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Synthesis and characterization of hybrid Anderson hexamolybdoaluminates(III) functionalized with indometacin or cinnamic acid

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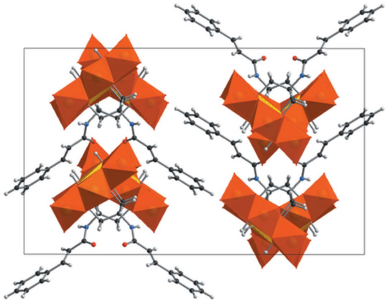
The single-side Al-centred tris-functionalized hybrid organic–inorganic Anderson polyoxomolybdates $(C_{16}H_{36}N)_3[Al(OH)_3Mo_6O_{18}(OCH_2)_3CNH(C_{10}H_8O)]\cdot C_9H_7N\cdot 4CH_3OH\cdot 5H_2O$ (**AlMo$_6$-NH-Cin**; Cin is cinnamic acid, $C_{10}H_9O_2$) and $(C_{16}H_{36}N)_3[Al(OH)_3Mo_6O_{18}(OCH_2)_3CNH(C_{19}H_{15}ClNO_3)]\cdot 9H_2O$ (**AlMo$_6$-NH-Indo**; Indo is indometacin, $C_{19}H_{16}ClNO_4$) have been prepared in a mild three-step synthesis and structurally characterized by single-crystal X-ray diffraction, ^{1}H NMR and IR spectroscopies and elemental analysis. Both **AlMo$_6$-NH-Cin** and **AlMo$_6$-NH-Indo** crystallize in the orthorhombic space group *Pbca*. The antibacterial activities of **AlMo$_6$-NH-Cin** and **AlMo$_6$-NH-Indo** against the Gram-negative human mucosal pathogen *Moraxella catarrhalis* were investigated by determination of the minimum inhibitory concentration, which is 32 µg ml^{-1} for **AlMo$_6$-NH-Cin** and 256 µg ml^{-1} for **AlMo$_6$-NH-Indo**.

1. Introduction

Polyoxometalates (POMs), an exceptional class of metal–oxide clusters with various compositions, exhibit an oxygen-rich surface with strong coordination potential (Pope, 1983). They have attracted much attention owing to their unique catalytic (Wang & Yang, 2015), redox (Gumerova & Rompel, 2018), magnetic (Clemente-Juan *et al.*, 2012) and bioactive properties (Bijelic & Rompel, 2015, 2017; Molitor *et al.*, 2017; Fu *et al.*, 2015; Bijelic *et al.*, 2018*a*,*b*) and constitute promising building blocks for advanced materials. Recently, increasing effort has been devoted to the introduction of organic and metal–organic units into the metal oxide frameworks in order to functionalize POM materials (Dolbecq *et al.*, 2010). Among the various synthetic strategies for the organic functionalization of POMs, alkoxylation has gained much attention due to the diversity and tunability of alkoxyl ligands, especially when using the disk-shaped Anderson-type anions $[X^{n+}H_m M_6O_{24}]^{(12-n-m)-}$ (M = Mo^{6+} and W^{6+}; X = heteroatom, *e.g.* Te^{6+} and I^{7+} for A-type with m = 0, or Al^{3+} and Ni^{2+} for B-type with m = 6), with a wide spectrum of central heteroatoms (Blazevic & Rompel, 2016; Zhang *et al.*, 2018). In particular, after Hasenknopf *et al.* (2002) had pioneered and established the synthesis of tris-derivatives of Anderson polyoxomolybdates (POMos), this archetype has been widely used as starting materials for the attachment of various tris [tris(hydroxymethyl)methane]-based organic ligands [$RC(CH_2OH)_3$, denoted R-Tris]. If the R group itself is reactive (–NH$_2$, –CH$_2$OH *etc.*), post-functionalization with a variety of organic mol-



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ecules, including ligands containing aromatic units (Al-Sayed *et al.*, 2015) or alkyl chains (Rosnes *et al.*, 2013) *via* imine, amide or ester-bond formation, is possible. The resulting hybrid materials were used in supramolecular self-assembly (Macdonell *et al.*, 2015) or for the formation of metal–organic frameworks (MOFs; Li *et al.*, 2016). Major application fields are bio-inorganic (Yvon *et al.*, 2014), nano-structured (Song *et al.*, 2009), energy storage (Ji *et al.*, 2015), optical (Boulmier *et al.*, 2018) and photochemical (Schaming *et al.*, 2010) materials.

Herein, two biologically active molecules, namely indometacin and cinnamic acid, were used to post-functionalize the Al-centred Anderson anion $[Al(OH)_3Mo_6O_{18}(OCH_2)_3CNH_2]^{3-}$ (Wu *et al.*, 2011) *via* amidation reaction, resulting in two novel single-side grafted hybrid organic–inorganic Anderson-type POMos, namely $(TBA)_3[Al(OH)_3Mo_6O_{18}(OCH_2)_3CNH(C_{10}H_8O)]\cdot C_9H_7N\cdot 4CH_3OH\cdot 5H_2O$ (**AlMo$_6$-NH-Cin**; Cin is cinnamic acid and TBA is tetrabutylammonium) and $(TBA)_3[Al(OH)_3Mo_6O_{18}(OCH_2)_3CNH(C_{19}H_{15}ClNO_3)]\cdot 9H_2O$ (**AlMo$_6$-NH-Indo**; Indo is indometacin). Both compounds were structurally characterized by single-crystal X-ray diffraction, IR spectroscopy and elemental analysis. Their antibacterial activity against *Moraxella catarrhalis* was investigated by determination of the minimum inhibitory concentration (MIC).

2. Experimental

2.1. Synthesis and crystallization

2.1.1. Synthesis of AlMo$_6$-NH-Indo. $Na_3(H_2O)_6[Al(OH)_6Mo_6O_{18}]\cdot 2H_2O$ (**AlMo$_6$**) was prepared according to a published procedure (Shivaiah & Das, 2005). The single-side attachment of Tris-NH_2 to **AlMo$_6$** was achieved through a modified published procedure (Wu *et al.*, 2011). **AlMo$_6$** (3.84 g, 3.28 mmol) was dissolved in water (20.5 ml) and heated to reflux, when Tris-NH_2 (0.735 g, 6.02 mmol) was added. After refluxing for 3 h, the solvent was removed by vacuum. The white powder obtained was redissolved with deionized H_2O and then centrifuged to remove unreacted educts. Tetrabutylammonium bromide (TBABr) (4.12 g, 12.8 mmol) was added to the solution and a white precipitate appeared. In order to functionalize **AlMo$_6$-NH$_2$** with indometacin, a mixture of indometacin (0.172 g, 0.500 mmol), **AlMo$_6$-NH$_2$** (1.05 g, 0.519 mmol) and EEDQ (*N*-ethoxycarbonyl-2-ethoxy-1,2-dihydroquinoline; 0.143 g, 0.570 mmol) in CH_3CN (9.00 ml) was stirred at 323 K for 24 h. The solvent was collected and removed by vacuum. The remaining yellow solid was redissolved in an MeOH–H_2O mixture (2:1 *v*/*v*), followed by the addition of TBABr (0.5 g). After several weeks, crystals suitable for single-crystal X-ray diffraction were obtained [yield 2.3 g, 32% (based on Mo)]. FT–IR (cm^{-1}): 324 (*s*), 368 (*s*), 395 (*m*), 442 (*s*), 484 (*s*), 505 (*m*), 534 (*m*, *sh*), 567 (*m*), 611 (*m*), 650 (*s*), 736 (*m*), 754 (*m*), 796 (*m*), 833 (*w*), 850 (*m*), 897 (*s*), 918 (*s*), 939 (*s*), 1012 (*w*, *sh*), 1027 (*m*), 1053 (*m*), 1072 (*m*), 1091 (*m*), 1122 (*m*), 1151 (*m*), 1174 (*w*), 1224 (*m*), 1290 (*w*), 1315 (*m*), 1336 (*w*, *sh*), 1361 (*m*), 1369 (*m*), 1396 (*sh*), 1458 (*m*), 1479 (*m*), 1552 (*m*), 1564 (*m*), 1610 (*m*), 1677 (*m*), 2871 (*m*), 2933 (*m*), 2960 (*m*), 3081 (*w*), 3322 (*m*, *br*). Elemental analysis for $C_{71}H_{145}AlClMo_6N_5O_{36}$ (calculated) (%): C 38.38 (37.27), H 6.75 (6.61), N 3.06 (3.06), Cl 1.29 (1.55), O 22.3 (25.17). ^{1}H NMR (500.32 MHz, CD_3CN, 298 K): δ 0.96 (*t*, 36H), 1.34 (*m*, 24H), 1.59 (*m*, 24H), 3.53 (*m*, 24H), 3.62 (*s*, 2H), 3.81 (*s*, 3H), 2.15 (*s*, 3H), 6.66 (*dd*, 1H), 6.85 (*d*, 1H), 6.96 (*d*, 1H), 7.02 (*d*, 1H), 7.55 (*d*, 2H), 7.64 (*d*, 2H), 64 (*s*, 6H in $CH_2-\mu_3$-O groups).

2.1.2. Synthesis of AlMo$_6$-NH-Cin. The preparation of **AlMo$_6$-NH-Cin** was similar to that of **AlMo$_6$-NH-Indo**, except that cinnamic acid (0.074 g, 0.500 mmol) was used instead of indometacin [yield 1.9 g, 27% (based on Mo)]. FT–IR (cm^{-1}): 324 (*s*), 368 (*s*), 441 (*s*), 482 (*s*), 503 (*m*), 518 (*m*), 534 (*m*), 565 (*m*), 578 (*m*), 607 (*m*), 649 (*s*), 832 (*w*), 898 (*s*), 916 (*s*), 939 (*s*), 983 (*w*), 1035 (*m*), 1060 (*m*), 1112 (*w*), 1118 (*m*), 1153 (*m*), 1193 (*w*), 1228 (*m*), 1284 (*w*), 1323 (*w*), 1348 (*m*), 1380 (*m*), 1458 (*m*), 1479 (*m*), 1548 (*m*, *br*), 1575 (*w*), 1627 (*m*), 1668 (*m*), 1720 (*w*), 1731 (*w*, *sh*), 2874 (*m*), 2933 (*m*), 2960 (*m*), 3062 (*w*), 3290 (*m*, *br*), 3404 (*m*, *br*). Elemental analysis for $C_{73}H_{154}AlMo_6N_5O_{32.6}$ (calculated) (%): C 36.48 (36.92), H 6.50 (7.00), N 2.92 (3.16), O 22.16 (23.10). ^{1}H NMR (500.32 MHz, CD_3CN, 298 K): δ 0.98 (*t*, 36H), 1.37 (*m*, 24H in TBA), 1.61 (*m*, 24H), 3.11 (*d*, 12H), 3.51 (*m*, 24H), 5.12 (*q*, 4H), 6.46 (*d*, 1H), 7.37 (*d*, 1H), 7.47–7.91 (*m*, 5H), 64 (*s*, 6H in $CH_2-\mu_3$-O groups).

2.2. IR spectroscopy

Both compounds were identified by IR measurements on a Bruker Vertex70 IR Spectrometer equipped with a single-reflection diamond-ATR (attenuated total reflectance) unit in the range 4000–300 cm^{-1}.

2.3. ^{1}H NMR

NMR spectra were recorded on a Bruker FT–NMR Avance III 500 MHz instrument at 500.32 (^{1}H) MHz in CD_3CN at ambient temperature. Chemical shifts were referenced relative to the solvent signal for ^{1}H nucleus.

2.4. Elemental analysis

The determination of C/H/N/O/Cl was carried out using an 'EA 1108 CHNS-O' elemental analyzer by Carlo Erba Instruments at the Mikroanalytisches Laboratorium, University of Vienna.

2.5. MIC determination

Minimum inhibitory concentrations (MICs) were determined by the broth microdilution method according to guidelines of the Clinical Laboratory Standards Institute (Wikler, 2009). Double dilutions of tested compounds in 96-well microtiter plates were prepared in the concentration range 1–256 µg ml^{-1}. *M. catarrhalis* (ATCC 23246) was grown on Columbia agar with 5% defibrinated sheep blood. Inocula were prepared by the direct colony suspension method and plates were inoculated with 5×10^{-4} CFU per well. Results were determined by visual inspection after 20–22 h of incubation at 310 K in ambient air. Testing was performed by the standard broth microdilution method with azithromycin

Table 1
Experimental details.

	$AlMo_6$-NH-Cin	**$AlMo_6$-NH-Indo**
Crystal data		
Chemical formula	$(C_{16}H_{36}N)_3[Al(OH)_3Mo_6O_{18}(OCH_2)_3CNH$-$(C_{10}H_8O)]\cdot C_9H_7N\cdot 4CH_3OH\cdot 5H_2O$	$(C_{16}H_{36}N)_3[Al(OH)_3Mo_6O_{18}(OCH_2)_3CNH$-$(C_{19}H_{15}ClNO_3)]\cdot 9H_2O$
M_r	2227.19	2288.02
Crystal system, space group	Orthorhombic, *Pbca*	Orthorhombic, *Pbca*
Temperature (K)	100	200
a, *b*, *c* (Å)	16.1062 (17), 26.512 (3), 45.569 (5)	21.8904 (6), 23.9848 (6), 37.719 (1)
V (Å^3)	19458 (3)	19803.9 (9)
Z	8	8
Radiation type	Mo *Kα*	Mo *Kα*
μ (mm^{-1})	0.84	0.85
Crystal size (mm)	0.23 × 0.15 × 0.03	0.15 × 0.12 × 0.05
Data collection		
Diffractometer	Bruker APEXII CCD	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2013)	Multi-scan (*SADABS*; Bruker, 2013)
T_{min}, T_{max}	0.666, 0.746	0.678, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	293657, 17800, 15423	374956, 18115, 15743
R_{int}	0.066	0.050
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602	0.602
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.066, 0.144, 1.24	0.029, 0.075, 1.06
No. of reflections	17800	18115
No. of parameters	1129	1166
No. of restraints	39	53
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.27, −1.04	1.18, −0.64

Computer programs: *APEX2* (Bruker, 2013), *SAINT* (Bruker, 2013), *SHELXS97* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

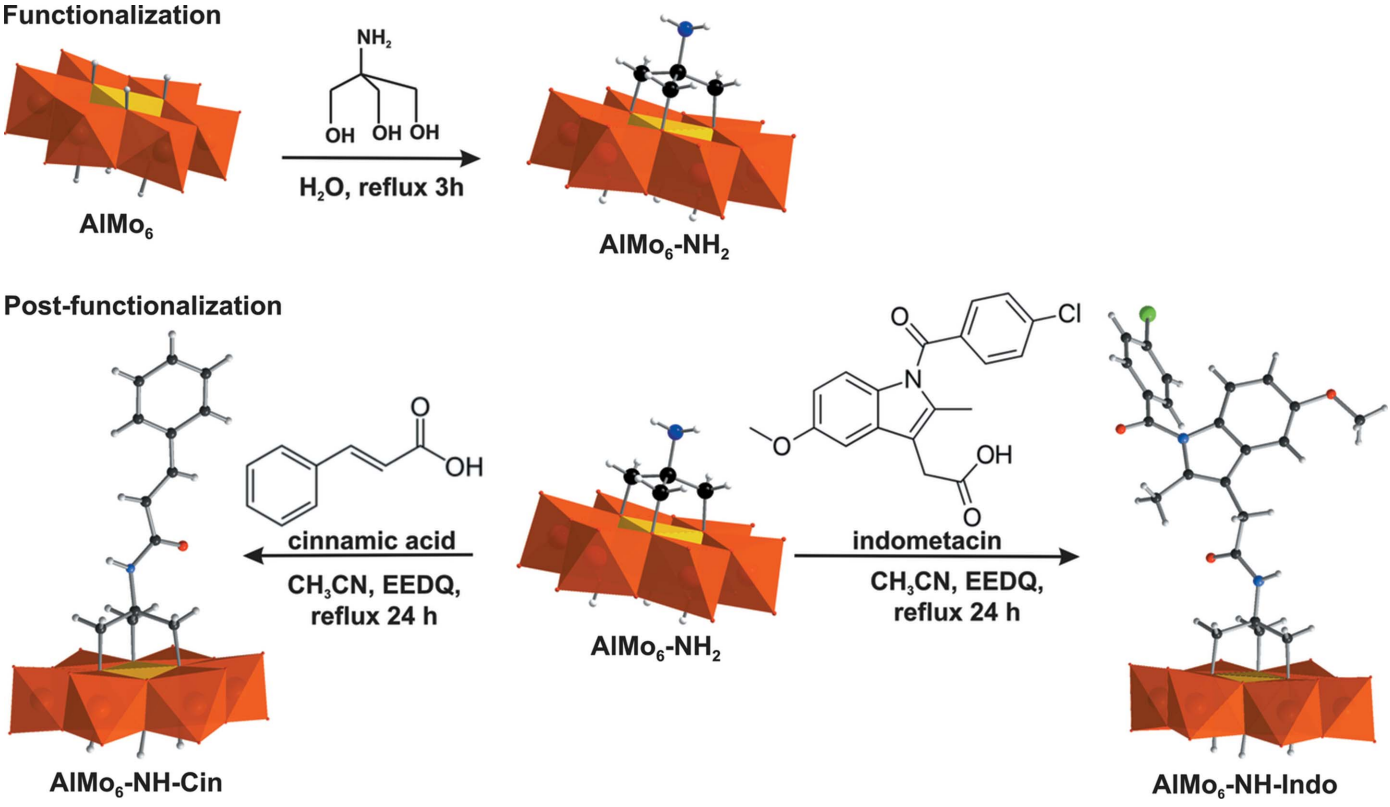

Figure 1
Functionalization of $[Al(OH)_6Mo_6O_{18}]^{3-}$ (**$AlMo_6$**) with the Tris-NH_2 ligand, followed by further post-functionalization of $[Al(OH)_3Mo_6O_{18}(OCH_2)_3$-$CNH_2]^{3-}$ (**$AlMo_6$-NH_2**) with indometacin or cinnamic acid, respectively. EEDQ is *N*-ethoxycarbonyl-2-ethoxy-1,2-dihydroquinoline. Colour code: {MoO_6} octahedra orange and {AlO_6} octahedra yellow, with C atoms black, N blue, Cl green, H grey and O red.

(Lode *et al.*, 1996) as the reference antibiotic to assess test validity. MIC determinatiom was performed at the School of Medicine, University of Zagreb, Croatia.

2.6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The positions of the independent H atoms were obtained by difference Fourier techniques and were refined with free isotropic displacement parameters. Fixed isotropic displacement parameters for all H atoms with a value equal to $1.5U_{eq}$ of the corresponding OH or H_2O group atom were assigned. Restrained distances for D—H bonds were applied to avoid short D—H···H—D interactions. In the case of disordered groups, some bonds were added to or deleted from the connectivity array.

3. Results and discussion

$AlMo_6$-NH-Cin and **$AlMo_6$-NH-Indo** were prepared *via* post-functionalization by pre-forming the hybrid cluster **$AlMo_6$-NH_2** which was modified by amidation reactions (Fig. 1). The fact that single-side grafted anions were obtained supports an earlier theory claiming that the aqueous solvent is a key factor for the formation of single-sided Anderson derivatives (Wu *et al.*, 2011; Blazevic *et al.*, 2015; Gumerova *et al.*, 2016).

