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ISSN 2414-3146

Synthesis and crystal structure of [Cs([2.2.2]crypt)]$_2$[Mo(CO)$_5$]

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Received 15 August 2019
Accepted 6 September 2019

Edited by M. Weil, Vienna University of Technology, Austria

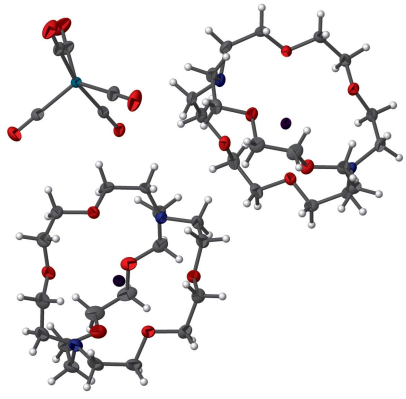
Keywords: crystal structure; liquid ammonia; carbonyl metalates; pentacarbonyl molybdate; metallic salt reduction.

CCDC reference: 1951927

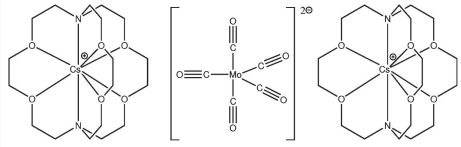
Structural data: full structural data are available from iucrdata.iucr.org

Reduction of the heteroleptic metal carbonyl complex Mo(CO)$_3$(η^5-Cp)H with the metallic salt Cs$_5$Bi$_4$ in the presence of [2.2.2]crypt (= 4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8.8.8]hexacosane) in liquid ammonia led to single crystals of bis[(4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8.8.8]hexacosane)-caesium] pentacarbonylmolybdate, [Cs(C$_{18}$H$_{36}$N$_2$O$_6$)]$_2$[Mo(CO)$_5$] or [Cs([2.2.2]crypt)]$_2$[Mo(CO)$_5$]. The twofold negatively charged anionic complex corresponds to the 18 valence electron rule. It consists of an Mo atom coordinated by five carbonyl ligands in a shape intermediate between trigonal–bipyramidal and square-pyramidal. The Mo—C distances range from 1.961 (3) to 2.017 (3) Å, and the C≡O distances from 1.164 (3) to 1.180 (4) Å.

3D view



Chemical scheme



Structure description

Synthetic routes and structural compositions of neutral metal carbonyl complexes for group 4 to 11 as well as negatively charged carbonyl metalates for group 4 to 10 are well known in the literature, and are extensively documented (Holleman *et al.*, 2016). For a detailed review of metal carbonyl anions, see: Ellis (2003). Only very recently, the first tricarbonyl nickelate, [Ni(CO)$_3$]$^{2-}$, could be synthesized *via* the reaction between Ni(CO)$_2$(PPh$_3$)$_2$, K$_6$Rb$_6$Ge$_{17}$ and chelating ligands in liquid ammonia (Lorenz *et al.*, 2018). Thus, it was again demonstrated that Zintl phases are suitable for the reduction of metal carbonyl complexes. This behaviour has previously been exemplified in the reduction of Mn$_2$(CO)$_{10}$ by K$_4$Ge$_9$ to yield [Mn(CO)$_5$]$^-$ (Härtl, 2012). In the field of group 6 homoleptic carbonyl metalates, crystal structures determined by single-crystal X-ray diffraction experiments are sporadically documented. The first crystal structure comprising [Cr(CO)$_5$]$^{2-}$ and documented in the Cambridge Crystal Structure Database (Groom *et al.*, 2016) resulted from the reaction between Cr(CO)$_6$, [2.2.2]crypt and the nominal phase K$_3$Cd$_2$Sb$_2$ in ethylenediamine (Zhai & Xu, 2011). Previously, in 1985, the

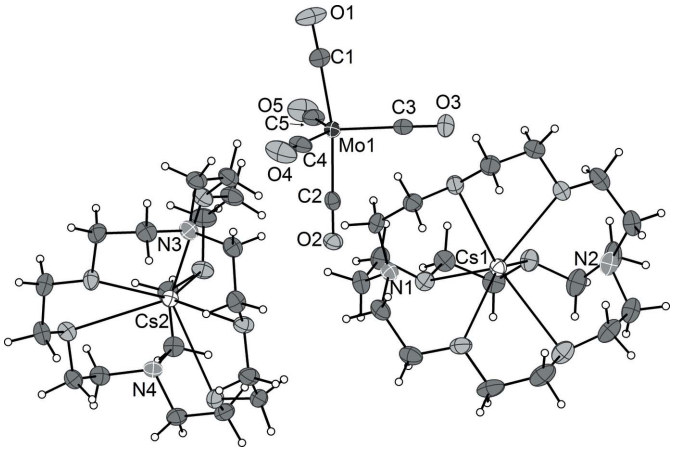


Figure 1
The asymmetric unit of $[Cs([2.2.2]crypt)]_2[Mo(CO)_5]$. Displacement ellipsoids are drawn at the 50% probability level.

heavier homologue $[W(CO)_5]^{2-}$ was obtained in the reaction between $W(CO)_2(NMe_3)$, $NaC_{10}H_8$ and [2.2.1]crypt (Maher *et al.*, 1985). Using the same route, the corresponding Mo species could be synthesized, but there was no documentation of its structural characterization (Maher *et al.*, 1982). To our knowledge, there is no detailed structure data of the $[Mo(CO)_5]^{2-}$ anion published so far. We here present the synthesis and crystal structure of the pentacarbonyl molybdate complex $[Cs([2.2.2]crypt)]_2[Mo(CO)_5]$.

