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Fully protonated B-type hexamolybdoplatinate $[H_6PtMo_6O_{24}]^{2-}$ and its adduct formation with $[Pt(OH)_6]^{2-}$

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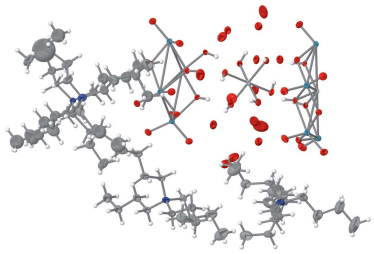
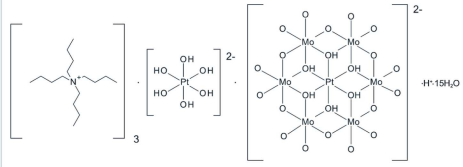
Structural data: full structural data are available from iucrdata.iucr.org

The crystral structure of tris(tetra-*n*-butylammonium) hydrogen hexahydroxidoplatinate(IV) [hexahydrogen α-hexamolybdoplatinate(IV)] pentadecahydrate, $(C_{16}H_{36}N)_3H[Pt(OH)_6][H_6PtMo_6O_{24}]\cdot 15H_2O$, was determined. The structural analysis revealed that all six triply-bridging O atoms of the hexamolybdoplatinate(IV) anion are protonated, making it formally the B-type Anderson anion $[H_6PtMo_6O_{24}]^{2-}$. The $[H_6PtMo_6O_{24}]^{2-}$ anions connect with the $[Pt(OH)_6]^{2-}$ anions through strong hydrogen bonds (O$\cdots$O = 2.45–2.62 Å) to form a linear polymer in the crystal.

3D view



Chemical scheme



Structure description

Anderson anions, where an octahedral XO_6 unit is surrounded by a planar M_6O_{18} ring, have traditionally been divided into two groups (Blazevic & Rompel, 2016). In type A, none of the O atoms in the structure is protonated. In type B, on the other hand, all six triply bridging μ_3-O atoms are protonated. However, the discovery of $[H_{4.5}PtMo_6O_{24}]^{3.5-}$ (Lee & Sasaki, 1984) and $[H_3PtW_6O_{24}]^{5-}$ (Lee *et al.*, 1983), together with a report of protonated $[IMo_6O_{24}]^{5-}$ (Honda *et al.*, 2007), which is considered typical type A Anderson anion, rendered this distinction blurred, if not meaningless. Many different Anderson-type molybdoplatinates of different degrees of protonation have been reported since the initial discovery of Lee and Sasaki (Lee & Sasaki, 1987, 1994; Lee, 1988, 1994; Lee & Joo, 2000, 2004, 2006*a*,*b*, 2007, 2010; Day *et al.*, 2009; Joo *et al.*, 2015*a*,*b*). Curiously, fully protonated $[H_6PtMo_6O_{24}]^{2-}$, where protons are attached to all six μ_3-O atoms, has not been reported with all those efforts. Formation of anions with the formula $[H_6PtMo_6O_{24}]^{2-}$ was observed in four occasions, but only four out of six μ_3-O atoms are protonated in all of them (Lee, 1994; Lee & Joo, 2006*a*,*b*, 2010).

Tris(tetra-*n*-butylammonium) hydrogen hexahydroxoplatinate(IV) [hexahydrogen α-hexamolybdoplatinate(IV)] pentadecahydrate crystallizes in the space group *C*2/*c*.

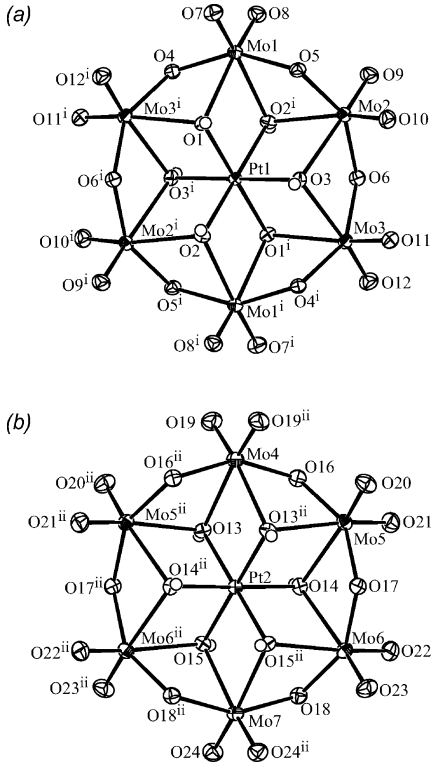


Figure 1
The structures of (*a*) anion A and (*b*) anion B with the atom labelling and displacement ellipsoids at the 50% probability level. [Symmetry codes: (i) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z$; (ii) $-x, y, -z+\frac{1}{2}$.]

X-ray structural analysis revealed the existence of $[H_6PtMo_6O_{24}]^{2-}$ and $[Pt(OH)_6]^{2-}$ anions, which form a hydrogen-bonded adduct (see below) in the crystal. There are two crystallographically independent $[H_6PtMo_6O_{24}]^{2-}$ anions in the crystal. They are depicted in Fig. 1. One of them (anion A) is centrosymmetric and the other (anion B) has a twofold symmetry. No significant structural difference other than the crystallographic symmetry is observed between these two anions. All six μ_3-O atoms that bridge the central Pt atom of the Anderson anion with the Mo atoms are protonated, and all bonds between Mo and μ_3-O atoms are anomaluosly long (Table 1). The current $[H_6PtMo_6O_{24}]^{2-}$ anion is the first example of hexamolybdoplatinate in which all six μ_3-O atoms are protonated.

Table 1
Selected bond lengths (Å).

Pt1—O3	1.993 (2)	Pt2—O14	2.005 (2)
Pt1—O3^{i}	1.993 (2)	Mo4—O19	1.711 (3)
Pt1—O2^{i}	1.995 (2)	Mo4—O16	1.944 (2)
Pt1—O2	1.995 (2)	Mo4—O13	2.300 (2)
Pt1—O1	2.002 (2)	Mo5—O20	1.705 (2)
Pt1—O1^{i}	2.002 (2)	Mo5—O21	1.717 (2)
Mo1—O8	1.711 (2)	Mo5—O16	1.932 (2)
Mo1—O7	1.716 (2)	Mo5—O17	1.949 (2)
Mo1—O4	1.937 (2)	Mo5—O13^{ii}	2.272 (2)
Mo1—O5	1.948 (2)	Mo5—O14	2.327 (2)
Mo1—O2^{i}	2.261 (2)	Mo6—O23	1.699 (2)
Mo1—O1	2.310 (2)	Mo6—O22	1.721 (2)
Mo2—O9	1.704 (2)	Mo6—O17	1.930 (2)
Mo2—O10	1.711 (2)	Mo6—O18	1.947 (2)
Mo2—O5	1.940 (2)	Mo6—O15^{ii}	2.252 (2)
Mo2—O6	1.952 (2)	Mo6—O14	2.354 (2)
Mo2—O2^{i}	2.238 (2)	Mo7—O24	1.716 (2)
Mo2—O3	2.342 (2)	Mo7—O18	1.952 (2)
Mo3—O11	1.714 (2)	Mo7—O15	2.273 (2)
Mo3—O12	1.714 (2)	Pt3—O27	1.995 (2)
Mo3—O6	1.916 (2)	Pt3—O29	1.996 (2)
Mo3—O4^{i}	1.945 (2)	Pt3—O28	1.998 (2)
Mo3—O1^{i}	2.287 (2)	Pt3—O25	1.999 (2)
Mo3—O3	2.317 (2)	Pt3—O26	2.000 (2)
Pt2—O15	1.999 (2)	Pt3—O30	2.010 (2)
Pt2—O13	2.000 (2)		

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O25	0.82 (2)	1.71 (2)	2.532 (3)	179 (4)
O2—H2···O26	0.83 (2)	1.62 (2)	2.446 (3)	171 (4)
O3—H3···O27	0.83 (2)	1.78 (2)	2.605 (3)	174 (4)
O13—H13···O28	0.81 (2)	1.67 (2)	2.474 (3)	174 (4)
O14—H14···O29	0.81 (2)	1.82 (2)	2.615 (3)	169 (4)
O15—H15···O30	0.81 (2)	1.70 (2)	2.506 (3)	176 (4)
O25—H25···O31	0.81 (2)	1.96 (2)	2.768 (4)	177 (4)
O26—H26···O32	0.81 (2)	2.01 (2)	2.786 (4)	163 (4)
O27—H27···O35	0.80 (2)	2.34 (3)	3.078 (4)	154 (4)
O28—H28···O34	0.81 (2)	2.17 (2)	2.972 (3)	175 (4)
O29—H29···O35	0.81 (2)	2.04 (2)	2.853 (4)	174 (4)
O30—H30···O36	0.81 (2)	2.03 (2)	2.830 (4)	172 (4)

There are $[Pt(OH)_6]^{2-}$ anions in addition to the $[H_6PtMo_6O_{24}]^{2-}$ anions, and they form a hydrogen-bonded polymer in the crystal (Fig. 2). The hydrogen bonds that hold

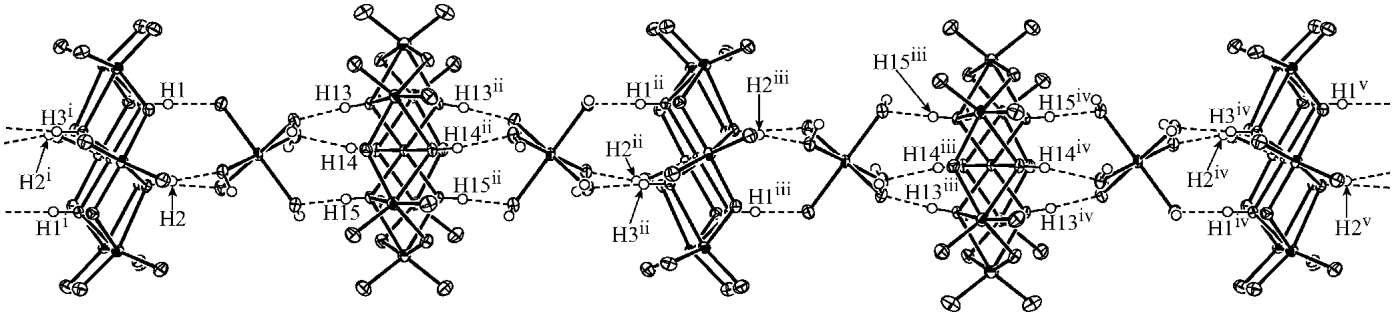


Figure 2
The hydrogen-bonded polymer formed by $[H_6PtMo_6O_{24}]^{2-}$ and $[Pt(OH)_6]^{2-}$ anions. [Symmetry codes: (i) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z$; (ii) $-x, y, -z+\frac{1}{2}$; (iii) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (iv) $-x-\frac{1}{2}, -y+\frac{1}{2}, -z+1$; (v) $x-1, y, z+1$.]

Table 3
Experimental details.

Crystal data	
Chemical formula	$(C_{16}H_{36}N)_3H[Pt(OH)_6]$-$[H_6PtMo_6O_{24}]\cdot 15H_2O$
M_r	2456.53
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	123
a, *b*, *c* (Å)	25.2749 (3), 27.2438 (3), 25.6038 (4)
β (°)	94.1516 (13)
V (Å^3)	17584.1 (4)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	4.08
Crystal size (mm)	0.18 × 0.08 × 0.08
Data collection	
Diffractometer	Rigaku VariMax Saturn724R
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.833, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	107516, 24393, 20469
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.719
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.030, 0.066, 1.08
No. of reflections	24393
No. of parameters	1056
No. of restraints	47
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
	$w = 1/[\sigma^2(F_o^2) + (0.0211P)^2 + 98.3848P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.06, −1.14

Computer programs: *CrystalClear* (Molecular Structure Corporation, 2001), *CrysAlis PRO* (Rigaku OD, 2015), *SHELXT2014* (Sheldrick, 2015*a*) and *SHELXL2016* (Sheldrick, 2015*b*).

the polymer together are relatively strong, with O···O distances in the range 2.45–2.62 Å (av. 2.53 Å, see also Table 2). Polymer formation by $X(OH)_6$ and XMo_6O_{24} units through hydrogen bonding is also known for $[\{Te(OH)_6\}(TeMo_6O_{24})]^{6-}$ (Evans, 1974). However, the hydrogen bonds are weaker in this Te complex, with O···O distances in the range 2.59–2.62 Å (av. 2.61 Å). In addition, only four of the six μ_3-O atoms of the $[TeMo_6O_{24}]^{6-}$ anion are hydrogen bonded to the $Te(OH)_6$ unit. Two OH groups of the $Te(OH)_6$ unit are hydrogen bonded to doubly bridging μ_2-O atoms of the Anderson anion. In the current Pt compound, on the other hand, all six μ_3-O atoms (and no μ_2-O atoms) of the Anderson anion are involved in hydrogen bonding with the $[Pt(OH)_6]^{2-}$ anion.