X-ray crystallographic analysis shows that the asymmetric units in **$AlMo_6$-NH-Cin** and **$AlMo_6$-NH-Indo** consist of the hybrid Anderson anion, three TBA counter-cations, solvent molecules and, in the case of **$AlMo_6$-NH-Cin**, one molecule of quinoline as a by-product from EEDQ decomposition. The structural analysis revealed that both compounds crystallize in the orthorhombic space group *Pbca*. **$AlMo_6$-NH-Cin** and **$AlMo_6$-NH-Indo** both show the characteristic Anderson-type structure, with a central $\{AlO_6\}$ octahedron surrounded by six edge-shared $\{MoO_6\}$ octahedra that form a planar array of distorted octahedra (Fig. 1). Three different coordination modes of O atoms are found in the structure: six triple-bridged O atoms (denoted μ_3-O) connect the heteroatom and two Mo atoms, six double-bridged O atoms (denoted μ_2-O) connect two Mo atoms and two terminal O atoms (denoted O_t) are connected to each of the six Mo atoms. The bond lengths of the three different binding modes are summarized in Table 2 and are in good agreement with other tris-functionalized Anderson POMos (Wu *et al.*, 2011; Al-Sayed *et al.*, 2015; Blazevic *et al.*, 2015).

Table 2
Selected bond lengths (Å) in **$AlMo_6$—NH-Cin** and **$AlMo_6$—NH-Indo**.

	$AlMo_6$—NH-Cin	**$AlMo_6$—NH-Indo**
Mo—μ_3-O	2.291 (4)–2.391 (4)	2.3068 (19)–2.3632 (18)
Mo—μ_2-O	1.910 (4)–1.941 (5)	1.912 (2)–1.944 (2)
Mo—O_t	1.694 (5)–1.722 (5)	1.696 (2)–1.711 (2)
Al—μ_3-O	1.864 (5)–1.923 (4)	1.863 (2)–1.927 (2)

The tris-ligand caps one side of the planar hexagon by binding to three μ_3-O atoms of the $\{AlO_6\}$ fragment, whereas on the other side of **$AlMo_6$-NH-Cin** and **$AlMo_6$-NH-Indo**, the respective μ_3-O atoms according to BVS calculations [−1.16 (O2), −1.20 (O4) and −1.19 (O6) for **$AlMo_6$-NH-Indo**, and −1.15 (O1), −1.16 (O3) and −1.18 (O5) for **$AlMo_6$-NH-Indo**, calculated according to (Brown & Altermatt, 1985)] are protonated.

The crystal packing of **$AlMo_6$-NH-Cin** can be described as alternate layers of POMo anions and TBA counter-cations, which are repeated along the *c* axis (Fig. 2). The orientations of the hybrid polyanions along the *c* and *b* axes also alternate with an angle of approximately 85° between the planes of the inorganic Anderson 'disks' (Fig. 2*a*). The attached ligands are turned towards each other along the *bc* plane. The distances between the inorganic POMo skeletons along the *a* axis are around 9.5 Å, and around 14 Å along the *b* axis. All four lattice water molecules are situated in front of the undecorated side of the anion and form strong intermolecular hydrogen bonds with μ_3-O—H fragments, with short distances in the region 1.85–1.94 Å.

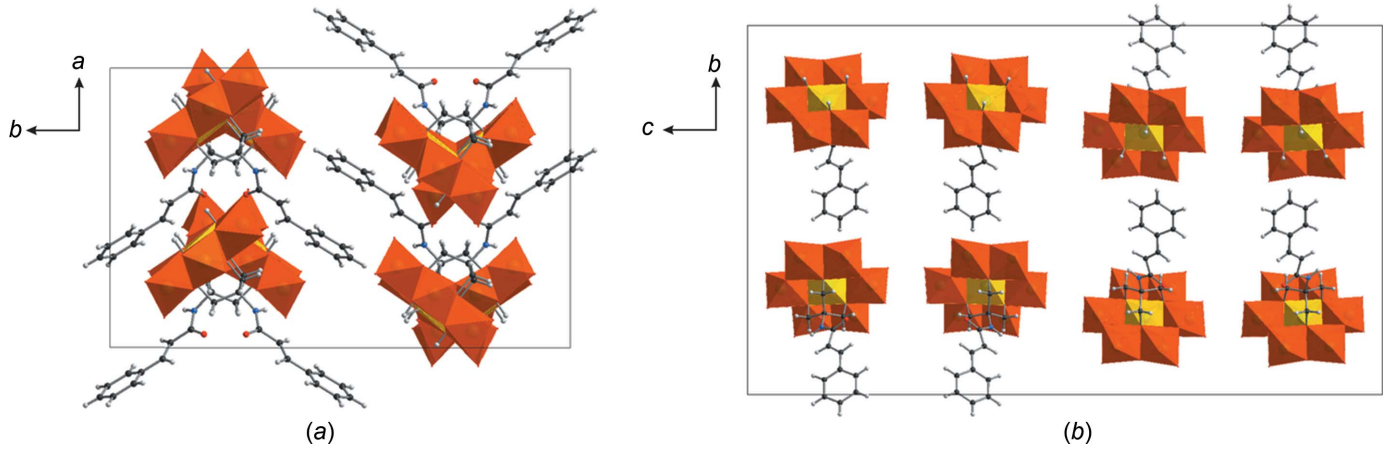

Figure 2
The crystal packing of **$AlMo_6$-NH-Cin**, viewed along (*a*) the *c* axis and (*b*) the *a* axis. The TBA counter-cations and the solvent molecules have been omitted for clarity. Colour code: $\{MoO_6\}$ octahedra orange and $\{AlO_6\}$ octahedra yellow, with C atoms black, N blue, H grey and O red.

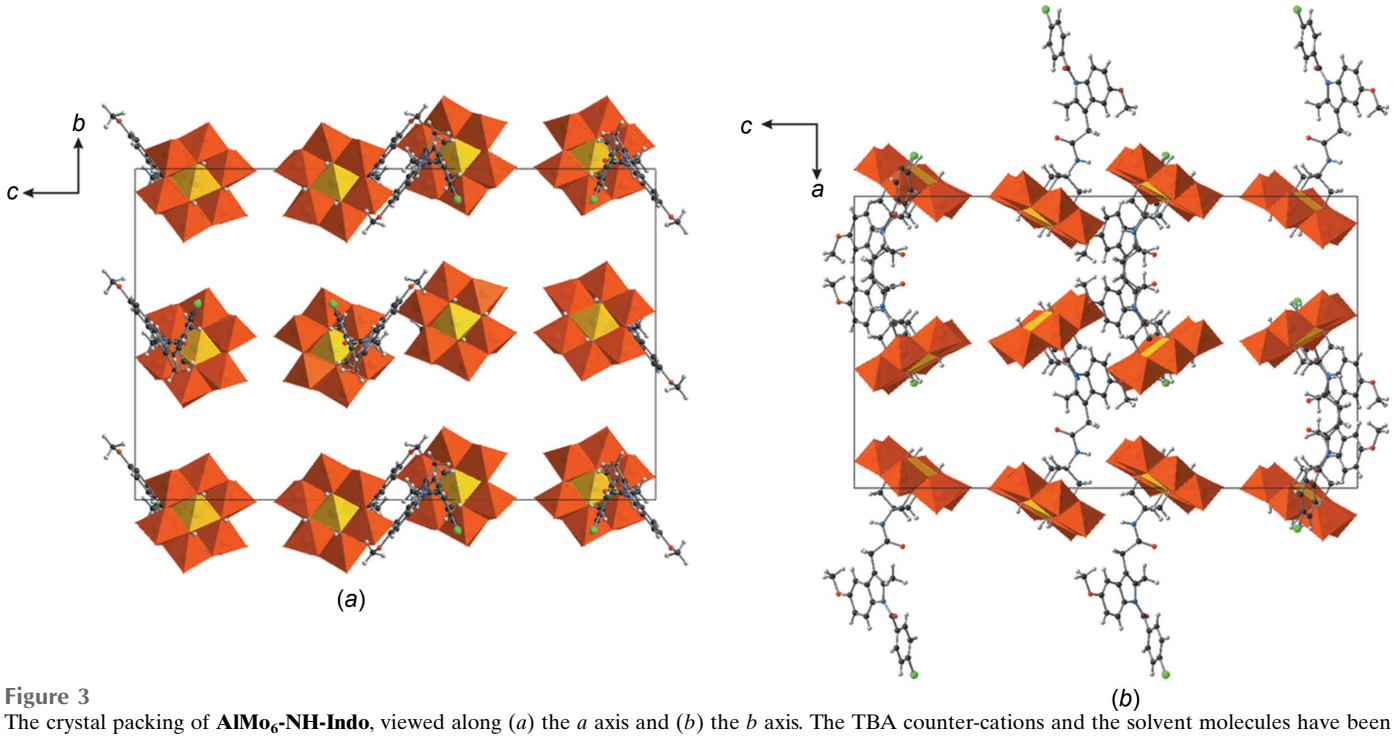

Figure 3
The crystal packing of **AlMo$_6$-NH-Indo**, viewed along (*a*) the *a* axis and (*b*) the *b* axis. The TBA counter-cations and the solvent molecules have been omitted for clarity. Colour code: {MoO$_6$} octahedra orange and {AlO$_6$} octahedra yellow, with C atoms black, N blue, H grey and O red.

The crystal packing of **AlMo$_6$-NH-Indo** is similar to that of **AlMo$_6$-NH-Cin** and can be described as alternate layers of POMo anions and TBA counter-cations, which are repeated along the *a* axis (Fig. 3). The orientation of the hybrid polyanions along the *c* and *b* axes is the same, with the grafted sides turned in different directions (Fig. 3*b*). The distances between inorganic POMos along the *a* axis are around 12 Å, around 11 Å along the *b* axis and approximately 5 Å along the *c* axis. Six of nine lattice water molecules are situated in front of the unfunctionalized side and form strong intermolecular hydrogen bonds with μ_3-O—H fragments and O$_t$ atoms, with distances in the range 1.86–2.08 Å. The crystallographic refinement results for both **AlMo$_6$-NH-Cin** and **AlMo$_6$-NH-Indo** suggest no π–π interactions between the aromatic ring and the C═C double bond based on geometry and separation.

The IR spectra of **AlMo$_6$-NH-Cin** and **AlMo$_6$-NH-Indo** (Fig. 4) are typical for Anderson-type POMos and the characteristic peaks of the core structure are all in agreement with the peaks observed in the spectrum of $Na_3(H_2O)_6[Al(OH)_6Mo_6O_{18}]\cdot 2H_2O$ (Shivaiah & Das, 2005). The stretching vibrations of the terminal Mo═O units appear at 939 cm^{-1}, whereas the peaks in the region from 300 to 920 cm^{-1} correspond to the antisymmetric and symmetric deformation vibrations of the Mo—O—Mo and Mo—O—Al bridging fragments. The peaks appearing in the region 1030–1125 cm^{-1} could be assigned to C—O stretching vibrations, indicating the successful grafting of the tris ligands.

The antibacterial activities of **AlMo$_6$-NH-Cin** and **AlMo$_6$-NH-Indo** against the Gram-negative human mucosal pathogen *Moraxella catarrhalis* (Karalus & Campagnari, 2000) were investigated by determination of the minimum inhibitory concentration (MIC). **AlMo$_6$-NH-Cin** shows a higher activity, with MIC values of 32 µg ml^{-1}, while **AlMo$_6$-NH-Indo** shows an MIC value of 256 µg ml^{-1}. The MIC values for both compounds are much higher than for the clinically applied

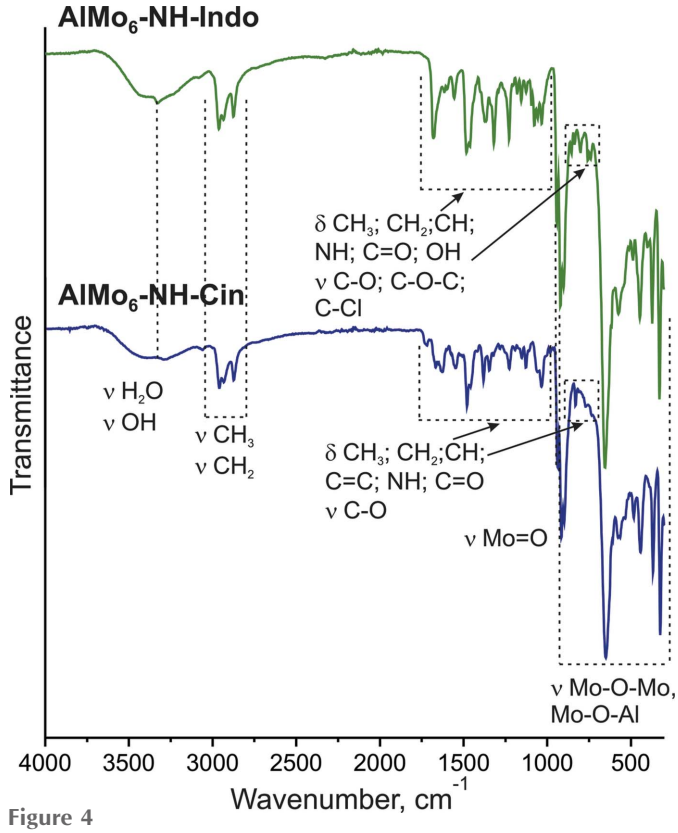

Figure 4
The IR spectra of **AlMo$_6$-NH-Cin** and **AlMo$_6$-NH-Indo** in the region from 4000 to 300 cm^{-1}.

drug azithromycin, which has an MIC value of 0.06 μg ml^{-1}. Taking into account that **AlMo$_6$-NH-Cin** and **AlMo$_6$-NH-Indo** have the same inorganic POMo part, counter-cations and net charge, it can be assumed that their antibacterial activities differs only due to the organic ligands attached. It is known that cinnamic acid and its derivatives exhibit antimicrobial activity against pathogenic and spoilage bacteria (Sova, 2012), indometacin in its turn, as a nonsteroidal anti-inflammatory drug (Lucas, 2016), showed bacteriostatic activity against *Helicobacter pylori* (Shirin *et al.*, 2006), whereas pure inorganic Ni- and Te-centred Anderson-type POMos and POTs are inactive (MIC > 256 μg ml^{-1}) against *M. catarrhalis* (Gumerova *et al.*, 2018). Thereby, the activity of **AlMo$_6$-NH-Cin** is caused by the synergistic effect of **AlMo$_6$** and cinnamic acid, which is not the case for **AlMo$_6$-NH-Indo**. The preliminary results obtained here show that not only does the activity of the attached ligand play a role, but also synergism with POMs strongly influences the properties of the hybrid compounds.

4. Conclusion

The success in synthesizing **AlMo$_6$-NH-Cin** and **AlMo$_6$-NH-Indo** shows the versatility and reproducibility of the post-functionalization protocol for the alkoxylation of Anderson POMs. The attachment of bioactive ligands makes the hybrid Anderson POMos reported herein potentially superior to pure inorganic structures for antibacterial applications.

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supporting information

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Synthesis and characterization of hybrid Anderson hexamolybdoaluminates(III) functionalized with indometacin or cinnamic acid

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Computing details

Data collection: *APEX2* (Bruker, 2013) for mo_ambl235_pbca; *'APEX2* (Bruker, 2013) for taco104_0m. For both structures, cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); 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).

(mo_ambl235_pbca)

Crystal data

$C_{13}H_{17}AlMo_6NO_{25}·4.73(H_2O)·3(CH_4O)·2(C_{16}H_{36}N)·C_{16}H_{35.5}N·CH_4N$
M_r = 2227.19
Orthorhombic, *Pbca*
a = 16.1062 (17) Å
b = 26.512 (3) Å
c = 45.569 (5) Å
V = 19458 (3) Å^3
Z = 8
F(000) = 9222
D_x = 1.521 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 9772 reflections
θ = 2.3–29.5°
μ = 0.84 mm^{-1}
T = 100 K
Plate, clear colourless
0.23 × 0.15 × 0.03 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2013)
T_{min} = 0.666, T_{max} = 0.746
293657 measured reflections
17800 independent reflections
15423 reflections with $I > 2\sigma(I)$
R_{int} = 0.066
θ_{max} = 25.4°, θ_{min} = 2.3°
h = −19→19
k = −31→31
l = −54→54

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.144
S = 1.24
17800 reflections
1129 parameters
39 restraints
Primary atom site location: heavy-atom method
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0201P)^2 + 204.0739P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.27 e Å^{-3}
$\Delta\rho_{min}$ = −1.04 e Å^{-3}

Special details

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

Refinement. _olex2_refinement_description
1. Fixed Uiso At 1.2 times of: All C(H) groups, All C(H,H) groups, All N(H) groups At 1.5 times of: All C(H,H,H) groups, All O(H) groups, All O(H,H) groups 2. Restrained distances O6-H6 = O2-H2 0.88 with sigma of 0.02 O4-H4 0.88 with sigma of 0.02 H1BB-H6 = H1BB-H1DB = H1AA-H4 2.2 with sigma of 0.04 H29S-O16_$1 1.9 with sigma of 0.08 O1C-H1DB 1.85 with sigma of 0.015 H2-H1CB 2.1 with sigma of 0.015 H1CB-O30S 1.95 with sigma of 0.03 O1A-H1CA 1.95 with sigma of 0.03 H73B-H1CB_$1 2.1 with sigma of 0.02 O30S-C74S ~ O27S-C72S ~ O29S-C73S with sigma of 0.02 C61-C60 ~ C49-C48 ~ C53-C52 ~ C57-C56 with sigma of 0.02 3. Uiso/Uaniso restraints and constraints Uanis(C59) ~ Ueq, Uanis(C60) ~ Ueq, Uanis(C61) ~ Ueq: with sigma of 0.01 and sigma for terminal atoms of 0.02 4. Others Sof(O30S)=Sof(H30S)=Sof(C74S)=Sof(H74A)=Sof(H74B)=Sof(H74C)=1-FVAR(1) Sof(O29S)=Sof(H29S)=Sof(C73S)=Sof(H73A)=Sof(H73B)=Sof(H73C)=FVAR(1) Sof(O28S)=Sof(H28C)=Sof(H28D)=FVAR(2) Fixed Sof: H58A(0.75) H58B(0.75) 5.a Free rotating group: O1A(H1AA,H1AB), O1B(H1BA,H1BB), O1C(H1CA,H1CB), O1D(H1DA,H1DB), O28S(H28C,H28D) 5.b Secondary CH2 refined with riding coordinates: C2(H2A,H2B), C3(H3A,H3B), C4(H4A,H4B), C14(H14A,H14B), C15(H15A,H15B), C16(H16A,H16B), C18(H18A,H18B), C19(H19A,H19B), C20(H20A,H20B), C22(H22A,H22B), C23(H23A,H23B), C24(H24A,H24B), C26(H26A,H26B), C27(H27A,H27B), C28(H28A, H28B), C30(H30A,H30B), C31(H31A,H31B), C32(H32A,H32B), C34(H34A,H34B), C35(H35A,H35B), C36(H36A,H36B), C38(H38A,H38B), C39(H39A,H39B), C40(H40A,H40B), C42(H42A,H42B), C43(H43A,H43B), C44(H44A,H44B), C46(H46A,H46B), C47(H47A, H47B), C48(H48A,H48B), C50(H50A,H50B), C51(H51A,H51B), C52(H52A,H52B), C54(H54A,H54B), C55(H55A,H55B), C56(H56A,H56B), C58(H58A,H58B), C59(H59A,H59B), C60(H60A,H60B) 5.c Aromatic/amide H refined with riding coordinates: N1(H1), C6(H6A), C7(H7), C9(H9), C10(H10), C11(H11), C12(H12), C13(H13), C62(H62), C63(H63), C64(H64), C66(H66), C67(H67), C68(H68), C69(H69) 5.d Tetrahedral OH refined with riding coordinates: O27S(H27S) 5.e Idealised Me refined as rotating group: C71S(H71A,H71B,H71C), C72S(H72A,H72B,H72C), C73S(H73A,H73B,H73C), C17(H17A, H17B,H17C), C21(H21A,H21B,H21C), C25(H25A,H25B,H25C), C29(H29A,H29B,H29C), C33(H33A,H33B,H33C), C37(H37A,H37B,H37C), C41(H41A,H41B,H41C), C45(H45A,H45B, H45C), C49(H49A,H49B,H49C), C53(H53A,H53B,H53C), C57(H57A,H57B,H57C), C61(H61A, H61B,H61C), C74S(H74A,H74B,H74C) 5.f Idealised tetrahedral OH refined as rotating group: O26S(H26S), O29S(H29S), O30S(H30S)

