporting information (Figs. S3 and S4). Characteristic stretches in the fingerprint region are assigned as the bridging, central and terminal tungsten–oxo stretches at 810, 902 and 947 cm^{-1}, respectively. A weak signal at 988 cm^{-1} is assigned to the B—O stretches in the templating {BO_4} group, with the remainder of the observed stretches originating from the organic ligand and the solvent water molecules. The TPT FT–IR spectrum contains peaks at 3040 cm^{-1} for ArH, 1590 cm^{-1} for C=N, and 1515 and 1370 cm^{-1} for C=C. The FT–IR spectrum of **1** contains an additional large solvent water peak centred at 3400 cm^{-1} which obscures the ArH peak of the coordinated TPT ligand. In the 2000–1200 cm^{-1} range, C=N (1620 cm^{-1}) and C=C (1524 and 1385 cm^{-1}) peaks are observed. These stretches are shifted to higher wavenumbers due to coordination of the POM.

2.4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The significant number of high-electron-density elements in the compound made locating the light elements in the structure a challenge. C, N and O atoms are refined isotropically, with H atoms not located from the difference map. H-atom positions on the organic ligand were included at geometrical estimates and refined with the riding model, with a C—H distance of 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C). The *OLEX2* (Dolomanov *et al.*, 2009) solvent mask procedure was used to calculate the volume of the solvent-accessible voids, which were capable of containing 21 molecules of solvent water per formula unit; however, there appeared little electron density in these voids in the crystal used for data collection.

3. Results and discussion

3.1. Synthesis

Herein, we present a reliable synthetic protocol for the preparation and crystallization of solution-stable polypyridyl coordination complexes of $[B^{III}W^{VI}{}_{11}O_{39}Co^{III}]^{6-}$, where the Lewis basic pyridyl nitrogen donor coordinates to the Co^{III} ion located within the polyoxotungstate framework of the Keggin anion. Our facile microwave-assisted synthetic protocol has enabled the preparation and crystallization of numerous examples of such compounds that are as yet unpublished, with the 2,4,6-tris(pyridin-4-yl)-1,3,5-triazine (TPT) derivative being reported in this article. A typical reaction involves mixing the transition-metal-substituted polyanion (TMSP) with the ligand of choice in a water–acetonitrile solvent system

Table 2
C—H···*OW* interactions (Å, °) for compound **1**.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O95	0.95	2.39	3.05 (5)	127
C4—H4···O1^{i}	0.95	2.36	3.23 (5)	152
C10—H10···O49^{i}	0.95	3.06	3.46 (4)	108
C12—H12···O1^{i}	0.95	2.83	3.37 (5)	117
C15—H15···O49^{i}	0.95	2.75	3.61 (4)	152
C17—H17···O67	0.95	2.65	3.17 (5)	115

Symmetry code: (i) $-x+1, y-\frac{1}{2}, -z-\frac{1}{2}$.

to yield a slurry of the reagents. The slurry is then sealed in a microwave reaction vessel and irradiated for 10 min with variable power to autogenously generate a pressure of 4 bar, while the temperature was maintained at 105 °C. On cooling to 4 °C, a dark-green crystalline product formed over the course of 4–8 h. Using this approach, we synthesised and subsequently characterized compound **1** by single-crystal X-ray diffraction, combustion analysis, IR spectroscopy, thermogravimetric analysis, NMR spectroscopy and UV–Vis spectroscopy.

3.2. Crystal description

The coordination complex $[(B^{III}W^{VI}_{11}O_{39}Co^{III})_3(C_{18}H_{12}N_6)]^{18-}$ found in compound **1** is constructed by coordination of one tritopic 2,4,6-tris(4-pyridyl)-1,3,5-triazine (TPT) ligand with three Co^{III} atoms incorporated in borotungstate polyanions (Fig. 1). Structural analysis of the resulting complex reveals distorted octahedral coordination environments for the cobalt ions, with four POM-based Co—μ_2-O [1.77 (4)–1.97 (5) Å] bonds and one Co—μ_4-O [1.98 (3)–2.00 (3) Å] bond originating from the central templating $\{BO_4\}$ tetrahedron. Completing the coordination sphere of the metal ion is the pyridyl nitrogen donor from the TPT ligand, with the three Co—N(py) bonds per molecule falling in the range 1.91 (2)–1.95 (2) Å. Tungsten–oxo bond lengths fall within the expected ranges based on extensive literature precedence (An *et al.*, 2010*a*,*b*; Liu *et al.*, 2016). A bond valence sum (BVS) (Hormillosa *et al.*, 1993) analysis of the three crystallographically independent cobalt ions is included in the supporting information (Table S1) and verifies that the cobalt ions are trivalent.

The use of Ba^{II} counter-ions has proven invaluable in our efforts to obtain crystalline products. In contrast, their high electron density and tendency to be disordered within the crystalline lattice has raised crystallographic challenges, such as several fractionally occupied cations across multiple crystallographically independent sites. Nonetheless, five of the barium cations (Ba5, Ba8, Ba9, Ba11 and Ba12) were located and refined anisotropically with occupancies of 1. The remaining four barium cations required for charge-balancing considerations are disordered throughout hydrated channels within the monoclinic crystalline lattice, while also being associated with the surface oxo ligands of the Keggin polyanions. Interactions between neighbouring coordination complexes are better defined, with the triazine of each TPT being capped above and below the aromatic plane by either a $\{W_4O_{18}\}$ or a $\{W_3O_{13}\}$ face (Fig. 2). Separations between planes defined by the terminal oxo ligands of the $\{W_4O_{18}\}$ and $\{W_3O_{13}\}$ faces and the triazine are 2.931 (1) and 3.385 (2) Å, respectively, with the corresponding angles between the planes measured as 7.2 (8) and 7.3 (8)°. To maximize the intermolecular interactions, two of the three TPT pyridyl groups within each complex are rotated approximately 20.57 and 27.78° out of planarity with respect to the central triazine ring, while the other pyridyl group deviates from coplanarity by 1.34° (Fig. 2*a*). All six pyridyl β-protons are involved in C—H···O*W* interactions, with four of these corresponding to two pairs of asymmetric bifurcated interactions with terminal tungsten–oxo ligand acceptors (W—O1 and W—O49)

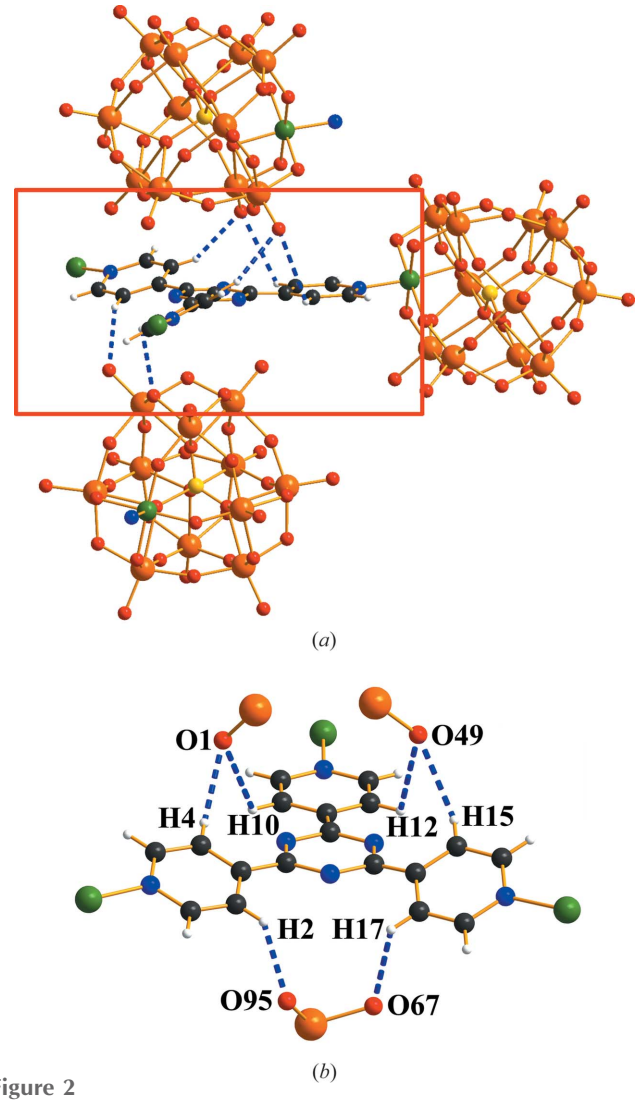


Figure 2
(*a*) The intermolecular interactions between neighbouring molecules of complex **1**. Two sets of bifurcated C—H···O*W* interactions between the TPT ligand and a $\{W_4O_{18}\}$ face of a neighbouring molecule above the plane of the triazine are indicated by dashed blue bonds. Additional C—H···O*W* interactions below the plane with a $\{W_3O_{13}\}$ face of a second polyanion are also indicated by dashed bonds. (*b*) An expanded view of the intermolecular interactions marked with a box in part (*a*), with only essential molecular fragments shown for clarity. Colour key: C atoms black, H white, N blue, B yellow, Co green, O red and W orange.

(Fig. 2*b*). Additional details of these interactions are listed in Table 2.

The crystallographic packing of compound **1**, viewed along the crystallographic *c* axis, is shown in Fig. 3, with cations and solvent molecules omitted for clarity. Interactions between the aromatic surface of the TPT ligand and the oxo-rich surface of neighbouring molecules are evident, with the highlighted region of Fig. 3(*a*) expanded and rotated to view along the crystallographic *a* axis in Fig. 3(*b*), showing two coordination complexes of **1** that are related by inversion symmetry. Despite significant disorder of the barium counter-cations and solvent water molecules, their predominant association with the surface of the polyoxotungstate moieties is discernible from the location of the voids in Fig. 3(*a*).

3.3. Solution-state characterization

A ^{1}H NMR spectrum of compound **1** dissolved in D_2O was collected, with two signals observed in the aromatic region at 8.81 and 8.60 ppm as expected for the highly symmetrical assembly. The more upfield resonance is assigned as the six α-pyridyl protons due to their closer proximity to the electron-withdrawing polyanion, with the signal at 8.60 ppm assigned as the β-pyridyl protons. Integrations of the peak areas are comparable, with signal broadening precluding observation of any splitting due to the increased size of the assembly on coordination to the polyanions. No evidence for any uncoordinated or partially coordinated TPT ligands is observed (see Fig. S1 in the supporting information). The UV–Vis spectra of compound **1** are typical for a pyridyl-coordinated $[BW_{11}O_{39}Co^{III}(py)]^{6-}$ polyanion (Weakley, 1973). An intense ligand-to-metal charge transfer (O→W; λ_{max} = 251 nm, ε = 1.85 × 10^5 M^{-1} cm^{-1}) and a much weaker *d*–*d* transition (Co→Co; λ_{max} = 609 nm, ε = 5.34 × 10^2 M^{-1} cm^{-1}) are observed. On coordination of TPT to $[BW_{11}O_{39}Co^{III}]^{6-}$, the absorption maximum of the broad *d*–*d* transition is hypsochromically shifted by 79 nm in line with that reported previously in the literature (Weakley, 1973) (see Figs. S4–S7 in the supporting information).

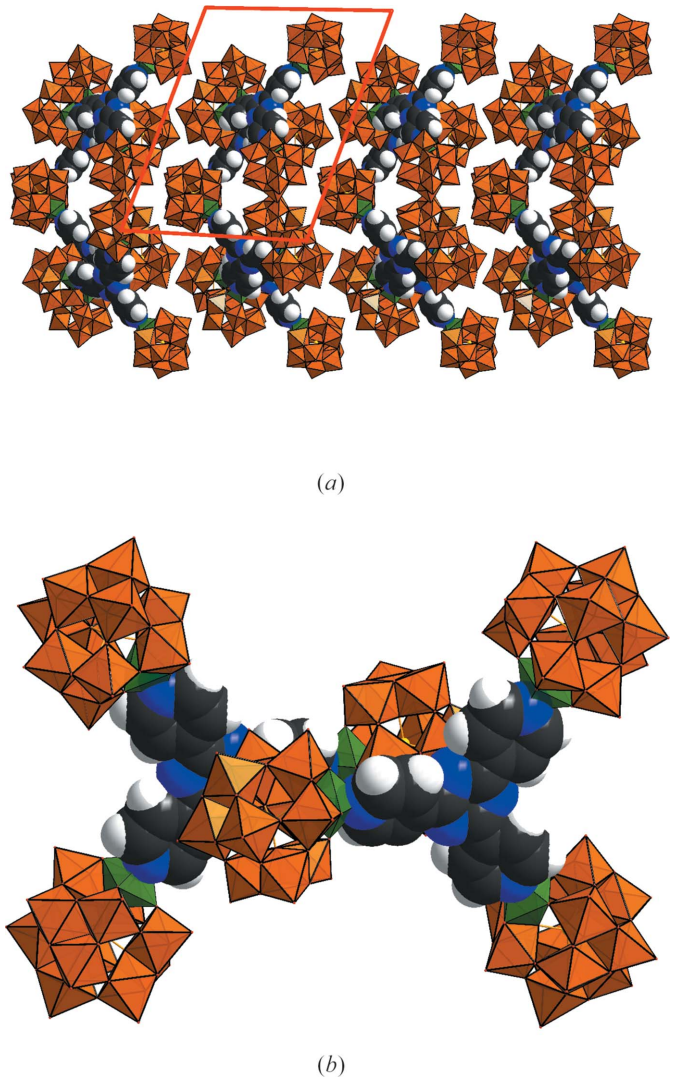


Figure 3
(*a*) Graphical representation of the crystallographic packing of **1**, viewed along the *c* axis. (*b*) An expanded view of the supramolecular dimer marked with a box in part (*a*), viewed along the crystallographic *a* axis. The colour scheme is as used previously.

4. Concluding remarks

We have successfully implemented a microwave-assisted approach towards the synthesis and crystallization of POM coordination complexes, with compound **1** discussed herein being the first reported example prepared using this synthetic method. The synthetic strategy offers a practical alternative to the typically less predictable traditional approaches (reflux and hydrothermal), with additional examples to be published in due course to validate this statement. Compound **1** was structurally characterized using single-crystal X-ray diffraction, with the molecular structure of the coordination complex therein being unambiguously determined. The complex was also studied in solution by NMR and UV–Vis spectroscopies with the molecular assembly being stable in hot water. An extension of this work targeting coordinatively unsaturated polyoxometalate–pyridyl ligands for the construction of elaborate molecular architectures is underway.