Synthesis and crystallization

To a solution of $H_2Pt(OH)_6$ (0.85 g, 2.8 mmol) in 15.9 ml of aqueous 0.40 *M* $(n\text{-}C_4H_9)_4NOH$ (6.4 mmol) was added 2.45 g (15.1 mmol) of H_2MoO_4. The mixture was stirred for 24 h, after which time the solid left undissolved was removed by filtration. Pale-yellow crystals started to form after allowing the filtrate to stand for several weeks.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

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full crystallographic data

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Fully protonated B-type hexamolybdoplatinate $[H_6PtMo_6O_{24}]^{2-}$ and its adduct formation with $[Pt(OH)_6]^{2-}$

Tomoji Ozeki and Atsushi Yagasaki

Tris(tetra-*n*-butylammonium) hydrogen hexahydroxidoplatinate(IV) [hexahydrogen α-hexamolybdoplatinate(IV)] pentadecahydrate

Crystal data

$(C_{16}H_{36}N)_3H[Pt(OH)_6][H_6PtMo_6O_{24}]\cdot 15H_2O$
M_r = 2456.53
Monoclinic, $C2/c$
a = 25.2749 (3) Å
b = 27.2438 (3) Å
c = 25.6038 (4) Å
β = 94.1516 (13)°
V = 17584.1 (4) Å^3
Z = 8
$F(000)$ = 9824
D_x = 1.856 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 37457 reflections
θ = 2.9–30.8°
μ = 4.08 mm^{-1}
T = 123 K
Block, translucent pale yellow
0.18 × 0.08 × 0.08 mm

Data collection

Rigaku VariMax Saturn724R diffractometer
Radiation source: fine-focus rotating anode generator with focusing mirror
oscillation method, ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2015)
T_{min} = 0.833, T_{max} = 1.000
107516 measured reflections
24393 independent reflections
20469 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 30.7°, θ_{min} = 2.5°
h = −32→34
k = −36→39
l = −34→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.066
S = 1.08
24393 reflections
1056 parameters
47 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0211P)^2 + 98.3848P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.06 e Å^{-3}
$\Delta\rho_{min}$ = −1.14 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. Hydrogen atom positions of the tetrabutylammonium cations were calculated and refined by using AFIX 23 and AFIX 33 of SHELXL. Hydrogen atoms of $[H_6PtMo_6O_{24}]^{2-}$ and $[Pt(OH)_6]^{2-}$ were located from the difference Fourier syntheses. Their positional parameters were refined with the restraint that O-H distances to be 0.82 Å and their isotropic displacement parameters were fixed to 1.5 times the equivalent isotropic displacement parameters to the oxygen atoms to which they attach. The hydrogen atoms of the water molecules of crystallization and the proton that is required by the charge neutrality condition were not located, the situation of which is frequently observed in polyoxometalate crystals. The tetrabutylammonium cation labeled as N1 and C1–C16 is disordered over three groups. The second most dominant group, labeled as N1B and C1B-C16B differs from the most dominant group (N1A, C1A-C16A) only at one terminal methyl group, labeled as C12B (and, consequently, hydrogen atoms on C11 and C12); and the other N and C atoms are at the same positions as those of the most dominant group (N1A, C1A-C16B). Due to the restriction of the SHELX PART command that do not allow nesting of disorder groups, N1B, C1B-C11B and C13B-C16B were given independent labels and their atomic parameters were fixed to those of N1A, C1A–C11A and C13A–C16B by using SHELX EXYZ and EADP commands. The least dominant group (N1C, C1C–C16C) is severely overlapped over the other groups and therefore DFIX and DANG restraints were applied to establish stable refinement. Another disorder is observed at the gamma C atom (C47A and C47B) of another tetrabutylammonium cation (N3 and C33-C48). The disorder of the corresponding terminal (or delta) C atom (C48) was not resolved. This unresolved disorder may account for somewhat large Hirshfeld difference between C47A and C48, to which an Alert level C was issued. Isotropic displacement parameters were applied to non-dominant components of the disordered atoms. Other non-hydrogen atoms were refined with anisotropic displacement parameters.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Pt1	0.250000	0.250000	0.000000	0.01126 (3)	
Mo1	0.30209 (2)	0.35811 (2)	0.03903 (2)	0.01476 (5)	
Mo2	0.35688 (2)	0.25448 (2)	0.08500 (2)	0.01477 (5)	
Mo3	0.30692 (2)	0.14552 (2)	0.04487 (2)	0.01522 (5)	
O1	0.22442 (9)	0.31330 (8)	0.02882 (8)	0.0148 (4)	
H1	0.2072 (14)	0.3127 (14)	0.0548 (11)	0.022*	
O2	0.17925 (8)	0.21732 (8)	−0.00840 (8)	0.0147 (4)	
H2	0.1612 (14)	0.2231 (14)	0.0168 (11)	0.022*	
O3	0.27228 (8)	0.22017 (8)	0.06920 (8)	0.0144 (4)	
H3	0.2480 (12)	0.2193 (14)	0.0891 (13)	0.022*	
O4	0.26768 (9)	0.37022 (8)	−0.02986 (9)	0.0169 (4)	
O5	0.31931 (9)	0.31479 (8)	0.09835 (9)	0.0169 (4)	
O6	0.36223 (8)	0.19366 (8)	0.04546 (9)	0.0167 (4)	
O7	0.27346 (10)	0.40292 (8)	0.07473 (9)	0.0231 (5)	
O8	0.36341 (9)	0.37985 (8)	0.02650 (9)	0.0212 (5)	
O9	0.41923 (9)	0.27585 (9)	0.07744 (10)	0.0221 (5)	
O10	0.35704 (10)	0.23143 (9)	0.14718 (9)	0.0229 (5)	
O11	0.31154 (9)	0.12676 (8)	0.10892 (9)	0.0224 (5)	
O12	0.33582 (10)	0.09983 (8)	0.01080 (10)	0.0241 (5)	
Pt2	0.000000	0.25869 (2)	0.250000	0.01291 (4)	
Mo4	0.000000	0.38261 (2)	0.250000	0.01960 (8)	
Mo5	0.07638 (2)	0.32171 (2)	0.33960 (2)	0.01753 (6)	
Mo6	0.07480 (2)	0.19698 (2)	0.34103 (2)	0.01783 (6)	
Mo7	0.000000	0.13593 (2)	0.250000	0.01688 (8)	
O13	0.00693 (9)	0.31364 (8)	0.19916 (9)	0.0156 (4)	
H13	0.0279 (13)	0.3086 (14)	0.1774 (13)	0.023*	
O14	0.07632 (9)	0.25934 (8)	0.27752 (9)	0.0158 (4)	

H14	0.0961 (14)	0.2615 (14)	0.2544 (12)	0.024*	
O15	0.00708 (8)	0.20373 (8)	0.19927 (8)	0.0148 (4)	
H15	0.0353 (10)	0.2021 (14)	0.1863 (14)	0.022*	
O16	0.07042 (9)	0.36452 (8)	0.27933 (9)	0.0196 (5)	
O17	0.05929 (9)	0.25949 (8)	0.37196 (9)	0.0186 (5)	
O18	0.07045 (9)	0.15308 (8)	0.28086 (9)	0.0192 (5)	
O19	0.01990 (11)	0.41979 (9)	0.20125 (11)	0.0308 (6)	
O20	0.05472 (10)	0.35931 (9)	0.38680 (10)	0.0271 (5)	
O21	0.14433 (10)	0.32146 (9)	0.34866 (10)	0.0265 (5)	
O22	0.14299 (10)	0.19649 (9)	0.34908 (10)	0.0269 (5)	
O23	0.05383 (11)	0.16022 (9)	0.38897 (10)	0.0277 (5)	
O24	0.02094 (10)	0.09821 (9)	0.20196 (10)	0.0256 (5)	
Pt3	0.13345 (2)	0.25409 (2)	0.13410 (2)	0.01389 (3)	
O25	0.17155 (9)	0.31295 (8)	0.10913 (9)	0.0193 (5)	
H25	0.1964 (12)	0.3168 (15)	0.1307 (13)	0.029*	
O26	0.11828 (9)	0.23409 (8)	0.05937 (9)	0.0178 (4)	
H26	0.0987 (14)	0.2108 (11)	0.0560 (16)	0.027*	
O27	0.20026 (9)	0.21491 (9)	0.13677 (9)	0.0194 (5)	
H27	0.2204 (14)	0.2187 (16)	0.1619 (11)	0.029*	
O28	0.06650 (9)	0.29332 (9)	0.12972 (9)	0.0190 (5)	
H28	0.0472 (14)	0.2805 (14)	0.1071 (13)	0.029*	
O29	0.14513 (9)	0.27650 (9)	0.20825 (9)	0.0188 (5)	
H29	0.1711 (12)	0.2629 (14)	0.2220 (16)	0.028*	
O30	0.09301 (9)	0.19532 (8)	0.15704 (9)	0.0193 (5)	
H30	0.1101 (15)	0.1823 (14)	0.1810 (12)	0.029*	
O31	0.25841 (10)	0.32422 (10)	0.18036 (10)	0.0309 (6)	
O32	0.04578 (12)	0.16150 (11)	0.02630 (13)	0.0419 (7)	
O33	0.17865 (10)	0.11520 (9)	0.11516 (10)	0.0276 (5)	
O34	−0.00400 (10)	0.25222 (9)	0.04254 (10)	0.0263 (5)	
O35	0.24133 (12)	0.23304 (12)	0.25127 (13)	0.0462 (8)	
O36	0.16174 (10)	0.15151 (10)	0.23588 (10)	0.0292 (6)	
O37	0.14510 (12)	0.38033 (10)	0.20602 (12)	0.0396 (7)	
O38	0.0823 (2)	0.39092 (15)	0.09682 (18)	0.0826 (14)	
O39	0.04806 (11)	0.33497 (11)	0.00474 (12)	0.0385 (7)	
O40	0.07003 (12)	0.09220 (14)	0.10122 (14)	0.0535 (9)	
O41	0.31430 (13)	0.16703 (12)	0.22367 (12)	0.0452 (8)	
O42	0.24120 (12)	0.08789 (11)	0.20585 (12)	0.0398 (7)	
O43	0.21516 (15)	0.44421 (12)	0.15548 (15)	0.0582 (10)	
O44	0.23310 (12)	0.25627 (11)	0.35535 (14)	0.0466 (8)	
O45	0.14619 (17)	0.47164 (13)	0.06749 (15)	0.0633 (11)	
N1A	0.58609 (17)	0.22036 (16)	0.10264 (18)	0.0320 (9)	0.545 (3)
C1A	0.6179 (2)	0.2327 (2)	0.1531 (2)	0.0297 (11)	0.545 (3)
H1A	0.654351	0.241473	0.144880	0.036*	0.545 (3)
H1B	0.620247	0.202954	0.175392	0.036*	0.545 (3)
C2A	0.5953 (3)	0.2744 (3)	0.1840 (3)	0.0414 (18)	0.545 (3)
H2A	0.560434	0.264517	0.195895	0.050*	0.545 (3)
H2B	0.589885	0.303531	0.161212	0.050*	0.545 (3)
C3A	0.6332 (2)	0.28756 (19)	0.23203 (19)	0.0329 (11)	0.545 (3)

H3A	0.636886	0.259005	0.255933	0.039*	0.545 (3)
H3B	0.668774	0.295351	0.220326	0.039*	0.545 (3)
C4A	0.6126 (2)	0.3311 (2)	0.2610 (2)	0.0462 (15)	0.545 (3)
H4A	0.637223	0.338773	0.291184	0.069*	0.545 (3)
H4B	0.609521	0.359467	0.237455	0.069*	0.545 (3)
H4C	0.577674	0.323168	0.273017	0.069*	0.545 (3)
C5A	0.6136 (2)	0.1772 (2)	0.0794 (2)	0.0391 (13)	0.545 (3)
H5A	0.615163	0.150143	0.105258	0.047*	0.545 (3)
H5B	0.650540	0.186893	0.073972	0.047*	0.545 (3)
C6A	0.5882 (2)	0.1579 (2)	0.0281 (2)	0.0456 (15)	0.545 (3)
H6A	0.579474	0.185652	0.004034	0.055*	0.545 (3)
H6B	0.554880	0.140541	0.034425	0.055*	0.545 (3)
C7A	0.6269 (3)	0.1223 (2)	0.0029 (3)	0.052 (2)	0.545 (3)
H7A	0.639674	0.097544	0.029235	0.063*	0.545 (3)
H7B	0.607590	0.104724	−0.026452	0.063*	0.545 (3)
C8A	0.6730 (3)	0.1480 (3)	−0.0167 (3)	0.062 (2)	0.545 (3)
H8A	0.696272	0.124130	−0.032226	0.093*	0.545 (3)
H8B	0.660639	0.172079	−0.043303	0.093*	0.545 (3)
H8C	0.692721	0.164900	0.012381	0.093*	0.545 (3)
C9A	0.5291 (2)	0.2075 (2)	0.1130 (3)	0.0421 (14)	0.545 (3)
H9A	0.511491	0.237545	0.124841	0.051*	0.545 (3)
H9B	0.510274	0.197358	0.079432	0.051*	0.545 (3)
C10A	0.5222 (3)	0.1673 (3)	0.1530 (3)	0.0562 (17)	0.545 (3)
H10A	0.541403	0.176222	0.186762	0.067*	0.545 (3)
H10B	0.537247	0.136128	0.140764	0.067*	0.545 (3)
C11A	0.4633 (3)	0.1605 (3)	0.1608 (4)	0.071 (2)	0.545 (3)
H11A	0.448716	0.192553	0.170894	0.085*	0.545 (3)
H11B	0.445077	0.151250	0.126629	0.085*	0.545 (3)
C12A	0.4499 (4)	0.1244 (4)	0.1992 (5)	0.067 (3)	0.545 (3)
H12A	0.411343	0.123151	0.200877	0.101*	0.545 (3)
H12B	0.462902	0.092056	0.189231	0.101*	0.545 (3)
H12C	0.466554	0.133496	0.233644	0.101*	0.545 (3)
C13A	0.5834 (2)	0.26396 (19)	0.0655 (2)	0.0344 (12)	0.545 (3)
H13A	0.558434	0.255785	0.035164	0.041*	0.545 (3)
H13B	0.568220	0.292130	0.083746	0.041*	0.545 (3)
C14A	0.6343 (3)	0.2799 (2)	0.0453 (2)	0.0451 (14)	0.545 (3)
H14A	0.646724	0.254943	0.020928	0.054*	0.545 (3)
H14B	0.661690	0.283561	0.074754	0.054*	0.545 (3)
C15A	0.6260 (3)	0.3289 (3)	0.0169 (3)	0.064 (2)	0.545 (3)
H15A	0.595987	0.325556	−0.009848	0.076*	0.545 (3)
H15B	0.616119	0.353977	0.042462	0.076*	0.545 (3)
C16A	0.6736 (5)	0.3468 (4)	−0.0092 (4)	0.091 (4)	0.545 (3)
H16A	0.665284	0.378249	−0.026523	0.137*	0.545 (3)
H16B	0.703379	0.351166	0.017058	0.137*	0.545 (3)
H16C	0.683218	0.322704	−0.035329	0.137*	0.545 (3)
N1B	0.58609 (17)	0.22036 (16)	0.10264 (18)	0.0320 (9)	0.251 (3)
C1B	0.6179 (2)	0.2327 (2)	0.1531 (2)	0.0297 (11)	0.251 (3)
H1C	0.654351	0.241473	0.144880	0.036*	0.251 (3)