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Mo1	0.28978 (3)	0.12375 (2)	0.15448 (2)	0.02046 (13)	
Mo2	0.26650 (4)	0.12931 (2)	0.08205 (2)	0.02403 (14)	
Mo3	0.14206 (4)	0.21510 (2)	0.05222 (2)	0.02528 (14)	
Mo4	0.03843 (3)	0.29405 (2)	0.09578 (2)	0.02120 (13)	
Mo5	0.05897 (3)	0.28718 (2)	0.16801 (2)	0.01787 (13)	
Mo6	0.19091 (3)	0.20442 (2)	0.19676 (2)	0.01845 (13)	
Al1	0.16091 (11)	0.20713 (7)	0.12491 (4)	0.0157 (4)	
O1	0.2752 (2)	0.18828 (16)	0.11964 (9)	0.0180 (9)	
O2	0.1387 (3)	0.16351 (17)	0.09338 (10)	0.0218 (10)	
H2	0.097 (3)	0.144 (2)	0.0881 (13)	0.012 (16)*	
O3	0.1719 (3)	0.25809 (16)	0.09537 (9)	0.0184 (9)	
O4	0.0525 (3)	0.23026 (17)	0.12979 (10)	0.0197 (9)	
H4	0.008 (3)	0.212 (3)	0.1280 (18)	0.04 (2)*	
O5	0.1917 (2)	0.25372 (16)	0.15493 (9)	0.0157 (9)	

O6	0.1597 (3)	0.15885 (16)	0.15511 (9)	0.0174 (9)
H6	0.118 (3)	0.1382 (19)	0.1566 (14)	0.017 (18)*
O7	0.2477 (3)	0.09393 (17)	0.11854 (10)	0.0245 (10)
O8	0.2519 (3)	0.18994 (18)	0.05924 (9)	0.0240 (10)
O9	0.0397 (3)	0.23830 (18)	0.06851 (10)	0.0258 (11)
O10	0.0778 (3)	0.32261 (16)	0.13199 (9)	0.0196 (9)
O11	0.0791 (3)	0.22767 (16)	0.19056 (9)	0.0185 (9)
O12	0.2936 (3)	0.18129 (17)	0.18001 (10)	0.0207 (10)
O13	0.2642 (3)	0.07662 (18)	0.17817 (11)	0.0292 (11)
O14	0.3934 (3)	0.11791 (18)	0.14810 (10)	0.0273 (11)
O15	0.3719 (3)	0.1254 (2)	0.07897 (11)	0.0331 (12)
O16	0.2271 (3)	0.0845 (2)	0.05880 (11)	0.0381 (13)
O17	0.1043 (3)	0.1703 (2)	0.02849 (11)	0.0400 (14)
O18	0.1693 (3)	0.2650 (2)	0.03089 (11)	0.0353 (13)
O19	0.0692 (3)	0.34262 (19)	0.07379 (10)	0.0301 (11)
O20	−0.0660 (3)	0.30034 (19)	0.09925 (11)	0.0303 (11)
O21	−0.0460 (3)	0.29147 (19)	0.17170 (11)	0.0290 (11)
O22	0.0991 (3)	0.33269 (17)	0.19056 (10)	0.0247 (10)
O23	0.2301 (3)	0.25227 (18)	0.21712 (10)	0.0251 (10)
O24	0.1690 (3)	0.15656 (18)	0.22111 (10)	0.0256 (10)
O25	0.4523 (3)	0.29582 (19)	0.15522 (11)	0.0295 (11)
N1	0.3683 (3)	0.3169 (2)	0.11673 (12)	0.0227 (12)
H1	0.3647	0.3368	0.1013	0.027*
C1	0.3020 (4)	0.2795 (2)	0.12057 (13)	0.0173 (13)
C2	0.3386 (4)	0.2264 (3)	0.11847 (14)	0.0226 (14)
H2A	0.3697	0.2231	0.0998	0.027*
H2B	0.3781	0.2211	0.1348	0.027*
C3	0.2426 (4)	0.2908 (3)	0.09541 (14)	0.0218 (14)
H3A	0.2235	0.3262	0.0970	0.026*
H3B	0.2726	0.2872	0.0766	0.026*
C4	0.2593 (4)	0.2878 (3)	0.15033 (13)	0.0195 (14)
H4A	0.3005	0.2834	0.1662	0.023*
H4B	0.2383	0.3229	0.1513	0.023*
C5	0.4350 (4)	0.3237 (3)	0.13473 (15)	0.0243 (15)
C6	0.4829 (4)	0.3685 (3)	0.12725 (16)	0.0257 (15)
H6A	0.4741	0.3855	0.1092	0.031*
C7	0.5408 (5)	0.3856 (3)	0.14672 (18)	0.0345 (18)
H7	0.5512	0.3645	0.1632	0.041*
C8	0.5883 (5)	0.4321 (4)	0.1454 (2)	0.047 (2)
C9	0.5936 (6)	0.4596 (4)	0.1207 (2)	0.056 (3)
H9	0.5675	0.4483	0.1032	0.067*
C10	0.6382 (7)	0.5054 (4)	0.1209 (3)	0.068 (3)
H10	0.6408	0.5252	0.1035	0.082*
C11	0.6775 (8)	0.5215 (4)	0.1456 (3)	0.075 (3)
H11	0.7070	0.5526	0.1455	0.090*
C12	0.6745 (9)	0.4930 (5)	0.1707 (3)	0.096 (5)
H12	0.7027	0.5037	0.1879	0.115*
C13	0.6298 (7)	0.4485 (5)	0.1704 (2)	0.075 (4)

H13	0.6273	0.4286	0.1878	0.090*	
O1A	−0.0631 (3)	0.1555 (2)	0.12810 (13)	0.0389 (13)	
H1AA	−0.1094	0.1724	0.1289	0.058*	
H1AB	−0.0568	0.1381	0.1441	0.058*	
O1B	0.0314 (3)	0.0941 (2)	0.16390 (12)	0.0348 (12)	
H1BA	0.0342	0.0875	0.1825	0.052*	
H1BB	0.0479	0.0678	0.1539	0.052*	
O1C	0.0080 (4)	0.0977 (2)	0.08468 (14)	0.0544 (17)	
H1CA	−0.0362	0.1078	0.0939	0.082*	
H1CB	0.0025	0.1043	0.0660	0.082*	
O1D	0.1030 (4)	0.0368 (2)	0.11923 (15)	0.0524 (16)	
H1DA	0.1536	0.0481	0.1206	0.079*	
H1DB	0.0741	0.0567	0.1080	0.079*	
O26S	0.0689 (4)	0.0732 (2)	0.22182 (15)	0.0498 (16)	
H26S	0.1019	0.0975	0.2238	0.075*	
C71S	0.1139 (7)	0.0279 (4)	0.2216 (3)	0.069 (3)	
H71A	0.0795	0.0010	0.2132	0.103*	
H71B	0.1293	0.0188	0.2417	0.103*	
H71C	0.1642	0.0321	0.2098	0.103*	
O27S	0.3490 (4)	0.3846 (3)	0.06798 (15)	0.071 (2)	
H27S	0.3748	0.4119	0.0698	0.106*	
O28S	0.4326 (6)	0.4679 (3)	0.0745 (2)	0.058 (3)	0.726 (18)
H28C	0.4399	0.4815	0.0917	0.087*	0.726 (18)
H28D	0.3981	0.4880	0.0656	0.087*	0.726 (18)
O29S	0.3705 (9)	0.5161 (5)	0.0291 (3)	0.033 (4)	0.395 (11)
H29S	0.3281	0.5285	0.0370	0.049*	0.395 (11)
C72S	0.2841 (9)	0.3912 (7)	0.0500 (4)	0.150 (9)	
H72A	0.2997	0.3813	0.0300	0.225*	
H72B	0.2677	0.4268	0.0501	0.225*	
H72C	0.2375	0.3704	0.0567	0.225*	
C73S	0.4340 (15)	0.5502 (9)	0.0303 (6)	0.090 (14)	0.395 (11)
H73A	0.4558	0.5559	0.0105	0.134*	0.395 (11)
H73B	0.4783	0.5369	0.0429	0.134*	0.395 (11)
H73C	0.4135	0.5821	0.0384	0.134*	0.395 (11)
N2	−0.0810 (5)	0.3123 (3)	0.00127 (15)	0.0482 (19)	
C14	−0.1458 (6)	0.3528 (4)	−0.0044 (2)	0.051 (2)	
H14A	−0.1235	0.3765	−0.0193	0.061*	
H14B	−0.1956	0.3366	−0.0130	0.061*	
C15	−0.1723 (7)	0.3829 (4)	0.0223 (2)	0.064 (3)	
H15A	−0.1241	0.4018	0.0301	0.077*	
H15B	−0.1922	0.3597	0.0378	0.077*	
C16	−0.2419 (8)	0.4202 (4)	0.0142 (2)	0.066 (3)	
H16A	−0.2205	0.4437	−0.0009	0.079*	
H16B	−0.2882	0.4010	0.0052	0.079*	
C17	−0.2762 (8)	0.4511 (4)	0.0399 (2)	0.075 (3)	
H17A	−0.2925	0.4283	0.0558	0.113*	
H17B	−0.3247	0.4704	0.0333	0.113*	
H17C	−0.2333	0.4743	0.0469	0.113*	

C18	0.0016 (6)	0.3362 (4)	0.01053 (19)	0.050 (2)
H18A	−0.0077	0.3562	0.0286	0.059*
H18B	0.0412	0.3089	0.0154	0.059*
C19	0.0413 (7)	0.3702 (4)	−0.0125 (2)	0.062 (3)
H19A	0.0439	0.3526	−0.0316	0.075*
H19B	0.0080	0.4013	−0.0149	0.075*
C20	0.1284 (7)	0.3834 (4)	−0.0020 (2)	0.063 (3)
H20A	0.1251	0.3979	0.0179	0.076*
H20B	0.1619	0.3521	−0.0009	0.076*
C21	0.1713 (8)	0.4207 (5)	−0.0222 (3)	0.082 (4)
H21A	0.1437	0.4535	−0.0209	0.122*
H21B	0.1684	0.4084	−0.0425	0.122*
H21C	0.2296	0.4242	−0.0164	0.122*
C22	−0.0701 (6)	0.2825 (3)	−0.02684 (18)	0.046 (2)
H22A	−0.1230	0.2652	−0.0314	0.055*
H22B	−0.0587	0.3064	−0.0430	0.055*
C23	−0.0022 (7)	0.2441 (4)	−0.0260 (2)	0.065 (3)
H23A	−0.0136	0.2199	−0.0100	0.079*
H23B	0.0509	0.2612	−0.0216	0.079*
C24	0.0066 (7)	0.2156 (4)	−0.0545 (2)	0.060 (3)
H24A	−0.0453	0.1967	−0.0581	0.072*
H24B	0.0134	0.2402	−0.0706	0.072*
C25	0.0783 (8)	0.1792 (4)	−0.0553 (2)	0.074 (3)
H25A	0.0817	0.1638	−0.0748	0.110*
H25B	0.0697	0.1528	−0.0405	0.110*
H25C	0.1300	0.1973	−0.0511	0.110*
C26	−0.1065 (6)	0.2782 (4)	0.0263 (2)	0.054 (3)
H26A	−0.1077	0.2983	0.0446	0.065*
H26B	−0.0635	0.2518	0.0287	0.065*
C27	−0.1914 (6)	0.2521 (4)	0.0226 (2)	0.058 (3)
H27A	−0.2357	0.2779	0.0215	0.070*
H27B	−0.1919	0.2325	0.0042	0.070*
C28	−0.2079 (6)	0.2179 (5)	0.0479 (2)	0.070 (3)
H28A	−0.2659	0.2058	0.0466	0.084*
H28B	−0.2025	0.2374	0.0663	0.084*
C29	−0.1502 (7)	0.1722 (5)	0.0495 (3)	0.087 (4)
H29A	−0.1533	0.1533	0.0310	0.130*
H29B	−0.1673	0.1503	0.0657	0.130*
H29C	−0.0930	0.1836	0.0527	0.130*
N3	0.4974 (4)	0.2232 (2)	0.22640 (13)	0.0315 (14)
C30	0.4703 (5)	0.1913 (3)	0.25231 (17)	0.0361 (18)
H30A	0.5107	0.1635	0.2548	0.043*
H30B	0.4726	0.2124	0.2702	0.043*
C31	0.3843 (5)	0.1688 (3)	0.24991 (18)	0.0368 (18)
H31A	0.3812	0.1476	0.2321	0.044*
H31B	0.3431	0.1963	0.2479	0.044*
C32	0.3622 (6)	0.1366 (3)	0.27686 (18)	0.043 (2)
H32A	0.3107	0.1175	0.2728	0.051*

H32B	0.4073	0.1119	0.2805	0.051*
C33	0.3500 (7)	0.1686 (4)	0.3039 (2)	0.064 (3)
H33A	0.4033	0.1832	0.3098	0.096*
H33B	0.3283	0.1476	0.3199	0.096*
H33C	0.3105	0.1957	0.2996	0.096*
C34	0.4381 (4)	0.2667 (3)	0.22307 (16)	0.0285 (16)
H34A	0.3829	0.2531	0.2178	0.034*
H34B	0.4572	0.2878	0.2065	0.034*
C35	0.4282 (5)	0.3001 (3)	0.2497 (2)	0.047 (2)
H35A	0.3937	0.2824	0.2645	0.057*
H35B	0.4835	0.3062	0.2585	0.057*
C36	0.3889 (6)	0.3494 (3)	0.2424 (2)	0.056 (3)
H36A	0.3324	0.3433	0.2346	0.067*
H36B	0.4217	0.3661	0.2268	0.067*
C37	0.3831 (7)	0.3852 (4)	0.2695 (3)	0.077 (4)
H37A	0.4390	0.3917	0.2771	0.116*
H37B	0.3494	0.3692	0.2848	0.116*
H37C	0.3573	0.4171	0.2636	0.116*
C38	0.5846 (4)	0.2430 (3)	0.23305 (16)	0.0318 (17)
H38A	0.5816	0.2657	0.2503	0.038*
H38B	0.6205	0.2141	0.2384	0.038*
C39	0.6246 (5)	0.2713 (3)	0.20769 (17)	0.0375 (19)
H39A	0.5814	0.2908	0.1972	0.045*
H39B	0.6485	0.2467	0.1937	0.045*
C40	0.6927 (5)	0.3071 (3)	0.21802 (17)	0.0363 (18)
H40A	0.7223	0.3207	0.2007	0.044*
H40B	0.7332	0.2881	0.2300	0.044*
C41	0.6581 (6)	0.3513 (3)	0.2363 (2)	0.049 (2)
H41A	0.7018	0.3765	0.2392	0.074*
H41B	0.6394	0.3387	0.2554	0.074*
H41C	0.6113	0.3666	0.2259	0.074*
C42	0.4946 (5)	0.1935 (3)	0.19805 (19)	0.0392 (19)
H42A	0.4356	0.1888	0.1926	0.047*
H42B	0.5204	0.2144	0.1825	0.047*
C43	0.5360 (7)	0.1423 (4)	0.1975 (3)	0.067 (3)
H43A	0.5143	0.1236	0.2147	0.080*
H43B	0.5149	0.1248	0.1799	0.080*
C44	0.6231 (7)	0.1355 (4)	0.1976 (2)	0.065 (3)
H44A	0.6450	0.1451	0.2171	0.078*
H44B	0.6481	0.1586	0.1830	0.078*
C45	0.6508 (6)	0.0804 (4)	0.1905 (2)	0.056 (3)
H45A	0.6324	0.0713	0.1708	0.084*
H45B	0.6260	0.0572	0.2048	0.084*
H45C	0.7115	0.0780	0.1916	0.084*
N4	0.4373 (5)	−0.0337 (3)	0.14557 (19)	0.052 (2)
C46	0.5074 (6)	−0.0727 (3)	0.1469 (2)	0.048 (2)
H46A	0.4946	−0.0967	0.1629	0.057*
H46B	0.5071	−0.0920	0.1283	0.057*

C47	0.5948 (6)	−0.0526 (3)	0.1518 (3)	0.059 (3)	
H47A	0.6020	−0.0431	0.1727	0.071*	
H47B	0.6038	−0.0222	0.1396	0.071*	
C48	0.6581 (7)	−0.0935 (4)	0.1435 (3)	0.068 (3)	
H48A	0.7112	−0.0866	0.1537	0.082*	
H48B	0.6376	−0.1267	0.1502	0.082*	
C49	0.6731 (9)	−0.0953 (5)	0.1110 (3)	0.104 (5)	
H49A	0.6940	−0.0626	0.1043	0.156*	
H49B	0.6210	−0.1031	0.1009	0.156*	
H49C	0.7142	−0.1215	0.1066	0.156*	
C50	0.4381 (5)	−0.0003 (3)	0.1722 (2)	0.044 (2)	
H50A	0.4935	0.0156	0.1736	0.053*	
H50B	0.3971	0.0270	0.1691	0.053*	
C51	0.4196 (6)	−0.0252 (3)	0.2009 (2)	0.049 (2)	
H51A	0.4594	−0.0530	0.2042	0.059*	
H51B	0.3630	−0.0396	0.2004	0.059*	
C52	0.4259 (7)	0.0129 (4)	0.2260 (2)	0.058 (3)	
H52A	0.4838	0.0251	0.2274	0.070*	
H52B	0.3900	0.0422	0.2216	0.070*	
C53	0.4009 (8)	−0.0088 (4)	0.2547 (2)	0.080 (4)	
H53A	0.4331	−0.0395	0.2584	0.120*	
H53B	0.3416	−0.0171	0.2542	0.120*	
H53C	0.4116	0.0158	0.2703	0.120*	
C54	0.3575 (6)	−0.0644 (3)	0.1442 (2)	0.053 (3)	
H54A	0.3593	−0.0861	0.1265	0.064*	
H54B	0.3551	−0.0868	0.1615	0.064*	
C55	0.2790 (6)	−0.0332 (3)	0.1432 (3)	0.074 (4)	
H55A	0.2756	−0.0152	0.1242	0.089*	
H55B	0.2802	−0.0077	0.1591	0.089*	
C56	0.2033 (6)	−0.0667 (3)	0.1469 (3)	0.064 (3)	
H56A	0.1531	−0.0473	0.1415	0.077*	
H56B	0.2078	−0.0955	0.1332	0.077*	
C57	0.1931 (7)	−0.0864 (4)	0.1772 (3)	0.074 (4)	
H57A	0.1840	−0.0582	0.1907	0.111*	
H57B	0.2433	−0.1048	0.1830	0.111*	
H57C	0.1452	−0.1092	0.1779	0.111*	
C58	0.4474 (8)	0.0003 (3)	0.1190 (2)	0.065 (3)	
H58A	0.4042	0.0268	0.1200	0.077*	0.75
H58B	0.5019	0.0173	0.1206	0.077*	0.75
C59	0.4426 (11)	−0.0235 (5)	0.0896 (3)	0.101 (4)	
H59A	0.4805	−0.0529	0.0892	0.121*	
H59B	0.3855	−0.0363	0.0866	0.121*	
C60	0.4634 (10)	0.0092 (5)	0.0652 (3)	0.090 (4)	
H60A	0.4369	0.0423	0.0687	0.108*	
H60B	0.5242	0.0145	0.0653	0.108*	
C61	0.4400 (14)	−0.0078 (7)	0.0365 (4)	0.161 (8)	
H61A	0.3797	−0.0128	0.0358	0.242*	
H61B	0.4680	−0.0398	0.0322	0.242*	