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Targeted synthesis of a polypyridyl polyoxometalate coordination complex using microwave-assisted reaction conditions

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Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2015); cell refinement: *CrysAlis PRO* (Rigaku OD, 2015); data reduction: *CrysAlis PRO* (Rigaku OD, 2015); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

(I)

Crystal data

$Ba_9[(BW_{11}O_{39}Co)_3(C_{18}H_{12}N_6)]\cdot 38H_2O$
M_r = 10381.18
Monoclinic, $P2_1/c$
a = 22.1764 (11) Å
b = 38.1422 (19) Å
c = 23.9668 (15) Å
β = 114.657 (7)°
V = 18424.1 (19) Å^3
Z = 4
$F(000)$ = 18888
D_x = 3.873 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 3524 reflections
θ = 3.9–62.2°
μ = 54.67 mm^{-1}
T = 130 K
Needle, light green
0.18 × 0.05 × 0.05 mm

Data collection

Agilent SuperNova Dual Source diffractometer with an Atlas detector
Radiation source: micro-focus sealed X-ray tube, SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.2273 pixels mm^{-1}
ω scans
Absorption correction: gaussian (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.029, T_{max} = 0.250
52897 measured reflections
30384 independent reflections
11689 reflections with $I > 2\sigma(I)$
R_{int} = 0.147
θ_{max} = 76.6°, θ_{min} = 3.7°
h = −27→27
k = −26→46
l = −29→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.120
$wR(F^2)$ = 0.334
S = 0.88
30384 reflections
1134 parameters
44 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1744P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 5.36 e Å^{-3}
$\Delta\rho_{min}$ = −4.51 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. Crystals were found to be disordered and twinned. Attempts to get beter crystals were not successful. The data was processed as a 2-component twin, and it was possible to carry out a refinement on the data from twin component 1. The OLEX2 solvent mask routine was used to account for solvent accessible voids, sufficient for 21 molecules of solvent water per formula unit, or 84 per unit cell. Little electron density was found in these solvent voids using the data collected from the crystal used for data collection. ADP were assigned to all atoms, except for oxygen, nitrogen and carbon. Hydrogen atoms were assigned to the carbons atoms of the ligand, none were able to be assigned to the oxygen atoms of the POM moieties or to the solvent water molecules. Five Ba atoms were fully occupied, the rest appeared to be distributed over multiple sites.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
W1	0.47183 (11)	0.40098 (7)	−0.44256 (10)	0.0524 (5)	
W2	0.77770 (10)	0.31644 (6)	−0.30904 (10)	0.0497 (5)	
W3	0.64200 (11)	0.28881 (6)	−0.26958 (10)	0.0505 (5)	
W4	0.61004 (10)	0.33650 (7)	−0.52043 (10)	0.0504 (5)	
W5	1.02583 (10)	−0.19838 (7)	−0.00242 (11)	0.0517 (5)	
W6	0.77436 (10)	−0.23599 (7)	0.01983 (11)	0.0543 (6)	
W7	0.76172 (11)	0.39774 (7)	−0.26887 (10)	0.0514 (5)	
W8	0.48873 (10)	0.30945 (6)	−0.48375 (10)	0.0507 (5)	
W9	0.63467 (10)	0.26972 (6)	−0.42289 (10)	0.0494 (5)	
W10	0.74975 (11)	0.38180 (7)	−0.40996 (10)	0.0523 (5)	
W11	0.89465 (10)	−0.21800 (7)	−0.15516 (11)	0.0512 (5)	
W12	0.90466 (10)	−0.17583 (7)	0.03701 (10)	0.0519 (5)	
W13	0.62475 (11)	0.37154 (7)	−0.23156 (10)	0.0520 (5)	
W14	0.60096 (11)	0.44292 (6)	−0.34245 (11)	0.0522 (5)	
W15	1.01843 (12)	−0.28465 (7)	−0.06970 (12)	0.0584 (6)	
W16	0.49539 (10)	0.32886 (7)	−0.33352 (10)	0.0512 (5)	
W17	0.82899 (12)	0.11482 (7)	−0.34049 (12)	0.0601 (6)	
W18	1.01921 (11)	−0.23428 (7)	0.12000 (11)	0.0585 (6)	
W19	0.75338 (12)	0.10549 (7)	−0.24812 (11)	0.0584 (6)	
W20	0.66653 (12)	0.10143 (7)	−0.40020 (11)	0.0575 (6)	
W21	0.77460 (13)	−0.27369 (7)	−0.17094 (11)	0.0600 (6)	
W22	0.60156 (11)	0.01734 (7)	−0.38728 (12)	0.0604 (6)	
W23	0.94215 (12)	0.04337 (8)	−0.26722 (12)	0.0633 (7)	
W24	0.88451 (13)	−0.29546 (8)	0.10297 (12)	0.0622 (6)	
W25	0.86720 (12)	0.03341 (7)	−0.17230 (11)	0.0592 (6)	
W26	0.68766 (13)	0.01868 (8)	−0.23526 (12)	0.0628 (6)	
W27	0.88032 (13)	−0.03408 (7)	−0.25553 (13)	0.0629 (6)	
W28	0.83974 (13)	0.04083 (8)	−0.43437 (13)	0.0652 (7)	
W29	0.77010 (14)	−0.31632 (8)	−0.03495 (13)	0.0666 (7)	
W30	0.77991 (14)	−0.03635 (8)	−0.42228 (13)	0.0654 (7)	
W31	1.01283 (15)	−0.32189 (8)	0.05361 (13)	0.0697 (7)	
W32	0.70222 (13)	−0.04841 (7)	−0.31527 (13)	0.0629 (6)	

W33	0.89732 (16)	−0.34082 (8)	−0.08637 (14)	0.0699 (7)	
Ba1	0.5081 (6)	0.2250 (4)	−0.3729 (7)	0.063 (5)	0.236 (12)
Ba2	0.8934 (7)	0.4147 (4)	−0.0769 (6)	0.084 (5)	0.331 (13)
Ba3	0.9353 (5)	−0.0707 (3)	0.1072 (6)	0.077 (5)	0.340 (12)
Ba4	0.5170 (4)	0.1924 (2)	−0.4929 (5)	0.057 (3)	0.343 (11)
Ba5	1.1868 (2)	−0.32906 (15)	0.0130 (2)	0.0999 (15)	
Ba8	0.96197 (16)	−0.13732 (9)	−0.23726 (17)	0.0623 (8)	
Ba9	0.6928 (2)	−0.31423 (16)	−0.3609 (2)	0.1000 (16)	
Ba11	0.67236 (14)	0.18625 (9)	−0.16897 (14)	0.0540 (7)	
Ba12	1.13016 (17)	−0.27826 (10)	−0.18079 (16)	0.0661 (9)	
Ba13	0.403 (3)	0.3748 (19)	−0.611 (3)	0.07 (2)*	0.054 (12)
Co1	0.5931 (4)	0.4180 (2)	−0.4668 (3)	0.0472 (17)	
Co2	0.7917 (3)	−0.2034 (2)	−0.1058 (3)	0.0506 (19)	
Co3	0.6935 (4)	0.0281 (3)	−0.4728 (4)	0.060 (2)	
O1	0.3950 (7)	0.4134 (11)	−0.4731 (18)	0.078 (11)*	
O2	0.502 (2)	0.4243 (12)	−0.493 (2)	0.086 (13)*	
O3	0.4677 (15)	0.3697 (9)	−0.3822 (15)	0.051 (7)*	
O4	0.4679 (15)	0.3575 (8)	−0.4832 (15)	0.049 (7)*	
O5	0.517 (3)	0.4344 (15)	−0.383 (3)	0.111 (17)*	
O6	0.5874 (14)	0.3907 (8)	−0.3979 (14)	0.047 (7)*	
O7	0.6959 (5)	0.3495 (6)	−0.4674 (15)	0.077 (11)*	
O8	0.8107 (16)	0.3516 (9)	−0.2510 (16)	0.057 (8)*	
O9	0.6246 (15)	0.2701 (9)	−0.3390 (15)	0.051 (7)*	
O10	0.5532 (7)	0.2924 (13)	−0.284 (2)	0.092 (14)*	
O11	0.6916 (15)	0.3568 (8)	−0.3560 (15)	0.050 (7)*	
O12	0.6616 (15)	0.2558 (9)	−0.2199 (15)	0.052 (8)*	
O13	0.6554 (15)	0.3226 (8)	−0.2080 (15)	0.049 (7)*	
O14	0.6033 (11)	0.3401 (6)	−0.3234 (12)	0.030 (5)*	
O15	0.5834 (18)	0.3784 (10)	−0.5209 (18)	0.066 (9)*	
O16	0.6134 (18)	0.3342 (10)	−0.5867 (8)	0.067 (10)*	
O17	0.5261 (12)	0.3177 (13)	−0.541 (2)	0.107 (17)*	
O18	0.634 (2)	0.2851 (11)	−0.4945 (19)	0.073 (11)*	
O19	0.6025 (12)	0.3272 (7)	−0.4258 (12)	0.036 (6)*	
O20	1.0836 (14)	−0.1737 (9)	−0.0062 (18)	0.072 (10)*	
O21	0.9809 (13)	−0.1647 (7)	0.0216 (13)	0.040 (6)*	
O22	1.0670 (16)	−0.2105 (9)	0.0811 (16)	0.057 (8)*	
O23	1.0478 (18)	−0.2459 (10)	−0.0177 (16)	0.061 (9)*	
O24	0.9401 (15)	−0.2289 (8)	0.0131 (15)	0.049 (7)*	
O25	0.7521 (18)	−0.2169 (10)	−0.0559 (17)	0.063 (9)*	
O26	0.7185 (12)	−0.2186 (8)	0.0384 (15)	0.056 (8)*	
O27	0.8474 (17)	−0.2039 (9)	0.0610 (16)	0.058 (8)*	
O28	0.8170 (19)	−0.2651 (11)	0.0961 (18)	0.071 (10)*	
O29	0.856 (2)	−0.2713 (11)	0.0107 (19)	0.075 (11)*	
O30	0.8149 (12)	0.4210 (7)	−0.2139 (11)	0.052 (8)*	
O31	0.688 (2)	0.4317 (12)	−0.308 (2)	0.085 (12)*	
O32	0.7067 (12)	0.3793 (10)	−0.2337 (15)	0.067 (10)*	
O33	0.4185 (11)	0.2927 (10)	−0.5296 (16)	0.078 (11)*	
O34	0.4834 (14)	0.3047 (8)	−0.4053 (14)	0.044 (7)*	

O35	0.650 (2)	0.2284 (3)	−0.4258 (19)	0.074 (11)*
O36	0.6854 (15)	0.4134 (9)	−0.4372 (15)	0.052 (8)*
O37	0.7998 (15)	0.3938 (10)	−0.4401 (16)	0.069 (10)*
O38	0.8047 (18)	0.3423 (10)	−0.3672 (18)	0.066 (9)*
O39	0.917 (2)	−0.1960 (12)	−0.202 (2)	0.080 (12)*
O40	0.966 (3)	−0.2571 (14)	−0.123 (2)	0.098 (15)*
O41	0.8288 (16)	−0.1878 (9)	−0.1554 (16)	0.054 (8)*
O42	0.8337 (13)	−0.2555 (7)	−0.2042 (12)	0.038 (6)*
O43	0.8567 (13)	−0.2427 (7)	−0.0881 (13)	0.040 (6)*
O44	0.8485 (15)	−0.1763 (10)	−0.0461 (5)	0.065 (9)*
O45	0.8917 (18)	−0.1377 (5)	0.0600 (17)	0.069 (10)*
O46	0.973 (2)	−0.1887 (12)	0.109 (2)	0.088 (13)*
O47	0.5422 (12)	0.3498 (12)	−0.265 (2)	0.103 (16)*
O48	0.5974 (15)	0.4125 (9)	−0.2785 (15)	0.052 (7)*
O49	0.6061 (14)	0.4802 (4)	−0.3080 (13)	0.047 (7)*
O50	0.6018 (14)	0.4562 (8)	−0.4138 (14)	0.044 (7)*
O51	0.642 (2)	0.3865 (11)	−0.1633 (8)	0.081 (12)*
O52	1.0774 (10)	−0.2887 (8)	−0.0926 (13)	0.045 (7)*
O53	1.0553 (19)	−0.3114 (11)	0.0039 (19)	0.070 (10)*
O54	0.9727 (16)	−0.3259 (9)	−0.1036 (16)	0.057 (8)*
O55	0.9383 (17)	−0.2853 (10)	−0.0307 (17)	0.061 (9)*
O56	0.4274 (9)	0.3170 (9)	−0.3288 (16)	0.058 (8)*
O57	0.940 (2)	−0.3190 (11)	0.0814 (19)	0.074 (11)*
O58	0.8706 (17)	0.1484 (7)	−0.3468 (19)	0.074 (11)*
O59	0.6078 (19)	0.1292 (11)	−0.4446 (18)	0.070 (10)*
O60	0.6774 (17)	0.0745 (9)	−0.4563 (16)	0.058 (8)*
O61	0.6223 (16)	0.0681 (9)	−0.3785 (16)	0.057 (8)*
O62	0.7172 (15)	−0.2900 (10)	−0.2327 (11)	0.073 (11)*
O63	0.7327 (18)	−0.2314 (10)	−0.1691 (17)	0.064 (9)*
O64	0.842 (3)	−0.3101 (16)	−0.142 (3)	0.121 (19)*
O65	0.5218 (4)	0.0185 (11)	−0.4259 (17)	0.075 (11)*
O66	0.6335 (19)	0.0147 (11)	−0.4464 (18)	0.070 (10)*
O67	0.6190 (18)	−0.0333 (10)	−0.3645 (18)	0.067 (10)*
O68	0.6096 (4)	0.0176 (11)	−0.3067 (2)	0.078 (11)*
O69	0.7143 (14)	0.0135 (8)	−0.3197 (14)	0.045 (7)*
O70	1.0188 (7)	0.0526 (11)	−0.2514 (19)	0.078 (11)*
O71	0.951 (2)	−0.0077 (11)	−0.2559 (19)	0.075 (11)*
O72	0.9364 (17)	0.0497 (9)	−0.1887 (16)	0.058 (8)*
O73	0.8396 (14)	0.0228 (8)	−0.2739 (14)	0.045 (7)*
O74	0.831 (2)	−0.3251 (11)	0.058 (2)	0.078 (11)*
O75	0.7799 (4)	0.0192 (14)	−0.194 (3)	0.17 (3)*
O76	0.9013 (13)	0.0393 (8)	−0.0986 (3)	0.045 (7)*
O77	0.8958 (16)	−0.0152 (9)	−0.1758 (16)	0.057 (8)*
O78	0.6641 (18)	0.0197 (10)	−0.1797 (12)	0.086 (13)*
O79	0.685 (2)	−0.0284 (12)	−0.247 (2)	0.086 (13)*
O80	0.9268 (14)	−0.0676 (8)	−0.2282 (15)	0.048 (7)*
O81	0.802 (3)	−0.0491 (14)	−0.257 (2)	0.098 (15)*
O82	0.851 (2)	−0.0414 (13)	−0.337 (2)	0.089 (13)*