H1D	0.620247	0.202954	0.175392	0.036*	0.251 (3)
C2B	0.5953 (3)	0.2744 (3)	0.1840 (3)	0.0414 (18)	0.251 (3)
H2C	0.560434	0.264517	0.195895	0.050*	0.251 (3)
H2D	0.589885	0.303531	0.161212	0.050*	0.251 (3)
C3B	0.6332 (2)	0.28756 (19)	0.23203 (19)	0.0329 (11)	0.251 (3)
H3C	0.636886	0.259005	0.255933	0.039*	0.251 (3)
H3D	0.668774	0.295351	0.220326	0.039*	0.251 (3)
C4B	0.6126 (2)	0.3311 (2)	0.2610 (2)	0.0462 (15)	0.251 (3)
H4D	0.637223	0.338773	0.291184	0.069*	0.251 (3)
H4E	0.609521	0.359467	0.237455	0.069*	0.251 (3)
H4F	0.577674	0.323168	0.273017	0.069*	0.251 (3)
C5B	0.6136 (2)	0.1772 (2)	0.0794 (2)	0.0391 (13)	0.251 (3)
H5C	0.615163	0.150143	0.105258	0.047*	0.251 (3)
H5D	0.650540	0.186893	0.073972	0.047*	0.251 (3)
C6B	0.5882 (2)	0.1579 (2)	0.0281 (2)	0.0456 (15)	0.251 (3)
H6C	0.579474	0.185652	0.004034	0.055*	0.251 (3)
H6D	0.554880	0.140541	0.034425	0.055*	0.251 (3)
C7B	0.6269 (3)	0.1223 (2)	0.0029 (3)	0.052 (2)	0.251 (3)
H7C	0.639674	0.097544	0.029235	0.063*	0.251 (3)
H7D	0.607590	0.104724	−0.026452	0.063*	0.251 (3)
C8B	0.6730 (3)	0.1480 (3)	−0.0167 (3)	0.062 (2)	0.251 (3)
H8D	0.696272	0.124130	−0.032226	0.093*	0.251 (3)
H8E	0.660639	0.172079	−0.043303	0.093*	0.251 (3)
H8F	0.692721	0.164900	0.012381	0.093*	0.251 (3)
C9B	0.5291 (2)	0.2075 (2)	0.1130 (3)	0.0421 (14)	0.251 (3)
H9C	0.511491	0.237545	0.124841	0.051*	0.251 (3)
H9D	0.510274	0.197358	0.079432	0.051*	0.251 (3)
C10B	0.5222 (3)	0.1673 (3)	0.1530 (3)	0.0562 (17)	0.251 (3)
H10C	0.541403	0.176222	0.186762	0.067*	0.251 (3)
H10D	0.537247	0.136128	0.140764	0.067*	0.251 (3)
C11B	0.4633 (3)	0.1605 (3)	0.1608 (4)	0.071 (2)	0.251 (3)
H11C	0.454831	0.126366	0.170556	0.085*	0.251 (3)
H11D	0.440540	0.170375	0.129413	0.085*	0.251 (3)
C12B	0.4585 (8)	0.2007 (7)	0.2120 (8)	0.060 (6)*	0.251 (3)
H12D	0.421980	0.201072	0.222475	0.090*	0.251 (3)
H12E	0.482505	0.190262	0.241744	0.090*	0.251 (3)
H12F	0.468383	0.233752	0.201087	0.090*	0.251 (3)
C13B	0.5834 (2)	0.26396 (19)	0.0655 (2)	0.0344 (12)	0.251 (3)
H13C	0.558434	0.255785	0.035164	0.041*	0.251 (3)
H13D	0.568220	0.292130	0.083746	0.041*	0.251 (3)
C14B	0.6343 (3)	0.2799 (2)	0.0453 (2)	0.0451 (14)	0.251 (3)
H14C	0.646724	0.254943	0.020928	0.054*	0.251 (3)
H14D	0.661690	0.283561	0.074754	0.054*	0.251 (3)
C15B	0.6260 (3)	0.3289 (3)	0.0169 (3)	0.064 (2)	0.251 (3)
H15C	0.595987	0.325556	−0.009848	0.076*	0.251 (3)
H15D	0.616119	0.353977	0.042462	0.076*	0.251 (3)
C16B	0.6736 (5)	0.3468 (4)	−0.0092 (4)	0.091 (4)	0.251 (3)
H16D	0.665284	0.378249	−0.026523	0.137*	0.251 (3)

H16E	0.703379	0.351166	0.017058	0.137*	0.251 (3)
H16F	0.683218	0.322704	−0.035329	0.137*	0.251 (3)
N1C	0.6036 (5)	0.2313 (4)	0.0847 (5)	0.017 (3)*	0.205 (3)
C1C	0.6315 (7)	0.2412 (7)	0.1391 (6)	0.024 (5)*	0.205 (3)
H1E	0.634053	0.209785	0.158550	0.029*	0.205 (3)
H1F	0.668179	0.252250	0.134336	0.029*	0.205 (3)
C2C	0.6053 (10)	0.2793 (8)	0.1734 (8)	0.017 (5)*	0.205 (3)
H2E	0.568366	0.285404	0.159300	0.021*	0.205 (3)
H2F	0.624990	0.310702	0.173007	0.021*	0.205 (3)
C3C	0.6054 (15)	0.2596 (12)	0.2310 (9)	0.083 (10)*	0.205 (3)
H3E	0.593559	0.224966	0.229847	0.099*	0.205 (3)
H3F	0.642335	0.260174	0.246858	0.099*	0.205 (3)
C4C	0.5712 (15)	0.2877 (14)	0.2653 (12)	0.102 (12)*	0.205 (3)
H4G	0.573581	0.273076	0.300371	0.122*	0.205 (3)
H4H	0.583254	0.321871	0.267594	0.122*	0.205 (3)
H4I	0.534390	0.286600	0.250552	0.122*	0.205 (3)
C5C	0.6346 (6)	0.1920 (5)	0.0584 (5)	0.015 (3)*	0.205 (3)
H5E	0.672296	0.202210	0.060293	0.018*	0.205 (3)
H5F	0.632662	0.161531	0.079287	0.018*	0.205 (3)
C6C	0.6182 (8)	0.1796 (6)	0.0022 (6)	0.031 (4)*	0.205 (3)
H6E	0.635709	0.201989	−0.021628	0.037*	0.205 (3)
H6F	0.579300	0.182972	−0.004495	0.037*	0.205 (3)
C7C	0.635 (2)	0.1264 (9)	−0.007 (2)	0.25 (5)*	0.205 (3)
H7E	0.634304	0.121086	−0.044987	0.300*	0.205 (3)
H7F	0.672760	0.123351	0.006962	0.300*	0.205 (3)
C8C	0.6053 (14)	0.0850 (11)	0.0160 (14)	0.085 (10)*	0.205 (3)
H8G	0.621250	0.053660	0.006713	0.102*	0.205 (3)
H8H	0.606915	0.088230	0.054212	0.102*	0.205 (3)
H8I	0.568227	0.085951	0.001950	0.102*	0.205 (3)
C9C	0.5455 (6)	0.2183 (7)	0.0860 (8)	0.031 (4)*	0.205 (3)
H9E	0.530705	0.212465	0.049712	0.038*	0.205 (3)
H9F	0.526649	0.246890	0.099732	0.038*	0.205 (3)
C10C	0.5339 (8)	0.1736 (9)	0.1190 (11)	0.055 (7)*	0.205 (3)
H10E	0.539556	0.143288	0.098763	0.066*	0.205 (3)
H10F	0.558385	0.172979	0.150933	0.066*	0.205 (3)
C11C	0.4774 (9)	0.1756 (9)	0.1339 (11)	0.052 (6)*	0.205 (3)
H11E	0.472313	0.207043	0.152256	0.063*	0.205 (3)
H11F	0.453835	0.176169	0.101266	0.063*	0.205 (3)
C12C	0.4596 (12)	0.1357 (11)	0.1671 (13)	0.060 (9)*	0.205 (3)
H12G	0.422434	0.141086	0.174066	0.072*	0.205 (3)
H12H	0.462995	0.104290	0.149055	0.072*	0.205 (3)
H12I	0.481543	0.135281	0.200239	0.072*	0.205 (3)
C13C	0.6062 (9)	0.2777 (7)	0.0516 (8)	0.033 (5)*	0.205 (3)
H13E	0.583655	0.272618	0.018753	0.040*	0.205 (3)
H13F	0.590347	0.304941	0.070744	0.040*	0.205 (3)
C14C	0.6605 (10)	0.2937 (10)	0.0373 (12)	0.062 (8)*	0.205 (3)
H14E	0.677081	0.266376	0.018795	0.074*	0.205 (3)
H14F	0.682933	0.300263	0.069849	0.074*	0.205 (3)

C15C	0.6600 (12)	0.3393 (11)	0.0027 (14)	0.054 (9)*	0.205 (3)
H15E	0.637656	0.333120	−0.029976	0.065*	0.205 (3)
H15F	0.644327	0.367052	0.021192	0.065*	0.205 (3)
C16C	0.7149 (13)	0.3525 (13)	−0.0104 (15)	0.088 (11)*	0.205 (3)
H16G	0.713521	0.381862	−0.032545	0.106*	0.205 (3)
H16H	0.736846	0.359109	0.021973	0.106*	0.205 (3)
H16I	0.730183	0.325218	−0.029132	0.106*	0.205 (3)
N2	0.38010 (12)	0.51048 (10)	0.14781 (12)	0.0232 (6)	
C17	0.41819 (15)	0.54048 (13)	0.11674 (14)	0.0266 (8)	
H17A	0.411078	0.575751	0.122379	0.032*	
H17B	0.454878	0.533777	0.131167	0.032*	
C18	0.41515 (17)	0.53080 (16)	0.05800 (15)	0.0340 (9)	
H18A	0.422150	0.495655	0.051498	0.041*	
H18B	0.379105	0.538637	0.042538	0.041*	
C19	0.45558 (17)	0.56203 (16)	0.03245 (16)	0.0347 (9)	
H19A	0.491433	0.554240	0.048444	0.042*	
H19B	0.448432	0.597073	0.039363	0.042*	
C20	0.4546 (2)	0.55390 (19)	−0.02669 (17)	0.0469 (12)	
H20A	0.481387	0.574837	−0.041358	0.070*	
H20B	0.462458	0.519400	−0.033774	0.070*	
H20C	0.419452	0.562238	−0.042857	0.070*	
C21	0.38624 (14)	0.45602 (12)	0.13760 (14)	0.0243 (7)	
H21A	0.360024	0.438045	0.157246	0.029*	
H21B	0.377419	0.449847	0.099870	0.029*	
C22	0.44079 (15)	0.43491 (13)	0.15238 (16)	0.0294 (8)	
H22A	0.446417	0.432446	0.190958	0.035*	
H22B	0.468325	0.456916	0.139797	0.035*	
C23	0.44559 (15)	0.38433 (13)	0.12808 (16)	0.0297 (8)	
H23A	0.415721	0.363604	0.137927	0.036*	
H23B	0.442960	0.387510	0.089464	0.036*	
C24	0.49757 (16)	0.35928 (15)	0.14557 (18)	0.0375 (10)	
H24A	0.498926	0.326920	0.129002	0.056*	
H24B	0.527276	0.379328	0.135264	0.056*	
H24C	0.500039	0.355424	0.183723	0.056*	
C25	0.39338 (14)	0.52239 (13)	0.20529 (14)	0.0251 (7)	
H25A	0.393302	0.558503	0.209544	0.030*	
H25B	0.429811	0.510704	0.215241	0.030*	
C26	0.35607 (16)	0.50030 (16)	0.24311 (15)	0.0316 (8)	
H26A	0.354789	0.464216	0.238594	0.038*	
H26B	0.319814	0.513339	0.235195	0.038*	
C27	0.37485 (16)	0.51264 (16)	0.29970 (15)	0.0330 (9)	
H27A	0.381258	0.548426	0.302486	0.040*	
H27B	0.346258	0.504377	0.322664	0.040*	
C28	0.42525 (19)	0.48566 (18)	0.31938 (18)	0.0437 (11)	
H28A	0.435041	0.495202	0.355699	0.066*	
H28B	0.419035	0.450176	0.317636	0.066*	
H28C	0.454071	0.494271	0.297438	0.066*	
C29	0.32286 (14)	0.52307 (14)	0.13131 (14)	0.0260 (7)	