H61C	0.4563	0.0175	0.0219	0.242*	
N5	0.7865 (4)	0.2020 (3)	0.12613 (16)	0.0459 (18)	
C62	0.7838 (6)	0.2503 (4)	0.13404 (19)	0.049 (2)	
H62	0.8343	0.2661	0.1397	0.059*	
C63	0.7122 (6)	0.2788 (4)	0.1345 (2)	0.055 (3)	
H63	0.7143	0.3136	0.1395	0.066*	
C64	0.6383 (6)	0.2566 (4)	0.1278 (2)	0.055 (3)	
H64	0.5884	0.2756	0.1283	0.066*	
C65	0.6365 (5)	0.2050 (4)	0.12010 (18)	0.042 (2)	
C66	0.5626 (5)	0.1773 (4)	0.1129 (2)	0.059 (3)	
H66	0.5105	0.1941	0.1132	0.071*	
C67	0.5655 (6)	0.1293 (4)	0.1057 (2)	0.062 (3)	
H67	0.5153	0.1119	0.1014	0.075*	
C68	0.6415 (6)	0.1031 (4)	0.1043 (2)	0.060 (3)	
H68	0.6424	0.0685	0.0987	0.072*	
C69	0.7135 (5)	0.1273 (4)	0.1109 (2)	0.053 (2)	
H69	0.7648	0.1097	0.1098	0.064*	
C70	0.7124 (5)	0.1789 (3)	0.11928 (18)	0.040 (2)	
O30S	0.0141 (8)	0.0886 (5)	0.0218 (3)	0.065 (4)	0.605 (11)
H30S	0.0502	0.1113	0.0199	0.098*	0.605 (11)
C74S	−0.0257 (18)	0.0828 (10)	−0.0032 (5)	0.167 (18)	0.605 (11)
H74A	−0.0008	0.1045	−0.0182	0.251*	0.605 (11)
H74B	−0.0842	0.0920	−0.0006	0.251*	0.605 (11)
H74C	−0.0219	0.0475	−0.0094	0.251*	0.605 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.0161 (3)	0.0229 (3)	0.0223 (3)	0.0046 (2)	0.0010 (2)	−0.0003 (2)
Mo2	0.0211 (3)	0.0289 (3)	0.0221 (3)	0.0041 (2)	0.0010 (2)	−0.0086 (3)
Mo3	0.0227 (3)	0.0367 (4)	0.0165 (3)	0.0047 (3)	−0.0047 (2)	−0.0081 (3)
Mo4	0.0172 (3)	0.0278 (3)	0.0185 (3)	0.0034 (2)	−0.0051 (2)	−0.0031 (2)
Mo5	0.0149 (3)	0.0217 (3)	0.0170 (3)	0.0027 (2)	0.0008 (2)	−0.0024 (2)
Mo6	0.0148 (3)	0.0246 (3)	0.0160 (3)	0.0024 (2)	0.0013 (2)	0.0003 (2)
Al1	0.0111 (9)	0.0198 (9)	0.0162 (9)	−0.0002 (7)	−0.0014 (7)	−0.0033 (7)
O1	0.011 (2)	0.024 (2)	0.019 (2)	0.0010 (18)	0.0003 (17)	−0.0041 (18)
O2	0.015 (2)	0.025 (2)	0.025 (2)	0.0002 (19)	−0.0025 (19)	−0.009 (2)
O3	0.011 (2)	0.026 (2)	0.018 (2)	−0.0008 (18)	−0.0026 (18)	−0.0009 (18)
O4	0.013 (2)	0.023 (2)	0.023 (2)	−0.0012 (19)	0.0014 (18)	−0.0048 (19)
O5	0.010 (2)	0.023 (2)	0.014 (2)	0.0003 (17)	0.0003 (17)	−0.0024 (17)
O6	0.013 (2)	0.018 (2)	0.022 (2)	−0.0017 (18)	0.0004 (18)	−0.0039 (18)
O7	0.022 (2)	0.022 (2)	0.030 (3)	0.0038 (19)	0.002 (2)	−0.005 (2)
O8	0.023 (2)	0.036 (3)	0.013 (2)	0.003 (2)	0.0029 (19)	−0.0043 (19)
O9	0.021 (2)	0.034 (3)	0.023 (2)	0.003 (2)	−0.009 (2)	−0.011 (2)
O10	0.021 (2)	0.022 (2)	0.015 (2)	0.0015 (19)	−0.0009 (18)	−0.0030 (18)
O11	0.014 (2)	0.025 (2)	0.017 (2)	0.0004 (18)	0.0037 (17)	0.0014 (18)
O12	0.012 (2)	0.027 (2)	0.023 (2)	−0.0006 (18)	−0.0023 (18)	−0.0005 (19)
O13	0.028 (3)	0.028 (3)	0.031 (3)	0.004 (2)	0.007 (2)	0.001 (2)

O14	0.020 (2)	0.034 (3)	0.028 (3)	0.009 (2)	0.000 (2)	−0.006 (2)
O15	0.025 (3)	0.043 (3)	0.031 (3)	0.008 (2)	0.005 (2)	−0.004 (2)
O16	0.042 (3)	0.038 (3)	0.034 (3)	0.005 (3)	−0.002 (2)	−0.011 (2)
O17	0.035 (3)	0.055 (4)	0.030 (3)	0.010 (3)	−0.013 (2)	−0.015 (3)
O18	0.031 (3)	0.053 (3)	0.021 (3)	0.011 (3)	0.002 (2)	−0.001 (2)
O19	0.034 (3)	0.035 (3)	0.021 (2)	0.008 (2)	−0.007 (2)	−0.001 (2)
O20	0.021 (2)	0.038 (3)	0.032 (3)	0.003 (2)	−0.008 (2)	−0.005 (2)
O21	0.018 (2)	0.037 (3)	0.032 (3)	0.002 (2)	0.004 (2)	0.000 (2)
O22	0.026 (3)	0.026 (3)	0.022 (2)	0.003 (2)	0.000 (2)	−0.003 (2)
O23	0.019 (2)	0.034 (3)	0.022 (2)	0.005 (2)	0.0000 (19)	−0.002 (2)
O24	0.025 (3)	0.031 (3)	0.020 (2)	0.006 (2)	0.003 (2)	0.002 (2)
O25	0.021 (2)	0.038 (3)	0.030 (3)	−0.004 (2)	−0.003 (2)	0.002 (2)
N1	0.018 (3)	0.035 (3)	0.015 (3)	−0.004 (2)	0.001 (2)	0.003 (2)
C1	0.011 (3)	0.026 (3)	0.015 (3)	−0.007 (3)	0.000 (2)	0.004 (3)
C2	0.013 (3)	0.036 (4)	0.019 (3)	−0.003 (3)	0.004 (3)	−0.003 (3)
C3	0.017 (3)	0.029 (4)	0.020 (3)	−0.006 (3)	0.003 (3)	0.002 (3)
C4	0.010 (3)	0.030 (4)	0.019 (3)	−0.010 (3)	0.000 (2)	−0.008 (3)
C5	0.013 (3)	0.032 (4)	0.029 (4)	−0.001 (3)	0.005 (3)	−0.007 (3)
C6	0.016 (3)	0.027 (4)	0.035 (4)	0.000 (3)	0.003 (3)	0.000 (3)
C7	0.027 (4)	0.033 (4)	0.044 (5)	−0.008 (3)	−0.008 (3)	−0.003 (3)
C8	0.035 (5)	0.055 (6)	0.050 (5)	−0.006 (4)	−0.001 (4)	0.004 (4)
C9	0.049 (6)	0.063 (6)	0.056 (6)	−0.018 (5)	−0.005 (5)	−0.002 (5)
C10	0.076 (8)	0.055 (6)	0.073 (7)	−0.020 (6)	−0.015 (6)	0.011 (6)
C11	0.087 (9)	0.068 (7)	0.070 (7)	−0.042 (7)	−0.002 (7)	−0.003 (6)
C12	0.123 (12)	0.099 (10)	0.066 (8)	−0.073 (9)	−0.020 (8)	−0.001 (7)
C13	0.082 (8)	0.092 (9)	0.052 (6)	−0.049 (7)	−0.021 (6)	0.005 (6)
O1A	0.026 (3)	0.039 (3)	0.052 (4)	−0.004 (2)	−0.004 (3)	0.006 (3)
O1B	0.030 (3)	0.035 (3)	0.039 (3)	−0.001 (2)	0.003 (3)	0.002 (2)
O1C	0.038 (3)	0.064 (4)	0.061 (4)	−0.010 (3)	0.005 (3)	−0.016 (3)
O1D	0.041 (4)	0.049 (4)	0.067 (4)	−0.004 (3)	−0.012 (3)	0.002 (3)
O26S	0.059 (4)	0.035 (3)	0.055 (4)	−0.003 (3)	0.010 (3)	0.002 (3)
C71S	0.071 (7)	0.044 (6)	0.091 (8)	0.014 (5)	0.034 (6)	0.003 (6)
O27S	0.064 (5)	0.089 (5)	0.059 (4)	−0.027 (4)	−0.024 (4)	0.025 (4)
O28S	0.067 (7)	0.041 (5)	0.065 (7)	−0.010 (4)	−0.001 (5)	−0.010 (5)
O29S	0.043 (9)	0.026 (7)	0.029 (8)	0.011 (6)	0.005 (6)	0.000 (6)
C72S	0.096 (11)	0.195 (19)	0.158 (16)	−0.062 (12)	−0.073 (11)	0.123 (15)
C73S	0.12 (3)	0.10 (3)	0.050 (17)	0.10 (3)	0.010 (18)	0.005 (17)
N2	0.057 (5)	0.056 (5)	0.032 (4)	0.001 (4)	−0.027 (3)	0.000 (3)
C14	0.057 (6)	0.053 (6)	0.042 (5)	0.003 (5)	−0.026 (4)	−0.003 (4)
C15	0.083 (8)	0.076 (7)	0.034 (5)	0.000 (6)	−0.019 (5)	−0.011 (5)
C16	0.088 (8)	0.059 (7)	0.051 (6)	0.018 (6)	−0.016 (6)	−0.011 (5)
C17	0.101 (10)	0.071 (8)	0.055 (6)	−0.005 (7)	0.007 (6)	−0.011 (6)
C18	0.061 (6)	0.052 (5)	0.035 (5)	−0.009 (5)	−0.028 (4)	0.005 (4)
C19	0.082 (8)	0.063 (6)	0.043 (5)	−0.018 (6)	−0.029 (5)	0.011 (5)
C20	0.065 (7)	0.060 (6)	0.065 (7)	−0.017 (5)	−0.026 (5)	0.011 (5)
C21	0.088 (9)	0.086 (9)	0.070 (8)	−0.012 (7)	−0.012 (7)	0.029 (7)
C22	0.052 (5)	0.054 (5)	0.032 (4)	−0.001 (4)	−0.023 (4)	−0.001 (4)
C23	0.075 (7)	0.066 (7)	0.056 (6)	0.020 (6)	−0.037 (6)	−0.015 (5)

C24	0.070 (7)	0.048 (6)	0.063 (6)	0.005 (5)	−0.031 (5)	−0.002 (5)
C25	0.092 (9)	0.071 (7)	0.058 (7)	0.022 (7)	−0.023 (6)	−0.015 (6)
C26	0.050 (6)	0.070 (7)	0.043 (5)	−0.005 (5)	−0.025 (4)	0.009 (5)
C27	0.042 (5)	0.078 (7)	0.055 (6)	−0.003 (5)	−0.020 (5)	0.006 (5)
C28	0.042 (6)	0.106 (9)	0.063 (7)	−0.016 (6)	−0.007 (5)	0.008 (7)
C29	0.063 (8)	0.106 (10)	0.091 (9)	−0.024 (7)	−0.016 (7)	0.037 (8)
N3	0.020 (3)	0.044 (4)	0.031 (3)	−0.003 (3)	−0.012 (3)	0.009 (3)
C30	0.034 (4)	0.046 (5)	0.028 (4)	−0.006 (4)	−0.009 (3)	0.013 (4)
C31	0.030 (4)	0.048 (5)	0.032 (4)	−0.005 (4)	−0.007 (3)	0.006 (4)
C32	0.043 (5)	0.043 (5)	0.041 (5)	−0.008 (4)	−0.002 (4)	0.010 (4)
C33	0.066 (7)	0.085 (8)	0.042 (5)	−0.024 (6)	0.004 (5)	−0.003 (5)
C34	0.023 (4)	0.035 (4)	0.027 (4)	0.001 (3)	−0.004 (3)	0.004 (3)
C35	0.030 (4)	0.055 (5)	0.056 (5)	−0.003 (4)	−0.006 (4)	−0.010 (5)
C36	0.048 (6)	0.044 (5)	0.076 (7)	−0.002 (4)	0.023 (5)	0.002 (5)
C37	0.062 (7)	0.066 (7)	0.103 (9)	−0.021 (6)	0.021 (7)	−0.024 (7)
C38	0.023 (4)	0.044 (5)	0.028 (4)	−0.006 (3)	−0.009 (3)	0.009 (3)
C39	0.028 (4)	0.054 (5)	0.030 (4)	−0.008 (4)	−0.009 (3)	0.005 (4)
C40	0.033 (4)	0.041 (5)	0.034 (4)	−0.004 (4)	−0.005 (3)	0.009 (4)
C41	0.056 (6)	0.041 (5)	0.051 (5)	−0.007 (4)	−0.009 (5)	0.004 (4)
C42	0.022 (4)	0.046 (5)	0.050 (5)	−0.003 (3)	−0.008 (4)	0.001 (4)
C43	0.059 (7)	0.062 (7)	0.079 (8)	0.008 (5)	0.007 (6)	−0.013 (6)
C44	0.070 (7)	0.066 (7)	0.060 (7)	0.001 (6)	0.011 (6)	0.006 (5)
C45	0.046 (5)	0.061 (6)	0.061 (6)	0.004 (5)	0.002 (5)	−0.009 (5)
N4	0.054 (5)	0.029 (4)	0.072 (6)	−0.005 (3)	−0.004 (4)	0.007 (4)
C46	0.056 (6)	0.022 (4)	0.066 (6)	0.001 (4)	0.006 (5)	0.003 (4)
C47	0.055 (6)	0.034 (5)	0.089 (8)	−0.006 (4)	0.010 (6)	−0.002 (5)
C48	0.053 (6)	0.046 (6)	0.106 (9)	−0.004 (5)	0.027 (6)	−0.003 (6)
C49	0.108 (11)	0.074 (9)	0.131 (13)	−0.025 (8)	0.062 (10)	−0.010 (8)
C50	0.037 (5)	0.024 (4)	0.072 (6)	−0.002 (3)	−0.010 (4)	0.004 (4)
C51	0.040 (5)	0.028 (4)	0.080 (7)	0.000 (4)	0.000 (5)	0.004 (4)
C52	0.059 (6)	0.042 (5)	0.073 (7)	−0.004 (5)	−0.002 (5)	0.005 (5)
C53	0.097 (9)	0.064 (7)	0.080 (9)	−0.025 (7)	0.012 (7)	−0.007 (6)
C54	0.052 (6)	0.020 (4)	0.088 (7)	0.000 (4)	−0.018 (5)	−0.002 (4)
C55	0.060 (7)	0.028 (5)	0.134 (11)	0.005 (5)	−0.031 (7)	−0.006 (6)
C56	0.058 (6)	0.031 (5)	0.103 (9)	0.007 (4)	−0.031 (6)	−0.006 (5)
C57	0.053 (6)	0.072 (8)	0.098 (9)	0.010 (6)	−0.003 (6)	−0.041 (7)
C58	0.094 (8)	0.030 (5)	0.070 (7)	−0.007 (5)	0.002 (6)	0.005 (5)
C59	0.146 (9)	0.063 (6)	0.093 (8)	−0.005 (7)	0.002 (7)	0.003 (6)
C60	0.114 (8)	0.078 (7)	0.079 (7)	−0.018 (6)	−0.003 (6)	0.013 (6)
C61	0.217 (17)	0.123 (13)	0.143 (14)	−0.039 (13)	−0.012 (13)	0.004 (11)
N5	0.023 (3)	0.067 (5)	0.048 (4)	0.001 (3)	−0.002 (3)	0.011 (4)
C62	0.041 (5)	0.067 (7)	0.040 (5)	−0.009 (5)	−0.002 (4)	−0.001 (4)
C63	0.047 (6)	0.073 (7)	0.045 (5)	0.009 (5)	0.007 (4)	−0.005 (5)
C64	0.035 (5)	0.074 (7)	0.056 (6)	0.019 (5)	0.006 (4)	0.000 (5)
C65	0.027 (4)	0.060 (6)	0.039 (5)	0.006 (4)	0.002 (3)	0.009 (4)
C66	0.018 (4)	0.089 (8)	0.071 (7)	0.007 (5)	−0.002 (4)	0.027 (6)
C67	0.035 (5)	0.071 (7)	0.081 (8)	−0.009 (5)	−0.012 (5)	0.023 (6)
C68	0.047 (6)	0.061 (6)	0.072 (7)	−0.018 (5)	0.005 (5)	0.007 (5)

C69	0.032 (5)	0.048 (5)	0.079 (7)	0.001 (4)	0.009 (5)	0.018 (5)
C70	0.021 (4)	0.059 (6)	0.040 (5)	−0.001 (4)	0.002 (3)	0.006 (4)
O30S	0.068 (9)	0.071 (9)	0.058 (8)	−0.031 (7)	−0.011 (6)	−0.003 (6)
C74S	0.19 (3)	0.16 (3)	0.15 (3)	−0.13 (3)	0.07 (2)	−0.11 (2)

Geometric parameters (Å, º)

Mo1—O1	2.346 (4)	O29S—C73S	1.37 (2)
Mo1—O6	2.293 (4)	N2—C14	1.520 (11)
Mo1—O7	1.941 (5)	N2—C18	1.533 (11)
Mo1—O12	1.920 (4)	N2—C22	1.515 (11)
Mo1—O13	1.702 (5)	N2—C26	1.513 (12)
Mo1—O14	1.702 (5)	C14—C15	1.518 (13)
Mo2—O1	2.324 (4)	C15—C16	1.539 (14)
Mo2—O2	2.307 (4)	C16—C17	1.532 (14)
Mo2—O7	1.933 (5)	C18—C19	1.523 (13)
Mo2—O8	1.929 (5)	C19—C20	1.522 (13)
Mo2—O15	1.707 (5)	C20—C21	1.518 (14)
Mo2—O16	1.713 (5)	C22—C23	1.494 (13)
Mo3—O2	2.322 (5)	C23—C24	1.507 (13)
Mo3—O3	2.323 (4)	C24—C25	1.504 (14)
Mo3—O8	1.917 (5)	C26—C27	1.540 (12)
Mo3—O9	1.910 (5)	C27—C28	1.489 (14)
Mo3—O17	1.718 (5)	C28—C29	1.528 (16)
Mo3—O18	1.699 (5)	N3—C30	1.516 (9)
Mo4—O3	2.352 (4)	N3—C34	1.505 (9)
Mo4—O4	2.305 (5)	N3—C38	1.530 (9)
Mo4—O9	1.931 (4)	N3—C42	1.513 (10)
Mo4—O10	1.923 (4)	C30—C31	1.513 (10)
Mo4—O19	1.705 (5)	C31—C32	1.537 (11)
Mo4—O20	1.697 (5)	C32—C33	1.509 (13)
Mo5—O4	2.307 (4)	C34—C35	1.510 (11)
Mo5—O5	2.390 (4)	C35—C36	1.490 (12)
Mo5—O10	1.915 (4)	C36—C37	1.562 (14)
Mo5—O11	1.911 (4)	C38—C39	1.521 (10)
Mo5—O21	1.703 (5)	C39—C40	1.526 (10)
Mo5—O22	1.711 (5)	C40—C41	1.540 (12)
Mo6—O5	2.311 (4)	C42—C43	1.512 (13)
Mo6—O6	2.305 (4)	C43—C44	1.415 (14)
Mo6—O11	1.924 (4)	C44—C45	1.562 (14)
Mo6—O12	1.922 (4)	N4—C46	1.532 (11)
Mo6—O23	1.694 (5)	N4—C50	1.501 (12)
Mo6—O24	1.722 (5)	N4—C54	1.522 (11)
Al1—O1	1.923 (4)	N4—C58	1.519 (12)
Al1—O2	1.879 (5)	C46—C47	1.521 (13)
Al1—O3	1.915 (5)	C47—C48	1.535 (13)
Al1—O4	1.865 (5)	C48—C49	1.503 (13)
Al1—O5	1.909 (4)	C50—C51	1.494 (12)