O83	0.8877 (18)	0.0492 (12)	−0.4686 (18)	0.087 (13)*
O84	0.9031 (16)	0.0380 (9)	−0.3483 (15)	0.053 (8)*
O85	0.7687 (14)	0.0198 (8)	−0.3922 (14)	0.047 (7)*
O86	0.7077 (14)	−0.3428 (9)	−0.054 (2)	0.079 (11)*
O87	0.736 (3)	−0.2936 (15)	−0.115 (2)	0.107 (16)*
O88	0.8335 (17)	−0.3422 (9)	−0.0530 (16)	0.059 (8)*
O89	0.712 (2)	−0.0205 (12)	−0.489 (2)	0.084 (12)*
O90	0.783 (2)	−0.0733 (7)	−0.454 (2)	0.093 (14)*
O91	0.7234 (16)	−0.0500 (9)	−0.3892 (15)	0.053 (8)*
O92	0.8415 (18)	−0.0091 (10)	−0.4413 (17)	0.064 (9)*
O93	1.0694 (16)	−0.3467 (9)	0.1029 (16)	0.080 (12)*
O94	0.9640 (16)	−0.3556 (9)	−0.0040 (16)	0.055 (8)*
O95	0.685 (3)	−0.0897 (4)	−0.315 (2)	0.104 (16)*
O96	0.763 (3)	0.0420 (14)	−0.495 (2)	0.103 (16)*
O97	0.874 (2)	−0.3763 (7)	−0.1271 (18)	0.084 (12)*
O98	0.900 (3)	−0.3156 (12)	0.1671 (12)	0.099 (15)*
O99	0.8385 (14)	0.2878 (8)	−0.2838 (14)	0.043 (7)*
O100	0.7225 (17)	0.3001 (9)	−0.2693 (16)	0.058 (8)*
O101	0.7192 (17)	0.2879 (9)	−0.3760 (16)	0.059 (9)*
O102	0.750 (2)	0.1286 (12)	−0.389 (2)	0.081 (12)*
O103	0.9004 (17)	0.0910 (9)	−0.2861 (16)	0.058 (8)*
O104	0.8136 (18)	0.1318 (10)	−0.2708 (17)	0.065 (9)*
O105	0.834 (2)	0.0848 (11)	−0.401 (2)	0.078 (11)*
O106	0.7651 (13)	0.0722 (7)	−0.3255 (13)	0.040 (6)*
O107	1.0745 (14)	−0.2330 (11)	0.1902 (6)	0.069 (10)*
O108	1.0400 (16)	−0.2760 (9)	0.0930 (16)	0.056 (8)*
O109	0.9498 (18)	−0.2609 (10)	0.1311 (17)	0.063 (9)*
O110	0.7510 (16)	0.1326 (7)	−0.1970 (12)	0.058 (8)*
O111	0.7053 (17)	0.0691 (9)	−0.2399 (16)	0.059 (9)*
O112	0.8253 (15)	0.0771 (9)	−0.2002 (15)	0.052 (8)*
O113	0.6816 (18)	0.1224 (10)	−0.3226 (17)	0.063 (9)*
O114	0.965 (2)	−0.1980 (11)	−0.082 (2)	0.076 (11)*
O115	0.7229 (18)	−0.2785 (10)	−0.0178 (18)	0.066 (10)*
O116	0.7915 (17)	0.4058 (10)	−0.3322 (17)	0.061 (9)*
O117	0.5438 (6)	0.2653 (15)	−0.469 (2)	0.111 (17)*
O118	0.5791 (18)	−0.2972 (10)	−0.3349 (17)	0.066 (9)*
O119	0.760 (2)	−0.2465 (12)	−0.325 (2)	0.088 (13)*
O120	1.263 (3)	−0.3800 (13)	0.026 (2)	0.096 (14)*
O121	1.181 (2)	−0.2594 (12)	0.022 (2)	0.088 (13)*
O122	1.196 (3)	−0.3020 (16)	0.129 (3)	0.120 (19)*
O123	0.6766 (18)	0.2380 (10)	−0.0829 (17)	0.066 (9)*
O124	0.769 (2)	0.1672 (11)	−0.054 (2)	0.078 (11)*
O125	1.324 (3)	−0.3047 (16)	0.094 (3)	0.120 (19)*
O126	0.4003 (11)	0.1578 (7)	−0.5912 (12)	0.032 (5)*
O127	0.596 (3)	0.1614 (16)	−0.556 (3)	0.115 (18)*
O128	0.8958 (14)	0.4577 (8)	−0.0910 (14)	0.044 (7)*
O129	1.0120 (19)	0.4278 (11)	0.0066 (19)	0.071 (10)*
O130	0.386 (3)	0.2467 (15)	−0.367 (3)	0.116 (18)*

O131	1.2286 (19)	−0.2910 (11)	−0.2159 (18)	0.071 (10)*
O132	1.075 (2)	−0.1680 (12)	−0.135 (2)	0.081 (12)*
O133	0.767 (2)	0.4433 (13)	−0.112 (2)	0.094 (14)*
O134	1.168 (2)	−0.2279 (13)	−0.086 (2)	0.092 (14)*
O135	0.621 (3)	0.1918 (16)	−0.201 (3)	0.121 (19)*
O136	0.823 (2)	−0.1327 (12)	−0.253 (2)	0.079 (12)*
O137	1.012 (3)	−0.2401 (17)	−0.231 (3)	0.13 (2)*
O138	0.838 (2)	0.1041 (12)	−0.064 (2)	0.082 (12)*
O139	0.8937 (19)	−0.0004 (11)	0.0044 (18)	0.072 (10)*
O140	0.956 (4)	−0.437 (2)	−0.140 (4)	0.17 (3)*
O141	1.053 (4)	−0.1678 (19)	−0.280 (3)	0.15 (3)*
O142	0.642 (2)	0.1842 (13)	−0.292 (2)	0.092 (14)*
O143	0.7929 (16)	0.2162 (9)	−0.1560 (16)	0.058 (8)*
O144	1.2409 (19)	−0.3068 (11)	−0.0710 (19)	0.071 (10)*
O145	1.067 (3)	−0.0941 (16)	−0.210 (3)	0.117 (19)*
O146	0.6546 (16)	−0.2667 (9)	−0.3594 (16)	0.058 (8)*
O147	0.994 (3)	0.1175 (16)	0.111 (3)	0.119 (19)*
O148	1.094 (3)	−0.3755 (14)	−0.036 (2)	0.099 (15)*
O149	0.602 (3)	0.1231 (17)	−0.192 (3)	0.13 (2)*
O150	0.708 (4)	−0.368 (2)	−0.448 (4)	0.17 (3)*
O151	0.920 (3)	−0.1078 (16)	−0.352 (3)	0.122 (19)*
N1	0.7316 (17)	−0.1642 (8)	−0.1318 (15)	0.087 (16)*
C1	0.7019 (16)	−0.1567 (8)	−0.1942 (14)	0.061 (13)*
H1	0.710978	−0.171043	−0.222284	0.073*
C2	0.6589 (15)	−0.1284 (9)	−0.2157 (11)	0.046 (10)*
H2	0.638659	−0.123324	−0.258365	0.056*
C3	0.6456 (15)	−0.1075 (8)	−0.1747 (14)	0.077 (17)*
C4	0.6753 (16)	−0.1149 (8)	−0.1122 (13)	0.044 (9)*
H4	0.666212	−0.100614	−0.084161	0.053*
C5	0.7183 (16)	−0.1433 (9)	−0.0908 (11)	0.073 (16)*
H5	0.738532	−0.148332	−0.048079	0.087*
N2	0.5579 (15)	−0.0738 (7)	−0.2506 (12)	0.074 (13)*
C6	0.6049 (13)	−0.0768 (6)	−0.1903 (13)	0.049 (10)*
N3	0.6100 (11)	−0.0510 (7)	−0.1477 (9)	0.046 (8)*
C7	0.5681 (13)	−0.0221 (6)	−0.1653 (12)	0.051 (11)*
N4	0.5211 (13)	−0.0190 (6)	−0.2256 (13)	0.071 (12)*
C8	0.5160 (13)	−0.0448 (8)	−0.2683 (10)	0.051 (11)*
N5	0.5911 (14)	0.0512 (7)	−0.0303 (12)	0.045 (8)*
C9	0.5434 (13)	0.0547 (7)	−0.0902 (13)	0.074 (16)*
H9	0.514439	0.074362	−0.101378	0.089*
C10	0.5382 (14)	0.0295 (8)	−0.1339 (10)	0.049 (10)*
H10	0.505587	0.031878	−0.174836	0.059*
C11	0.5806 (15)	0.0007 (7)	−0.1176 (13)	0.056 (12)*
C12	0.6283 (14)	−0.0028 (7)	−0.0576 (14)	0.058 (12)*
H12	0.657241	−0.022391	−0.046481	0.069*
C13	0.6335 (13)	0.0225 (8)	−0.0140 (10)	0.059 (12)*
H13	0.666094	0.020092	0.026979	0.071*
N6	0.3739 (14)	−0.0332 (10)	−0.4431 (12)	0.072 (13)*

C14	0.3651 (14)	−0.0188 (11)	−0.3938 (16)	0.11 (2)*	
H14	0.326323	−0.005623	−0.400656	0.126*	
C15	0.4132 (16)	−0.0237 (10)	−0.3343 (14)	0.082 (18)*	
H15	0.407161	−0.013830	−0.300598	0.099*	
C16	0.4699 (13)	−0.0430 (8)	−0.3243 (11)	0.029 (7)*	
C17	0.4787 (13)	−0.0574 (9)	−0.3736 (14)	0.084 (19)*	
H17	0.517523	−0.070577	−0.366756	0.101*	
C18	0.4307 (16)	−0.0525 (10)	−0.4331 (12)	0.057 (12)*	
H18	0.436686	−0.062369	−0.466815	0.069*	
B25	0.900 (2)	−0.2568 (14)	−0.021 (2)	0.043 (10)*	
B44	0.625 (2)	0.3548 (12)	−0.379 (2)	0.035 (9)*	
B69	0.766 (3)	0.0344 (17)	−0.327 (3)	0.058 (14)*	
Ba6	0.8698 (4)	−0.4199 (2)	−0.2268 (4)	0.076 (3)	0.472 (12)
Ba7	0.9666 (5)	0.0955 (3)	−0.0108 (5)	0.089 (2)	0.442 (8)
Ba14	0.593 (3)	−0.0553 (17)	−0.503 (3)	0.10 (2)*	0.084 (14)
Ba7A	0.8958 (6)	0.0618 (4)	0.0205 (6)	0.089 (2)	0.373 (8)
Ba7B	0.9147 (13)	0.0961 (7)	0.0535 (12)	0.089 (2)	0.185 (8)
Ba10	0.484 (3)	0.348 (2)	−0.162 (3)	0.18 (3)	0.140 (16)
O201	0.389 (2)	0.1299 (11)	−0.4846 (19)	0.076 (11)*	
O202	0.727 (3)	0.4933 (14)	−0.203 (2)	0.098 (15)*	
O203	0.402 (3)	0.4664 (15)	−0.579 (3)	0.113 (18)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
W1	0.0528 (10)	0.0632 (14)	0.0418 (12)	0.0114 (10)	0.0202 (9)	0.0067 (10)
W2	0.0464 (9)	0.0617 (14)	0.0394 (12)	0.0084 (9)	0.0165 (9)	0.0058 (10)
W3	0.0513 (10)	0.0588 (14)	0.0412 (12)	0.0089 (9)	0.0190 (9)	0.0086 (10)
W4	0.0503 (10)	0.0668 (15)	0.0346 (11)	0.0100 (10)	0.0183 (9)	0.0055 (10)
W5	0.0427 (9)	0.0669 (15)	0.0428 (12)	0.0019 (9)	0.0151 (9)	0.0003 (10)
W6	0.0452 (10)	0.0750 (16)	0.0445 (13)	−0.0021 (10)	0.0206 (9)	−0.0006 (11)
W7	0.0504 (10)	0.0625 (14)	0.0410 (12)	0.0005 (10)	0.0188 (9)	−0.0017 (10)
W8	0.0449 (9)	0.0639 (14)	0.0409 (12)	0.0058 (9)	0.0155 (9)	0.0018 (10)
W9	0.0482 (10)	0.0596 (13)	0.0388 (12)	0.0071 (9)	0.0165 (9)	0.0039 (10)
W10	0.0523 (10)	0.0675 (15)	0.0385 (12)	0.0077 (10)	0.0204 (9)	0.0055 (10)
W11	0.0462 (10)	0.0634 (14)	0.0439 (13)	0.0017 (9)	0.0187 (9)	0.0014 (10)
W12	0.0428 (9)	0.0646 (14)	0.0430 (12)	0.0010 (9)	0.0127 (9)	−0.0026 (10)
W13	0.0584 (11)	0.0640 (14)	0.0352 (12)	0.0050 (10)	0.0212 (10)	0.0052 (10)
W14	0.0609 (11)	0.0560 (13)	0.0416 (12)	0.0076 (10)	0.0232 (10)	0.0033 (10)
W15	0.0609 (12)	0.0655 (15)	0.0554 (15)	0.0094 (11)	0.0308 (11)	0.0052 (11)
W16	0.0473 (9)	0.0650 (14)	0.0432 (12)	0.0086 (9)	0.0209 (9)	0.0069 (10)
W17	0.0616 (12)	0.0645 (15)	0.0535 (15)	−0.0037 (11)	0.0234 (11)	0.0052 (12)
W18	0.0486 (10)	0.0795 (17)	0.0455 (13)	0.0089 (11)	0.0177 (10)	0.0078 (11)
W19	0.0578 (11)	0.0681 (16)	0.0456 (13)	0.0070 (11)	0.0178 (10)	0.0015 (11)
W20	0.0567 (11)	0.0656 (15)	0.0425 (13)	0.0026 (11)	0.0131 (10)	0.0021 (11)
W21	0.0644 (13)	0.0722 (16)	0.0451 (14)	−0.0117 (12)	0.0246 (11)	−0.0099 (11)
W22	0.0518 (11)	0.0740 (17)	0.0515 (14)	−0.0041 (11)	0.0179 (10)	−0.0006 (12)
W23	0.0520 (11)	0.0751 (17)	0.0587 (16)	0.0017 (11)	0.0189 (11)	0.0091 (13)