H29A	0.316378	0.516007	0.093454	0.031*
H29B	0.299580	0.501116	0.150240	0.031*
C30	0.30696 (17)	0.57497 (15)	0.14079 (17)	0.0376 (10)
H30A	0.324466	0.597087	0.116671	0.045*
H30B	0.318510	0.584511	0.177152	0.045*
C31	0.2462 (2)	0.5802 (2)	0.1319 (2)	0.0607 (15)
H31A	0.235730	0.576167	0.094158	0.073*
H31B	0.229051	0.553710	0.151056	0.073*
C32	0.2270 (3)	0.6281 (2)	0.1496 (2)	0.0727 (18)
H32A	0.188338	0.629702	0.143188	0.109*
H32B	0.236605	0.632036	0.187162	0.109*
H32C	0.243285	0.654495	0.130260	0.109*
N3	0.16227 (13)	0.48302 (11)	0.35298 (13)	0.0298 (7)
C33	0.20126 (17)	0.50701 (13)	0.39315 (15)	0.0320 (9)
H33A	0.185631	0.538254	0.404396	0.038*
H33B	0.233876	0.515217	0.375796	0.038*
C34	0.21694 (19)	0.47672 (15)	0.44180 (16)	0.0390 (10)
H34A	0.230222	0.444279	0.431231	0.047*
H34B	0.185395	0.471281	0.461843	0.047*
C35	0.25990 (19)	0.50280 (15)	0.47650 (17)	0.0409 (10)
H35A	0.247649	0.536454	0.483822	0.049*
H35B	0.264788	0.485207	0.510335	0.049*
C36	0.3128 (2)	0.50593 (18)	0.4527 (2)	0.0520 (13)
H36A	0.338399	0.523011	0.476907	0.078*
H36B	0.325800	0.472753	0.446123	0.078*
H36C	0.308641	0.524059	0.419580	0.078*
C37	0.18408 (17)	0.43504 (14)	0.33315 (17)	0.0344 (9)
H37A	0.156124	0.419176	0.309882	0.041*
H37B	0.191882	0.412999	0.363477	0.041*
C38	0.2340 (2)	0.43964 (18)	0.3034 (2)	0.0487 (12)
H38A	0.258785	0.463297	0.321529	0.058*
H38B	0.224609	0.452002	0.267612	0.058*
C39	0.2607 (2)	0.3892 (2)	0.3007 (2)	0.0569 (14)
H39A	0.233299	0.364177	0.291223	0.068*
H39B	0.285710	0.389781	0.272648	0.068*
C40	0.2898 (3)	0.3749 (2)	0.3504 (2)	0.0730 (18)
H40A	0.305990	0.342565	0.346369	0.109*
H40B	0.317583	0.399134	0.359581	0.109*
H40C	0.265149	0.373518	0.378165	0.109*
C41	0.11105 (18)	0.47056 (16)	0.37643 (18)	0.0397 (10)
H41A	0.118312	0.445206	0.403706	0.048*
H41B	0.086473	0.456060	0.348755	0.048*
C42	0.0833 (2)	0.5140 (2)	0.4008 (2)	0.0592 (14)
H42A	0.104910	0.525945	0.432045	0.071*
H42B	0.078961	0.541218	0.375292	0.071*
C43	0.0294 (3)	0.4972 (3)	0.4164 (3)	0.085 (2)
H43A	0.033761	0.469424	0.441258	0.102*
H43B	0.007575	0.485898	0.385026	0.102*

C44	0.0018 (4)	0.5399 (4)	0.4420 (4)	0.135 (4)	
H44A	−0.033056	0.529121	0.452045	0.202*	
H44B	0.023390	0.550691	0.473150	0.202*	
H44C	−0.002728	0.567122	0.417063	0.202*	
C45	0.15373 (19)	0.51962 (15)	0.30840 (16)	0.0375 (10)	
H45A	0.141874	0.551044	0.323060	0.045*	
H45B	0.188331	0.525704	0.293763	0.045*	
C46	0.1144 (2)	0.50496 (19)	0.2642 (2)	0.0539 (13)	
H46A	0.077782	0.507875	0.275161	0.065*	0.797 (16)
H46B	0.120472	0.470506	0.253886	0.065*	0.797 (16)
H46C	0.132945	0.481488	0.242320	0.065*	0.203 (16)
H46D	0.086193	0.486165	0.280154	0.065*	0.203 (16)
C47A	0.1228 (4)	0.5413 (3)	0.2158 (3)	0.065 (3)	0.797 (16)
H47A	0.120489	0.575755	0.227681	0.078*	0.797 (16)
H47B	0.158501	0.536055	0.203341	0.078*	0.797 (16)
C47B	0.0877 (10)	0.5399 (7)	0.2284 (8)	0.030 (6)*	0.203 (16)
H47C	0.051225	0.543799	0.239505	0.036*	0.203 (16)
H47D	0.105679	0.571901	0.234616	0.036*	0.203 (16)
C48	0.0830 (3)	0.5326 (3)	0.1733 (3)	0.092 (2)	
H48A	0.088830	0.555009	0.144381	0.138*	0.797 (16)
H48B	0.085648	0.498587	0.161261	0.138*	0.797 (16)
H48C	0.047687	0.538234	0.185569	0.138*	0.797 (16)
H48D	0.063791	0.560209	0.156419	0.138*	0.203 (16)
H48E	0.118484	0.530385	0.160339	0.138*	0.203 (16)
H48F	0.063599	0.502061	0.165267	0.138*	0.203 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.01088 (7)	0.01183 (7)	0.01131 (7)	−0.00033 (6)	0.00239 (5)	0.00048 (5)
Mo1	0.01494 (13)	0.01407 (12)	0.01536 (13)	−0.00181 (10)	0.00165 (9)	−0.00082 (9)
Mo2	0.01338 (12)	0.01612 (12)	0.01473 (13)	−0.00069 (10)	0.00058 (9)	0.00013 (9)
Mo3	0.01466 (13)	0.01328 (12)	0.01780 (14)	0.00075 (9)	0.00173 (10)	0.00115 (9)
O1	0.0185 (11)	0.0136 (10)	0.0128 (11)	0.0009 (8)	0.0054 (8)	−0.0004 (8)
O2	0.0143 (11)	0.0164 (10)	0.0138 (11)	−0.0038 (8)	0.0041 (8)	−0.0011 (8)
O3	0.0143 (11)	0.0164 (10)	0.0129 (11)	−0.0002 (8)	0.0032 (8)	0.0030 (8)
O4	0.0166 (11)	0.0151 (10)	0.0189 (12)	−0.0027 (8)	0.0012 (8)	0.0025 (8)
O5	0.0201 (11)	0.0148 (10)	0.0158 (11)	−0.0001 (9)	0.0017 (9)	−0.0021 (8)
O6	0.0131 (11)	0.0168 (10)	0.0204 (12)	0.0000 (8)	0.0037 (8)	−0.0006 (8)
O7	0.0248 (13)	0.0187 (11)	0.0259 (13)	−0.0001 (10)	0.0032 (10)	−0.0021 (9)
O8	0.0198 (12)	0.0216 (11)	0.0221 (12)	−0.0046 (9)	0.0013 (9)	0.0012 (9)
O9	0.0155 (11)	0.0220 (12)	0.0288 (13)	−0.0026 (9)	0.0016 (9)	−0.0019 (10)
O10	0.0264 (13)	0.0228 (12)	0.0191 (12)	0.0016 (10)	−0.0008 (9)	0.0010 (9)
O11	0.0241 (12)	0.0180 (11)	0.0246 (13)	−0.0009 (9)	−0.0008 (10)	0.0037 (9)
O12	0.0231 (13)	0.0187 (11)	0.0306 (14)	0.0025 (10)	0.0035 (10)	−0.0026 (10)
Pt2	0.01203 (7)	0.01370 (7)	0.01345 (8)	0.000	0.00410 (5)	0.000
Mo4	0.01857 (19)	0.01647 (18)	0.0238 (2)	0.000	0.00176 (15)	0.000
Mo5	0.01739 (13)	0.01843 (13)	0.01689 (14)	−0.00287 (10)	0.00213 (10)	−0.00036 (10)

Mo6	0.01845 (14)	0.01780 (13)	0.01738 (14)	0.00069 (10)	0.00226 (10)	0.00250 (10)
Mo7	0.01417 (18)	0.01452 (17)	0.0223 (2)	0.000	0.00368 (14)	0.000
O13	0.0175 (11)	0.0162 (10)	0.0141 (11)	−0.0002 (8)	0.0068 (8)	0.0026 (8)
O14	0.0128 (10)	0.0207 (11)	0.0144 (11)	−0.0017 (8)	0.0046 (8)	−0.0002 (8)
O15	0.0128 (10)	0.0163 (10)	0.0159 (11)	0.0007 (8)	0.0054 (8)	−0.0028 (8)
O16	0.0171 (11)	0.0208 (11)	0.0212 (12)	−0.0044 (9)	0.0040 (9)	0.0030 (9)
O17	0.0237 (12)	0.0190 (11)	0.0136 (11)	−0.0024 (9)	0.0041 (9)	0.0010 (8)
O18	0.0163 (11)	0.0197 (11)	0.0219 (12)	0.0024 (9)	0.0033 (9)	−0.0008 (9)
O19	0.0304 (14)	0.0248 (13)	0.0367 (16)	−0.0057 (11)	−0.0014 (11)	0.0090 (11)
O20	0.0328 (14)	0.0256 (13)	0.0236 (13)	−0.0036 (11)	0.0065 (10)	−0.0058 (10)
O21	0.0208 (13)	0.0288 (13)	0.0297 (14)	−0.0061 (10)	−0.0009 (10)	0.0042 (10)
O22	0.0220 (13)	0.0277 (13)	0.0302 (14)	0.0033 (10)	−0.0031 (10)	−0.0007 (10)
O23	0.0355 (15)	0.0239 (12)	0.0242 (13)	0.0006 (11)	0.0057 (11)	0.0074 (10)
O24	0.0240 (13)	0.0237 (12)	0.0296 (14)	0.0039 (10)	0.0040 (10)	−0.0054 (10)
Pt3	0.01283 (5)	0.01678 (6)	0.01251 (6)	−0.00079 (4)	0.00394 (4)	−0.00042 (4)
O25	0.0210 (12)	0.0212 (11)	0.0160 (12)	−0.0049 (9)	0.0043 (9)	−0.0005 (9)
O26	0.0166 (11)	0.0216 (11)	0.0155 (11)	−0.0039 (9)	0.0040 (8)	−0.0036 (9)
O27	0.0156 (11)	0.0240 (12)	0.0189 (12)	0.0038 (9)	0.0033 (9)	0.0010 (9)
O28	0.0192 (12)	0.0227 (12)	0.0156 (12)	0.0045 (9)	0.0044 (9)	−0.0011 (9)
O29	0.0182 (11)	0.0269 (12)	0.0113 (11)	−0.0015 (9)	0.0022 (8)	−0.0003 (9)
O30	0.0191 (12)	0.0214 (11)	0.0183 (12)	−0.0013 (9)	0.0064 (9)	0.0011 (9)
O31	0.0260 (14)	0.0442 (16)	0.0231 (14)	−0.0011 (12)	0.0050 (10)	−0.0068 (11)
O32	0.0397 (17)	0.0340 (16)	0.055 (2)	−0.0084 (13)	0.0217 (14)	−0.0102 (14)
O33	0.0269 (13)	0.0313 (14)	0.0255 (14)	−0.0030 (11)	0.0083 (10)	−0.0012 (10)
O34	0.0257 (13)	0.0318 (14)	0.0219 (13)	−0.0008 (11)	0.0047 (10)	0.0028 (10)
O35	0.0339 (17)	0.053 (2)	0.049 (2)	0.0067 (14)	−0.0118 (14)	−0.0004 (15)
O36	0.0227 (13)	0.0341 (14)	0.0318 (15)	0.0032 (11)	0.0098 (11)	0.0010 (11)
O37	0.0410 (17)	0.0329 (15)	0.0478 (18)	−0.0055 (13)	0.0222 (14)	−0.0079 (13)
O38	0.117 (4)	0.054 (2)	0.076 (3)	−0.018 (2)	0.006 (3)	0.006 (2)
O39	0.0274 (15)	0.0378 (16)	0.0518 (19)	0.0035 (12)	0.0141 (13)	0.0044 (13)
O40	0.0298 (17)	0.080 (3)	0.051 (2)	−0.0042 (17)	0.0013 (14)	0.0086 (18)
O41	0.0468 (19)	0.0518 (19)	0.0387 (18)	0.0025 (15)	0.0151 (14)	0.0104 (14)
O42	0.0421 (17)	0.0343 (15)	0.0432 (18)	0.0150 (13)	0.0051 (13)	0.0042 (13)
O43	0.066 (2)	0.0424 (19)	0.070 (2)	−0.0150 (17)	0.036 (2)	−0.0197 (17)
O44	0.0280 (15)	0.0432 (18)	0.068 (2)	0.0001 (13)	0.0006 (15)	−0.0055 (15)
O45	0.090 (3)	0.0408 (19)	0.063 (2)	−0.0050 (19)	0.035 (2)	−0.0160 (17)
N1A	0.028 (2)	0.029 (2)	0.037 (3)	0.0055 (18)	−0.0057 (19)	−0.0030 (18)
C1A	0.027 (3)	0.034 (3)	0.028 (3)	0.005 (2)	−0.004 (2)	0.007 (2)
C2A	0.037 (4)	0.063 (4)	0.025 (3)	0.020 (3)	0.005 (3)	0.007 (3)
C3A	0.035 (3)	0.035 (3)	0.027 (3)	0.006 (2)	−0.011 (2)	0.0000 (19)
C4A	0.035 (3)	0.066 (4)	0.035 (3)	0.017 (3)	−0.015 (2)	−0.021 (3)
C5A	0.038 (3)	0.034 (3)	0.043 (3)	0.012 (2)	−0.007 (2)	−0.010 (2)
C6A	0.041 (3)	0.040 (3)	0.053 (4)	0.014 (3)	−0.012 (3)	−0.018 (3)
C7A	0.048 (4)	0.039 (3)	0.067 (4)	0.014 (3)	−0.022 (3)	−0.027 (3)
C8A	0.061 (4)	0.081 (5)	0.045 (4)	0.016 (4)	0.010 (3)	−0.030 (3)
C9A	0.026 (3)	0.041 (3)	0.059 (4)	0.000 (2)	−0.002 (3)	−0.009 (3)
C10A	0.050 (4)	0.049 (4)	0.070 (5)	−0.007 (3)	0.003 (3)	−0.001 (3)
C11A	0.048 (4)	0.060 (5)	0.109 (7)	0.004 (4)	0.032 (4)	0.005 (5)