Al1—O6	1.880 (5)	C51—C52	1.528 (13)
O1—C2	1.437 (8)	C52—C53	1.482 (12)
O3—C3	1.432 (7)	C54—C55	1.511 (13)
O5—C4	1.431 (7)	C55—C56	1.518 (14)
O25—C5	1.223 (8)	C56—C57	1.485 (12)
N1—C1	1.469 (8)	C58—C59	1.484 (16)
N1—C5	1.363 (8)	C59—C60	1.447 (17)
C1—C2	1.529 (9)	C60—C61	1.432 (14)
C1—C3	1.523 (8)	N5—C62	1.331 (12)
C1—C4	1.537 (8)	N5—C70	1.377 (10)
C5—C6	1.458 (9)	C62—C63	1.379 (13)
C6—C7	1.364 (10)	C63—C64	1.363 (14)
C7—C8	1.452 (11)	C64—C65	1.412 (14)
C8—C9	1.345 (13)	C65—C66	1.436 (13)
C8—C13	1.391 (13)	C65—C70	1.405 (11)
C9—C10	1.410 (13)	C66—C67	1.316 (15)
C10—C11	1.364 (15)	C67—C68	1.409 (14)
C11—C12	1.369 (16)	C68—C69	1.361 (13)
C12—C13	1.384 (14)	C69—C70	1.422 (13)
O26S—C71S	1.403 (11)	O30S—C74S	1.315 (19)
O27S—C72S	1.340 (12)		

O6—Mo1—O1	67.73 (15)	Al1—O3—Mo3	103.28 (19)
O7—Mo1—O1	72.00 (17)	Al1—O3—Mo4	101.29 (18)
O7—Mo1—O6	81.74 (17)	C3—O3—Mo3	117.6 (4)
O12—Mo1—O1	80.43 (17)	C3—O3—Mo4	118.8 (4)
O12—Mo1—O6	72.48 (16)	C3—O3—Al1	120.0 (4)
O12—Mo1—O7	147.80 (19)	Mo4—O4—Mo5	91.85 (16)
O13—Mo1—O1	160.16 (19)	Al1—O4—Mo4	104.7 (2)
O13—Mo1—O6	94.0 (2)	Al1—O4—Mo5	105.2 (2)
O13—Mo1—O7	98.7 (2)	Mo6—O5—Mo5	89.97 (14)
O13—Mo1—O12	101.9 (2)	Al1—O5—Mo5	100.75 (17)
O14—Mo1—O1	92.80 (19)	Al1—O5—Mo6	102.93 (19)
O14—Mo1—O6	159.3 (2)	C4—O5—Mo5	118.8 (4)
O14—Mo1—O7	99.3 (2)	C4—O5—Mo6	118.9 (3)
O14—Mo1—O12	98.3 (2)	C4—O5—Al1	120.1 (3)
O14—Mo1—O13	106.2 (2)	Mo1—O6—Mo6	91.36 (15)
O2—Mo2—O1	67.94 (15)	Al1—O6—Mo1	104.94 (19)
O7—Mo2—O1	72.65 (17)	Al1—O6—Mo6	104.10 (19)
O7—Mo2—O2	81.84 (18)	Mo2—O7—Mo1	118.2 (2)
O8—Mo2—O1	81.02 (17)	Mo3—O8—Mo2	119.5 (2)
O8—Mo2—O2	71.58 (18)	Mo3—O9—Mo4	120.4 (2)
O8—Mo2—O7	148.07 (18)	Mo5—O10—Mo4	119.3 (2)
O15—Mo2—O1	92.3 (2)	Mo5—O11—Mo6	120.2 (2)
O15—Mo2—O2	158.3 (2)	Mo1—O12—Mo6	117.8 (2)
O15—Mo2—O7	101.4 (2)	C5—N1—C1	126.2 (6)
O15—Mo2—O8	97.3 (2)	N1—C1—C2	109.5 (5)
O15—Mo2—O16	106.0 (3)	N1—C1—C3	103.5 (5)

O16—Mo2—O1	160.9 (2)	N1—C1—C4	109.5 (5)
O16—Mo2—O2	94.6 (2)	C2—C1—C4	111.2 (5)
O16—Mo2—O7	97.9 (2)	C3—C1—C2	112.2 (5)
O16—Mo2—O8	101.5 (2)	C3—C1—C4	110.8 (5)
O2—Mo3—O3	67.05 (15)	O1—C2—C1	111.7 (5)
O8—Mo3—O2	71.43 (17)	O3—C3—C1	112.3 (5)
O8—Mo3—O3	80.71 (16)	O5—C4—C1	112.2 (5)
O9—Mo3—O2	81.71 (18)	O25—C5—N1	124.0 (6)
O9—Mo3—O3	72.05 (16)	O25—C5—C6	123.4 (6)
O9—Mo3—O8	147.53 (19)	N1—C5—C6	112.6 (6)
O17—Mo3—O2	95.3 (2)	C7—C6—C5	118.7 (7)
O17—Mo3—O3	161.0 (2)	C6—C7—C8	128.0 (8)
O17—Mo3—O8	101.0 (2)	C9—C8—C7	121.9 (9)
O17—Mo3—O9	99.3 (2)	C9—C8—C13	119.1 (9)
O18—Mo3—O2	157.9 (2)	C13—C8—C7	119.0 (9)
O18—Mo3—O3	92.8 (2)	C8—C9—C10	119.7 (10)
O18—Mo3—O8	97.4 (2)	C11—C10—C9	120.8 (10)
O18—Mo3—O9	101.2 (2)	C10—C11—C12	120.0 (10)
O18—Mo3—O17	105.6 (3)	C11—C12—C13	118.9 (11)
O4—Mo4—O3	67.56 (15)	C12—C13—C8	121.5 (11)
O9—Mo4—O3	71.04 (17)	C14—N2—C18	110.6 (7)
O9—Mo4—O4	82.54 (18)	C22—N2—C14	107.6 (6)
O10—Mo4—O3	82.24 (17)	C22—N2—C18	110.4 (7)
O10—Mo4—O4	71.32 (17)	C26—N2—C14	111.4 (8)
O10—Mo4—O9	148.23 (19)	C26—N2—C18	106.0 (6)
O19—Mo4—O3	92.1 (2)	C26—N2—C22	110.9 (7)
O19—Mo4—O4	157.0 (2)	C15—C14—N2	115.3 (7)
O19—Mo4—O9	101.4 (2)	C14—C15—C16	110.4 (7)
O19—Mo4—O10	96.4 (2)	C17—C16—C15	115.0 (9)
O20—Mo4—O3	161.1 (2)	C19—C18—N2	114.8 (7)
O20—Mo4—O4	96.1 (2)	C20—C19—C18	107.9 (7)
O20—Mo4—O9	98.4 (2)	C21—C20—C19	112.3 (9)
O20—Mo4—O10	102.0 (2)	C23—C22—N2	114.8 (7)
O20—Mo4—O19	105.6 (2)	C22—C23—C24	113.0 (8)
O4—Mo5—O5	67.02 (14)	C25—C24—C23	114.6 (8)
O10—Mo5—O4	71.39 (17)	N2—C26—C27	115.4 (7)
O10—Mo5—O5	80.02 (16)	C28—C27—C26	110.4 (8)
O11—Mo5—O4	82.74 (17)	C27—C28—C29	114.3 (10)
O11—Mo5—O5	71.07 (16)	C30—N3—C38	107.5 (5)
O11—Mo5—O10	147.03 (18)	C34—N3—C30	108.9 (6)
O21—Mo5—O4	94.2 (2)	C34—N3—C38	109.9 (6)
O21—Mo5—O5	159.6 (2)	C34—N3—C42	107.1 (5)
O21—Mo5—O10	102.1 (2)	C42—N3—C30	111.5 (6)
O21—Mo5—O11	99.8 (2)	C42—N3—C38	112.0 (6)
O21—Mo5—O22	105.6 (2)	C31—C30—N3	115.3 (6)
O22—Mo5—O4	158.70 (19)	C30—C31—C32	111.9 (6)
O22—Mo5—O5	94.24 (18)	C33—C32—C31	111.7 (7)
O22—Mo5—O10	96.3 (2)	N3—C34—C35	115.8 (6)

O22—Mo5—O11	101.3 (2)	C36—C35—C34	112.2 (8)
O6—Mo6—O5	67.59 (15)	C35—C36—C37	112.4 (9)
O11—Mo6—O5	72.71 (16)	C39—C38—N3	114.0 (6)
O11—Mo6—O6	80.97 (16)	C38—C39—C40	112.2 (6)
O12—Mo6—O5	81.27 (16)	C39—C40—C41	112.4 (7)
O12—Mo6—O6	72.15 (16)	C43—C42—N3	117.9 (7)
O12—Mo6—O11	148.13 (18)	C44—C43—C42	123.5 (10)
O23—Mo6—O5	91.50 (19)	C43—C44—C45	113.7 (10)
O23—Mo6—O6	157.64 (19)	C50—N4—C46	111.0 (7)
O23—Mo6—O11	100.9 (2)	C50—N4—C54	110.9 (7)
O23—Mo6—O12	97.8 (2)	C50—N4—C58	107.1 (7)
O23—Mo6—O24	106.0 (2)	C54—N4—C46	105.3 (6)
O24—Mo6—O5	161.67 (19)	C58—N4—C46	110.7 (8)
O24—Mo6—O6	95.72 (19)	C58—N4—C54	111.9 (8)
O24—Mo6—O11	98.0 (2)	C47—C46—N4	116.9 (7)
O24—Mo6—O12	101.3 (2)	C46—C47—C48	109.4 (8)
O2—Al1—O1	85.8 (2)	C49—C48—C47	111.9 (10)
O2—Al1—O3	85.1 (2)	C51—C50—N4	116.5 (7)
O2—Al1—O5	174.8 (2)	C50—C51—C52	110.6 (7)
O2—Al1—O6	98.0 (2)	C53—C52—C51	112.7 (8)
O3—Al1—O1	90.41 (19)	C55—C54—N4	114.5 (7)
O4—Al1—O1	175.9 (2)	C54—C55—C56	110.4 (8)
O4—Al1—O2	96.6 (2)	C57—C56—C55	113.4 (10)
O4—Al1—O3	86.5 (2)	C59—C58—N4	117.6 (8)
O4—Al1—O5	86.85 (19)	C60—C59—C58	115.2 (11)
O4—Al1—O6	97.3 (2)	C61—C60—C59	116.8 (13)
O5—Al1—O1	90.51 (19)	C62—N5—C70	117.4 (8)
O5—Al1—O3	91.3 (2)	N5—C62—C63	123.9 (9)
O6—Al1—O1	85.7 (2)	C64—C63—C62	119.3 (10)
O6—Al1—O3	174.8 (2)	C63—C64—C65	119.5 (9)
O6—Al1—O5	85.33 (19)	C64—C65—C66	124.6 (8)
Mo2—O1—Mo1	90.82 (15)	C70—C65—C64	117.7 (8)
Al1—O1—Mo1	101.59 (19)	C70—C65—C66	117.7 (9)
Al1—O1—Mo2	102.06 (18)	C67—C66—C65	121.5 (9)
C2—O1—Mo1	117.8 (4)	C66—C67—C68	121.3 (9)
C2—O1—Mo2	119.2 (3)	C69—C68—C67	119.9 (10)
C2—O1—Al1	120.1 (4)	C68—C69—C70	120.2 (9)
Mo2—O2—Mo3	91.73 (16)	N5—C70—C65	122.0 (8)
Al1—O2—Mo2	104.1 (2)	N5—C70—C69	118.5 (8)
Al1—O2—Mo3	104.5 (2)	C65—C70—C69	119.5 (8)
Mo3—O3—Mo4	90.94 (14)		

Mo1—O1—C2—C1	−127.0 (4)	C18—N2—C22—C23	53.5 (11)
Mo2—O1—C2—C1	124.7 (4)	C18—N2—C26—C27	176.6 (9)
Mo3—O3—C3—C1	−127.1 (4)	C18—C19—C20—C21	−175.5 (10)
Mo4—O3—C3—C1	125.0 (5)	C22—N2—C14—C15	173.4 (8)
Mo5—O5—C4—C1	−127.3 (4)	C22—N2—C18—C19	56.7 (10)
Mo6—O5—C4—C1	125.1 (4)	C22—N2—C26—C27	−63.6 (11)

Al1—O1—C2—C1	−2.3 (7)	C22—C23—C24—C25	175.8 (10)
Al1—O3—C3—C1	−0.1 (7)	C26—N2—C14—C15	51.6 (11)
Al1—O5—C4—C1	−2.9 (7)	C26—N2—C18—C19	176.9 (9)
O1—Al1—O2—Mo2	2.7 (2)	C26—N2—C22—C23	−63.6 (11)
O1—Al1—O2—Mo3	−92.9 (2)	C26—C27—C28—C29	−67.1 (13)
O1—Al1—O6—Mo1	−2.42 (19)	N3—C30—C31—C32	179.4 (7)
O1—Al1—O6—Mo6	92.89 (19)	N3—C34—C35—C36	163.6 (7)
O2—Al1—O4—Mo4	−83.4 (2)	N3—C38—C39—C40	157.5 (7)
O2—Al1—O4—Mo5	−179.5 (2)	N3—C42—C43—C44	−72.4 (14)
O2—Al1—O6—Mo1	82.7 (2)	C30—N3—C34—C35	56.5 (8)
O2—Al1—O6—Mo6	178.01 (19)	C30—N3—C38—C39	173.8 (7)
O3—Al1—O2—Mo2	93.5 (2)	C30—N3—C42—C43	−49.6 (9)
O3—Al1—O2—Mo3	−2.11 (19)	C30—C31—C32—C33	69.6 (10)
O3—Al1—O4—Mo4	1.2 (2)	C34—N3—C30—C31	60.3 (9)
O3—Al1—O4—Mo5	−94.8 (2)	C34—N3—C38—C39	−67.8 (8)
O4—Al1—O2—Mo2	179.3 (2)	C34—N3—C42—C43	−168.7 (7)
O4—Al1—O2—Mo3	83.7 (2)	C34—C35—C36—C37	−176.8 (7)
O4—Al1—O6—Mo1	−179.50 (19)	C38—N3—C30—C31	179.3 (7)
O4—Al1—O6—Mo6	−84.2 (2)	C38—N3—C34—C35	−61.0 (8)
O5—Al1—O4—Mo4	92.8 (2)	C38—N3—C42—C43	70.9 (9)
O5—Al1—O4—Mo5	−3.3 (2)	C38—C39—C40—C41	−67.2 (9)
O5—Al1—O6—Mo1	−93.29 (19)	C42—N3—C30—C31	−57.7 (9)
O5—Al1—O6—Mo6	2.02 (19)	C42—N3—C34—C35	177.2 (7)
O6—Al1—O2—Mo2	−82.3 (2)	C42—N3—C38—C39	51.1 (9)
O6—Al1—O2—Mo3	−177.89 (19)	C42—C43—C44—C45	−168.2 (9)
O6—Al1—O4—Mo4	177.64 (19)	N4—C46—C47—C48	−163.2 (9)
O6—Al1—O4—Mo5	81.6 (2)	N4—C50—C51—C52	177.9 (8)
O25—C5—C6—C7	−12.0 (10)	N4—C54—C55—C56	−170.7 (10)
N1—C1—C2—O1	−175.2 (5)	N4—C58—C59—C60	−172.3 (12)
N1—C1—C3—O3	−179.5 (5)	C46—N4—C50—C51	−65.6 (10)
N1—C1—C4—O5	177.7 (5)	C46—N4—C54—C55	179.0 (10)
N1—C5—C6—C7	166.9 (6)	C46—N4—C58—C59	63.1 (14)
C1—N1—C5—O25	7.2 (11)	C46—C47—C48—C49	81.4 (11)
C1—N1—C5—C6	−171.7 (6)	C50—N4—C46—C47	−53.6 (11)
C2—C1—C3—O3	62.6 (7)	C50—N4—C54—C55	58.8 (11)
C2—C1—C4—O5	−61.2 (7)	C50—N4—C58—C59	−175.8 (11)
C3—C1—C2—O1	−60.9 (7)	C50—C51—C52—C53	175.0 (9)
C3—C1—C4—O5	64.2 (7)	C54—N4—C46—C47	−173.6 (9)
C4—C1—C2—O1	63.8 (6)	C54—N4—C50—C51	51.1 (10)
C4—C1—C3—O3	−62.3 (7)	C54—N4—C58—C59	−54.0 (14)
C5—N1—C1—C2	−63.3 (8)	C54—C55—C56—C57	72.1 (13)
C5—N1—C1—C3	176.9 (6)	C58—N4—C46—C47	65.2 (11)
C5—N1—C1—C4	58.8 (8)	C58—N4—C50—C51	173.5 (8)
C5—C6—C7—C8	−172.3 (8)	C58—N4—C54—C55	−60.7 (12)
C6—C7—C8—C9	−15.1 (15)	C58—C59—C60—C61	−164.9 (16)
C6—C7—C8—C13	165.2 (10)	N5—C62—C63—C64	3.0 (15)
C7—C8—C9—C10	177.8 (9)	C62—N5—C70—C65	0.8 (12)
C7—C8—C13—C12	−178.6 (12)	C62—N5—C70—C69	−179.8 (8)

C8—C9—C10—C11	1.5 (18)	C62—C63—C64—C65	−0.8 (15)
C9—C8—C13—C12	1.7 (19)	C63—C64—C65—C66	179.4 (9)
C9—C10—C11—C12	0 (2)	C63—C64—C65—C70	−1.0 (14)
C10—C11—C12—C13	−1 (2)	C64—C65—C66—C67	179.6 (10)
C11—C12—C13—C8	0 (2)	C64—C65—C70—N5	1.0 (13)
C13—C8—C9—C10	−2.5 (16)	C64—C65—C70—C69	−178.3 (8)
N2—C14—C15—C16	−176.3 (9)	C65—C66—C67—C68	−1.3 (17)
N2—C18—C19—C20	−170.5 (9)	C66—C65—C70—N5	−179.4 (8)
N2—C22—C23—C24	−179.7 (9)	C66—C65—C70—C69	1.3 (13)
N2—C26—C27—C28	177.4 (9)	C66—C67—C68—C69	1.2 (17)
C14—N2—C18—C19	−62.2 (11)	C67—C68—C69—C70	0.3 (16)
C14—N2—C22—C23	174.3 (9)	C68—C69—C70—N5	179.2 (9)
C14—N2—C26—C27	56.2 (11)	C68—C69—C70—C65	−1.5 (14)
C14—C15—C16—C17	177.5 (10)	C70—N5—C62—C63	−2.9 (14)
C18—N2—C14—C15	−66.0 (11)	C70—C65—C66—C67	0.1 (14)

(taco104_0m)

Crystal data

$C_{23}H_{25}AlClMo_6N_2O_{27}·9(H_2O)·2(C_{16}H_{36}N)·C_{16}H_{35}N$
M_r = 2288.02
Orthorhombic, *Pbca*
a = 21.8904 (6) Å
b = 23.9848 (6) Å
c = 37.719 (1) Å
V = 19803.9 (9) Å^3
Z = 8
F(000) = 9448
D_x = 1.535 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9039 reflections
θ = 2.5–29.1°
μ = 0.85 mm^{-1}
T = 200 K
Plate, clear dark green
0.15 × 0.12 × 0.05 mm