W24	0.0696 (13)	0.0705 (17)	0.0525 (15)	0.0056 (12)	0.0314 (12)	0.0087 (12)
W25	0.0616 (12)	0.0648 (15)	0.0427 (13)	0.0023 (11)	0.0133 (10)	0.0049 (11)
W26	0.0630 (12)	0.0765 (18)	0.0541 (15)	−0.0034 (12)	0.0295 (12)	0.0040 (13)
W27	0.0637 (13)	0.0614 (15)	0.0621 (16)	0.0098 (11)	0.0248 (12)	0.0100 (12)
W28	0.0661 (13)	0.0808 (19)	0.0564 (16)	−0.0035 (13)	0.0332 (12)	0.0041 (13)
W29	0.0808 (16)	0.0669 (17)	0.0638 (17)	−0.0101 (13)	0.0416 (14)	−0.0077 (13)
W30	0.0746 (14)	0.0664 (16)	0.0588 (16)	−0.0005 (13)	0.0314 (13)	−0.0030 (12)
W31	0.0823 (16)	0.0789 (19)	0.0610 (17)	0.0251 (14)	0.0428 (14)	0.0188 (13)
W32	0.0651 (13)	0.0636 (16)	0.0625 (16)	−0.0025 (11)	0.0292 (12)	0.0056 (12)
W33	0.0930 (18)	0.0594 (16)	0.0722 (19)	0.0009 (13)	0.0491 (16)	−0.0035 (13)
Ba1	0.048 (6)	0.083 (11)	0.051 (9)	0.002 (6)	0.013 (6)	0.002 (7)
Ba2	0.094 (8)	0.109 (11)	0.063 (8)	0.001 (7)	0.046 (7)	−0.016 (7)
Ba3	0.057 (5)	0.063 (7)	0.086 (9)	−0.007 (4)	0.004 (5)	−0.016 (6)
Ba4	0.039 (4)	0.055 (5)	0.077 (7)	0.007 (3)	0.025 (4)	0.005 (4)
Ba5	0.082 (2)	0.119 (4)	0.107 (4)	0.028 (3)	0.048 (3)	0.034 (3)
Ba8	0.0575 (15)	0.063 (2)	0.067 (2)	−0.0017 (14)	0.0263 (15)	−0.0007 (16)
Ba9	0.069 (2)	0.155 (5)	0.069 (3)	−0.005 (3)	0.022 (2)	−0.012 (3)
Ba11	0.0526 (14)	0.071 (2)	0.0369 (15)	0.0011 (13)	0.0174 (12)	0.0038 (14)
Ba12	0.0663 (17)	0.080 (2)	0.053 (2)	−0.0002 (16)	0.0261 (16)	0.0087 (17)
Co1	0.056 (4)	0.048 (4)	0.040 (4)	0.008 (3)	0.022 (3)	0.007 (3)
Co2	0.037 (3)	0.076 (6)	0.040 (4)	0.001 (3)	0.016 (3)	0.003 (4)
Co3	0.054 (4)	0.077 (6)	0.038 (5)	0.004 (4)	0.009 (4)	0.000 (4)
Ba6	0.063 (4)	0.087 (6)	0.087 (6)	−0.006 (4)	0.039 (4)	−0.029 (5)
Ba7	0.094 (4)	0.094 (5)	0.076 (5)	0.004 (4)	0.033 (4)	0.000 (4)
Ba7A	0.094 (4)	0.094 (5)	0.076 (5)	0.004 (4)	0.033 (4)	0.000 (4)
Ba7B	0.094 (4)	0.094 (5)	0.076 (5)	0.004 (4)	0.033 (4)	0.000 (4)
Ba10	0.11 (3)	0.28 (9)	0.16 (5)	0.00 (4)	0.07 (4)	−0.06 (5)

Geometric parameters (Å, º)

W1—Ba13	3.81 (7)	W30—O91	1.82 (3)
W1—Co1	3.049 (8)	W30—O92	1.92 (4)
W1—O1	1.619 (5)	W30—Ba14	3.84 (6)
W1—O2	1.84 (5)	W31—O53	1.84 (4)
W1—O3	1.91 (3)	W31—O55	2.44 (4)
W1—O4	1.91 (3)	W31—O57	2.00 (4)
W1—O5	1.86 (6)	W31—O93	1.621 (5)
W1—O6	2.36 (3)	W31—O94	1.87 (3)
W2—O8	1.85 (3)	W31—O108	1.96 (3)
W2—O11	2.34 (3)	W32—O67	1.82 (4)
W2—O38	1.99 (4)	W32—O69	2.38 (3)
W2—O99	1.64 (3)	W32—O79	1.98 (5)
W2—O100	1.94 (4)	W32—O81	2.07 (5)
W2—O101	1.93 (4)	W32—O91	2.01 (3)
W3—O9	1.70 (3)	W32—O95	1.621 (5)
W3—O10	1.859 (5)	W33—O54	1.97 (3)
W3—O12	1.66 (3)	W33—O55	2.46 (4)
W3—O13	1.89 (3)	W33—O64	1.81 (6)

W3—O14	2.30 (2)	W33—O88	1.90 (4)
W3—O100	1.83 (3)	W33—O94	1.99 (3)
W4—O7	1.862 (5)	W33—O97	1.621 (5)
W4—O15	1.70 (4)	Ba1—O9	2.92 (3)
W4—O16	1.623 (5)	Ba1—O10	3.22 (5)
W4—O17	1.860 (5)	Ba1—O34	3.13 (3)
W4—O18	2.06 (4)	Ba1—O117	3.14 (6)
W4—O19	2.37 (3)	Ba1—O130	2.89 (6)
W5—O20	1.622 (5)	Ba1—O142	3.20 (5)
W5—O21	1.86 (3)	Ba2—O30	3.02 (3)
W5—O22	1.88 (3)	Ba2—O83^{ii}	2.99 (3)
W5—O23	1.95 (4)	Ba2—O93^{i}	2.87 (4)
W5—O24	2.39 (3)	Ba2—O128	1.68 (3)
W5—O114	1.81 (4)	Ba2—O129	2.60 (4)
W5—Ba7^{i}	3.936 (12)	Ba2—O133	2.78 (5)
W6—O25	1.82 (4)	Ba2—O148^{i}	3.01 (5)
W6—O26	1.623 (5)	Ba3—O45	2.80 (2)
W6—O27	1.94 (3)	Ba3—O70^{i}	3.24 (4)
W6—O28	2.01 (4)	Ba3—O72^{i}	2.81 (4)
W6—O29	2.35 (4)	Ba3—Ba7^{i}	3.893 (18)
W6—O115	1.97 (4)	Ba4—O35	3.04 (4)
W7—O8	2.02 (3)	Ba4—O59	3.04 (4)
W7—O11	2.55 (3)	Ba4—O117	2.85 (6)
W7—O30	1.617 (5)	Ba4—O126	2.98 (3)
W7—O31	1.99 (5)	Ba4—O127	2.99 (6)
W7—O32	1.883 (16)	Ba5—O52	3.09 (3)
W7—O116	1.92 (4)	Ba5—O53	2.91 (4)
W8—Ba13	3.79 (7)	Ba5—O120	2.50 (5)
W8—O4	1.89 (3)	Ba5—O121	2.67 (5)
W8—O17	1.90 (5)	Ba5—O122	2.90 (6)
W8—O19	2.41 (2)	Ba5—O125	3.00 (6)
W8—O33	1.617 (5)	Ba5—O144	2.87 (4)
W8—O34	1.94 (3)	Ba5—O148	2.60 (5)
W8—O117	2.02 (5)	Ba8—O39	2.73 (5)
W9—O9	2.11 (3)	Ba8—O80	2.80 (3)
W9—O18	1.81 (4)	Ba8—O98^{iii}	2.78 (2)
W9—O19	2.30 (3)	Ba8—O132	2.92 (4)
W9—O35	1.621 (5)	Ba8—O136	2.95 (4)
W9—O101	1.87 (3)	Ba8—O141	2.86 (7)
W9—O117	1.859 (5)	Ba8—O145	2.70 (6)
W10—O7	1.862 (5)	Ba8—O147^{i}	2.86 (6)
W10—O11	2.37 (3)	Ba8—O151	2.76 (6)
W10—O36	1.77 (3)	Ba9—Ba13^{iv}	3.01 (7)
W10—O37	1.622 (5)	Ba9—O26^{iii}	2.98 (2)
W10—O38	1.94 (4)	Ba9—O33^{iv}	2.87 (3)
W10—O116	1.93 (4)	Ba9—O62	3.03 (3)
W11—O39	1.63 (5)	Ba9—O118	2.91 (4)
W11—O40	2.07 (5)	Ba9—O119	2.93 (5)

W11—O41	1.86 (3)	Ba9—O146	2.01 (4)
W11—O42	1.98 (3)	Ba9—O150	3.06 (8)
W11—O43	2.30 (3)	Ba11—O12	2.89 (3)
W11—O114	1.96 (4)	Ba11—O16^{ii}	2.892 (18)
W12—O21	1.92 (3)	Ba11—O110	2.94 (2)
W12—O24	2.33 (3)	Ba11—O123	2.83 (4)
W12—O27	1.92 (4)	Ba11—O124	2.79 (4)
W12—O44	1.857 (5)	Ba11—O135	1.10 (6)
W12—O45	1.622 (5)	Ba11—O142	2.73 (5)
W12—O46	1.83 (5)	Ba11—O143	2.80 (3)
W13—O13	1.99 (3)	Ba11—O149	2.80 (6)
W13—O14	2.37 (3)	Ba12—O52	2.839 (16)
W13—O32	1.864 (15)	Ba12—O58^{v}	2.88 (3)
W13—O47	1.860 (5)	Ba12—O99^{v}	2.84 (3)
W13—O48	1.87 (3)	Ba12—O107^{iii}	2.842 (16)
W13—O51	1.621 (5)	Ba12—O131	2.69 (4)
W14—O5	1.73 (6)	Ba12—O134	2.82 (5)
W14—O6	2.34 (3)	Ba12—O137	2.79 (7)
W14—O31	1.80 (5)	Ba12—O144	2.96 (4)
W14—O48	1.95 (3)	Ba13—O4	2.87 (8)
W14—O49	1.622 (5)	Ba13—O118^{iv}	3.32 (8)
W14—O50	1.79 (3)	Co1—O2	1.87 (5)
W15—O23	1.87 (4)	Co1—O6	2.00 (3)
W15—O40	1.69 (5)	Co1—O15	1.94 (4)
W15—O52	1.623 (5)	Co1—O36	1.87 (3)
W15—O53	1.90 (4)	Co1—O50	1.89 (3)
W15—O54	1.87 (3)	Co1—N5^{vi}	1.91 (2)
W15—O55	2.33 (4)	Co2—O25	1.83 (4)
W16—O3	1.89 (3)	Co2—O41	1.81 (4)
W16—O10	1.93 (4)	Co2—O43	2.00 (3)
W16—O14	2.34 (2)	Co2—O44	1.79 (2)
W16—O34	1.87 (3)	Co2—O63	1.87 (4)
W16—O47	1.72 (4)	Co2—N1	1.93 (2)
W16—O56	1.621 (5)	Co3—O60	1.88 (4)
W17—O58	1.621 (5)	Co3—O66	1.77 (4)
W17—O102	1.73 (4)	Co3—O85	1.98 (3)
W17—O103	1.82 (3)	Co3—O89	1.97 (5)
W17—O104	1.95 (4)	Co3—O96	1.89 (6)
W17—O105	1.88 (4)	Co3—N6^{iv}	1.95 (2)
W17—O106	2.28 (3)	Co3—Ba14	3.77 (7)
W18—O22	1.91 (4)	O6—B44	1.57 (5)
W18—O24	2.44 (3)	O11—B44	1.34 (5)
W18—O46	1.98 (5)	O14—B44	1.70 (5)
W18—O107	1.618 (5)	O19—B44	1.46 (5)
W18—O108	1.85 (4)	O20—Ba7^{i}	3.27 (4)
W18—O109	1.95 (4)	O20—Ba7B^{i}	3.18 (4)
W19—O104	1.92 (4)	O21—Ba7^{i}	2.94 (3)
W19—O106	2.35 (3)	O24—B25	1.41 (6)

W19—O110	1.621 (5)	O29—B25	1.55 (6)
W19—O111	1.81 (4)	O37—Ba7A^{vi}	3.158 (19)
W19—O112	1.87 (3)	O37—Ba7B^{vi}	2.64 (3)
W19—O113	1.94 (4)	O43—B25	1.59 (6)
W20—O59	1.67 (4)	O47—Ba10	3.22 (8)
W20—O60	1.79 (4)	O55—B25	1.46 (6)
W20—O61	1.81 (3)	O65—Ba14^{iv}	2.79 (7)
W20—O102	2.04 (4)	O66—Ba14	2.96 (8)
W20—O106	2.44 (3)	O67—Ba14	3.23 (8)
W20—O113	1.92 (4)	O69—B69	1.46 (7)
W21—O42	1.93 (3)	O70—Ba6^{vii}	2.926 (19)
W21—O43	2.37 (3)	O73—B69	1.66 (7)
W21—O62	1.619 (5)	O76—Ba7	2.93 (2)
W21—O63	1.87 (4)	O76—Ba7A	3.03 (2)
W21—O64	1.95 (6)	O85—B69	1.68 (7)
W21—O87	2.02 (6)	O89—Ba14	2.85 (8)
W22—O61	1.98 (3)	O91—Ba14	3.04 (7)
W22—O65	1.618 (5)	O97—Ba6	2.88 (2)
W22—O66	1.83 (4)	O106—B69	1.44 (7)
W22—O67	2.00 (4)	O126—Ba10^{vi}	3.02 (6)
W22—O68	1.864 (5)	O127—Ba10^{vi}	2.73 (8)
W22—O69	2.35 (3)	O132—Ba7B^{i}	3.32 (5)
W22—Ba14	3.87 (7)	O138—Ba7	2.61 (5)
W23—Ba3^{i}	3.807 (11)	O138—Ba7A	2.49 (5)
W23—O70	1.619 (5)	O138—Ba7B	2.64 (5)
W23—O71	1.96 (4)	O139—Ba7A	2.40 (4)
W23—O72	1.95 (4)	O140—Ba6	2.24 (8)
W23—O73	2.35 (3)	O147—Ba7	2.86 (6)
W23—O84	1.78 (3)	O147—Ba7A	3.17 (6)
W23—O103	2.00 (4)	O147—Ba7B	1.91 (6)
W24—O28	1.84 (4)	N1—C1	1.3900
W24—O29	2.23 (4)	N1—C5	1.3900
W24—O57	1.76 (4)	C1—H1	0.9500
W24—O74	1.67 (4)	C1—C2	1.3900
W24—O98	1.622 (5)	C2—H2	0.9500
W24—O109	1.87 (4)	C2—C3	1.3900
W25—O72	1.84 (4)	C3—C4	1.3900
W25—O73	2.28 (3)	C3—C6	1.43 (3)
W25—O75	1.864 (5)	C4—H4	0.9500
W25—O76	1.620 (5)	C4—C5	1.3900
W25—O77	1.97 (3)	C5—H5	0.9500
W25—O112	1.89 (3)	N2—C6	1.3900
W26—O68	1.860 (5)	N2—C8	1.3900
W26—O69	2.34 (3)	C6—N3	1.3900
W26—O75	1.865 (5)	N3—C7	1.3900
W26—O78	1.621 (5)	C7—N4	1.3900
W26—O79	1.81 (5)	C7—C11	1.37 (3)
W26—O111	1.97 (4)	N4—C8	1.3900