C12A	0.059 (7)	0.072 (7)	0.072 (8)	−0.021 (6)	0.015 (6)	−0.002 (6)
C13A	0.045 (3)	0.031 (3)	0.026 (3)	0.009 (2)	−0.007 (2)	−0.001 (2)
C14A	0.054 (4)	0.048 (4)	0.033 (3)	0.002 (3)	0.004 (3)	0.003 (2)
C15A	0.076 (5)	0.061 (4)	0.053 (4)	−0.009 (4)	−0.001 (4)	0.019 (3)
C16A	0.106 (9)	0.104 (8)	0.064 (7)	−0.031 (7)	0.011 (6)	0.021 (5)
N1B	0.028 (2)	0.029 (2)	0.037 (3)	0.0055 (18)	−0.0057 (19)	−0.0030 (18)
C1B	0.027 (3)	0.034 (3)	0.028 (3)	0.005 (2)	−0.004 (2)	0.007 (2)
C2B	0.037 (4)	0.063 (4)	0.025 (3)	0.020 (3)	0.005 (3)	0.007 (3)
C3B	0.035 (3)	0.035 (3)	0.027 (3)	0.006 (2)	−0.011 (2)	0.0000 (19)
C4B	0.035 (3)	0.066 (4)	0.035 (3)	0.017 (3)	−0.015 (2)	−0.021 (3)
C5B	0.038 (3)	0.034 (3)	0.043 (3)	0.012 (2)	−0.007 (2)	−0.010 (2)
C6B	0.041 (3)	0.040 (3)	0.053 (4)	0.014 (3)	−0.012 (3)	−0.018 (3)
C7B	0.048 (4)	0.039 (3)	0.067 (4)	0.014 (3)	−0.022 (3)	−0.027 (3)
C8B	0.061 (4)	0.081 (5)	0.045 (4)	0.016 (4)	0.010 (3)	−0.030 (3)
C9B	0.026 (3)	0.041 (3)	0.059 (4)	0.000 (2)	−0.002 (3)	−0.009 (3)
C10B	0.050 (4)	0.049 (4)	0.070 (5)	−0.007 (3)	0.003 (3)	−0.001 (3)
C11B	0.048 (4)	0.060 (5)	0.109 (7)	0.004 (4)	0.032 (4)	0.005 (5)
C13B	0.045 (3)	0.031 (3)	0.026 (3)	0.009 (2)	−0.007 (2)	−0.001 (2)
C14B	0.054 (4)	0.048 (4)	0.033 (3)	0.002 (3)	0.004 (3)	0.003 (2)
C15B	0.076 (5)	0.061 (4)	0.053 (4)	−0.009 (4)	−0.001 (4)	0.019 (3)
C16B	0.106 (9)	0.104 (8)	0.064 (7)	−0.031 (7)	0.011 (6)	0.021 (5)
N2	0.0242 (15)	0.0208 (14)	0.0241 (16)	−0.0024 (12)	−0.0013 (12)	−0.0041 (11)
C17	0.0265 (19)	0.0256 (18)	0.027 (2)	−0.0058 (14)	−0.0005 (14)	−0.0046 (14)
C18	0.034 (2)	0.039 (2)	0.030 (2)	−0.0116 (17)	0.0056 (16)	−0.0081 (16)
C19	0.036 (2)	0.037 (2)	0.032 (2)	−0.0100 (18)	0.0070 (17)	−0.0066 (17)
C20	0.052 (3)	0.055 (3)	0.036 (3)	−0.012 (2)	0.016 (2)	−0.012 (2)
C21	0.0248 (18)	0.0208 (16)	0.0265 (19)	−0.0039 (14)	−0.0032 (14)	−0.0049 (13)
C22	0.0277 (19)	0.0243 (18)	0.035 (2)	0.0000 (15)	−0.0065 (15)	−0.0064 (15)
C23	0.030 (2)	0.0228 (17)	0.035 (2)	0.0024 (15)	−0.0098 (16)	−0.0040 (15)
C24	0.034 (2)	0.029 (2)	0.048 (3)	0.0048 (17)	−0.0075 (18)	−0.0065 (17)
C25	0.0242 (18)	0.0259 (17)	0.0243 (19)	−0.0028 (14)	−0.0038 (14)	−0.0055 (14)
C26	0.028 (2)	0.040 (2)	0.026 (2)	−0.0060 (17)	−0.0015 (15)	−0.0013 (16)
C27	0.033 (2)	0.041 (2)	0.024 (2)	−0.0032 (17)	−0.0012 (15)	−0.0005 (16)
C28	0.046 (3)	0.045 (3)	0.039 (3)	0.006 (2)	−0.009 (2)	0.0044 (19)
C29	0.0215 (17)	0.0318 (19)	0.0240 (19)	0.0009 (14)	−0.0032 (14)	−0.0030 (14)
C30	0.036 (2)	0.037 (2)	0.038 (2)	0.0096 (18)	−0.0118 (18)	−0.0090 (17)
C31	0.052 (3)	0.048 (3)	0.079 (4)	0.020 (2)	−0.017 (3)	−0.016 (3)
C32	0.072 (4)	0.071 (4)	0.072 (4)	0.035 (3)	−0.018 (3)	−0.011 (3)
N3	0.0381 (19)	0.0199 (14)	0.0316 (18)	−0.0077 (13)	0.0031 (14)	−0.0027 (12)
C33	0.045 (2)	0.0197 (17)	0.030 (2)	−0.0104 (16)	−0.0031 (17)	−0.0017 (14)
C34	0.059 (3)	0.0263 (19)	0.031 (2)	−0.0073 (19)	−0.0029 (19)	0.0011 (16)
C35	0.061 (3)	0.0253 (19)	0.034 (2)	0.0012 (19)	−0.010 (2)	−0.0023 (16)
C36	0.055 (3)	0.040 (3)	0.058 (3)	0.003 (2)	−0.017 (2)	0.004 (2)
C37	0.041 (2)	0.0199 (17)	0.042 (2)	−0.0060 (16)	0.0009 (18)	−0.0094 (16)
C38	0.053 (3)	0.042 (3)	0.052 (3)	−0.005 (2)	0.010 (2)	−0.010 (2)
C39	0.057 (3)	0.055 (3)	0.059 (3)	0.000 (3)	0.007 (3)	−0.023 (3)
C40	0.086 (5)	0.062 (4)	0.071 (4)	0.019 (3)	0.003 (3)	−0.005 (3)
C41	0.045 (3)	0.032 (2)	0.042 (3)	−0.0094 (19)	0.007 (2)	0.0015 (18)

C42	0.068 (4)	0.054 (3)	0.059 (3)	−0.002 (3)	0.028 (3)	−0.008 (3)
C43	0.075 (5)	0.091 (5)	0.093 (5)	0.013 (4)	0.043 (4)	−0.008 (4)
C44	0.119 (7)	0.144 (9)	0.152 (9)	0.017 (6)	0.084 (7)	−0.041 (7)
C45	0.052 (3)	0.028 (2)	0.031 (2)	−0.0066 (18)	−0.0041 (19)	0.0010 (16)
C46	0.066 (3)	0.045 (3)	0.047 (3)	−0.002 (2)	−0.019 (2)	−0.004 (2)
C47A	0.073 (6)	0.067 (5)	0.052 (5)	−0.019 (4)	−0.016 (4)	−0.002 (3)
C48	0.116 (6)	0.076 (5)	0.079 (5)	0.007 (4)	−0.021 (4)	−0.006 (4)

Geometric parameters (Å, º)

Pt1—O3	1.993 (2)	C15B—H15C	0.9900
Pt1—O3^{i}	1.993 (2)	C15B—H15D	0.9900
Pt1—O2^{i}	1.995 (2)	C16B—H16D	0.9800
Pt1—O2	1.995 (2)	C16B—H16E	0.9800
Pt1—O1	2.002 (2)	C16B—H16F	0.9800
Pt1—O1^{i}	2.002 (2)	N1C—C5C	1.513 (13)
Mo1—O8	1.711 (2)	N1C—C9C	1.514 (14)
Mo1—O7	1.716 (2)	N1C—C13C	1.525 (15)
Mo1—O4	1.937 (2)	N1C—C1C	1.540 (15)
Mo1—O5	1.948 (2)	C1C—C2C	1.540 (17)
Mo1—O2^{i}	2.261 (2)	C1C—H1E	0.9900
Mo1—O1	2.310 (2)	C1C—H1F	0.9900
Mo2—O9	1.704 (2)	C2C—C3C	1.568 (18)
Mo2—O10	1.711 (2)	C2C—H2E	0.9900
Mo2—O5	1.940 (2)	C2C—H2F	0.9900
Mo2—O6	1.952 (2)	C3C—C4C	1.488 (18)
Mo2—O2^{i}	2.238 (2)	C3C—H3E	0.9900
Mo2—O3	2.342 (2)	C3C—H3F	0.9900
Mo3—O11	1.714 (2)	C4C—H4G	0.9800
Mo3—O12	1.714 (2)	C4C—H4H	0.9800
Mo3—O6	1.916 (2)	C4C—H4I	0.9800
Mo3—O4^{i}	1.945 (2)	C5C—C6C	1.506 (15)
Mo3—O1^{i}	2.287 (2)	C5C—H5E	0.9900
Mo3—O3	2.317 (2)	C5C—H5F	0.9900
O1—H1	0.821 (18)	C6C—C7C	1.535 (19)
O2—H2	0.832 (18)	C6C—H6E	0.9900
O3—H3	0.826 (18)	C6C—H6F	0.9900
Pt2—O15	1.999 (2)	C7C—C8C	1.50 (2)
Pt2—O15^{ii}	1.999 (2)	C7C—H7E	0.9900
Pt2—O13	2.000 (2)	C7C—H7F	0.9900
Pt2—O13^{ii}	2.000 (2)	C8C—H8G	0.9800
Pt2—O14^{ii}	2.005 (2)	C8C—H8H	0.9800
Pt2—O14	2.005 (2)	C8C—H8I	0.9800
Mo4—O19^{ii}	1.711 (3)	C9C—C10C	1.522 (17)
Mo4—O19	1.711 (3)	C9C—H9E	0.9900
Mo4—O16	1.944 (2)	C9C—H9F	0.9900
Mo4—O16^{ii}	1.944 (2)	C10C—C11C	1.507 (18)
Mo4—O13^{ii}	2.300 (2)	C10C—H10E	0.9900