Data collection

Bruker APEX-II CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2013)
T_{min} = 0.678, T_{max} = 0.746
374956 measured reflections
18115 independent reflections
15743 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 25.4°, θ_{min} = 2.2°
h = −26→26
k = −28→28
l = −45→45

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.075
S = 1.06
18115 reflections
1166 parameters
53 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0307P)^2 + 38.9537P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.005
$\Delta\rho_{max}$ = 1.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

Special details

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

Refinement. _olex2_refinement_description 1. Fixed Uiso At 1.2 times of: All C(H) groups, All C(H,H) groups, All C(H,H,H,H) groups, All N(H) groups At 1.5 times of: All C(H,H,H) groups, All C(H,H,H,H,H,H) groups, All O(H,H) groups 2. Restrained distances H32C-H36E 2.1 with sigma of 0.02 H34D-H33D 2.1 with sigma of 0.02 H37D-H29B 2.1 with sigma of 0.02 H29B-H37C 2.1 with sigma of 0.02 H28C-H35E_$1 2.1 with sigma of 0.02 C38-C37 ~ C37-C36 ~ C36-C37A ~ C37A-C38A ~ C38A-C39A ~ C39-C38 with sigma of 0.02 O3-H3 ~ O5-H5 ~ O1-H1 with sigma of 0.01 C31A-C30 ~ C31-C30 ~ C30-C29 ~ C28-C29 with sigma of 0.02 3. Rigid bond restraints C36, C37, C38, C37A, C38A with sigma for 1-2 distances of 0.01 and sigma for 1-3 distances of 0.01 4. Uiso/Uaniso restraints and constraints C37 ~ C37A: within 1.7A with sigma of 0.04 and sigma for terminal atoms of 0.08 Uanis(C37A) ~ Ueq, Uanis(C37) ~ Ueq: with sigma of 0.01 and sigma for terminal atoms of 0.02 5. Others
Sof(C37A)=Sof(H37C)=Sof(H37D)=Sof(C38A)=Sof(H38C)=Sof(H38D)=Sof(C39A)=
Sof(H39D)=Sof(H39E)=Sof(H39F)=1-FVAR(1)
Sof(C37)=Sof(H37A)=Sof(H37B)=Sof(C38)=Sof(H38A)=Sof(H38B)=Sof(C39)=Sof(H39A)=
Sof(H39B)=Sof(H39C)=FVAR(1) Sof(H30C)=Sof(H30D)=Sof(C31A)=Sof(H31D)=Sof(H31E)=Sof(H31F)=1-FVAR(2)
Sof(H30A)=Sof(H30B)=Sof(C31)=Sof(H31A)=Sof(H31B)=Sof(H31C)=FVAR(2) Fixed Sof: H36A(0.5) H36B(0.5)
H36C(0.5) H36D(0.5) 6.a Free rotating group: O28(H28C,H28D), O29(H29C,H29D), O30(H30E,H30F),
O31(H31G,H31H), O32(H32C, H32D), O33(H33C,H33D), O34(H34C,H34D), O35(H35D,H35E), O36(H36E,H36F)
6.b Secondary CH2 refined with riding coordinates: C1(H1B,H1C), C2(H2A,H2B), C3(H3A,H3B), C6(H6A,H6B),
C56(H56A,H56B), C57(H57A, H57B), C58(H58A,H58B), C60(H60A,H60B), C61(H61A,H61B), C62(H62A,H62B),
C64(H64A,H64B), C65(H65A,H65B), C66(H66A,H66B), C68(H68A,H68B), C69(H69A,H69B), C70(H70A,H70B),
C40(H40A,H40B), C41(H41A,H41B), C44(H44A,H44B), C45(H45A, H45B), C46(H46A,H46B), C48(H48A,H48B),
C49(H49A,H49B), C50(H50A,H50B), C52(H52A,H52B), C53(H53A,H53B), C54(H54A,H54B), C24(H24A,H24B),
C25(H25A,H25B), C26(H26A,H26B), C28(H28A,H28B), C29(H29A,H29B), C30(H30A,H30B), C30(H30C, H30D),
C32(H32A,H32B), C33(H33A,H33B), C34(H34A,H34B), C36(H36A,H36B), C36(H36C,H36D), C37(H37A,H37B),
C38(H38A,H38B), C37A(H37C,H37D), C38A(H38C, H38D) 6.c Aromatic/amide H refined with riding coordinates:
N1(H1A), C11(H11), C13(H13), C14(H14), C18(H18), C19(H19), C21(H21), C22(H22), C42(H42) 6.d Idealised Me
refined as rotating group: C9(H9A,H9B,H9C), C23(H23A,H23B,H23C), C59(H59A,H59B,H59C), C63(H63A,H63B,
H63C), C67(H67A,H67B,H67C), C71(H71A,H71B,H71C), C43(H43A,H43B,H43C), C47(H47A, H47B,H47C),
C51(H51A,H51B,H51C), C55(H55A,H55B,H55C), C27(H27A,H27B,H27C), C35(H35A,H35B,H35C),
C31(H31A,H31B,H31C), C39(H39A,H39B,H39C), C31A(H31D,H31E, H31F), C39A(H39D,H39E,H39F)

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Mo1	0.38344 (2)	0.54750 (2)	0.56120 (2)	0.01876 (6)	
Mo2	0.38949 (2)	0.41213 (2)	0.54338 (2)	0.01851 (6)	
Mo3	0.46290 (2)	0.32597 (2)	0.59697 (2)	0.01923 (6)	
Mo4	0.52407 (2)	0.37445 (2)	0.67227 (2)	0.01915 (6)	
Mo5	0.51712 (2)	0.50938 (2)	0.69045 (2)	0.01967 (6)	
Mo6	0.45106 (2)	0.59683 (2)	0.63343 (2)	0.01943 (6)	
Cl1	1.13904 (6)	0.59166 (7)	0.61924 (4)	0.0835 (4)	
Al1	0.45154 (3)	0.46060 (3)	0.61741 (2)	0.01350 (16)	
O1	0.39852 (8)	0.40276 (8)	0.60405 (5)	0.0177 (4)	
O2	0.45671 (8)	0.47740 (7)	0.56841 (4)	0.0143 (4)	
O3	0.39356 (8)	0.51857 (8)	0.61928 (5)	0.0173 (4)	
O4	0.51078 (8)	0.51710 (7)	0.62810 (5)	0.0152 (4)	
O5	0.45153 (8)	0.44436 (8)	0.66574 (5)	0.0169 (4)	
O6	0.51547 (8)	0.40570 (7)	0.61360 (5)	0.0150 (4)	

O7	0.44728 (9)	0.59114 (8)	0.58283 (5)	0.0218 (4)
O8	0.32102 (10)	0.58856 (9)	0.56881 (6)	0.0320 (5)
O9	0.40337 (10)	0.55811 (8)	0.51813 (5)	0.0266 (5)
O10	0.34218 (9)	0.47671 (8)	0.55733 (5)	0.0220 (4)
O11	0.33243 (10)	0.36470 (9)	0.53945 (6)	0.0342 (5)
O12	0.40874 (10)	0.43100 (9)	0.50130 (5)	0.0286 (5)
O13	0.45839 (9)	0.36411 (8)	0.55234 (5)	0.0196 (4)
O14	0.40467 (10)	0.27903 (9)	0.59318 (6)	0.0322 (5)
O15	0.52805 (10)	0.28995 (9)	0.58878 (6)	0.0312 (5)
O16	0.46295 (9)	0.33037 (8)	0.64844 (5)	0.0219 (4)
O17	0.50269 (11)	0.35904 (9)	0.71477 (5)	0.0325 (5)
O18	0.58728 (10)	0.33537 (9)	0.66424 (6)	0.0322 (5)
O19	0.49588 (11)	0.49390 (10)	0.73261 (5)	0.0349 (5)
O20	0.56449 (9)	0.44463 (8)	0.67753 (5)	0.0204 (4)
O21	0.57620 (10)	0.55541 (9)	0.69410 (6)	0.0317 (5)
O22	0.45133 (9)	0.56024 (8)	0.67924 (5)	0.0217 (4)
O23	0.51442 (10)	0.63746 (8)	0.63623 (5)	0.0298 (5)
O24	0.39050 (10)	0.63988 (9)	0.64191 (6)	0.0330 (5)
O25	0.69976 (10)	0.47434 (11)	0.59651 (5)	0.0362 (6)
O26	0.93869 (12)	0.38839 (11)	0.58143 (9)	0.0575 (8)
O27	0.86240 (12)	0.64512 (12)	0.46946 (8)	0.0553 (8)
N1	0.62325 (10)	0.48441 (10)	0.55628 (6)	0.0191 (5)
H1A	0.6167	0.4937	0.5340	0.023*
N2	0.88830 (11)	0.46349 (11)	0.55840 (7)	0.0314 (6)
C1	0.51561 (12)	0.48452 (12)	0.55214 (7)	0.0180 (6)
H1B	0.5179	0.5222	0.5416	0.022*
H1C	0.5201	0.4571	0.5327	0.022*
C2	0.56650 (12)	0.52145 (11)	0.60751 (7)	0.0185 (6)
H2A	0.6022	0.5169	0.6234	0.022*
H2B	0.5689	0.5589	0.5966	0.022*
C3	0.57029 (12)	0.41818 (11)	0.59373 (7)	0.0192 (6)
H3A	0.5747	0.3910	0.5741	0.023*
H3B	0.6063	0.4143	0.6094	0.023*
C4	0.56869 (11)	0.47718 (11)	0.57842 (7)	0.0158 (5)
C5	0.68201 (13)	0.47852 (12)	0.56591 (7)	0.0214 (6)
C6	0.72449 (13)	0.47496 (14)	0.53373 (8)	0.0275 (7)
H6A	0.7173	0.4387	0.5219	0.033*
H6B	0.7126	0.5046	0.5168	0.033*
C7	0.79175 (13)	0.48032 (13)	0.54075 (8)	0.0270 (7)
C8	0.82712 (14)	0.44402 (13)	0.55882 (8)	0.0286 (7)
C9	0.80915 (15)	0.39129 (14)	0.57705 (9)	0.0351 (8)
H9A	0.7646	0.3877	0.5768	0.053*
H9B	0.8237	0.3921	0.6016	0.053*
H9C	0.8274	0.3595	0.5647	0.053*
C10	0.83021 (14)	0.52331 (14)	0.52617 (9)	0.0315 (7)
C11	0.81826 (15)	0.56815 (15)	0.50339 (9)	0.0367 (8)
H11	0.7777	0.5764	0.4962	0.044*
C12	0.86663 (16)	0.59999 (16)	0.49172 (10)	0.0415 (8)

C13	0.92668 (16)	0.58762 (17)	0.50235 (10)	0.0446 (9)
H13	0.9593	0.6103	0.4942	0.054*
C14	0.93910 (16)	0.54318 (16)	0.52437 (10)	0.0424 (9)
H14	0.9799	0.5341	0.5307	0.051*
C15	0.89037 (14)	0.51210 (15)	0.53705 (9)	0.0348 (8)
C16	0.93806 (15)	0.43818 (15)	0.57565 (10)	0.0364 (8)
C17	0.98805 (15)	0.47540 (15)	0.58653 (9)	0.0351 (8)
C18	0.97462 (16)	0.52781 (16)	0.60125 (10)	0.0430 (9)
H18	0.9333	0.5391	0.6039	0.052*
C19	1.02114 (18)	0.56307 (19)	0.61185 (11)	0.0515 (10)
H19	1.0124	0.5985	0.6220	0.062*
C20	1.08094 (18)	0.5453 (2)	0.60731 (10)	0.0537 (11)
C21	1.09508 (17)	0.49361 (19)	0.59434 (11)	0.0524 (10)
H21	1.1364	0.4818	0.5924	0.063*
C22	1.04770 (17)	0.45893 (18)	0.58412 (11)	0.0484 (10)
H22	1.0568	0.4228	0.5752	0.058*
C23	0.80267 (18)	0.65923 (19)	0.45721 (13)	0.0606 (12)
H23A	0.8052	0.6914	0.4412	0.091*
H23B	0.7767	0.6686	0.4775	0.091*
H23C	0.7851	0.6274	0.4445	0.091*
O28	0.72919 (13)	0.34330 (13)	0.37814 (8)	0.0554 (7)
H28C	0.7099	0.3189	0.3901	0.083*
H28D	0.7338	0.3705	0.3923	0.083*
O29	0.71747 (12)	0.46184 (11)	0.34943 (7)	0.0434 (6)
H29C	0.7279	0.4289	0.3550	0.065*
H29D	0.7061	0.4593	0.3279	0.065*
O30	0.65908 (11)	0.57515 (10)	0.30301 (6)	0.0368 (5)
H30E	0.6477	0.6013	0.2893	0.055*
H30F	0.6796	0.5913	0.3191	0.055*
O31	0.34120 (12)	0.53722 (11)	0.71708 (7)	0.0461 (6)
H31G	0.3437	0.5021	0.7144	0.069*
H31H	0.3740	0.5499	0.7081	0.069*
O32	0.38081 (14)	0.34181 (13)	0.73972 (7)	0.0538 (7)
H32C	0.3784	0.3170	0.7237	0.081*
H32D	0.4177	0.3528	0.7389	0.081*
O33	0.24067 (12)	0.45998 (13)	0.60128 (7)	0.0529 (7)
H33C	0.2685	0.4700	0.5869	0.079*
H33D	0.2167	0.4399	0.5890	0.079*
O34	0.29073 (11)	0.37358 (11)	0.63812 (7)	0.0427 (6)
H34C	0.2827	0.3397	0.6335	0.064*
H34D	0.2650	0.3920	0.6259	0.064*
O35	0.29529 (13)	0.25727 (12)	0.62754 (8)	0.0576 (8)
H35D	0.3306	0.2689	0.6220	0.086*
H35E	0.2892	0.2293	0.6142	0.086*
O36	0.38207 (12)	0.26705 (11)	0.68514 (7)	0.0463 (6)
H36E	0.4089	0.2862	0.6744	0.070*
H36F	0.3531	0.2594	0.6710	0.070*
N3	0.47841 (12)	0.68789 (11)	0.76002 (7)	0.0323 (6)

C56	0.51693 (16)	0.63516 (14)	0.76153 (10)	0.0387 (8)
H56A	0.4953	0.6074	0.7763	0.046*
H56B	0.5200	0.6196	0.7373	0.046*
C57	0.58083 (17)	0.64259 (17)	0.77610 (12)	0.0504 (10)
H57A	0.6054	0.6651	0.7593	0.060*
H57B	0.5789	0.6629	0.7989	0.060*
C58	0.61104 (17)	0.58654 (18)	0.78167 (11)	0.0500 (10)
H58A	0.6063	0.5637	0.7600	0.060*
H58B	0.5905	0.5668	0.8014	0.060*
C59	0.67895 (19)	0.5929 (2)	0.79017 (12)	0.0646 (13)
H59A	0.7000	0.6093	0.7698	0.097*
H59B	0.6965	0.5562	0.7954	0.097*
H59C	0.6839	0.6173	0.8108	0.097*
C60	0.46558 (16)	0.71026 (14)	0.79697 (8)	0.0329 (7)
H60A	0.5052	0.7176	0.8087	0.039*
H60B	0.4442	0.7465	0.7946	0.039*
C61	0.42781 (18)	0.67314 (15)	0.82113 (10)	0.0415 (8)
H61A	0.4457	0.6353	0.8217	0.050*
H61B	0.3857	0.6702	0.8118	0.050*
C62	0.4264 (2)	0.69740 (16)	0.85848 (10)	0.0535 (11)
H62A	0.4684	0.6974	0.8682	0.064*
H62B	0.4125	0.7366	0.8572	0.064*
C63	0.3855 (3)	0.6660 (2)	0.88324 (13)	0.0811 (17)
H63A	0.3431	0.6688	0.8750	0.122*
H63B	0.3887	0.6820	0.9071	0.122*
H63C	0.3978	0.6268	0.8839	0.122*
C64	0.41939 (15)	0.67164 (14)	0.74125 (9)	0.0345 (8)
H64A	0.4299	0.6570	0.7175	0.041*
H64B	0.4002	0.6408	0.7547	0.041*
C65	0.37283 (17)	0.71747 (16)	0.73678 (10)	0.0419 (9)
H65A	0.3900	0.7476	0.7219	0.050*
H65B	0.3624	0.7335	0.7602	0.050*
C66	0.31578 (17)	0.69402 (18)	0.71944 (11)	0.0516 (10)
H66A	0.3269	0.6781	0.6961	0.062*
H66B	0.2997	0.6634	0.7343	0.062*
C67	0.2661 (2)	0.7370 (2)	0.71425 (13)	0.0716 (14)
H67A	0.2823	0.7684	0.7004	0.107*
H67B	0.2522	0.7505	0.7374	0.107*
H67C	0.2318	0.7201	0.7015	0.107*
C68	0.51168 (17)	0.73400 (15)	0.74029 (9)	0.0391 (8)*
H68A	0.4851	0.7674	0.7400	0.047*
H68B	0.5488	0.7437	0.7539	0.047*
C69	0.53056 (19)	0.72149 (19)	0.70252 (10)	0.0526 (10)
H69A	0.4943	0.7103	0.6885	0.063*
H69B	0.5601	0.6902	0.7023	0.063*
C70	0.5606 (3)	0.7747 (3)	0.68556 (12)	0.0858 (19)
H70A	0.5296	0.8047	0.6843	0.103*
H70B	0.5939	0.7878	0.7012	0.103*

C71	0.5856 (3)	0.7650 (2)	0.64974 (14)	0.0824 (16)
H71A	0.6173	0.7362	0.6509	0.124*
H71B	0.6034	0.7996	0.6406	0.124*
H71C	0.5528	0.7527	0.6339	0.124*
N4	0.74296 (12)	0.43812 (12)	0.70443 (7)	0.0327 (6)
C40	0.71554 (16)	0.48719 (15)	0.68431 (9)	0.0389 (8)
H40A	0.7308	0.4859	0.6596	0.047*
H40B	0.6707	0.4820	0.6834	0.047*
C41	0.7282 (2)	0.54375 (17)	0.69883 (11)	0.0530 (10)
H41A	0.7715	0.5466	0.7061	0.064*
H41B	0.7023	0.5506	0.7199	0.064*
C42	0.7141 (2)	0.58707 (19)	0.67008 (15)	0.0698 (14)
H42	0.7039	0.5775	0.6464	0.084*
C43	0.7178 (4)	0.6430 (3)	0.6824 (2)	0.122 (3)
H43A	0.7079	0.6686	0.6630	0.183*
H43B	0.7594	0.6506	0.6908	0.183*
H43C	0.6889	0.6485	0.7019	0.183*
C44	0.81231 (14)	0.44254 (16)	0.70681 (9)	0.0354 (8)
H44A	0.8226	0.4776	0.7193	0.042*
H44B	0.8274	0.4113	0.7216	0.042*
C45	0.84656 (16)	0.44170 (17)	0.67194 (9)	0.0431 (9)
H45A	0.8303	0.4709	0.6560	0.052*
H45B	0.8411	0.4051	0.6602	0.052*
C46	0.91481 (17)	0.45219 (17)	0.67907 (10)	0.0456 (9)
H46A	0.9287	0.4270	0.6982	0.055*
H46B	0.9384	0.4430	0.6574	0.055*
C47	0.9282 (2)	0.51121 (19)	0.68954 (11)	0.0562 (11)
H47A	0.9109	0.5366	0.6719	0.084*
H47B	0.9725	0.5167	0.6908	0.084*
H47C	0.9099	0.5189	0.7128	0.084*
C48	0.72107 (15)	0.43645 (16)	0.74266 (8)	0.0371 (8)
H48A	0.7443	0.4070	0.7552	0.044*
H48B	0.7317	0.4724	0.7539	0.044*
C49	0.65392 (16)	0.42599 (18)	0.74872 (9)	0.0447 (9)
H49A	0.6416	0.3909	0.7369	0.054*
H49B	0.6297	0.4568	0.7384	0.054*
C50	0.64140 (18)	0.4219 (2)	0.78812 (10)	0.0536 (11)
H50A	0.6670	0.3919	0.7983	0.064*
H50B	0.6534	0.4574	0.7996	0.064*
C51	0.5753 (2)	0.4101 (2)	0.79644 (13)	0.0756 (16)
H51A	0.5640	0.3735	0.7868	0.113*
H51B	0.5495	0.4389	0.7857	0.113*
H51C	0.5693	0.4101	0.8222	0.113*
C52	0.72437 (16)	0.38665 (15)	0.68374 (9)	0.0390 (8)
H52A	0.6792	0.3844	0.6836	0.047*
H52B	0.7380	0.3912	0.6589	0.047*
C53	0.7494 (2)	0.33229 (17)	0.69768 (12)	0.0555 (11)
H53A	0.7393	0.3287	0.7232	0.067*