W27—O71	1.86 (4)	C8—C16	1.31 (3)
W27—O73	2.32 (3)	N5—C9	1.3900
W27—O77	1.93 (4)	N5—C13	1.3900
W27—O80	1.60 (3)	C9—H9	0.9500
W27—O81	1.81 (5)	C9—C10	1.3900
W27—O82	1.79 (5)	C10—H10	0.9500
W28—O83	1.622 (5)	C10—C11	1.3900
W28—O84	1.96 (3)	C11—C12	1.3900
W28—O85	2.34 (3)	C12—H12	0.9500
W28—O92	1.91 (4)	C12—C13	1.3900
W28—O96	1.72 (5)	C13—H13	0.9500
W28—O105	1.89 (4)	N6—C14	1.3900
W29—O29	2.46 (4)	N6—C18	1.3900
W29—O74	2.09 (4)	C14—H14	0.9500
W29—O86	1.618 (5)	C14—C15	1.3900
W29—O87	1.95 (5)	C15—H15	0.9500
W29—O88	1.91 (4)	C15—C16	1.3900
W29—O115	1.93 (4)	C16—C17	1.3900
W30—O82	2.01 (5)	C17—H17	0.9500
W30—O85	2.31 (3)	C17—C18	1.3900
W30—O89	1.78 (4)	C18—H18	0.9500
W30—O90	1.623 (5)	Ba14—O201^{iv}	2.90 (8)

Co1—W1—Ba13	81.4 (11)	O120—Ba5—O125	73.2 (16)
O1—W1—Ba13	73.5 (19)	O120—Ba5—O144	81.9 (14)
O1—W1—Co1	134.2 (16)	O120—Ba5—O148	83.8 (16)
O1—W1—O2	99 (2)	O121—Ba5—O52	61.5 (11)
O1—W1—O3	98.7 (18)	O121—Ba5—O53	72.6 (13)
O1—W1—O4	102.0 (18)	O121—Ba5—O122	63.8 (16)
O1—W1—O5	106 (2)	O121—Ba5—O125	73.0 (15)
O1—W1—O6	172.5 (17)	O121—Ba5—O144	78.7 (13)
O2—W1—Ba13	61.5 (18)	O122—Ba5—O52	108.9 (13)
O2—W1—Co1	34.9 (14)	O122—Ba5—O125	68.1 (17)
O2—W1—O3	161.5 (17)	O125—Ba5—O52	127.9 (13)
O2—W1—O4	92.1 (18)	O144—Ba5—O52	72.1 (8)
O2—W1—O5	87 (2)	O144—Ba5—O122	133.4 (15)
O2—W1—O6	75.8 (16)	O144—Ba5—O125	75.5 (14)
O3—W1—Ba13	121.1 (15)	O148—Ba5—O52	76.3 (13)
O3—W1—Co1	127.1 (9)	O148—Ba5—O53	62.9 (14)
O3—W1—O4	80.7 (14)	O148—Ba5—O121	131.3 (15)
O3—W1—O5	92 (2)	O148—Ba5—O122	113.9 (17)
O3—W1—O6	86.5 (12)	O148—Ba5—O125	154.9 (17)
O4—W1—Ba13	47.0 (15)	O148—Ba5—O144	111.5 (14)
O4—W1—Co1	86.8 (9)	O39—Ba8—O80	127.2 (12)
O4—W1—O5	152 (2)	O39—Ba8—O98^{iii}	66.9 (14)
O4—W1—O6	84.1 (12)	O39—Ba8—O132	73.1 (12)
O5—W1—Ba13	147 (2)	O39—Ba8—O136	65.9 (12)
O5—W1—Co1	76.0 (18)	O39—Ba8—O141	100.5 (17)

O5—W1—O6	68.0 (19)	O39—Ba8—O145	144.6 (15)
O6—W1—Ba13	108.5 (13)	O39—Ba8—O147^{i}	84.1 (15)
O6—W1—Co1	41.0 (8)	O80—Ba8—O98^{iii}	128.2 (12)
O8—W2—O11	82.6 (13)	O80—Ba8—O132	119.0 (11)
O8—W2—O38	91.6 (16)	O80—Ba8—O136	69.2 (10)
O8—W2—O100	89.8 (15)	O80—Ba8—O141	132.3 (16)
O8—W2—O101	162.6 (15)	O80—Ba8—O147^{i}	69.6 (14)
O38—W2—O11	76.2 (14)	O98^{iii}—Ba8—O132	112.8 (14)
O99—W2—O8	101.6 (15)	O98^{iii}—Ba8—O136	78.5 (13)
O99—W2—O11	173.4 (14)	O98^{iii}—Ba8—O141	67.7 (18)
O99—W2—O38	98.5 (15)	O98^{iii}—Ba8—O147^{i}	151.0 (16)
O99—W2—O100	101.2 (15)	O132—Ba8—O136	128.4 (12)
O99—W2—O101	95.4 (15)	O132—Ba8—O147^{i}	55.0 (15)
O100—W2—O11	83.8 (13)	O136—Ba8—O147^{i}	90.1 (15)
O100—W2—O38	159.6 (15)	O141—Ba8—O132	69.6 (17)
O101—W2—O11	80.8 (13)	O141—Ba8—O136	146.1 (17)
O101—W2—O38	89.5 (16)	O141—Ba8—O147^{i}	120.4 (19)
O101—W2—O100	83.3 (15)	O145—Ba8—O80	69.0 (14)
O9—W3—O10	93.6 (18)	O145—Ba8—O98^{iii}	132.4 (16)
O9—W3—O13	161.6 (15)	O145—Ba8—O132	71.8 (15)
O9—W3—O14	85.9 (13)	O145—Ba8—O136	138.1 (15)
O9—W3—O100	85.7 (15)	O145—Ba8—O141	71 (2)
O10—W3—O13	84.3 (18)	O145—Ba8—O147^{i}	72.5 (18)
O10—W3—O14	73.6 (16)	O151—Ba8—O39	129.3 (16)
O12—W3—O9	105.6 (16)	O151—Ba8—O80	72.7 (14)
O12—W3—O10	97.2 (19)	O151—Ba8—O98^{iii}	66.1 (16)
O12—W3—O13	92.8 (15)	O151—Ba8—O132	144.4 (16)
O12—W3—O14	165.9 (13)	O151—Ba8—O136	87.1 (16)
O12—W3—O100	102.2 (16)	O151—Ba8—O141	78.3 (19)
O13—W3—O14	76.0 (12)	O151—Ba8—O145	83.7 (18)
O100—W3—O10	160.0 (19)	O151—Ba8—O147^{i}	140.5 (18)
O100—W3—O13	90.1 (15)	Ba13^{iv}—Ba9—O62	105.6 (16)
O100—W3—O14	86.4 (12)	Ba13^{iv}—Ba9—O150	67 (2)
O7—W4—O18	89.2 (15)	O26^{iii}—Ba9—Ba13^{iv}	119.9 (16)
O7—W4—O19	81.2 (14)	O26^{iii}—Ba9—O62	132.7 (10)
O15—W4—O7	90.5 (14)	O26^{iii}—Ba9—O150	67.3 (16)
O15—W4—O17	93 (2)	O33^{iv}—Ba9—Ba13^{iv}	76.2 (15)
O15—W4—O18	160.2 (18)	O33^{iv}—Ba9—O26^{iii}	61.4 (10)
O15—W4—O19	89.1 (15)	O33^{iv}—Ba9—O62	124.1 (12)
O16—W4—O7	103.4 (17)	O33^{iv}—Ba9—O119	98.8 (11)
O16—W4—O15	101.6 (19)	O33^{iv}—Ba9—O150	82.3 (17)
O16—W4—O17	100 (2)	O62—Ba9—O150	151.1 (17)
O16—W4—O18	97.7 (19)	O118—Ba9—Ba13^{iv}	68.1 (16)
O16—W4—O19	168.2 (15)	O118—Ba9—O26^{iii}	123.7 (10)
O17—W4—O7	155 (2)	O118—Ba9—O33^{iv}	69.0 (11)
O17—W4—O18	79 (2)	O118—Ba9—O62	61.3 (10)
O17—W4—O19	74.6 (18)	O118—Ba9—O119	96.7 (12)
O18—W4—O19	71.3 (14)	O118—Ba9—O150	130.8 (18)

O20—W5—O21	98.9 (17)	O119—Ba9—Ba13^{iv}	164.8 (17)
O20—W5—O22	99.1 (17)	O119—Ba9—O26^{iii}	67.8 (11)
O20—W5—O23	105.3 (18)	O119—Ba9—O62	65.0 (11)
O20—W5—O24	172.1 (17)	O119—Ba9—O150	127.5 (18)
O20—W5—O114	101.1 (19)	O146—Ba9—Ba13^{iv}	115.7 (17)
O20—W5—Ba7^{i}	54.4 (14)	O146—Ba9—O26^{iii}	81.9 (13)
O21—W5—O23	155.3 (14)	O146—Ba9—O33^{iv}	63.3 (13)
O21—W5—O24	74.0 (12)	O146—Ba9—O62	66.7 (13)
O21—W5—Ba7^{i}	45.2 (9)	O146—Ba9—O118	52.1 (13)
O22—W5—O21	85.8 (14)	O146—Ba9—O119	50.4 (13)
O22—W5—O23	85.5 (15)	O146—Ba9—O150	142.2 (18)
O22—W5—O24	77.2 (13)	O12—Ba11—O16^{ii}	123.7 (10)
O22—W5—O114	159.6 (17)	O12—Ba11—O110	119.6 (10)
O22—W5—Ba7^{i}	100.1 (11)	O12—Ba11—O123	68.8 (10)
O23—W5—O24	81.5 (13)	O16^{ii}—Ba11—O110	116.6 (10)
O23—W5—Ba7^{i}	159.4 (11)	O123—Ba11—O16^{ii}	65.0 (11)
O24—W5—Ba7^{i}	119.0 (8)	O123—Ba11—O110	144.0 (9)
O114—W5—O21	93.5 (16)	O124—Ba11—O12	123.4 (11)
O114—W5—O23	86.8 (17)	O124—Ba11—O16^{ii}	68.6 (11)
O114—W5—O24	83.0 (16)	O124—Ba11—O110	76.2 (11)
O114—W5—Ba7^{i}	93.7 (14)	O124—Ba11—O123	71.5 (12)
O25—W6—O27	94.5 (16)	O135—Ba11—O12	69 (3)
O25—W6—O28	163.2 (17)	O135—Ba11—O16^{ii}	84 (3)
O25—W6—O29	92.0 (16)	O135—Ba11—O110	121 (3)
O25—W6—O115	90.5 (16)	O135—Ba11—O123	95 (3)
O26—W6—O25	100.9 (17)	O135—Ba11—O124	153 (3)
O26—W6—O27	100.0 (16)	O135—Ba11—O142	62 (3)
O26—W6—O28	95.7 (17)	O135—Ba11—O143	131 (3)
O26—W6—O29	166.1 (16)	O135—Ba11—O149	72 (4)
O26—W6—O115	95.6 (17)	O142—Ba11—O12	68.4 (12)
O27—W6—O28	84.8 (16)	O142—Ba11—O16^{ii}	138.5 (12)
O27—W6—O29	83.9 (14)	O142—Ba11—O110	68.7 (12)
O27—W6—O115	162.4 (15)	O142—Ba11—O123	136.4 (13)
O28—W6—O29	71.2 (16)	O142—Ba11—O124	143.0 (14)
O115—W6—O28	85.6 (16)	O142—Ba11—O143	85.7 (13)
O115—W6—O29	79.0 (15)	O142—Ba11—O149	84.3 (17)
O8—W7—O11	74.4 (12)	O143—Ba11—O12	65.1 (9)
O30—W7—O8	99.3 (15)	O143—Ba11—O16^{ii}	135.8 (10)
O30—W7—O11	172.2 (13)	O143—Ba11—O110	71.3 (10)
O30—W7—O31	101.7 (17)	O143—Ba11—O123	84.0 (11)
O30—W7—O32	103.2 (16)	O143—Ba11—O124	72.1 (11)
O30—W7—O116	100.5 (16)	O149—Ba11—O12	140.2 (15)
O31—W7—O8	158.8 (16)	O149—Ba11—O16^{ii}	61.6 (15)
O31—W7—O11	85.0 (15)	O149—Ba11—O110	72.2 (15)
O31—W7—O116	90.8 (17)	O149—Ba11—O123	126.0 (15)
O32—W7—O8	88.4 (15)	O149—Ba11—O124	95.9 (16)
O32—W7—O11	81.4 (14)	O149—Ba11—O143	143.3 (15)
O32—W7—O31	83.7 (17)	O52—Ba12—O99^{v}	125.2 (9)