Mo4—O13	2.300 (2)	C10C—H10F	0.9900
Mo5—O20	1.705 (2)	C11C—C12C	1.469 (18)
Mo5—O21	1.717 (2)	C11C—H11E	0.9900
Mo5—O16	1.932 (2)	C11C—H11F	0.9900
Mo5—O17	1.949 (2)	C12C—H12G	0.9800
Mo5—O13^{ii}	2.272 (2)	C12C—H12H	0.9800
Mo5—O14	2.327 (2)	C12C—H12I	0.9800
Mo6—O23	1.699 (2)	C13C—C14C	1.512 (17)
Mo6—O22	1.721 (2)	C13C—H13E	0.9900
Mo6—O17	1.930 (2)	C13C—H13F	0.9900
Mo6—O18	1.947 (2)	C14C—C15C	1.524 (18)
Mo6—O15^{ii}	2.252 (2)	C14C—H14E	0.9900
Mo6—O14	2.354 (2)	C14C—H14F	0.9900
Mo7—O24	1.716 (2)	C15C—C16C	1.494 (18)
Mo7—O24^{ii}	1.716 (2)	C15C—H15E	0.9900
Mo7—O18	1.952 (2)	C15C—H15F	0.9900
Mo7—O18^{ii}	1.952 (2)	C16C—H16G	0.9800
Mo7—O15^{ii}	2.272 (2)	C16C—H16H	0.9800
Mo7—O15	2.273 (2)	C16C—H16I	0.9800
O13—H13	0.809 (18)	N2—C21	1.517 (4)
O14—H14	0.805 (18)	N2—C29	1.517 (4)
O15—H15	0.810 (18)	N2—C25	1.521 (4)
Pt3—O27	1.995 (2)	N2—C17	1.529 (5)
Pt3—O29	1.996 (2)	C17—C18	1.524 (5)
Pt3—O28	1.998 (2)	C17—H17A	0.9900
Pt3—O25	1.999 (2)	C17—H17B	0.9900
Pt3—O26	2.000 (2)	C18—C19	1.514 (5)
Pt3—O30	2.010 (2)	C18—H18A	0.9900
O25—H25	0.812 (19)	C18—H18B	0.9900
O26—H26	0.806 (18)	C19—C20	1.529 (6)
O27—H27	0.797 (19)	C19—H19A	0.9900
O28—H28	0.809 (19)	C19—H19B	0.9900
O29—H29	0.812 (19)	C20—H20A	0.9800
O30—H30	0.806 (19)	C20—H20B	0.9800
N1A—C1A	1.508 (6)	C20—H20C	0.9800
N1A—C5A	1.509 (6)	C21—C22	1.516 (5)
N1A—C13A	1.520 (7)	C21—H21A	0.9900
N1A—C9A	1.525 (7)	C21—H21B	0.9900
C1A—C2A	1.520 (8)	C22—C23	1.520 (5)
C1A—H1A	0.9900	C22—H22A	0.9900
C1A—H1B	0.9900	C22—H22B	0.9900
C2A—C3A	1.546 (9)	C23—C24	1.519 (5)
C2A—H2A	0.9900	C23—H23A	0.9900
C2A—H2B	0.9900	C23—H23B	0.9900
C3A—C4A	1.510 (7)	C24—H24A	0.9800
C3A—H3A	0.9900	C24—H24B	0.9800
C3A—H3B	0.9900	C24—H24C	0.9800
C4A—H4A	0.9800	C25—C26	1.524 (5)

C4A—H4B	0.9800	C25—H25A	0.9900
C4A—H4C	0.9800	C25—H25B	0.9900
C5A—C6A	1.513 (7)	C26—C27	1.529 (5)
C5A—H5A	0.9900	C26—H26A	0.9900
C5A—H5B	0.9900	C26—H26B	0.9900
C6A—C7A	1.551 (8)	C27—C28	1.524 (6)
C6A—H6A	0.9900	C27—H27A	0.9900
C6A—H6B	0.9900	C27—H27B	0.9900
C7A—C8A	1.480 (12)	C28—H28A	0.9800
C7A—H7A	0.9900	C28—H28B	0.9800
C7A—H7B	0.9900	C28—H28C	0.9800
C8A—H8A	0.9800	C29—C30	1.495 (5)
C8A—H8B	0.9800	C29—H29A	0.9900
C8A—H8C	0.9800	C29—H29B	0.9900
C9A—C10A	1.520 (9)	C30—C31	1.542 (6)
C9A—H9A	0.9900	C30—H30A	0.9900
C9A—H9B	0.9900	C30—H30B	0.9900
C10A—C11A	1.528 (10)	C31—C32	1.476 (7)
C10A—H10A	0.9900	C31—H31A	0.9900
C10A—H10B	0.9900	C31—H31B	0.9900
C11A—C12A	1.449 (14)	C32—H32A	0.9800
C11A—H11A	0.9900	C32—H32B	0.9800
C11A—H11B	0.9900	C32—H32C	0.9800
C12A—H12A	0.9800	N3—C41	1.505 (5)
C12A—H12B	0.9800	N3—C45	1.519 (5)
C12A—H12C	0.9800	N3—C33	1.520 (5)
C13A—C14A	1.487 (9)	N3—C37	1.520 (5)
C13A—H13A	0.9900	C33—C34	1.523 (5)
C13A—H13B	0.9900	C33—H33A	0.9900
C14A—C15A	1.527 (9)	C33—H33B	0.9900
C14A—H14A	0.9900	C34—C35	1.528 (6)
C14A—H14B	0.9900	C34—H34A	0.9900
C15A—C16A	1.499 (12)	C34—H34B	0.9900
C15A—H15A	0.9900	C35—C36	1.513 (7)
C15A—H15B	0.9900	C35—H35A	0.9900
C16A—H16A	0.9800	C35—H35B	0.9900
C16A—H16B	0.9800	C36—H36A	0.9800
C16A—H16C	0.9800	C36—H36B	0.9800
N1B—C1B	1.508 (6)	C36—H36C	0.9800
N1B—C5B	1.509 (6)	C37—C38	1.525 (6)
N1B—C13B	1.520 (7)	C37—H37A	0.9900
N1B—C9B	1.525 (7)	C37—H37B	0.9900
C1B—C2B	1.520 (8)	C38—C39	1.535 (7)
C1B—H1C	0.9900	C38—H38A	0.9900
C1B—H1D	0.9900	C38—H38B	0.9900
C2B—C3B	1.546 (9)	C39—C40	1.475 (8)
C2B—H2C	0.9900	C39—H39A	0.9900
C2B—H2D	0.9900	C39—H39B	0.9900

C3B—C4B	1.510 (7)	C40—H40A	0.9800
C3B—H3C	0.9900	C40—H40B	0.9800
C3B—H3D	0.9900	C40—H40C	0.9800
C4B—H4D	0.9800	C41—C42	1.532 (7)
C4B—H4E	0.9800	C41—H41A	0.9900
C4B—H4F	0.9800	C41—H41B	0.9900
C5B—C6B	1.513 (7)	C42—C43	1.517 (8)
C5B—H5C	0.9900	C42—H42A	0.9900
C5B—H5D	0.9900	C42—H42B	0.9900
C6B—C7B	1.551 (8)	C43—C44	1.527 (9)
C6B—H6C	0.9900	C43—H43A	0.9900
C6B—H6D	0.9900	C43—H43B	0.9900
C7B—C8B	1.480 (12)	C44—H44A	0.9800
C7B—H7C	0.9900	C44—H44B	0.9800
C7B—H7D	0.9900	C44—H44C	0.9800
C8B—H8D	0.9800	C45—C46	1.505 (6)
C8B—H8E	0.9800	C45—H45A	0.9900
C8B—H8F	0.9800	C45—H45B	0.9900
C9B—C10B	1.520 (9)	C46—C47B	1.45 (2)
C9B—H9C	0.9900	C46—C47A	1.611 (9)
C9B—H9D	0.9900	C46—H46A	0.9900
C10B—C11B	1.528 (10)	C46—H46B	0.9900
C10B—H10C	0.9900	C46—H46C	0.9900
C10B—H10D	0.9900	C46—H46D	0.9900
C11B—C12B	1.72 (2)	C47A—C48	1.446 (9)
C11B—H11C	0.9900	C47A—H47A	0.9900
C11B—H11D	0.9900	C47A—H47B	0.9900
C12B—H12D	0.9800	C47B—C48	1.42 (2)
C12B—H12E	0.9800	C47B—H47C	0.9900
C12B—H12F	0.9800	C47B—H47D	0.9900
C13B—C14B	1.487 (9)	C48—H48A	0.9800
C13B—H13C	0.9900	C48—H48B	0.9800
C13B—H13D	0.9900	C48—H48C	0.9800
C14B—C15B	1.527 (9)	C48—H48D	0.9800
C14B—H14C	0.9900	C48—H48E	0.9800
C14B—H14D	0.9900	C48—H48F	0.9800
C15B—C16B	1.499 (12)		

O3—Pt1—O3^{i}	180.0	C9B—C10B—H10D	109.8
O3—Pt1—O2^{i}	83.84 (9)	C11B—C10B—H10D	109.8
O3^{i}—Pt1—O2^{i}	96.16 (9)	H10C—C10B—H10D	108.2
O3—Pt1—O2	96.16 (9)	C10B—C11B—C12B	98.3 (9)
O3^{i}—Pt1—O2	83.84 (9)	C10B—C11B—H11C	112.1
O2^{i}—Pt1—O2	180.00 (5)	C12B—C11B—H11C	112.1
O3—Pt1—O1	95.83 (9)	C10B—C11B—H11D	112.1
O3^{i}—Pt1—O1	84.17 (9)	C12B—C11B—H11D	112.1
O2^{i}—Pt1—O1	83.49 (9)	H11C—C11B—H11D	109.7
O2—Pt1—O1	96.51 (9)	C11B—C12B—H12D	109.5

O3—Pt1—O1^{i}	84.17 (9)	C11B—C12B—H12E	109.5
O3^{i}—Pt1—O1^{i}	95.83 (9)	H12D—C12B—H12E	109.5
O2^{i}—Pt1—O1^{i}	96.51 (9)	C11B—C12B—H12F	109.5
O2—Pt1—O1^{i}	83.49 (9)	H12D—C12B—H12F	109.5
O1—Pt1—O1^{i}	180.0	H12E—C12B—H12F	109.5
O8—Mo1—O7	106.03 (11)	C14B—C13B—N1B	116.5 (4)
O8—Mo1—O4	97.09 (10)	C14B—C13B—H13C	108.2
O7—Mo1—O4	100.67 (11)	N1B—C13B—H13C	108.2
O8—Mo1—O5	101.62 (10)	C14B—C13B—H13D	108.2
O7—Mo1—O5	95.43 (10)	N1B—C13B—H13D	108.2
O4—Mo1—O5	150.85 (9)	H13C—C13B—H13D	107.3
O8—Mo1—O2^{i}	92.01 (10)	C13B—C14B—C15B	109.2 (6)
O7—Mo1—O2^{i}	159.66 (10)	C13B—C14B—H14C	109.8
O4—Mo1—O2^{i}	86.00 (9)	C15B—C14B—H14C	109.8
O5—Mo1—O2^{i}	71.29 (8)	C13B—C14B—H14D	109.8
O8—Mo1—O1	159.30 (10)	C15B—C14B—H14D	109.8
O7—Mo1—O1	92.79 (10)	H14C—C14B—H14D	108.3
O4—Mo1—O1	70.45 (8)	C16B—C15B—C14B	114.2 (8)
O5—Mo1—O1	84.73 (8)	C16B—C15B—H15C	108.7
O2^{i}—Mo1—O1	71.18 (7)	C14B—C15B—H15C	108.7
O9—Mo2—O10	106.92 (12)	C16B—C15B—H15D	108.7
O9—Mo2—O5	101.49 (10)	C14B—C15B—H15D	108.7
O10—Mo2—O5	96.61 (10)	H15C—C15B—H15D	107.6
O9—Mo2—O6	97.57 (10)	C15B—C16B—H16D	109.5
O10—Mo2—O6	100.10 (10)	C15B—C16B—H16E	109.5
O5—Mo2—O6	149.72 (9)	H16D—C16B—H16E	109.5
O9—Mo2—O2^{i}	96.05 (10)	C15B—C16B—H16F	109.5
O10—Mo2—O2^{i}	156.13 (10)	H16D—C16B—H16F	109.5
O5—Mo2—O2^{i}	71.94 (9)	H16E—C16B—H16F	109.5
O6—Mo2—O2^{i}	82.89 (9)	C5C—N1C—C9C	112.3 (12)
O9—Mo2—O3	163.15 (10)	C5C—N1C—C13C	107.2 (12)
O10—Mo2—O3	87.41 (10)	C9C—N1C—C13C	106.7 (12)
O5—Mo2—O3	85.19 (8)	C5C—N1C—C1C	108.0 (11)
O6—Mo2—O3	70.62 (8)	C9C—N1C—C1C	113.6 (12)
O2^{i}—Mo2—O3	71.11 (7)	C13C—N1C—C1C	108.8 (13)
O11—Mo3—O12	105.57 (12)	C2C—C1C—N1C	116.5 (15)
O11—Mo3—O6	101.39 (10)	C2C—C1C—H1E	108.2
O12—Mo3—O6	99.41 (10)	N1C—C1C—H1E	108.2
O11—Mo3—O4^{i}	96.97 (10)	C2C—C1C—H1F	108.2
O12—Mo3—O4^{i}	100.48 (11)	N1C—C1C—H1F	108.2
O6—Mo3—O4^{i}	148.10 (9)	H1E—C1C—H1F	107.3
O11—Mo3—O1^{i}	158.68 (10)	C1C—C2C—C3C	109.4 (16)
O12—Mo3—O1^{i}	94.08 (10)	C1C—C2C—H2E	109.8
O6—Mo3—O1^{i}	83.09 (9)	C3C—C2C—H2E	109.8
O4^{i}—Mo3—O1^{i}	70.86 (8)	C1C—C2C—H2F	109.8
O11—Mo3—O3	90.32 (9)	C3C—C2C—H2F	109.8
O12—Mo3—O3	163.27 (10)	H2E—C2C—H2F	108.2
O6—Mo3—O3	71.75 (8)	C4C—C3C—C2C	115 (2)