H53B	0.7944	0.3322	0.6953	0.067*	
C54	0.7232 (2)	0.28321 (18)	0.67774 (12)	0.0573 (11)	
H54A	0.7419	0.2486	0.6871	0.069*	
H54B	0.6788	0.2813	0.6825	0.069*	
C55	0.7328 (2)	0.2850 (2)	0.63830 (14)	0.0755 (15)	
H55A	0.7213	0.2491	0.6279	0.113*	
H55B	0.7759	0.2926	0.6332	0.113*	
H55C	0.7075	0.3146	0.6280	0.113*	
N5	0.48691 (14)	0.27269 (12)	0.47164 (7)	0.0367 (7)	
C24	0.51075 (17)	0.22825 (14)	0.44666 (9)	0.0351 (8)	
H24A	0.4753	0.2091	0.4358	0.042*	
H24B	0.5334	0.2003	0.4608	0.042*	
C25	0.55219 (17)	0.24845 (14)	0.41711 (9)	0.0380 (8)	
H25A	0.5306	0.2768	0.4027	0.046*	
H25B	0.5891	0.2661	0.4274	0.046*	
C26	0.57075 (18)	0.19998 (15)	0.39381 (10)	0.0427 (9)	
H26A	0.5336	0.1835	0.3831	0.051*	
H26B	0.5902	0.1710	0.4087	0.051*	
C27	0.6145 (2)	0.21623 (18)	0.36452 (11)	0.0591 (12)	
H27A	0.6232	0.1836	0.3497	0.089*	
H27B	0.6526	0.2300	0.3749	0.089*	
H27C	0.5961	0.2456	0.3500	0.089*	
C28	0.45485 (18)	0.24536 (16)	0.50351 (10)	0.0449 (9)	
H28A	0.4867	0.2341	0.5207	0.054*	
H28B	0.4294	0.2742	0.5152	0.054*	
C29	0.4153 (2)	0.19582 (17)	0.49664 (10)	0.0535 (11)	
H29A	0.4406	0.1651	0.4871	0.064*	
H29B	0.3842	0.2055	0.4786	0.064*	
C30	0.3834 (3)	0.1764 (2)	0.53010 (12)	0.0849 (19)	
H30A	0.3781	0.1355	0.5297	0.102*	0.126 (11)
H30B	0.4079	0.1865	0.5512	0.102*	0.126 (11)
H30C	0.4148	0.1665	0.5479	0.102*	0.874 (11)
H30D	0.3592	0.2078	0.5398	0.102*	0.874 (11)
C32	0.53868 (18)	0.30782 (14)	0.48615 (10)	0.0420 (9)	
H32A	0.5561	0.3300	0.4664	0.050*	
H32B	0.5216	0.3344	0.5036	0.050*	
C33	0.5899 (2)	0.27594 (17)	0.50367 (10)	0.0533 (11)	
H33A	0.5744	0.2580	0.5255	0.064*	
H33B	0.6041	0.2461	0.4875	0.064*	
C34	0.6431 (2)	0.3132 (2)	0.51296 (14)	0.0690 (13)	
H34A	0.6601	0.3293	0.4909	0.083*	
H34B	0.6281	0.3445	0.5278	0.083*	
C35	0.6928 (3)	0.2834 (3)	0.53243 (17)	0.115 (3)	
H35A	0.7091	0.2534	0.5175	0.172*	
H35B	0.6764	0.2675	0.5544	0.172*	
H35C	0.7256	0.3097	0.5381	0.172*	
C36	0.44488 (18)	0.31485 (16)	0.45387 (12)	0.0513 (10)	
H36A	0.4462	0.3491	0.4685	0.062*	0.5

H36B	0.4636	0.3243	0.4308	0.062*	0.5
H36C	0.4341	0.3439	0.4714	0.062*	0.5
H36D	0.4676	0.3332	0.4344	0.062*	0.5
C31	0.3223 (14)	0.205 (2)	0.5313 (12)	0.10 (2)	0.126 (11)
H31A	0.3045	0.2005	0.5550	0.156*	0.126 (11)
H31B	0.2951	0.1882	0.5136	0.156*	0.126 (11)
H31C	0.3275	0.2447	0.5262	0.156*	0.126 (11)
C37	0.3822 (5)	0.3033 (6)	0.4472 (4)	0.056 (4)	0.413 (15)
H37A	0.3613	0.2948	0.4698	0.068*	0.413 (15)
H37B	0.3788	0.2702	0.4317	0.068*	0.413 (15)
C38	0.3522 (4)	0.3517 (4)	0.4299 (3)	0.033 (3)	0.413 (15)
H38A	0.3705	0.3580	0.4063	0.040*	0.413 (15)
H38B	0.3586	0.3856	0.4444	0.040*	0.413 (15)
C39	0.2842 (4)	0.3406 (6)	0.4261 (4)	0.058 (4)	0.413 (15)
H39A	0.2778	0.3094	0.4098	0.087*	0.413 (15)
H39B	0.2641	0.3740	0.4167	0.087*	0.413 (15)
H39C	0.2668	0.3314	0.4493	0.087*	0.413 (15)
C31A	0.3421 (4)	0.1275 (3)	0.52492 (15)	0.113 (4)	0.874 (11)
H31D	0.3085	0.1379	0.5091	0.169*	0.874 (11)
H31E	0.3254	0.1159	0.5479	0.169*	0.874 (11)
H31F	0.3652	0.0966	0.5144	0.169*	0.874 (11)
H1	0.370 (3)	0.395 (3)	0.6145 (19)	0.169*	
H3	0.367 (3)	0.516 (3)	0.6318 (18)	0.169*	
H5	0.421 (2)	0.436 (3)	0.6739 (19)	0.169*	
C37A	0.3872 (5)	0.2911 (5)	0.4390 (4)	0.100 (5)	0.587 (15)
H37C	0.3624	0.2769	0.4591	0.120*	0.587 (15)
H37D	0.3982	0.2586	0.4241	0.120*	0.587 (15)
C38A	0.3468 (5)	0.3299 (5)	0.4169 (3)	0.076 (3)	0.587 (15)
H38C	0.3731	0.3530	0.4014	0.091*	0.587 (15)
H38D	0.3202	0.3071	0.4014	0.091*	0.587 (15)
C39A	0.3079 (8)	0.3671 (6)	0.4389 (3)	0.100 (5)	0.587 (15)
H39D	0.2783	0.3862	0.4237	0.149*	0.587 (15)
H39E	0.3337	0.3947	0.4508	0.149*	0.587 (15)
H39F	0.2862	0.3448	0.4566	0.149*	0.587 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.01950 (12)	0.02207 (13)	0.01470 (11)	0.00500 (10)	−0.00147 (9)	0.00069 (9)
Mo2	0.01694 (12)	0.02293 (13)	0.01566 (12)	−0.00276 (9)	−0.00218 (9)	−0.00190 (9)
Mo3	0.02231 (13)	0.01587 (12)	0.01950 (12)	−0.00241 (9)	0.00034 (10)	−0.00050 (9)
Mo4	0.02074 (13)	0.01765 (12)	0.01906 (12)	−0.00023 (9)	−0.00347 (9)	0.00331 (9)
Mo5	0.02338 (13)	0.02119 (13)	0.01444 (11)	0.00208 (10)	−0.00390 (9)	−0.00292 (9)
Mo6	0.02484 (13)	0.01597 (12)	0.01748 (12)	0.00340 (10)	−0.00096 (9)	−0.00195 (9)
Cl1	0.0554 (7)	0.1203 (12)	0.0748 (8)	−0.0373 (7)	−0.0177 (6)	−0.0061 (8)
Al1	0.0129 (4)	0.0155 (4)	0.0121 (4)	−0.0001 (3)	0.0007 (3)	−0.0001 (3)
O1	0.0144 (9)	0.0216 (10)	0.0172 (9)	−0.0034 (8)	0.0012 (7)	−0.0003 (8)
O2	0.0113 (9)	0.0187 (9)	0.0129 (9)	−0.0003 (7)	0.0017 (7)	0.0006 (7)

O3	0.0168 (10)	0.0207 (10)	0.0146 (9)	0.0023 (8)	0.0015 (7)	−0.0006 (8)
O4	0.0151 (9)	0.0168 (9)	0.0138 (9)	−0.0005 (7)	0.0006 (7)	−0.0015 (7)
O5	0.0181 (10)	0.0199 (10)	0.0127 (9)	0.0002 (8)	0.0006 (7)	0.0023 (7)
O6	0.0136 (9)	0.0164 (9)	0.0149 (9)	−0.0008 (7)	0.0017 (7)	0.0007 (7)
O7	0.0274 (11)	0.0186 (10)	0.0193 (10)	0.0014 (8)	−0.0007 (8)	0.0022 (8)
O8	0.0284 (12)	0.0374 (13)	0.0304 (12)	0.0137 (10)	−0.0032 (9)	−0.0035 (10)
O9	0.0333 (12)	0.0282 (11)	0.0183 (10)	0.0009 (9)	−0.0015 (9)	0.0016 (8)
O10	0.0162 (10)	0.0300 (11)	0.0199 (10)	0.0007 (8)	−0.0018 (8)	0.0002 (8)
O11	0.0259 (12)	0.0374 (13)	0.0394 (13)	−0.0099 (10)	−0.0066 (10)	−0.0029 (10)
O12	0.0341 (12)	0.0342 (12)	0.0177 (10)	0.0011 (10)	−0.0009 (9)	−0.0014 (9)
O13	0.0212 (10)	0.0210 (10)	0.0166 (9)	−0.0011 (8)	0.0023 (8)	−0.0029 (8)
O14	0.0386 (13)	0.0264 (11)	0.0317 (12)	−0.0127 (10)	0.0004 (10)	−0.0014 (9)
O15	0.0368 (13)	0.0251 (11)	0.0316 (12)	0.0083 (10)	0.0026 (10)	0.0000 (9)
O16	0.0258 (11)	0.0193 (10)	0.0207 (10)	−0.0055 (8)	0.0007 (8)	0.0039 (8)
O17	0.0433 (13)	0.0318 (12)	0.0223 (11)	−0.0066 (10)	−0.0040 (10)	0.0074 (9)
O18	0.0274 (12)	0.0214 (11)	0.0480 (14)	0.0031 (9)	−0.0071 (10)	−0.0008 (10)
O19	0.0456 (14)	0.0420 (14)	0.0170 (10)	0.0093 (11)	0.0006 (10)	0.0006 (9)
O20	0.0190 (10)	0.0211 (10)	0.0211 (10)	0.0012 (8)	−0.0044 (8)	−0.0005 (8)
O21	0.0308 (12)	0.0287 (12)	0.0355 (12)	−0.0007 (9)	−0.0101 (10)	−0.0098 (10)
O22	0.0257 (11)	0.0237 (10)	0.0156 (9)	0.0048 (8)	0.0003 (8)	−0.0030 (8)
O23	0.0403 (13)	0.0223 (11)	0.0269 (11)	−0.0045 (9)	−0.0024 (10)	−0.0033 (9)
O24	0.0386 (13)	0.0295 (12)	0.0310 (12)	0.0125 (10)	0.0007 (10)	−0.0037 (9)
O25	0.0191 (11)	0.0684 (17)	0.0210 (11)	0.0004 (11)	−0.0012 (9)	−0.0013 (11)
O26	0.0437 (16)	0.0367 (16)	0.092 (2)	0.0063 (12)	−0.0173 (15)	0.0000 (15)
O27	0.0347 (14)	0.0613 (18)	0.0700 (19)	−0.0108 (13)	−0.0082 (13)	0.0301 (15)
N1	0.0136 (11)	0.0282 (13)	0.0155 (11)	−0.0016 (10)	0.0018 (9)	0.0046 (10)
N2	0.0154 (13)	0.0341 (15)	0.0447 (16)	0.0010 (11)	−0.0015 (11)	0.0029 (12)
C1	0.0136 (13)	0.0267 (15)	0.0137 (13)	−0.0018 (11)	0.0018 (10)	0.0022 (11)
C2	0.0140 (13)	0.0219 (14)	0.0197 (13)	−0.0042 (11)	0.0036 (11)	−0.0016 (11)
C3	0.0139 (13)	0.0208 (14)	0.0229 (14)	0.0006 (11)	0.0064 (11)	0.0007 (11)
C4	0.0114 (12)	0.0213 (14)	0.0147 (12)	−0.0011 (10)	0.0036 (10)	0.0013 (11)
C5	0.0168 (14)	0.0251 (15)	0.0222 (15)	−0.0047 (11)	0.0012 (11)	−0.0008 (12)
C6	0.0168 (15)	0.0442 (19)	0.0215 (15)	−0.0047 (13)	0.0032 (12)	−0.0012 (13)
C7	0.0174 (15)	0.0351 (17)	0.0285 (16)	−0.0030 (13)	0.0054 (12)	−0.0035 (13)
C8	0.0205 (15)	0.0342 (17)	0.0310 (16)	−0.0029 (13)	0.0037 (13)	−0.0047 (14)
C9	0.0301 (18)	0.0369 (19)	0.0384 (19)	−0.0035 (14)	0.0013 (15)	0.0010 (15)
C10	0.0187 (15)	0.0377 (18)	0.0382 (18)	−0.0012 (13)	0.0019 (13)	−0.0003 (15)
C11	0.0197 (16)	0.046 (2)	0.045 (2)	−0.0002 (14)	−0.0001 (14)	0.0068 (16)
C12	0.0315 (19)	0.049 (2)	0.044 (2)	−0.0056 (16)	−0.0024 (16)	0.0085 (17)
C13	0.0237 (17)	0.058 (2)	0.052 (2)	−0.0135 (16)	0.0010 (16)	0.0096 (19)
C14	0.0219 (17)	0.055 (2)	0.050 (2)	−0.0046 (16)	−0.0032 (15)	0.0091 (18)
C15	0.0219 (16)	0.0409 (19)	0.0417 (19)	−0.0025 (14)	−0.0006 (14)	0.0031 (15)
C16	0.0258 (17)	0.040 (2)	0.044 (2)	0.0066 (15)	−0.0003 (15)	−0.0056 (16)
C17	0.0253 (17)	0.047 (2)	0.0334 (18)	0.0015 (15)	−0.0057 (14)	0.0047 (15)
C18	0.0294 (19)	0.053 (2)	0.047 (2)	0.0037 (16)	0.0020 (16)	−0.0115 (18)
C19	0.045 (2)	0.062 (3)	0.047 (2)	−0.003 (2)	−0.0016 (18)	−0.013 (2)
C20	0.038 (2)	0.082 (3)	0.041 (2)	−0.015 (2)	−0.0067 (17)	0.002 (2)
C21	0.0215 (18)	0.073 (3)	0.062 (3)	0.0067 (18)	−0.0075 (17)	0.001 (2)

C22	0.034 (2)	0.057 (2)	0.055 (2)	0.0104 (18)	−0.0048 (18)	0.003 (2)
C23	0.036 (2)	0.065 (3)	0.081 (3)	−0.006 (2)	−0.014 (2)	0.030 (2)
O28	0.0456 (17)	0.0564 (18)	0.0642 (18)	0.0168 (14)	−0.0026 (14)	−0.0194 (15)
O29	0.0352 (14)	0.0543 (16)	0.0408 (14)	0.0130 (12)	0.0089 (12)	0.0034 (12)
O30	0.0332 (13)	0.0448 (14)	0.0325 (13)	0.0012 (11)	0.0066 (10)	0.0043 (11)
O31	0.0462 (16)	0.0498 (16)	0.0424 (14)	0.0070 (13)	0.0147 (12)	0.0002 (13)
O32	0.0570 (18)	0.0613 (19)	0.0432 (16)	0.0130 (15)	0.0113 (14)	0.0132 (13)
O33	0.0294 (14)	0.0673 (19)	0.0619 (17)	−0.0017 (13)	0.0063 (13)	−0.0007 (15)
O34	0.0338 (14)	0.0498 (15)	0.0445 (15)	−0.0052 (12)	0.0011 (11)	0.0027 (12)
O35	0.0497 (17)	0.0565 (18)	0.0666 (19)	−0.0248 (14)	0.0159 (15)	−0.0166 (15)
O36	0.0396 (15)	0.0506 (16)	0.0489 (15)	−0.0131 (12)	0.0062 (12)	0.0208 (13)
N3	0.0312 (15)	0.0295 (15)	0.0360 (15)	0.0020 (12)	−0.0051 (12)	−0.0153 (12)
C56	0.0354 (19)	0.0304 (18)	0.050 (2)	0.0061 (15)	−0.0058 (16)	−0.0188 (16)
C57	0.038 (2)	0.047 (2)	0.066 (3)	0.0032 (18)	−0.0128 (19)	−0.016 (2)
C58	0.042 (2)	0.058 (3)	0.050 (2)	0.0125 (19)	−0.0120 (18)	−0.0142 (19)
C59	0.047 (2)	0.092 (4)	0.055 (3)	0.017 (2)	−0.016 (2)	−0.015 (2)
C60	0.0390 (19)	0.0280 (17)	0.0317 (17)	0.0023 (14)	−0.0062 (14)	−0.0122 (14)
C61	0.051 (2)	0.0313 (19)	0.042 (2)	0.0018 (16)	−0.0018 (17)	−0.0082 (16)
C62	0.085 (3)	0.037 (2)	0.039 (2)	0.013 (2)	0.003 (2)	−0.0036 (17)
C63	0.121 (5)	0.059 (3)	0.064 (3)	0.033 (3)	0.031 (3)	0.015 (2)
C64	0.0294 (18)	0.0362 (18)	0.0379 (18)	−0.0007 (14)	−0.0058 (14)	−0.0161 (15)
C65	0.042 (2)	0.043 (2)	0.040 (2)	0.0092 (17)	−0.0086 (16)	−0.0101 (16)
C66	0.039 (2)	0.068 (3)	0.048 (2)	0.010 (2)	−0.0102 (18)	−0.013 (2)
C67	0.056 (3)	0.094 (4)	0.065 (3)	0.024 (3)	−0.023 (2)	−0.011 (3)
C69	0.050 (2)	0.067 (3)	0.041 (2)	−0.001 (2)	0.0001 (18)	−0.013 (2)
C70	0.081 (4)	0.129 (5)	0.048 (3)	−0.053 (4)	0.010 (2)	−0.027 (3)
C71	0.085 (4)	0.094 (4)	0.068 (3)	−0.019 (3)	0.003 (3)	0.001 (3)
N4	0.0243 (14)	0.0468 (17)	0.0270 (14)	−0.0042 (12)	−0.0065 (11)	0.0073 (12)
C40	0.0317 (18)	0.053 (2)	0.0325 (18)	−0.0006 (16)	−0.0054 (15)	0.0146 (16)
C41	0.057 (3)	0.050 (2)	0.052 (2)	0.000 (2)	−0.007 (2)	0.0052 (19)
C42	0.071 (3)	0.052 (3)	0.087 (4)	−0.012 (2)	−0.018 (3)	0.016 (3)
C43	0.138 (6)	0.082 (5)	0.145 (7)	−0.005 (4)	−0.035 (5)	0.008 (4)
C44	0.0240 (17)	0.050 (2)	0.0321 (17)	−0.0031 (15)	−0.0069 (14)	0.0018 (15)
C45	0.036 (2)	0.056 (2)	0.0367 (19)	−0.0070 (17)	−0.0003 (16)	−0.0043 (17)
C46	0.033 (2)	0.058 (2)	0.046 (2)	−0.0041 (17)	0.0021 (17)	0.0051 (19)
C47	0.048 (2)	0.071 (3)	0.050 (2)	−0.019 (2)	−0.0023 (19)	0.006 (2)
C48	0.0327 (18)	0.054 (2)	0.0248 (16)	0.0000 (16)	−0.0055 (14)	0.0076 (15)
C49	0.0332 (19)	0.068 (3)	0.0334 (18)	−0.0007 (18)	−0.0028 (15)	0.0175 (18)
C50	0.043 (2)	0.079 (3)	0.039 (2)	0.002 (2)	0.0006 (17)	0.020 (2)
C51	0.048 (3)	0.120 (5)	0.059 (3)	0.009 (3)	0.017 (2)	0.037 (3)
C52	0.0327 (18)	0.049 (2)	0.0354 (18)	−0.0070 (16)	−0.0087 (15)	−0.0002 (16)
C53	0.052 (2)	0.053 (2)	0.062 (3)	0.000 (2)	−0.015 (2)	0.006 (2)
C54	0.047 (2)	0.048 (2)	0.077 (3)	−0.0021 (19)	−0.007 (2)	0.006 (2)
C55	0.081 (4)	0.062 (3)	0.083 (4)	−0.016 (3)	0.012 (3)	−0.017 (3)
N5	0.0461 (17)	0.0298 (15)	0.0343 (15)	−0.0003 (13)	0.0116 (13)	0.0032 (12)
C24	0.047 (2)	0.0279 (17)	0.0299 (17)	−0.0041 (15)	0.0003 (15)	−0.0010 (14)
C25	0.049 (2)	0.0325 (18)	0.0322 (18)	−0.0042 (16)	0.0031 (16)	−0.0021 (14)
C26	0.053 (2)	0.035 (2)	0.040 (2)	−0.0020 (17)	0.0025 (17)	−0.0048 (16)