$[Cs([2.2.2]crypt)]_2[Mo(CO)_5]$ was obtained by the reduction of $Mo(CO)_3(\eta^5\text{-Cp})H$ with Cs_5Bi_4 in the presence of [2.2.2]crypt in liquid ammonia. The asymmetric unit contains two $[Cs([2.2.2]crypt)]^+$ cation complexes and a twofold negatively charged $[Mo(CO)_5]^{2-}$ unit which follows the 18 valence electron rule (Fig. 1). The Mo—C bonds in the anionic unit range from 1.961 (3) to 2.017 (3) Å and the C≡O bonds from 1.164 (3) to 1.180 (4) Å. The former bonds are slightly shorter and the latter bonds are slightly longer than the corresponding bonds in $Mo(CO)_6$ (Mak, 1984). This can be explained by the high π-acceptor characteristics of the carbonyl ligands, which leads to a partial electron transfer into their π^* orbitals and consequently to a weakening of the C≡O bonds. As expected, this effect is stronger in the negatively charged pentacarbonyl molybdate than in the neutral complex. The $[Mo(CO)_5]^{2-}$ anion shows a shape intermediate between a trigonal bipyramid (TP) and a square pyramid (SP) (τ_5 = 0.49; extreme forms: τ_5 = 0 for SP and 1 for TP; Addison *et al.*, 1984), with the following C—Mo—C angles: C1—Mo1—C2 = 168.11 (11)°, C3—Mo1—C4 = 108.89 (13)°, C3—Mo1—C5 = 112.35 (13)°, C4—Mo1—C5 = 138.76 (14)°. The carbonyl ligands point almost linearly towards the central metal atoms, with angular values in the range between 177.3 (2)° for Mo1—C2≡O2 and 179.2 (3)° for Mo1—C3≡O3. The overall charge of the anionic unit is compensated by two $[Cs([2.2.2]crypt)]^+$ cation complexes. The caesium cations therein are located in the centre of the chelating molecules and are coordinated by

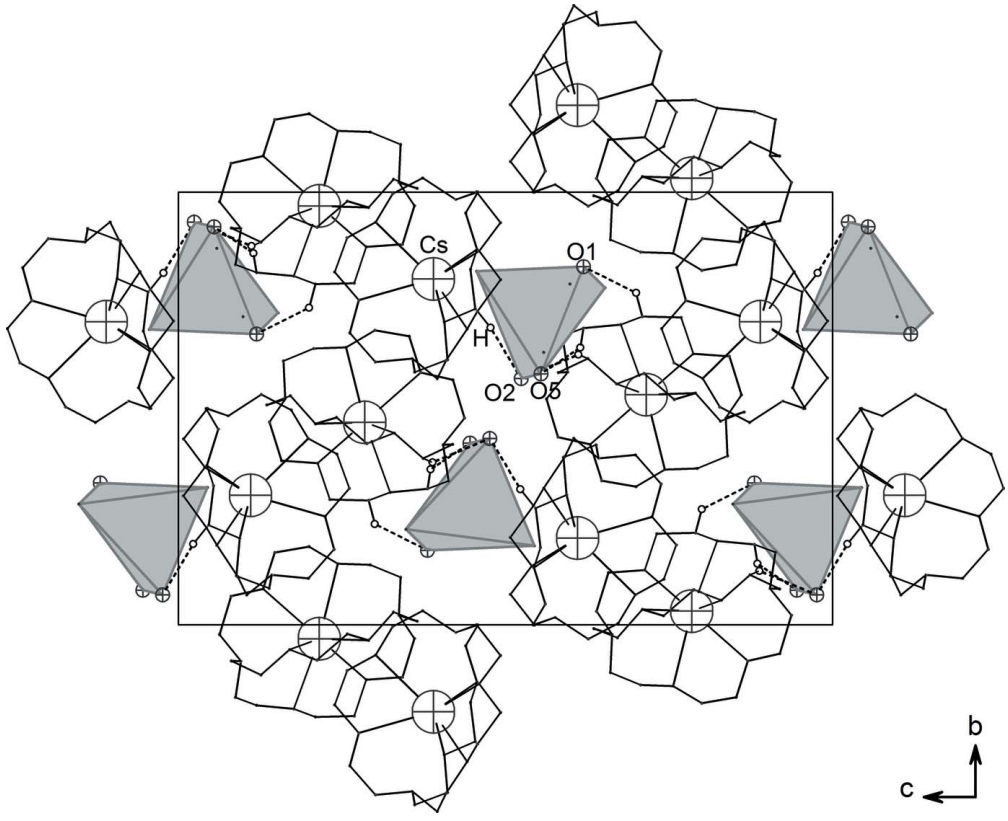


Figure 2
The crystal structure of $[Cs([2.2.2]crypt)]_2[Mo(CO)_5]$ in a projection onto the *bc* plane, including the shortest C—H···O hydrogen bonds. $[Mo(CO)_5]^{2-}$ anions are drawn as polyhedra and hydrogen bonds as dashed lines.