O4^{i}—Mo3—O3	82.36 (8)	C4C—C3C—H3E	108.6
O1^{i}—Mo3—O3	71.12 (7)	C2C—C3C—H3E	108.6
Pt1—O1—Mo3^{i}	102.72 (9)	C4C—C3C—H3F	108.6
Pt1—O1—Mo1	101.68 (9)	C2C—C3C—H3F	108.6
Mo3^{i}—O1—Mo1	94.29 (8)	H3E—C3C—H3F	107.6
Pt1—O1—H1	119 (3)	C3C—C4C—H4G	109.5
Mo3^{i}—O1—H1	120 (3)	C3C—C4C—H4H	109.5
Mo1—O1—H1	114 (3)	H4G—C4C—H4H	109.5
Pt1—O2—Mo2^{i}	104.30 (9)	C3C—C4C—H4I	109.5
Pt1—O2—Mo1^{i}	103.60 (9)	H4G—C4C—H4I	109.5
Mo2^{i}—O2—Mo1^{i}	95.17 (8)	H4H—C4C—H4I	109.5
Pt1—O2—H2	112 (3)	C6C—C5C—N1C	117.8 (12)
Mo2^{i}—O2—H2	114 (3)	C6C—C5C—H5E	107.8
Mo1^{i}—O2—H2	125 (3)	N1C—C5C—H5E	107.8
Pt1—O3—Mo3	101.94 (9)	C6C—C5C—H5F	107.8
Pt1—O3—Mo2	100.74 (9)	N1C—C5C—H5F	107.8
Mo3—O3—Mo2	92.22 (8)	H5E—C5C—H5F	107.2
Pt1—O3—H3	113 (3)	C5C—C6C—C7C	107 (2)
Mo3—O3—H3	117 (3)	C5C—C6C—H6E	110.3
Mo2—O3—H3	128 (3)	C7C—C6C—H6E	110.3
Mo1—O4—Mo3^{i}	120.49 (11)	C5C—C6C—H6F	110.3
Mo2—O5—Mo1	117.40 (11)	C7C—C6C—H6F	110.3
Mo3—O6—Mo2	120.48 (11)	H6E—C6C—H6F	108.6
O15—Pt2—O15^{ii}	82.96 (12)	C8C—C7C—C6C	120 (3)
O15—Pt2—O13	96.99 (9)	C8C—C7C—H7E	107.3
O15^{ii}—Pt2—O13	179.87 (11)	C6C—C7C—H7E	107.3
O15—Pt2—O13^{ii}	179.87 (11)	C8C—C7C—H7F	107.3
O15^{ii}—Pt2—O13^{ii}	96.99 (9)	C6C—C7C—H7F	107.3
O13—Pt2—O13^{ii}	83.06 (13)	H7E—C7C—H7F	106.9
O15—Pt2—O14^{ii}	84.68 (9)	C7C—C8C—H8G	109.5
O15^{ii}—Pt2—O14^{ii}	96.08 (9)	C7C—C8C—H8H	109.5
O13—Pt2—O14^{ii}	83.80 (9)	H8G—C8C—H8H	109.5
O13^{ii}—Pt2—O14^{ii}	95.44 (9)	C7C—C8C—H8I	109.5
O15—Pt2—O14	96.07 (9)	H8G—C8C—H8I	109.5
O15^{ii}—Pt2—O14	84.68 (9)	H8H—C8C—H8I	109.5
O13—Pt2—O14	95.44 (9)	N1C—C9C—C10C	115.2 (14)
O13^{ii}—Pt2—O14	83.80 (9)	N1C—C9C—H9E	108.5
O14^{ii}—Pt2—O14	178.99 (13)	C10C—C9C—H9E	108.5
O19^{ii}—Mo4—O19	107.40 (19)	N1C—C9C—H9F	108.5
O19^{ii}—Mo4—O16	100.22 (11)	C10C—C9C—H9F	108.5
O19—Mo4—O16	97.04 (11)	H9E—C9C—H9F	107.5
O19^{ii}—Mo4—O16^{ii}	97.04 (11)	C11C—C10C—C9C	109.6 (17)
O19—Mo4—O16^{ii}	100.22 (11)	C11C—C10C—H10E	109.7
O16—Mo4—O16^{ii}	150.64 (13)	C9C—C10C—H10E	109.7
O19^{ii}—Mo4—O13^{ii}	91.86 (11)	C11C—C10C—H10F	109.7
O19—Mo4—O13^{ii}	159.23 (11)	C9C—C10C—H10F	109.7
O16—Mo4—O13^{ii}	71.30 (9)	H10E—C10C—H10F	108.2
O16^{ii}—Mo4—O13^{ii}	84.63 (9)	C12C—C11C—C10C	117 (2)

O19^{ii}—Mo4—O13	159.23 (11)	C12C—C11C—H11E	108.0
O19—Mo4—O13	91.86 (11)	C10C—C11C—H11E	108.0
O16—Mo4—O13	84.63 (9)	C12C—C11C—H11F	108.0
O16^{ii}—Mo4—O13	71.30 (9)	C10C—C11C—H11F	108.0
O13^{ii}—Mo4—O13	70.42 (10)	H11E—C11C—H11F	107.3
O20—Mo5—O21	106.02 (13)	C11C—C12C—H12G	109.5
O20—Mo5—O16	101.13 (11)	C11C—C12C—H12H	109.5
O21—Mo5—O16	97.45 (11)	H12G—C12C—H12H	109.5
O20—Mo5—O17	97.41 (11)	C11C—C12C—H12I	109.5
O21—Mo5—O17	100.92 (11)	H12G—C12C—H12I	109.5
O16—Mo5—O17	149.10 (10)	H12H—C12C—H12I	109.5
O20—Mo5—O13^{ii}	91.89 (10)	C14C—C13C—N1C	116.7 (16)
O21—Mo5—O13^{ii}	160.92 (10)	C14C—C13C—H13E	108.1
O16—Mo5—O13^{ii}	72.14 (9)	N1C—C13C—H13E	108.1
O17—Mo5—O13^{ii}	82.81 (9)	C14C—C13C—H13F	108.1
O20—Mo5—O14	159.88 (10)	N1C—C13C—H13F	108.1
O21—Mo5—O14	92.32 (10)	H13E—C13C—H13F	107.3
O16—Mo5—O14	84.21 (9)	C13C—C14C—C15C	113.9 (19)
O17—Mo5—O14	70.49 (8)	C13C—C14C—H14E	108.8
O13^{ii}—Mo5—O14	71.11 (8)	C15C—C14C—H14E	108.8
O23—Mo6—O22	105.73 (13)	C13C—C14C—H14F	108.8
O23—Mo6—O17	98.07 (11)	C15C—C14C—H14F	108.8
O22—Mo6—O17	100.89 (11)	H14E—C14C—H14F	107.7
O23—Mo6—O18	101.94 (11)	C16C—C15C—C14C	111 (2)
O22—Mo6—O18	95.09 (11)	C16C—C15C—H15E	109.5
O17—Mo6—O18	149.89 (10)	C14C—C15C—H15E	109.5
O23—Mo6—O15^{ii}	93.14 (11)	C16C—C15C—H15F	109.5
O22—Mo6—O15^{ii}	159.16 (10)	C14C—C15C—H15F	109.5
O17—Mo6—O15^{ii}	84.77 (9)	H15E—C15C—H15F	108.0
O18—Mo6—O15^{ii}	71.96 (9)	C15C—C16C—H16G	109.5
O23—Mo6—O14	161.14 (10)	C15C—C16C—H16H	109.5
O22—Mo6—O14	91.26 (10)	H16G—C16C—H16H	109.5
O17—Mo6—O14	70.16 (8)	C15C—C16C—H16I	109.5
O18—Mo6—O14	84.24 (9)	H16G—C16C—H16I	109.5
O15^{ii}—Mo6—O14	71.64 (7)	H16H—C16C—H16I	109.5
O24—Mo7—O24^{ii}	106.41 (17)	C21—N2—C29	106.3 (3)
O24—Mo7—O18	96.54 (11)	C21—N2—C25	110.9 (3)
O24^{ii}—Mo7—O18	99.96 (11)	C29—N2—C25	111.1 (3)
O24—Mo7—O18^{ii}	99.96 (11)	C21—N2—C17	110.9 (3)
O24^{ii}—Mo7—O18^{ii}	96.54 (11)	C29—N2—C17	111.0 (3)
O18—Mo7—O18^{ii}	152.30 (13)	C25—N2—C17	106.6 (3)
O24—Mo7—O15^{ii}	159.68 (10)	C18—C17—N2	115.6 (3)
O24^{ii}—Mo7—O15^{ii}	92.06 (10)	C18—C17—H17A	108.4
O18—Mo7—O15^{ii}	71.42 (9)	N2—C17—H17A	108.4
O18^{ii}—Mo7—O15^{ii}	85.96 (9)	C18—C17—H17B	108.4
O24—Mo7—O15	92.06 (10)	N2—C17—H17B	108.4
O24^{ii}—Mo7—O15	159.68 (10)	H17A—C17—H17B	107.4
O18—Mo7—O15	85.96 (9)	C19—C18—C17	110.0 (3)

O18^{ii}—Mo7—O15	71.42 (9)	C19—C18—H18A	109.7
O15^{ii}—Mo7—O15	71.26 (11)	C17—C18—H18A	109.7
Pt2—O13—Mo5^{ii}	103.57 (9)	C19—C18—H18B	109.7
Pt2—O13—Mo4	103.26 (9)	C17—C18—H18B	109.7
Mo5^{ii}—O13—Mo4	93.56 (8)	H18A—C18—H18B	108.2
Pt2—O13—H13	114 (3)	C18—C19—C20	112.6 (3)
Mo5^{ii}—O13—H13	110 (3)	C18—C19—H19A	109.1
Mo4—O13—H13	128 (3)	C20—C19—H19A	109.1
Pt2—O14—Mo5	101.51 (9)	C18—C19—H19B	109.1
Pt2—O14—Mo6	99.96 (9)	C20—C19—H19B	109.1
Mo5—O14—Mo6	93.12 (8)	H19A—C19—H19B	107.8
Pt2—O14—H14	112 (3)	C19—C20—H20A	109.5
Mo5—O14—H14	119 (3)	C19—C20—H20B	109.5
Mo6—O14—H14	127 (3)	H20A—C20—H20B	109.5
Pt2—O15—Mo6^{ii}	103.67 (9)	C19—C20—H20C	109.5
Pt2—O15—Mo7	102.89 (9)	H20A—C20—H20C	109.5
Mo6^{ii}—O15—Mo7	95.03 (8)	H20B—C20—H20C	109.5
Pt2—O15—H15	116 (3)	C22—C21—N2	115.5 (3)
Mo6^{ii}—O15—H15	128 (3)	C22—C21—H21A	108.4
Mo7—O15—H15	107 (3)	N2—C21—H21A	108.4
Mo5—O16—Mo4	118.54 (11)	C22—C21—H21B	108.4
Mo6—O17—Mo5	122.35 (11)	N2—C21—H21B	108.4
Mo6—O18—Mo7	117.70 (11)	H21A—C21—H21B	107.5
O27—Pt3—O29	93.70 (10)	C21—C22—C23	109.9 (3)
O27—Pt3—O28	178.75 (9)	C21—C22—H22A	109.7
O29—Pt3—O28	87.48 (9)	C23—C22—H22A	109.7
O27—Pt3—O25	90.80 (10)	C21—C22—H22B	109.7
O29—Pt3—O25	91.00 (9)	C23—C22—H22B	109.7
O28—Pt3—O25	88.78 (10)	H22A—C22—H22B	108.2
O27—Pt3—O26	89.44 (9)	C24—C23—C22	112.3 (3)
O29—Pt3—O26	176.85 (10)	C24—C23—H23A	109.1
O28—Pt3—O26	89.38 (9)	C22—C23—H23A	109.1
O25—Pt3—O26	88.63 (9)	C24—C23—H23B	109.1
O27—Pt3—O30	90.62 (10)	C22—C23—H23B	109.1
O29—Pt3—O30	90.51 (9)	H23A—C23—H23B	107.9
O28—Pt3—O30	89.77 (10)	C23—C24—H24A	109.5
O25—Pt3—O30	177.86 (10)	C23—C24—H24B	109.5
O26—Pt3—O30	89.78 (9)	H24A—C24—H24B	109.5
Pt3—O25—H25	105 (3)	C23—C24—H24C	109.5
Pt3—O26—H26	113 (3)	H24A—C24—H24C	109.5
Pt3—O27—H27	117 (3)	H24B—C24—H24C	109.5
Pt3—O28—H28	106 (3)	N2—C25—C26	115.3 (3)
Pt3—O29—H29	109 (3)	N2—C25—H25A	108.4
Pt3—O30—H30	109 (3)	C26—C25—H25A	108.4
C1A—N1A—C5A	106.2 (4)	N2—C25—H25B	108.4
C1A—N1A—C13A	111.0 (4)	C26—C25—H25B	108.4
C5A—N1A—C13A	111.3 (4)	H25A—C25—H25B	107.5
C1A—N1A—C9A	110.7 (5)	C25—C26—C27	110.6 (3)