O32—W7—O116	156.3 (15)	O52—Ba12—O134	65.0 (12)
O116—W7—O8	88.6 (15)	O52—Ba12—O144	74.5 (10)
O116—W7—O11	75.1 (13)	O58^{v}—Ba12—O52	69.4 (9)
O4—W8—Ba13	47.6 (15)	O58^{v}—Ba12—O99^{v}	163.4 (8)
O4—W8—O17	91.5 (19)	O58^{v}—Ba12—O134	120.5 (13)
O4—W8—O19	85.6 (11)	O58^{v}—Ba12—O144	61.3 (11)
O4—W8—O34	88.3 (13)	O99^{v}—Ba12—O144	112.1 (10)
O4—W8—O117	159.5 (12)	O107^{iii}—Ba12—O52	134.8 (9)
O17—W8—Ba13	62.2 (19)	O107^{iii}—Ba12—O58^{v}	110.8 (11)
O17—W8—O19	72.8 (12)	O107^{iii}—Ba12—O99^{v}	65.8 (10)
O17—W8—O117	81 (2)	O107^{iii}—Ba12—O134	128.3 (13)
O19—W8—Ba13	109.5 (12)	O107^{iii}—Ba12—O144	147.7 (11)
O33—W8—Ba13	72.2 (19)	O131—Ba12—O52	147.9 (10)
O33—W8—O4	102.7 (18)	O131—Ba12—O58^{v}	88.8 (10)
O33—W8—O17	99.3 (18)	O131—Ba12—O99^{v}	74.6 (10)
O33—W8—O19	168.8 (17)	O131—Ba12—O107^{iii}	74.2 (11)
O33—W8—O34	101.0 (18)	O131—Ba12—O134	111.3 (13)
O33—W8—O117	97.4 (17)	O131—Ba12—O137	134.0 (15)
O34—W8—Ba13	129.1 (14)	O131—Ba12—O144	74.4 (12)
O34—W8—O17	159.3 (13)	O134—Ba12—O99^{v}	66.7 (12)
O34—W8—O19	86.6 (11)	O134—Ba12—O144	71.2 (13)
O34—W8—O117	91.9 (18)	O137—Ba12—O52	78.1 (14)
O117—W8—Ba13	138.6 (19)	O137—Ba12—O58^{v}	120.9 (15)
O117—W8—O19	73.9 (10)	O137—Ba12—O99^{v}	73.1 (14)
O9—W9—O19	82.4 (11)	O137—Ba12—O107^{iii}	63.0 (15)
O18—W9—O9	159.8 (16)	O137—Ba12—O134	84.6 (16)
O18—W9—O19	77.4 (15)	O137—Ba12—O144	149.1 (15)
O18—W9—O101	93.5 (17)	W8—Ba13—W1	58.1 (11)
O18—W9—O117	83 (2)	Ba9^{iv}—Ba13—W1	112 (2)
O35—W9—O9	99.0 (18)	Ba9^{iv}—Ba13—W8	75.2 (16)
O35—W9—O18	101 (2)	Ba9^{iv}—Ba13—O118^{iv}	54.5 (14)
O35—W9—O19	174.5 (16)	O4—Ba13—W1	29.0 (10)
O35—W9—O101	102.0 (18)	O4—Ba13—W8	29.1 (10)
O35—W9—O117	95 (2)	O4—Ba13—Ba9^{iv}	93 (2)
O101—W9—O9	84.4 (14)	O4—Ba13—O118^{iv}	97 (2)
O101—W9—O19	83.4 (13)	O118^{iv}—Ba13—W1	126 (2)
O117—W9—O9	93.0 (19)	O118^{iv}—Ba13—W8	67.9 (15)
O117—W9—O19	79.8 (19)	O2—Co1—W1	34.3 (15)
O117—W9—O101	163 (2)	O2—Co1—O6	85.0 (17)
O7—W10—O11	79.1 (15)	O2—Co1—O15	94.1 (19)
O7—W10—O38	86.8 (14)	O2—Co1—O36	177.0 (19)
O36—W10—O7	90.4 (12)	O2—Co1—O50	85.4 (17)
O36—W10—O11	86.4 (13)	O2—Co1—N5^{vi}	89.4 (17)
O36—W10—O38	162.8 (16)	O6—Co1—W1	50.8 (8)
O36—W10—O116	91.2 (15)	O15—Co1—W1	95.7 (12)
O37—W10—O7	101.8 (18)	O15—Co1—O6	96.8 (15)
O37—W10—O11	169.6 (16)	O36—Co1—W1	145.1 (11)
O37—W10—O36	103.9 (18)	O36—Co1—O6	94.3 (14)

O37—W10—O38	93.3 (18)	O36—Co1—O15	88.9 (15)
O37—W10—O116	98.9 (18)	O36—Co1—N5^{vi}	91.0 (14)
O38—W10—O11	76.4 (14)	O50—Co1—W1	83.5 (9)
O116—W10—O7	158.2 (17)	O50—Co1—O6	82.5 (13)
O116—W10—O11	79.4 (13)	O50—Co1—O15	179.2 (16)
O116—W10—O38	85.2 (16)	O50—Co1—O36	91.7 (14)
O39—W11—O40	103 (2)	O50—Co1—N5^{vi}	91.3 (14)
O39—W11—O41	98.2 (19)	N5^{vi}—Co1—W1	123.6 (9)
O39—W11—O42	106.9 (17)	N5^{vi}—Co1—O6	172.0 (14)
O39—W11—O43	172.9 (17)	N5^{vi}—Co1—O15	89.3 (15)
O39—W11—O114	93 (2)	O25—Co2—O41	177.0 (17)
O40—W11—O43	83.5 (16)	O25—Co2—O43	98.7 (15)
O41—W11—O40	157.2 (17)	O25—Co2—O63	90.3 (17)
O41—W11—O42	96.1 (13)	O25—Co2—N1	88.5 (16)
O41—W11—O43	75.0 (13)	O41—Co2—O43	84.2 (14)
O41—W11—O114	95.5 (16)	O41—Co2—O63	90.6 (16)
O42—W11—O40	85.9 (16)	O41—Co2—N1	88.6 (16)
O42—W11—O43	76.2 (11)	O44—Co2—O25	90.5 (17)
O114—W11—O40	75.1 (19)	O44—Co2—O41	88.5 (16)
O114—W11—O42	154.9 (15)	O44—Co2—O43	93.3 (14)
O114—W11—O43	85.4 (15)	O44—Co2—O63	179.1 (18)
O21—W12—O24	74.4 (11)	O44—Co2—N1	88.3 (16)
O21—W12—O27	157.5 (13)	O63—Co2—O43	86.7 (14)
O27—W12—O24	85.5 (13)	O63—Co2—N1	91.5 (16)
O44—W12—O21	92.7 (14)	N1—Co2—O43	172.6 (15)
O44—W12—O24	82.6 (14)	O60—Co3—O85	95.8 (14)
O44—W12—O27	94.8 (16)	O60—Co3—O89	178.7 (18)
O45—W12—O21	99.2 (16)	O60—Co3—O96	92 (2)
O45—W12—O24	171.4 (15)	O60—Co3—N6^{iv}	89.5 (16)
O45—W12—O27	99.6 (18)	O60—Co3—Ba14	133.3 (15)
O45—W12—O44	103.8 (18)	O66—Co3—O60	87.7 (18)
O45—W12—O46	97 (2)	O66—Co3—O85	93.4 (16)
O46—W12—O21	78.1 (17)	O66—Co3—O89	93 (2)
O46—W12—O24	76.6 (17)	O66—Co3—O96	176 (2)
O46—W12—O27	87.5 (18)	O66—Co3—N6^{iv}	91.8 (17)
O46—W12—O44	158.9 (19)	O66—Co3—Ba14	49.8 (17)
O13—W13—O14	72.7 (11)	O85—Co3—O89	83.1 (16)
O32—W13—O13	86.3 (14)	O85—Co3—N6^{iv}	172.7 (16)
O32—W13—O14	82.8 (13)	O85—Co3—Ba14	104.0 (14)
O32—W13—O48	85.7 (14)	O89—Co3—Ba14	47.8 (17)
O47—W13—O13	82.1 (19)	O96—Co3—O85	82.3 (19)
O47—W13—O14	65.9 (18)	O96—Co3—O89	87 (2)
O47—W13—O32	149 (2)	O96—Co3—N6^{iv}	92.5 (19)
O47—W13—O48	95.6 (19)	O96—Co3—Ba14	132 (2)
O48—W13—O13	160.3 (14)	N6^{iv}—Co3—O89	91.5 (18)
O48—W13—O14	88.5 (12)	N6^{iv}—Co3—Ba14	75.6 (15)
O51—W13—O13	97.8 (18)	W1—O2—Co1	111 (2)
O51—W13—O14	170.2 (17)	W16—O3—W1	151.4 (19)

O51—W13—O32	98.8 (19)	W1—O4—Ba13	104.0 (19)
O51—W13—O47	112 (2)	W8—O4—W1	152.5 (19)
O51—W13—O48	101.2 (19)	W8—O4—Ba13	103.3 (19)
O5—W14—O6	70 (2)	W14—O5—W1	132 (3)
O5—W14—O31	155 (2)	W1—O6—W14	88.5 (10)
O5—W14—O48	87 (2)	Co1—O6—W1	88.3 (11)
O5—W14—O50	87 (2)	Co1—O6—W14	89.4 (12)
O31—W14—O6	85.4 (16)	B44—O6—W1	129 (2)
O31—W14—O48	83.2 (17)	B44—O6—W14	131 (2)
O48—W14—O6	84.4 (13)	B44—O6—Co1	118 (3)
O49—W14—O5	107 (2)	W4—O7—W10	147.0 (8)
O49—W14—O6	176.1 (13)	W2—O8—W7	117.7 (17)
O49—W14—O31	98.0 (18)	W3—O9—W9	149.7 (19)
O49—W14—O48	98.0 (15)	W3—O9—Ba1	109.4 (15)
O49—W14—O50	102.2 (15)	W9—O9—Ba1	99.4 (12)
O50—W14—O6	75.4 (12)	W3—O10—W16	123 (2)
O50—W14—O31	94.2 (17)	W3—O10—Ba1	94.2 (16)
O50—W14—O48	159.8 (14)	W16—O10—Ba1	102.8 (17)
O23—W15—O53	84.8 (16)	W2—O11—W7	85.0 (10)
O23—W15—O54	159.0 (16)	W2—O11—W10	90.4 (11)
O23—W15—O55	81.5 (14)	W10—O11—W7	85.2 (10)
O40—W15—O23	87 (2)	B44—O11—W2	134 (3)
O40—W15—O53	158 (2)	B44—O11—W7	124 (3)
O40—W15—O54	97 (2)	B44—O11—W10	123 (3)
O40—W15—O55	85 (2)	W3—O12—Ba11	161.7 (17)
O52—W15—O23	101.3 (16)	W3—O13—W13	119.7 (16)
O52—W15—O40	102 (2)	W3—O14—W13	91.5 (9)
O52—W15—O53	99.6 (16)	W3—O14—W16	91.6 (9)
O52—W15—O54	98.1 (15)	W16—O14—W13	89.4 (9)
O52—W15—O55	172.9 (14)	B44—O14—W3	123.9 (19)
O53—W15—O55	74.1 (15)	B44—O14—W13	124 (2)
O54—W15—O53	84.1 (16)	B44—O14—W16	126.6 (19)
O54—W15—O55	78.3 (14)	W4—O15—Co1	142 (2)
O3—W16—O10	159.6 (13)	W4—O16—Ba11^{vi}	154 (2)
O3—W16—O14	88.1 (11)	W4—O17—W8	124 (3)
O3—W16—O34	87.3 (14)	W9—O18—W4	120 (2)
O10—W16—O14	71.5 (10)	W4—O19—W8	88.0 (9)
O34—W16—O10	91.0 (17)	W9—O19—W4	91.6 (10)
O34—W16—O14	86.1 (11)	W9—O19—W8	89.3 (9)
O47—W16—O3	97 (2)	B44—O19—W4	119 (2)
O47—W16—O10	76 (2)	B44—O19—W8	126 (2)
O47—W16—O14	68.5 (14)	B44—O19—W9	131 (2)
O47—W16—O34	154.0 (16)	W5—O20—Ba7^{i}	101.8 (16)
O56—W16—O3	101.6 (16)	W5—O20—Ba7B^{i}	133 (2)
O56—W16—O10	98.8 (15)	W5—O21—W12	122.3 (15)
O56—W16—O14	169.4 (14)	W5—O21—Ba7^{i}	108.1 (12)
O56—W16—O34	98.5 (15)	W12—O21—Ba7^{i}	128.9 (13)
O56—W16—O47	105.8 (18)	W5—O22—W18	121.0 (18)

O58—W17—O102	99 (2)	W15—O23—W5	145 (2)
O58—W17—O103	95.8 (18)	W5—O24—W18	86.2 (10)
O58—W17—O104	97.3 (19)	W12—O24—W5	89.2 (11)
O58—W17—O105	101 (2)	W12—O24—W18	89.0 (11)
O58—W17—O106	172.9 (17)	B25—O24—W5	129 (3)
O102—W17—O103	165.3 (19)	B25—O24—W12	127 (3)
O102—W17—O104	89.2 (19)	B25—O24—W18	123 (3)
O102—W17—O105	92 (2)	W6—O25—Co2	139 (2)
O102—W17—O106	78.5 (17)	W6—O26—Ba9^{viii}	145.2 (17)
O103—W17—O104	87.9 (16)	W12—O27—W6	136 (2)
O103—W17—O105	86.1 (17)	W24—O28—W6	119 (2)
O103—W17—O106	86.8 (13)	W6—O29—W29	87.3 (14)
O104—W17—O106	76.1 (13)	W24—O29—W6	93.0 (16)
O105—W17—O104	161.4 (18)	W24—O29—W29	89.8 (15)
O105—W17—O106	85.9 (15)	B25—O29—W6	120 (3)
O22—W18—O24	75.5 (13)	B25—O29—W24	131 (3)
O22—W18—O46	83.3 (17)	B25—O29—W29	124 (3)
O46—W18—O24	71.5 (16)	W7—O30—Ba2	137.4 (17)
O107—W18—O22	99.1 (18)	W14—O31—W7	152 (3)
O107—W18—O24	172.9 (16)	W13—O32—W7	153.3 (19)
O107—W18—O46	104 (2)	W8—O33—Ba9^{iv}	136 (2)
O107—W18—O108	101.5 (18)	W8—O34—Ba1	104.9 (12)
O107—W18—O109	100.0 (18)	W16—O34—W8	143.4 (17)
O108—W18—O22	88.1 (15)	W16—O34—Ba1	107.8 (13)
O108—W18—O24	83.1 (13)	W9—O35—Ba4	106.5 (17)
O108—W18—O46	154.5 (17)	W10—O36—Co1	142 (2)
O108—W18—O109	85.8 (15)	W10—O37—Ba7A^{vi}	163 (2)
O109—W18—O22	160.8 (15)	W10—O37—Ba7B^{vi}	157 (2)
O109—W18—O24	85.6 (13)	W10—O38—W2	116.6 (19)
O109—W18—O46	94.5 (18)	W11—O39—Ba8	153 (2)
O104—W19—O106	75.0 (13)	W15—O40—W11	156 (3)
O104—W19—O113	88.1 (16)	W11—O41—Co2	111.6 (18)
O110—W19—O104	97.2 (17)	W21—O42—W11	115.3 (14)
O110—W19—O106	172.1 (14)	W11—O43—W21	89.8 (10)
O110—W19—O111	101.6 (17)	Co2—O43—W11	89.2 (11)
O110—W19—O112	101.2 (16)	Co2—O43—W21	87.8 (10)
O110—W19—O113	102.1 (17)	B25—O43—W11	128 (2)
O111—W19—O104	160.3 (16)	B25—O43—W21	127 (2)
O111—W19—O106	86.3 (14)	B25—O43—Co2	123 (3)
O111—W19—O112	83.1 (15)	Co2—O44—W12	143 (2)
O111—W19—O113	93.5 (16)	W12—O45—Ba3	151 (2)
O112—W19—O104	87.8 (15)	W12—O46—W18	123 (2)
O112—W19—O106	79.9 (12)	W13—O47—Ba10	108 (2)
O112—W19—O113	156.6 (15)	W16—O47—W13	135 (3)
O113—W19—O106	76.8 (13)	W16—O47—Ba10	116.5 (15)
O59—W20—O60	101.5 (18)	W13—O48—W14	149.3 (19)
O59—W20—O61	104.8 (17)	W14—O50—Co1	112.6 (16)
O59—W20—O102	100.7 (18)	W15—O52—Ba5	103.9 (12)