C27	0.078 (3)	0.052 (3)	0.047 (2)	−0.004 (2)	0.019 (2)	−0.011 (2)
C28	0.057 (2)	0.044 (2)	0.0336 (19)	−0.0107 (18)	0.0117 (17)	0.0011 (16)
C29	0.075 (3)	0.047 (2)	0.038 (2)	−0.018 (2)	0.012 (2)	−0.0029 (18)
C30	0.126 (5)	0.084 (4)	0.045 (3)	−0.062 (4)	0.022 (3)	−0.007 (2)
C32	0.059 (2)	0.0246 (17)	0.043 (2)	−0.0065 (16)	0.0166 (18)	−0.0089 (15)
C33	0.079 (3)	0.044 (2)	0.037 (2)	−0.019 (2)	−0.008 (2)	0.0011 (17)
C34	0.071 (3)	0.059 (3)	0.076 (3)	−0.019 (2)	−0.002 (3)	−0.019 (2)
C35	0.129 (6)	0.110 (5)	0.105 (5)	−0.049 (4)	−0.072 (4)	0.017 (4)
C36	0.054 (2)	0.039 (2)	0.061 (3)	0.0075 (18)	0.018 (2)	0.0090 (19)
C31	0.09 (4)	0.16 (6)	0.07 (3)	−0.02 (4)	0.00 (3)	−0.02 (3)
C37	0.042 (5)	0.070 (7)	0.056 (6)	0.011 (5)	0.029 (4)	0.031 (5)
C38	0.040 (5)	0.019 (5)	0.040 (6)	−0.005 (4)	0.009 (4)	−0.006 (4)
C39	0.039 (6)	0.063 (8)	0.072 (9)	−0.012 (5)	−0.005 (5)	0.007 (6)
C31A	0.174 (8)	0.117 (6)	0.047 (3)	−0.099 (6)	0.015 (4)	−0.003 (3)
C37A	0.080 (7)	0.083 (7)	0.137 (9)	0.003 (5)	−0.021 (6)	0.040 (6)
C38A	0.078 (7)	0.041 (6)	0.109 (9)	−0.001 (5)	−0.026 (6)	0.006 (6)
C39A	0.111 (12)	0.111 (10)	0.077 (7)	0.015 (9)	−0.004 (7)	−0.007 (7)

Geometric parameters (Å, º)

Mo1—O2	2.3395 (18)	C10—C15	1.405 (4)
Mo1—O3	2.3087 (18)	C11—C12	1.378 (5)
Mo1—O7	1.927 (2)	C12—C13	1.406 (5)
Mo1—O8	1.708 (2)	C13—C14	1.378 (5)
Mo1—O9	1.7014 (19)	C14—C15	1.387 (5)
Mo1—O10	1.929 (2)	C16—C17	1.471 (5)
Mo2—O1	2.3078 (19)	C17—C18	1.405 (5)
Mo2—O2	2.3467 (18)	C17—C22	1.367 (5)
Mo2—O10	1.936 (2)	C18—C19	1.383 (5)
Mo2—O11	1.696 (2)	C19—C20	1.387 (6)
Mo2—O12	1.703 (2)	C20—C21	1.368 (6)
Mo2—O13	1.9275 (19)	C21—C22	1.384 (6)
Mo3—O1	2.3343 (19)	N3—C56	1.521 (4)
Mo3—O6	2.3183 (18)	N3—C60	1.520 (4)
Mo3—O13	1.9182 (19)	N3—C64	1.524 (4)
Mo3—O14	1.707 (2)	N3—C68	1.519 (4)
Mo3—O15	1.696 (2)	C56—C57	1.513 (5)
Mo3—O16	1.9442 (19)	C57—C58	1.513 (5)
Mo4—O5	2.3224 (19)	C58—C59	1.528 (5)
Mo4—O6	2.3440 (17)	C60—C61	1.519 (5)
Mo4—O16	1.9276 (19)	C61—C62	1.525 (5)
Mo4—O17	1.711 (2)	C62—C63	1.497 (6)
Mo4—O18	1.698 (2)	C64—C65	1.509 (5)
Mo4—O20	1.9119 (19)	C65—C66	1.518 (5)
Mo5—O4	2.3633 (17)	C66—C67	1.511 (6)
Mo5—O5	2.3156 (19)	C68—C69	1.514 (5)
Mo5—O19	1.698 (2)	C69—C70	1.572 (7)
Mo5—O20	1.9299 (19)	C70—C71	1.476 (7)

Mo5—O21	1.706 (2)	N4—C40	1.524 (4)
Mo5—O22	1.9341 (19)	N4—C44	1.525 (4)
Mo6—O3	2.3222 (19)	N4—C48	1.520 (4)
Mo6—O4	2.3251 (18)	N4—C52	1.516 (4)
Mo6—O7	1.9152 (19)	C40—C41	1.489 (5)
Mo6—O22	1.9380 (19)	C41—C42	1.533 (6)
Mo6—O23	1.698 (2)	C42—C43	1.423 (8)
Mo6—O24	1.711 (2)	C44—C45	1.514 (5)
Cl1—C20	1.749 (4)	C45—C46	1.539 (5)
Al1—O1	1.878 (2)	C46—C47	1.498 (6)
Al1—O2	1.8950 (19)	C48—C49	1.509 (5)
Al1—O3	1.884 (2)	C49—C50	1.514 (5)
Al1—O4	1.9183 (19)	C50—C51	1.508 (6)
Al1—O5	1.8639 (19)	C52—C53	1.509 (5)
Al1—O6	1.9269 (19)	C53—C54	1.510 (6)
O2—C1	1.438 (3)	C54—C55	1.503 (6)
O4—C2	1.450 (3)	N5—C24	1.515 (4)
O6—C3	1.446 (3)	N5—C28	1.539 (4)
O25—C5	1.222 (3)	N5—C32	1.515 (5)
O26—C16	1.214 (4)	N5—C36	1.523 (5)
O27—C12	1.373 (4)	C24—C25	1.517 (5)
O27—C23	1.427 (4)	C25—C26	1.513 (5)
N1—C4	1.468 (3)	C26—C27	1.513 (5)
N1—C5	1.344 (4)	C28—C29	1.493 (5)
N2—C8	1.418 (4)	C29—C30	1.514 (5)
N2—C15	1.418 (4)	C30—C31	1.504 (16)
N2—C16	1.407 (4)	C30—C31A	1.495 (6)
C1—C4	1.538 (4)	C32—C33	1.510 (6)
C2—C4	1.528 (4)	C33—C34	1.509 (6)
C3—C4	1.529 (4)	C34—C35	1.496 (8)
C5—C6	1.531 (4)	C36—C37	1.422 (11)
C6—C7	1.502 (4)	C36—C37A	1.494 (11)
C7—C8	1.350 (4)	C37—C38	1.484 (11)
C7—C10	1.440 (4)	C38—C39	1.518 (11)
C8—C9	1.493 (4)	C37A—C38A	1.533 (10)
C10—C11	1.401 (5)	C38A—C39A	1.485 (12)

O3—Mo1—O2	66.92 (6)	Mo5—O5—Mo4	91.12 (7)
O7—Mo1—O2	81.02 (7)	Al1—O5—Mo4	104.75 (8)
O7—Mo1—O3	72.06 (7)	Al1—O5—Mo5	104.65 (8)
O7—Mo1—O10	148.18 (8)	Mo3—O6—Mo4	91.80 (6)
O8—Mo1—O2	160.56 (9)	Al1—O6—Mo3	102.91 (8)
O8—Mo1—O3	95.20 (9)	Al1—O6—Mo4	101.91 (8)
O8—Mo1—O7	101.29 (10)	C3—O6—Mo3	116.26 (15)
O8—Mo1—O10	98.37 (10)	C3—O6—Mo4	119.26 (15)
O9—Mo1—O2	92.45 (8)	C3—O6—Al1	120.00 (15)
O9—Mo1—O3	157.90 (9)	Mo6—O7—Mo1	119.47 (10)
O9—Mo1—O7	97.88 (9)	Mo1—O10—Mo2	118.32 (10)

O9—Mo1—O8	106.21 (10)	Mo3—O13—Mo2	118.63 (9)
O9—Mo1—O10	100.34 (9)	Mo4—O16—Mo3	119.71 (9)
O10—Mo1—O2	72.37 (7)	Mo4—O20—Mo5	119.08 (10)
O10—Mo1—O3	81.50 (7)	Mo5—O22—Mo6	118.87 (10)
O1—Mo2—O2	67.19 (6)	C12—O27—C23	116.5 (3)
O10—Mo2—O1	81.62 (7)	C5—N1—C4	127.8 (2)
O10—Mo2—O2	72.08 (7)	C15—N2—C8	107.9 (2)
O11—Mo2—O1	94.85 (9)	C16—N2—C8	125.7 (3)
O11—Mo2—O2	160.81 (9)	C16—N2—C15	126.4 (3)
O11—Mo2—O10	99.58 (10)	O2—C1—C4	112.9 (2)
O11—Mo2—O12	106.20 (11)	O4—C2—C4	111.2 (2)
O11—Mo2—O13	101.00 (10)	O6—C3—C4	111.6 (2)
O12—Mo2—O1	158.22 (9)	N1—C4—C1	103.6 (2)
O12—Mo2—O2	92.44 (8)	N1—C4—C2	110.6 (2)
O12—Mo2—O10	99.96 (9)	N1—C4—C3	107.8 (2)
O12—Mo2—O13	97.39 (9)	C2—C4—C1	111.1 (2)
O13—Mo2—O1	72.59 (7)	C2—C4—C3	111.9 (2)
O13—Mo2—O2	80.65 (7)	C3—C4—C1	111.5 (2)
O13—Mo2—O10	148.09 (8)	O25—C5—N1	124.6 (3)
O6—Mo3—O1	67.54 (6)	O25—C5—C6	123.4 (3)
O13—Mo3—O1	72.13 (7)	N1—C5—C6	111.9 (2)
O13—Mo3—O6	82.51 (7)	C7—C6—C5	116.8 (2)
O13—Mo3—O16	148.25 (8)	C8—C7—C6	126.6 (3)
O14—Mo3—O1	94.54 (9)	C8—C7—C10	108.6 (3)
O14—Mo3—O6	159.64 (9)	C10—C7—C6	124.5 (3)
O14—Mo3—O13	101.68 (9)	N2—C8—C9	122.2 (3)
O14—Mo3—O16	96.88 (9)	C7—C8—N2	108.9 (3)
O15—Mo3—O1	158.52 (9)	C7—C8—C9	128.9 (3)
O15—Mo3—O6	92.99 (9)	C11—C10—C7	132.4 (3)
O15—Mo3—O13	97.27 (9)	C11—C10—C15	120.1 (3)
O15—Mo3—O14	106.06 (11)	C15—C10—C7	107.4 (3)
O15—Mo3—O16	102.07 (9)	C12—C11—C10	118.5 (3)
O16—Mo3—O1	80.98 (7)	O27—C12—C11	125.5 (3)
O16—Mo3—O6	71.63 (7)	O27—C12—C13	113.8 (3)
O5—Mo4—O6	67.30 (6)	C11—C12—C13	120.7 (3)
O16—Mo4—O5	82.64 (8)	C14—C13—C12	121.3 (3)
O16—Mo4—O6	71.31 (7)	C13—C14—C15	118.2 (3)
O17—Mo4—O5	93.91 (9)	C10—C15—N2	107.0 (3)
O17—Mo4—O6	158.74 (9)	C14—C15—N2	131.5 (3)
O17—Mo4—O16	97.38 (9)	C14—C15—C10	121.2 (3)
O17—Mo4—O20	102.68 (9)	O26—C16—N2	121.1 (3)
O18—Mo4—O5	159.49 (9)	O26—C16—C17	122.6 (3)
O18—Mo4—O6	94.23 (9)	N2—C16—C17	116.3 (3)
O18—Mo4—O16	100.35 (9)	C18—C17—C16	119.8 (3)
O18—Mo4—O17	105.71 (11)	C22—C17—C16	121.1 (3)
O18—Mo4—O20	97.32 (9)	C22—C17—C18	119.0 (3)
O20—Mo4—O5	72.05 (7)	C19—C18—C17	120.5 (3)
O20—Mo4—O6	81.59 (7)	C18—C19—C20	118.1 (4)

O20—Mo4—O16	148.49 (8)	C19—C20—Cl1	117.3 (4)
O5—Mo5—O4	67.40 (6)	C21—C20—Cl1	120.3 (3)
O19—Mo5—O4	158.93 (9)	C21—C20—C19	122.4 (4)
O19—Mo5—O5	93.44 (9)	C20—C21—C22	118.3 (4)
O19—Mo5—O20	101.99 (10)	C17—C22—C21	121.6 (4)
O19—Mo5—O21	105.88 (11)	C56—N3—C64	105.9 (2)
O19—Mo5—O22	97.98 (10)	C60—N3—C56	111.2 (3)
O20—Mo5—O4	80.99 (7)	C60—N3—C64	111.1 (2)
O20—Mo5—O5	71.91 (7)	C68—N3—C56	111.0 (3)
O20—Mo5—O22	148.48 (8)	C68—N3—C60	106.3 (2)
O21—Mo5—O4	94.25 (9)	C68—N3—C64	111.4 (3)
O21—Mo5—O5	159.77 (9)	C57—C56—N3	115.3 (3)
O21—Mo5—O20	97.69 (9)	C58—C57—C56	110.5 (3)
O21—Mo5—O22	100.01 (9)	C57—C58—C59	111.4 (4)
O22—Mo5—O4	71.90 (7)	C61—C60—N3	116.3 (3)
O22—Mo5—O5	82.83 (8)	C60—C61—C62	110.0 (3)
O3—Mo6—O4	67.67 (6)	C63—C62—C61	113.4 (4)
O7—Mo6—O3	71.94 (7)	C65—C64—N3	116.0 (3)
O7—Mo6—O4	83.07 (7)	C64—C65—C66	109.5 (3)
O7—Mo6—O22	148.91 (8)	C67—C66—C65	113.2 (4)
O22—Mo6—O3	80.82 (7)	C69—C68—N3	116.6 (3)
O22—Mo6—O4	72.72 (7)	C68—C69—C70	109.6 (3)
O23—Mo6—O3	157.03 (9)	C71—C70—C69	113.5 (4)
O23—Mo6—O4	91.04 (8)	C40—N4—C44	111.6 (3)
O23—Mo6—O7	97.93 (9)	C48—N4—C40	111.6 (3)
O23—Mo6—O22	101.66 (9)	C48—N4—C44	105.1 (2)
O23—Mo6—O24	105.97 (11)	C52—N4—C40	105.5 (2)
O24—Mo6—O3	96.35 (9)	C52—N4—C44	110.7 (3)
O24—Mo6—O4	161.50 (9)	C52—N4—C48	112.5 (3)
O24—Mo6—O7	101.30 (9)	C41—C40—N4	116.6 (3)
O24—Mo6—O22	96.25 (9)	C40—C41—C42	108.7 (3)
O1—Al1—O2	86.11 (8)	C43—C42—C41	113.4 (5)
O1—Al1—O3	97.99 (9)	C45—C44—N4	116.2 (3)
O1—Al1—O4	174.93 (9)	C44—C45—C46	109.1 (3)
O1—Al1—O6	85.64 (8)	C47—C46—C45	113.0 (3)
O2—Al1—O4	90.82 (8)	C49—C48—N4	117.1 (3)
O2—Al1—O6	91.67 (8)	C48—C49—C50	109.6 (3)
O3—Al1—O2	85.40 (8)	C51—C50—C49	113.0 (4)
O3—Al1—O4	85.77 (8)	C53—C52—N4	115.3 (3)
O3—Al1—O6	175.16 (9)	C52—C53—C54	111.2 (3)
O4—Al1—O6	90.43 (8)	C55—C54—C53	114.7 (4)
O5—Al1—O1	96.20 (9)	C24—N5—C28	110.1 (3)
O5—Al1—O2	176.58 (9)	C24—N5—C36	113.7 (3)
O5—Al1—O3	96.75 (9)	C32—N5—C24	111.0 (3)
O5—Al1—O4	86.69 (8)	C32—N5—C28	107.2 (3)
O5—Al1—O6	86.00 (8)	C32—N5—C36	104.0 (3)
Mo2—O1—Mo3	90.87 (7)	C36—N5—C28	110.6 (3)
Al1—O1—Mo2	104.31 (8)	N5—C24—C25	116.0 (3)

Al1—O1—Mo3	103.91 (8)	C26—C25—C24	110.0 (3)
Mo1—O2—Mo2	90.16 (6)	C25—C26—C27	113.3 (3)
Al1—O2—Mo1	103.02 (8)	C29—C28—N5	117.9 (3)
Al1—O2—Mo2	102.31 (8)	C28—C29—C30	111.5 (3)
C1—O2—Mo1	118.66 (15)	C31—C30—C29	107 (2)
C1—O2—Mo2	118.01 (15)	C31A—C30—C29	114.2 (4)
C1—O2—Al1	119.67 (15)	C33—C32—N5	115.6 (3)
Mo1—O3—Mo6	91.56 (7)	C34—C33—C32	112.0 (3)
Al1—O3—Mo1	104.53 (8)	C35—C34—C33	113.1 (4)
Al1—O3—Mo6	103.88 (8)	C37—C36—N5	122.1 (6)
Mo6—O4—Mo5	90.65 (6)	C37A—C36—N5	114.9 (5)
Al1—O4—Mo5	101.15 (8)	C36—C37—C38	110.7 (9)
Al1—O4—Mo6	102.66 (8)	C37—C38—C39	109.9 (9)
C2—O4—Mo5	119.28 (15)	C36—C37A—C38A	117.4 (9)
C2—O4—Mo6	117.40 (15)	C39A—C38A—C37A	113.0 (11)
C2—O4—Al1	120.47 (15)		