C5A—N1A—C9A	110.9 (4)	C25—C26—H26A	109.5
C13A—N1A—C9A	106.8 (4)	C27—C26—H26A	109.5
N1A—C1A—C2A	114.6 (4)	C25—C26—H26B	109.5
N1A—C1A—H1A	108.6	C27—C26—H26B	109.5
C2A—C1A—H1A	108.6	H26A—C26—H26B	108.1
N1A—C1A—H1B	108.6	C28—C27—C26	113.7 (4)
C2A—C1A—H1B	108.6	C28—C27—H27A	108.8
H1A—C1A—H1B	107.6	C26—C27—H27A	108.8
C1A—C2A—C3A	110.7 (5)	C28—C27—H27B	108.8
C1A—C2A—H2A	109.5	C26—C27—H27B	108.8
C3A—C2A—H2A	109.5	H27A—C27—H27B	107.7
C1A—C2A—H2B	109.5	C27—C28—H28A	109.5
C3A—C2A—H2B	109.5	C27—C28—H28B	109.5
H2A—C2A—H2B	108.1	H28A—C28—H28B	109.5
C4A—C3A—C2A	110.9 (4)	C27—C28—H28C	109.5
C4A—C3A—H3A	109.5	H28A—C28—H28C	109.5
C2A—C3A—H3A	109.5	H28B—C28—H28C	109.5
C4A—C3A—H3B	109.5	C30—C29—N2	115.5 (3)
C2A—C3A—H3B	109.5	C30—C29—H29A	108.4
H3A—C3A—H3B	108.1	N2—C29—H29A	108.4
C3A—C4A—H4A	109.5	C30—C29—H29B	108.4
C3A—C4A—H4B	109.5	N2—C29—H29B	108.4
H4A—C4A—H4B	109.5	H29A—C29—H29B	107.5
C3A—C4A—H4C	109.5	C29—C30—C31	109.9 (4)
H4A—C4A—H4C	109.5	C29—C30—H30A	109.7
H4B—C4A—H4C	109.5	C31—C30—H30A	109.7
N1A—C5A—C6A	115.7 (4)	C29—C30—H30B	109.7
N1A—C5A—H5A	108.3	C31—C30—H30B	109.7
C6A—C5A—H5A	108.3	H30A—C30—H30B	108.2
N1A—C5A—H5B	108.3	C32—C31—C30	112.5 (5)
C6A—C5A—H5B	108.3	C32—C31—H31A	109.1
H5A—C5A—H5B	107.4	C30—C31—H31A	109.1
C5A—C6A—C7A	109.8 (5)	C32—C31—H31B	109.1
C5A—C6A—H6A	109.7	C30—C31—H31B	109.1
C7A—C6A—H6A	109.7	H31A—C31—H31B	107.8
C5A—C6A—H6B	109.7	C31—C32—H32A	109.5
C7A—C6A—H6B	109.7	C31—C32—H32B	109.5
H6A—C6A—H6B	108.2	H32A—C32—H32B	109.5
C8A—C7A—C6A	112.4 (5)	C31—C32—H32C	109.5
C8A—C7A—H7A	109.1	H32A—C32—H32C	109.5
C6A—C7A—H7A	109.1	H32B—C32—H32C	109.5
C8A—C7A—H7B	109.1	C41—N3—C45	111.6 (3)
C6A—C7A—H7B	109.1	C41—N3—C33	111.2 (3)
H7A—C7A—H7B	107.9	C45—N3—C33	106.0 (3)
C7A—C8A—H8A	109.5	C41—N3—C37	106.4 (3)
C7A—C8A—H8B	109.5	C45—N3—C37	110.4 (3)
H8A—C8A—H8B	109.5	C33—N3—C37	111.3 (3)
C7A—C8A—H8C	109.5	N3—C33—C34	116.0 (3)

H8A—C8A—H8C	109.5	N3—C33—H33A	108.3
H8B—C8A—H8C	109.5	C34—C33—H33A	108.3
C10A—C9A—N1A	116.0 (5)	N3—C33—H33B	108.3
C10A—C9A—H9A	108.3	C34—C33—H33B	108.3
N1A—C9A—H9A	108.3	H33A—C33—H33B	107.4
C10A—C9A—H9B	108.3	C33—C34—C35	110.8 (3)
N1A—C9A—H9B	108.3	C33—C34—H34A	109.5
H9A—C9A—H9B	107.4	C35—C34—H34A	109.5
C9A—C10A—C11A	109.5 (6)	C33—C34—H34B	109.5
C9A—C10A—H10A	109.8	C35—C34—H34B	109.5
C11A—C10A—H10A	109.8	H34A—C34—H34B	108.1
C9A—C10A—H10B	109.8	C36—C35—C34	113.8 (4)
C11A—C10A—H10B	109.8	C36—C35—H35A	108.8
H10A—C10A—H10B	108.2	C34—C35—H35A	108.8
C12A—C11A—C10A	116.5 (8)	C36—C35—H35B	108.8
C12A—C11A—H11A	108.2	C34—C35—H35B	108.8
C10A—C11A—H11A	108.2	H35A—C35—H35B	107.7
C12A—C11A—H11B	108.2	C35—C36—H36A	109.5
C10A—C11A—H11B	108.2	C35—C36—H36B	109.5
H11A—C11A—H11B	107.3	H36A—C36—H36B	109.5
C11A—C12A—H12A	109.5	C35—C36—H36C	109.5
C11A—C12A—H12B	109.5	H36A—C36—H36C	109.5
H12A—C12A—H12B	109.5	H36B—C36—H36C	109.5
C11A—C12A—H12C	109.5	N3—C37—C38	115.4 (3)
H12A—C12A—H12C	109.5	N3—C37—H37A	108.4
H12B—C12A—H12C	109.5	C38—C37—H37A	108.4
C14A—C13A—N1A	116.5 (4)	N3—C37—H37B	108.4
C14A—C13A—H13A	108.2	C38—C37—H37B	108.4
N1A—C13A—H13A	108.2	H37A—C37—H37B	107.5
C14A—C13A—H13B	108.2	C37—C38—C39	109.4 (4)
N1A—C13A—H13B	108.2	C37—C38—H38A	109.8
H13A—C13A—H13B	107.3	C39—C38—H38A	109.8
C13A—C14A—C15A	109.2 (6)	C37—C38—H38B	109.8
C13A—C14A—H14A	109.8	C39—C38—H38B	109.8
C15A—C14A—H14A	109.8	H38A—C38—H38B	108.2
C13A—C14A—H14B	109.8	C40—C39—C38	113.0 (4)
C15A—C14A—H14B	109.8	C40—C39—H39A	109.0
H14A—C14A—H14B	108.3	C38—C39—H39A	109.0
C16A—C15A—C14A	114.2 (8)	C40—C39—H39B	109.0
C16A—C15A—H15A	108.7	C38—C39—H39B	109.0
C14A—C15A—H15A	108.7	H39A—C39—H39B	107.8
C16A—C15A—H15B	108.7	C39—C40—H40A	109.5
C14A—C15A—H15B	108.7	C39—C40—H40B	109.5
H15A—C15A—H15B	107.6	H40A—C40—H40B	109.5
C15A—C16A—H16A	109.5	C39—C40—H40C	109.5
C15A—C16A—H16B	109.5	H40A—C40—H40C	109.5
H16A—C16A—H16B	109.5	H40B—C40—H40C	109.5
C15A—C16A—H16C	109.5	N3—C41—C42	114.9 (4)

H16A—C16A—H16C	109.5	N3—C41—H41A	108.5
H16B—C16A—H16C	109.5	C42—C41—H41A	108.5
C1B—N1B—C5B	106.2 (4)	N3—C41—H41B	108.5
C1B—N1B—C13B	111.0 (4)	C42—C41—H41B	108.5
C5B—N1B—C13B	111.3 (4)	H41A—C41—H41B	107.5
C1B—N1B—C9B	110.7 (5)	C43—C42—C41	108.7 (5)
C5B—N1B—C9B	110.9 (4)	C43—C42—H42A	109.9
C13B—N1B—C9B	106.8 (4)	C41—C42—H42A	109.9
N1B—C1B—C2B	114.6 (4)	C43—C42—H42B	109.9
N1B—C1B—H1C	108.6	C41—C42—H42B	109.9
C2B—C1B—H1C	108.6	H42A—C42—H42B	108.3
N1B—C1B—H1D	108.6	C42—C43—C44	109.3 (6)
C2B—C1B—H1D	108.6	C42—C43—H43A	109.8
H1C—C1B—H1D	107.6	C44—C43—H43A	109.8
C1B—C2B—C3B	110.7 (5)	C42—C43—H43B	109.8
C1B—C2B—H2C	109.5	C44—C43—H43B	109.8
C3B—C2B—H2C	109.5	H43A—C43—H43B	108.3
C1B—C2B—H2D	109.5	C43—C44—H44A	109.5
C3B—C2B—H2D	109.5	C43—C44—H44B	109.5
H2C—C2B—H2D	108.1	H44A—C44—H44B	109.5
C4B—C3B—C2B	110.9 (4)	C43—C44—H44C	109.5
C4B—C3B—H3C	109.5	H44A—C44—H44C	109.5
C2B—C3B—H3C	109.5	H44B—C44—H44C	109.5
C4B—C3B—H3D	109.5	C46—C45—N3	116.2 (4)
C2B—C3B—H3D	109.5	C46—C45—H45A	108.2
H3C—C3B—H3D	108.1	N3—C45—H45A	108.2
C3B—C4B—H4D	109.5	C46—C45—H45B	108.2
C3B—C4B—H4E	109.5	N3—C45—H45B	108.2
H4D—C4B—H4E	109.5	H45A—C45—H45B	107.4
C3B—C4B—H4F	109.5	C47B—C46—C45	123.5 (9)
H4D—C4B—H4F	109.5	C45—C46—C47A	107.4 (4)
H4E—C4B—H4F	109.5	C45—C46—H46A	110.2
N1B—C5B—C6B	115.7 (4)	C47A—C46—H46A	110.2
N1B—C5B—H5C	108.3	C45—C46—H46B	110.2
C6B—C5B—H5C	108.3	C47A—C46—H46B	110.2
N1B—C5B—H5D	108.3	H46A—C46—H46B	108.5
C6B—C5B—H5D	108.3	C47B—C46—H46C	106.5
H5C—C5B—H5D	107.4	C45—C46—H46C	106.5
C5B—C6B—C7B	109.8 (5)	C47B—C46—H46D	106.5
C5B—C6B—H6C	109.7	C45—C46—H46D	106.5
C7B—C6B—H6C	109.7	H46C—C46—H46D	106.5
C5B—C6B—H6D	109.7	C48—C47A—C46	110.8 (6)
C7B—C6B—H6D	109.7	C48—C47A—H47A	109.5
H6C—C6B—H6D	108.2	C46—C47A—H47A	109.5
C8B—C7B—C6B	112.4 (5)	C48—C47A—H47B	109.5
C8B—C7B—H7C	109.1	C46—C47A—H47B	109.5
C6B—C7B—H7C	109.1	H47A—C47A—H47B	108.1
C8B—C7B—H7D	109.1	C48—C47B—C46	122.3 (15)

C6B—C7B—H7D	109.1	C48—C47B—H47C	106.7
H7C—C7B—H7D	107.9	C46—C47B—H47C	106.7
C7B—C8B—H8D	109.5	C48—C47B—H47D	106.7
C7B—C8B—H8E	109.5	C46—C47B—H47D	106.7
H8D—C8B—H8E	109.5	H47C—C47B—H47D	106.6
C7B—C8B—H8F	109.5	C47A—C48—H48A	109.5
H8D—C8B—H8F	109.5	C47A—C48—H48B	109.5
H8E—C8B—H8F	109.5	H48A—C48—H48B	109.5
C10B—C9B—N1B	116.0 (5)	C47A—C48—H48C	109.5
C10B—C9B—H9C	108.3	H48A—C48—H48C	109.5
N1B—C9B—H9C	108.3	H48B—C48—H48C	109.5
C10B—C9B—H9D	108.3	C47B—C48—H48D	109.5
N1B—C9B—H9D	108.3	C47B—C48—H48E	109.5
H9C—C9B—H9D	107.4	H48D—C48—H48E	109.5
C9B—C10B—C11B	109.5 (6)	C47B—C48—H48F	109.5
C9B—C10B—H10C	109.8	H48D—C48—H48F	109.5
C11B—C10B—H10C	109.8	H48E—C48—H48F	109.5

Symmetry codes: (i) $-x+1/2, -y+1/2, -z$; (ii) $-x, y, -z+1/2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O25	0.82 (2)	1.71 (2)	2.532 (3)	179 (4)
O2—H2···O26	0.83 (2)	1.62 (2)	2.446 (3)	171 (4)
O3—H3···O27	0.83 (2)	1.78 (2)	2.605 (3)	174 (4)
O13—H13···O28	0.81 (2)	1.67 (2)	2.474 (3)	174 (4)
O14—H14···O29	0.81 (2)	1.82 (2)	2.615 (3)	169 (4)
O15—H15···O30	0.81 (2)	1.70 (2)	2.506 (3)	176 (4)
O25—H25···O31	0.81 (2)	1.96 (2)	2.768 (4)	177 (4)
O26—H26···O32	0.81 (2)	2.01 (2)	2.786 (4)	163 (4)
O27—H27···O35	0.80 (2)	2.34 (3)	3.078 (4)	154 (4)
O28—H28···O34	0.81 (2)	2.17 (2)	2.972 (3)	175 (4)
O29—H29···O35	0.81 (2)	2.04 (2)	2.853 (4)	174 (4)
O30—H30···O36	0.81 (2)	2.03 (2)	2.830 (4)	172 (4)