O59—W20—O106	167.9 (15)	W15—O52—Ba12	151.4 (16)
O59—W20—O113	97.3 (18)	Ba12—O52—Ba5	104.7 (4)
O60—W20—O61	94.1 (16)	W15—O53—Ba5	102.9 (16)
O60—W20—O102	89.4 (17)	W31—O53—W15	125 (2)
O60—W20—O106	85.9 (13)	W31—O53—Ba5	131.8 (19)
O60—W20—O113	160.8 (15)	W33—O54—W15	120.5 (18)
O61—W20—O102	153.0 (16)	W15—O55—W31	88.4 (12)
O61—W20—O106	84.0 (12)	W15—O55—W33	87.9 (12)
O61—W20—O113	84.9 (16)	W31—O55—W33	85.8 (12)
O102—W20—O106	69.5 (14)	B25—O55—W15	131 (3)
O113—W20—O102	83.2 (17)	B25—O55—W31	122 (3)
O113—W20—O106	74.9 (13)	B25—O55—W33	128 (3)
O42—W21—O43	75.5 (11)	W24—O57—W31	153 (3)
O42—W21—O64	81 (2)	W17—O58—Ba12^{vii}	134 (2)
O42—W21—O87	164.2 (17)	W20—O59—Ba4	164 (2)
O62—W21—O42	99.8 (17)	W20—O60—Co3	143 (2)
O62—W21—O43	172.3 (16)	W20—O61—W22	142 (2)
O62—W21—O63	98.2 (19)	W21—O62—Ba9	142 (2)
O62—W21—O64	104 (2)	Co2—O63—W21	109.0 (18)
O62—W21—O87	94 (2)	W33—O64—W21	155 (4)
O63—W21—O42	97.5 (14)	W22—O65—Ba14^{iv}	150 (3)
O63—W21—O43	76.5 (13)	W22—O66—Ba14	105 (2)
O63—W21—O64	157 (2)	Co3—O66—W22	148 (2)
O63—W21—O87	87 (2)	Co3—O66—Ba14	103 (2)
O64—W21—O43	81.2 (19)	W22—O67—Ba14	92.3 (18)
O64—W21—O87	88 (2)	W32—O67—W22	121 (2)
O87—W21—O43	91.2 (17)	W32—O67—Ba14	106 (2)
O61—W22—O67	154.8 (14)	W26—O68—W22	127.1 (5)
O61—W22—O69	81.6 (12)	W22—O69—W32	89.2 (10)
O61—W22—Ba14	135.7 (14)	W26—O69—W22	90.7 (10)
O65—W22—O61	100.7 (18)	W26—O69—W32	88.4 (10)
O65—W22—O66	104 (2)	B69—O69—W22	123 (3)
O65—W22—O67	102.9 (19)	B69—O69—W26	123 (3)
O65—W22—O68	101.6 (15)	B69—O69—W32	131 (3)
O65—W22—O69	172.1 (17)	W23—O70—Ba3^{i}	97.4 (16)
O65—W22—Ba14	84.0 (18)	W23—O70—Ba6^{vii}	157 (2)
O66—W22—O61	89.3 (17)	Ba6^{vii}—O70—Ba3^{i}	101.6 (8)
O66—W22—O67	93.7 (17)	W27—O71—W23	120 (2)
O66—W22—O68	154.3 (13)	W23—O72—Ba3^{i}	104.5 (14)
O66—W22—O69	83.5 (14)	W25—O72—W23	123.9 (18)
O66—W22—Ba14	47.5 (16)	W25—O72—Ba3^{i}	129.6 (17)
O67—W22—O69	73.9 (13)	W25—O73—W23	92.7 (10)
O67—W22—Ba14	56.6 (15)	W25—O73—W27	93.1 (11)
O68—W22—O61	88.1 (17)	W27—O73—W23	90.6 (10)
O68—W22—O67	78.4 (18)	B69—O73—W23	125 (3)
O68—W22—O69	70.8 (8)	B69—O73—W25	121 (3)
O68—W22—Ba14	134.5 (17)	B69—O73—W27	125 (3)
O69—W22—Ba14	99.7 (12)	W24—O74—W29	123 (2)

O70—W23—Ba3^{i}	57.7 (15)	W25—O75—W26	158.8 (13)
O70—W23—O71	99 (2)	W25—O76—Ba7	138.7 (15)
O70—W23—O72	103.4 (18)	W25—O76—Ba7A	151.8 (15)
O70—W23—O73	169.0 (17)	W27—O77—W25	117.7 (17)
O70—W23—O84	105.5 (19)	W26—O79—W32	120 (2)
O70—W23—O103	101.4 (18)	W27—O80—Ba8	151.5 (17)
O71—W23—Ba3^{i}	98.4 (12)	W27—O81—W32	140 (3)
O71—W23—O72	91.8 (16)	W30—O82—W27	150 (3)
O71—W23—O73	73.3 (14)	W28—O83—Ba2^{vi}	143 (2)
O71—W23—O103	159.9 (16)	W23—O84—W28	163 (2)
O72—W23—Ba3^{i}	45.7 (10)	W30—O85—W28	90.2 (11)
O72—W23—O73	69.9 (12)	Co3—O85—W28	88.3 (12)
O73—W23—Ba3^{i}	115.1 (8)	Co3—O85—W30	90.0 (12)
O84—W23—Ba3^{i}	161.8 (11)	B69—O85—W28	126 (3)
O84—W23—O71	90.6 (17)	B69—O85—W30	130 (3)
O84—W23—O72	150.3 (14)	B69—O85—Co3	121 (3)
O84—W23—O73	82.6 (13)	W29—O87—W21	136 (3)
O84—W23—O103	83.7 (15)	W33—O88—W29	146 (2)
O103—W23—Ba3^{i}	92.7 (10)	W30—O89—Co3	108 (2)
O103—W23—O72	84.0 (15)	W30—O89—Ba14	110 (2)
O103—W23—O73	86.8 (12)	Co3—O89—Ba14	101 (2)
O28—W24—O29	76.8 (17)	W30—O91—W32	146.3 (19)
O28—W24—O109	93.9 (17)	W30—O91—Ba14	101.4 (19)
O57—W24—O28	158.7 (19)	W32—O91—Ba14	107.9 (18)
O57—W24—O29	82.0 (18)	W30—O92—W28	118.5 (19)
O57—W24—O109	86.3 (18)	W31—O93—Ba2^{i}	125 (2)
O74—W24—O28	91.8 (19)	W31—O94—W33	120.0 (18)
O74—W24—O29	79.0 (19)	W28—O96—Co3	113 (3)
O74—W24—O57	82 (2)	W33—O97—Ba6	150 (2)
O74—W24—O109	161.6 (19)	W24—O98—Ba8^{viii}	157 (3)
O98—W24—O28	103 (2)	W2—O99—Ba12^{vii}	138.4 (15)
O98—W24—O29	175 (2)	W3—O100—W2	152 (2)
O98—W24—O57	98 (2)	W2—O101—W9	150 (2)
O98—W24—O74	96 (2)	W17—O102—W20	123 (2)
O98—W24—O109	100 (2)	W17—O103—W23	143 (2)
O109—W24—O29	85.4 (16)	W19—O104—W17	117.3 (19)
O72—W25—O73	73.1 (13)	W28—O105—W17	155 (3)
O72—W25—O75	154.2 (19)	W17—O106—W19	91.1 (10)
O72—W25—O77	89.9 (15)	W17—O106—W20	89.1 (10)
O72—W25—O112	87.5 (15)	W19—O106—W20	88.4 (9)
O75—W25—O73	82 (2)	B69—O106—W17	134 (3)
O75—W25—O77	92 (2)	B69—O106—W19	125 (3)
O75—W25—O112	81.9 (16)	B69—O106—W20	117 (3)
O76—W25—O72	97.7 (15)	W18—O107—Ba12^{viii}	159 (2)
O76—W25—O73	168.9 (13)	W18—O108—W31	150.0 (19)
O76—W25—O75	107 (2)	W24—O109—W18	149 (2)
O76—W25—O77	99.5 (15)	W19—O110—Ba11	145.7 (17)
O76—W25—O112	101.6 (15)	W19—O111—W26	153 (2)

O77—W25—O73	74.7 (13)	W19—O112—W25	153.4 (19)
O112—W25—O73	84.5 (13)	W20—O113—W19	119.8 (19)
O112—W25—O77	158.9 (14)	W5—O114—W11	155 (3)
O68—W26—O69	71.1 (8)	W29—O115—W6	116.8 (19)
O68—W26—O75	152 (2)	W10—O116—W7	120.2 (18)
O68—W26—O79	83 (2)	W8—O117—Ba1	102.3 (19)
O68—W26—O111	95.7 (16)	W8—O117—Ba4	135.8 (6)
O75—W26—O69	81 (2)	W9—O117—W8	117 (3)
O75—W26—O79	93 (2)	W9—O117—Ba1	98.4 (19)
O75—W26—O111	79.7 (17)	W9—O117—Ba4	107 (2)
O78—W26—O68	105.1 (14)	Ba4—O117—Ba1	64.7 (12)
O78—W26—O69	174.9 (14)	Ba9—O118—Ba13^{iv}	57.4 (14)
O78—W26—O75	103 (2)	Ba4—O126—Ba10^{vi}	86.8 (15)
O78—W26—O79	99 (2)	Ba10^{vi}—O127—Ba4	92 (2)
O78—W26—O111	99.3 (17)	Ba8—O132—Ba7B^{i}	89.2 (12)
O79—W26—O69	77.6 (17)	Ba11—O142—Ba1	113.0 (16)
O79—W26—O111	161.6 (18)	Ba5—O144—Ba12	107.3 (13)
O111—W26—O69	84.6 (13)	Ba8^{i}—O147—Ba7A	138 (2)
O71—W27—O73	75.7 (15)	Ba7—O147—Ba8^{i}	173 (2)
O71—W27—O77	90.0 (17)	Ba5—O148—Ba2^{i}	99.7 (16)
O71—W27—O82	90 (2)	C1—N1—Co2	117.3 (19)
O77—W27—O73	74.5 (13)	C1—N1—C5	120.0
O80—W27—O71	92.1 (17)	C5—N1—Co2	122.7 (19)
O80—W27—O73	163.3 (13)	N1—C1—H1	120.0
O80—W27—O77	94.3 (15)	C2—C1—N1	120.0
O80—W27—O81	102 (2)	C2—C1—H1	120.0
O80—W27—O82	101.5 (19)	C1—C2—H2	120.0
O81—W27—O71	166 (2)	C1—C2—C3	120.0
O81—W27—O73	89.9 (18)	C3—C2—H2	120.0
O81—W27—O77	85.2 (19)	C2—C3—C6	126 (2)
O81—W27—O82	91 (2)	C4—C3—C2	120.0
O82—W27—O73	90.2 (17)	C4—C3—C6	114 (2)
O82—W27—O77	164.1 (18)	C3—C4—H4	120.0
O83—W28—O84	102.1 (19)	C5—C4—C3	120.0
O83—W28—O85	170.7 (18)	C5—C4—H4	120.0
O83—W28—O92	96 (2)	N1—C5—H5	120.0
O83—W28—O96	102 (2)	C4—C5—N1	120.0
O83—W28—O105	102 (2)	C4—C5—H5	120.0
O84—W28—O85	80.9 (12)	C6—N2—C8	120.0
O92—W28—O84	90.3 (15)	N2—C6—C3	117 (2)
O92—W28—O85	74.8 (14)	N2—C6—N3	120.0
O96—W28—O84	156 (2)	N3—C6—C3	123 (2)
O96—W28—O85	76 (2)	C7—N3—C6	120.0
O96—W28—O92	90 (2)	N4—C7—N3	120.0
O96—W28—O105	97 (2)	C11—C7—N3	112 (2)
O105—W28—O84	75.1 (16)	C11—C7—N4	128 (2)
O105—W28—O85	86.9 (16)	C8—N4—C7	120.0
O105—W28—O92	158.3 (18)	N4—C8—N2	120.0

O74—W29—O29	66.6 (16)	C16—C8—N2	120 (2)
O86—W29—O29	167.2 (19)	C16—C8—N4	120 (2)
O86—W29—O74	107.0 (19)	C9—N5—Co1^{ii}	121.3 (16)
O86—W29—O87	94 (2)	C9—N5—C13	120.0
O86—W29—O88	103.8 (19)	C13—N5—Co1^{ii}	118.2 (16)
O86—W29—O115	92.9 (19)	N5—C9—H9	120.0
O87—W29—O29	92.1 (19)	C10—C9—N5	120.0
O87—W29—O74	159 (2)	C10—C9—H9	120.0
O87—W29—O88	92 (2)	C9—C10—H10	120.0
O88—W29—O29	87.3 (14)	C9—C10—C11	120.0
O88—W29—O74	87.2 (16)	C11—C10—H10	120.0
O115—W29—O29	76.9 (15)	C7—C11—C10	113 (2)
O115—W29—O74	93.3 (17)	C7—C11—C12	127 (2)
O115—W29—O87	82 (2)	C10—C11—C12	120.0
O115—W29—O88	162.4 (16)	C11—C12—H12	120.0
O82—W30—O85	84.8 (16)	C13—C12—C11	120.0
O82—W30—O92	87.9 (18)	C13—C12—H12	120.0
O82—W30—Ba14	135.8 (17)	N5—C13—H13	120.0
O85—W30—Ba14	95.7 (12)	C12—C13—N5	120.0
O89—W30—O82	163 (2)	C12—C13—H13	120.0
O89—W30—O85	78.7 (17)	C14—N6—Co3^{iv}	121 (2)
O89—W30—O91	90.8 (18)	C14—N6—C18	120.0
O89—W30—O92	91.0 (19)	C18—N6—Co3^{iv}	119 (2)
O89—W30—Ba14	44.4 (18)	N6—C14—H14	120.0
O90—W30—O82	103 (2)	N6—C14—C15	120.0
O90—W30—O85	170.9 (19)	C15—C14—H14	120.0
O90—W30—O89	93 (2)	C14—C15—H15	120.0
O90—W30—O91	98 (2)	C16—C15—C14	120.0
O90—W30—O92	100 (2)	C16—C15—H15	120.0
O90—W30—Ba14	82 (2)	C8—C16—C15	118 (2)
O91—W30—O82	85.1 (17)	C8—C16—C17	122 (2)
O91—W30—O85	86.9 (13)	C15—C16—C17	120.0
O91—W30—O92	161.7 (16)	C16—C17—H17	120.0
O91—W30—Ba14	50.9 (14)	C18—C17—C16	120.0
O92—W30—O85	75.6 (14)	C18—C17—H17	120.0
O92—W30—Ba14	135.2 (15)	N6—C18—H18	120.0
O53—W31—O55	72.1 (15)	C17—C18—N6	120.0
O53—W31—O57	155.2 (17)	C17—C18—H18	120.0
O53—W31—O108	88.9 (16)	O24—B25—O29	111 (4)
O57—W31—O55	83.2 (15)	O24—B25—O43	107 (4)
O93—W31—O53	99 (2)	O24—B25—O55	112 (4)
O93—W31—O55	170.5 (18)	O43—B25—O29	113 (3)
O93—W31—O57	106 (2)	O55—B25—O29	110 (4)
O93—W31—O94	99.8 (19)	O55—B25—O43	103 (4)
O93—W31—O108	100.4 (18)	O6—B44—O14	102 (3)
O94—W31—O53	88.1 (17)	O11—B44—O6	116 (4)
O94—W31—O55	78.3 (14)	O11—B44—O14	108 (3)
O94—W31—O57	89.1 (16)	O11—B44—O19	109 (4)

O94—W31—O108	159.7 (14)	O19—B44—O6	116 (3)
O108—W31—O55	81.7 (13)	O19—B44—O14	104 (3)
O108—W31—O57	85.4 (16)	O69—B69—O73	109 (4)
O67—W32—O69	76.1 (14)	O69—B69—O85	106 (4)
O67—W32—O79	85.3 (18)	O73—B69—O85	103 (4)
O67—W32—O81	162.2 (19)	O106—B69—O69	122 (5)
O67—W32—O91	89.1 (16)	O106—B69—O73	105 (4)
O79—W32—O69	73.6 (16)	O106—B69—O85	111 (4)
O79—W32—O81	89 (2)	O97—Ba6—O70^{v}	128.4 (12)
O79—W32—O91	159.0 (17)	O140—Ba6—O70^{v}	67 (2)
O81—W32—O69	86.2 (16)	O140—Ba6—O97	71 (2)
O91—W32—O69	85.4 (12)	Ba3^{i}—Ba7—W5^{i}	105.9 (3)
O91—W32—O81	90.6 (17)	O20^{i}—Ba7—W5^{i}	23.78 (19)
O95—W32—O67	97 (2)	O20^{i}—Ba7—Ba3^{i}	126.8 (6)
O95—W32—O69	173 (2)	O21^{i}—Ba7—W5^{i}	26.7 (6)
O95—W32—O79	104 (2)	O21^{i}—Ba7—Ba3^{i}	79.9 (6)
O95—W32—O81	100 (2)	O21^{i}—Ba7—O20^{i}	50.2 (6)
O95—W32—O91	97 (2)	O76—Ba7—W5^{i}	141.2 (6)
O54—W33—O55	73.2 (13)	O76—Ba7—Ba3^{i}	68.1 (6)
O54—W33—O94	86.9 (14)	O76—Ba7—O20^{i}	131.7 (9)
O64—W33—O54	92 (2)	O76—Ba7—O21^{i}	133.5 (8)
O64—W33—O55	80 (2)	O138—Ba7—W5^{i}	85.1 (10)
O64—W33—O88	86 (2)	O138—Ba7—Ba3^{i}	120.2 (11)
O64—W33—O94	155 (2)	O138—Ba7—O20^{i}	65.7 (11)
O88—W33—O54	161.3 (15)	O138—Ba7—O21^{i}	103.5 (12)
O88—W33—O55	88.1 (14)	O138—Ba7—O76	68.2 (12)
O88—W33—O94	87.2 (14)	O138—Ba7—O147	101.0 (16)
O94—W33—O55	75.7 (13)	O147—Ba7—W5^{i}	69.0 (12)
O97—W33—O54	102 (2)	O147—Ba7—Ba3^{i}	138.3 (13)
O97—W33—O55	174.7 (19)	O147—Ba7—O20^{i}	62.7 (14)
O97—W33—O64	98 (2)	O147—Ba7—O21^{i}	84.5 (14)
O97—W33—O88	97 (2)	O147—Ba7—O76	141.4 (14)
O97—W33—O94	106.3 (19)	W22—Ba14—W30	77.6 (12)
O9—Ba1—O10	49.7 (8)	Co3—Ba14—W22	53.9 (9)
O9—Ba1—O34	62.6 (9)	Co3—Ba14—W30	47.1 (8)
O9—Ba1—O117	56.7 (8)	O65^{iv}—Ba14—W22	80.5 (18)
O9—Ba1—O142	68.2 (11)	O65^{iv}—Ba14—W30	137 (2)
O34—Ba1—O10	50.6 (10)	O65^{iv}—Ba14—Co3	90.4 (19)
O34—Ba1—O142	130.3 (11)	O65^{iv}—Ba14—O66	81 (2)
O117—Ba1—O10	89.7 (13)	O65^{iv}—Ba14—O67	103 (2)
O117—Ba1—O34	54.1 (12)	O65^{iv}—Ba14—O89	114 (3)
O117—Ba1—O142	103.4 (11)	O65^{iv}—Ba14—O91	143 (3)
O130—Ba1—O9	123.9 (14)	O65^{iv}—Ba14—O201^{iv}	124 (3)
O130—Ba1—O10	77.3 (12)	O66—Ba14—W22	27.2 (10)
O130—Ba1—O34	70.4 (13)	O66—Ba14—W30	62.8 (14)
O130—Ba1—O117	115.1 (14)	O66—Ba14—Co3	27.2 (10)
O130—Ba1—O142	139.7 (15)	O66—Ba14—O67	53.6 (15)
O142—Ba1—O10	91.8 (11)	O66—Ba14—O91	62.4 (16)

O30—Ba2—W31^{i}	104.6 (6)	O67—Ba14—W22	31.1 (9)
O83^{ii}—Ba2—W31^{i}	119.5 (10)	O67—Ba14—W30	75.1 (14)
O83^{ii}—Ba2—O30	133.9 (11)	O67—Ba14—Co3	75.4 (15)
O83^{ii}—Ba2—O148^{i}	57.8 (14)	O89—Ba14—W22	79.5 (18)
O93^{i}—Ba2—W31^{i}	19.2 (5)	O89—Ba14—W30	25.9 (11)
O93^{i}—Ba2—O30	85.6 (8)	O89—Ba14—Co3	30.8 (12)
O93^{i}—Ba2—O83^{ii}	136.6 (12)	O89—Ba14—O66	55.8 (17)
O93^{i}—Ba2—O148^{i}	79.6 (13)	O89—Ba14—O67	90 (2)
O128—Ba2—W31^{i}	146.0 (12)	O89—Ba14—O91	51.4 (16)
O128—Ba2—O30	75.8 (12)	O89—Ba14—O201^{iv}	108 (2)
O128—Ba2—O83^{ii}	75.0 (15)	O91—Ba14—W22	64.3 (14)
O128—Ba2—O93^{i}	143.5 (15)	O91—Ba14—W30	27.7 (9)
O128—Ba2—O129	82.0 (14)	O91—Ba14—Co3	60.6 (13)
O128—Ba2—O133	70.6 (15)	O91—Ba14—O67	50.8 (14)
O128—Ba2—O148^{i}	131.9 (16)	O201^{iv}—Ba14—W22	144 (2)
O129—Ba2—W31^{i}	76.4 (10)	O201^{iv}—Ba14—W30	94.2 (18)
O129—Ba2—O30	139.5 (12)	O201^{iv}—Ba14—Co3	139 (2)
O129—Ba2—O83^{ii}	68.9 (12)	O201^{iv}—Ba14—O66	155 (3)
O129—Ba2—O93^{i}	92.9 (12)	O201^{iv}—Ba14—O67	113 (2)
O129—Ba2—O133	136.2 (15)	O201^{iv}—Ba14—O91	92 (2)
O129—Ba2—O148^{i}	73.6 (14)	O76—Ba7A—O37^{ii}	136.9 (9)
O133—Ba2—W31^{i}	141.5 (11)	O76—Ba7A—O147	123.4 (13)
O133—Ba2—O30	65.8 (12)	O138—Ba7A—O37^{ii}	73.6 (13)
O133—Ba2—O83^{ii}	71.3 (13)	O138—Ba7A—O76	67.8 (12)
O133—Ba2—O93^{i}	129.2 (13)	O138—Ba7A—O147	95.6 (15)
O133—Ba2—O148^{i}	99.9 (15)	O139—Ba7A—O37^{ii}	127.5 (13)
O148^{i}—Ba2—W31^{i}	65.7 (10)	O139—Ba7A—O76	64.9 (12)
O148^{i}—Ba2—O30	144.7 (12)	O139—Ba7A—O138	122.7 (15)
W23^{i}—Ba3—Ba7^{i}	108.9 (3)	O139—Ba7A—O147	137.2 (15)
O45—Ba3—W23^{i}	129.7 (9)	O147—Ba7A—O37^{ii}	77.9 (13)
O45—Ba3—O70^{i}	121.8 (12)	O20^{i}—Ba7B—Ba8^{i}	85.9 (9)
O45—Ba3—Ba7^{i}	73.9 (8)	O20^{i}—Ba7B—O132^{i}	55.5 (12)
O70^{i}—Ba3—W23^{i}	24.94 (16)	O37^{ii}—Ba7B—Ba8^{i}	95.8 (10)
O70^{i}—Ba3—Ba7^{i}	132.8 (4)	O37^{ii}—Ba7B—O20^{i}	92.3 (13)
O72^{i}—Ba3—W23^{i}	29.8 (8)	O37^{ii}—Ba7B—O132^{i}	71.0 (12)
O72^{i}—Ba3—O45	128.3 (11)	O37^{ii}—Ba7B—O138	80.9 (14)
O72^{i}—Ba3—O70^{i}	54.7 (8)	O132^{i}—Ba7B—Ba8^{i}	41.6 (8)
O72^{i}—Ba3—Ba7^{i}	80.1 (8)	O138—Ba7B—Ba8^{i}	152.3 (13)
O35—Ba4—O59	79.3 (8)	O138—Ba7B—O20^{i}	66.9 (13)
O117—Ba4—O35	51.6 (5)	O138—Ba7B—O132^{i}	113.1 (15)
O117—Ba4—O59	130.4 (9)	O147—Ba7B—Ba8^{i}	28.2 (19)
O117—Ba4—O126	129.0 (8)	O147—Ba7B—O20^{i}	74 (2)
O117—Ba4—O127	111.7 (15)	O147—Ba7B—O37^{ii}	121 (2)
O126—Ba4—O35	161.7 (10)	O147—Ba7B—O132^{i}	53 (2)
O126—Ba4—O59	99.7 (9)	O147—Ba7B—O138	136 (2)
O126—Ba4—O127	85.5 (13)	O47—Ba10—Ba4^{ii}	143 (2)
O127—Ba4—O35	78.7 (13)	O47—Ba10—C2^{ix}	82 (7)
O127—Ba4—O59	56.4 (14)	O126^{ii}—Ba10—Ba4^{ii}	46.3 (11)

O53—Ba5—O52	53.4 (8)	O126^{ii}—Ba10—O47	166 (2)
O53—Ba5—O122	69.7 (14)	O126^{ii}—Ba10—C2^{ix}	86 (7)
O53—Ba5—O125	134.0 (14)	O127^{ii}—Ba10—Ba4^{ii}	46.5 (17)
O53—Ba5—O144	125.3 (11)	O127^{ii}—Ba10—O47	103 (2)
O120—Ba5—O52	138.1 (12)	O127^{ii}—Ba10—O126^{ii}	90 (2)
O120—Ba5—O53	142.1 (14)	O127^{ii}—Ba10—C2^{ix}	171 (6)
O120—Ba5—O121	144.3 (16)	C2^{ix}—Ba10—Ba4^{ii}	131 (6)
O120—Ba5—O122	112.8 (17)		

Symmetry codes: (i) −*x*+2, −*y*, −*z*; (ii) *x*, −*y*+1/2, *z*+1/2; (iii) *x*, −*y*−1/2, *z*−1/2; (iv) −*x*+1, −*y*, −*z*−1; (v) −*x*+2, *y*−1/2, −*z*−1/2; (vi) *x*, −*y*+1/2, *z*−1/2; (vii) −*x*+2, *y*+1/2, −*z*−1/2; (viii) *x*, −*y*−1/2, *z*+1/2; (ix) −*x*+1, *y*+1/2, −*z*−1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O95	0.95	2.39	3.05 (5)	127
C4—H4···O1^{x}	0.95	2.36	3.23 (5)	152
C10—H10···O49^{x}	0.95	3.06	3.46 (4)	108
C12—H12···O1^{x}	0.95	2.83	3.37 (5)	117
C15—H15···O49^{x}	0.95	2.75	3.61 (4)	152
C17—H17···O67	0.95	2.65	3.17 (5)	115

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