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Cs(C_{18}H_{36}N_2O_6)]_2[Mo(CO)_5]$
M_r	1254.78
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	123
a, b, c (Å)	13.2243 (1), 16.1431 (2), 24.3966 (3)
β (°)	90.958 (1)
V (Å^3)	5207.49 (10)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.70
Crystal size (mm)	0.16 × 0.12 × 0.12
Data collection	
Diffractometer	Rigaku Oxford DiffractionSuper-Nova Single source at offset/far, Eos
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2017)
T_{min}, T_{max}	0.798, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	33230, 11436, 9742
R_{int}	0.032
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.641
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.030, 0.065, 1.07
No. of reflections	11436
No. of parameters	586
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.94, −0.54

Computer programs: *CrysAlis PRO* (Rigaku OD, 2017), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2016* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

two nitrogen atoms and six oxygen atoms, respectively. The Cs—N and the Cs—O distances in the two cationic units range from 3.053 (2) to 3.107 (3) Å and from 2.9457 (19) to 3.022 (2) Å, and agree with corresponding values in the compound [Cs([2.2.2]crypt)]SCN·H_2O (Moras *et al.*, 1973). The positions of the cationic complexes in the crystal structure are determined by weak hydrogen bonds between the donor C—H fragments of the [2.2.2]crypt molecules and the acceptor O atoms of the carbonyl ligands. The shortest distances are found between C32—H32*B* ··· O2 [2.486 (2) Å], C22—H22*B*···O5 [2.663 (3) Å], C21—H21*B*···O1 [2.682 (3) Å] and C16—H16H···O2 [2.688 (2) Å] (Fig. 2).

Synthesis and crystallization

$Mo(CO)_3(\eta^5\text{-Cp})H$ was prepared *via* the route documented in the literature (Fischer *et al.*, 1955) Cs_5Bi_4 was prepared by high-temperature synthesis from the elements (Gascoin & Sevov, 2001). 13 mg (0.05 mmol) $Mo(CO)_3(\eta^5\text{-Cp})H$, 40 mg (0.026 mmol) Cs_5Bi_4 and 50 mg (0.13 mmol) [2.2.2]crypt were dissolved in dry liquid ammonia in a baked-out reaction vessel. Liquid ammonia was previously dried over sodium metal and condensed using a standard Schlenk line. The mixture was stored at 237 K for crystallization. After several weeks, crystals appeared as red blocks in an orange solution.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Acknowledgements

We thank the group of Professor Scheer (University of Regensburg) for providing the heteroleptic molybdenum carbonyl complex.

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full crystallographic data

IUCrData (2019). **4**, x191244 [https://doi.org/10.1107/S2414314619012446]

Synthesis and crystal structure of $[Cs([2.2.2]crypt)]_2[Mo(CO)_5]$

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Bis[(4,7,13,16,21,24-hexaoxa-1,10-diazabicyclo[8.8.8]hexacosane)caesium] pentacarbonylmolybdate

Crystal data

$[Cs(C_{18}H_{36}N_2O_6)]_2[Mo(CO)_5]$
M_r = 1254.78
Monoclinic, $P2_1/n$
a = 13.2243 (1) Å
b = 16.1431 (2) Å
c = 24.3966 (3) Å
β = 90.958 (1)°
V = 5207.49 (10) Å^3
Z = 4
$F(000)$ = 2536
D_x = 1.600 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 16518 reflections
θ = 3.4–30.2°
μ = 1.70 mm^{-1}
T = 123 K
Block, dark red
0.16 × 0.12 × 0.12 mm

Data collection

Rigaku Oxford DiffractionSuperNova Single source at offset/far, Eos diffractometer
Radiation source: micro-focus sealed X-ray tube
Detector resolution: 15.9702 pixels mm^{-1}
ω scans
Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2017)
T_{min} = 0.798, T_{max} = 1.000
33230 measured reflections
11436 independent reflections
9742 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 27.1°, θ_{min} = 3.3°
h = −16→16
k = −19→20
l = −31→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.065
S = 1.07
11436 reflections
586 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0225P)^2 + 4.0699P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.94 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 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. All H-atoms could be located from difference Fourier maps, but were positioned with idealized geometry.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cs2	0.74432 (2)	0.20064 (2)	0.38970 (2)	0.02053 (5)
Cs1	0.76188 (2)	0.46807 (2)	0.71525 (2)	0.02300 (5)
Mo1	0.75814 (2)	0.71499 (2)	0.43570 (2)	0.01903 (6)
O12	0.69040 (15)	0.24956 (12)	0.27581 (8)	0.0262 (4)
O16	0.93080 (15)	0.30030 (12)	0.40639 (9)	0.0285 (5)
O15	0.57629 (15)	0.13611 (12)	0.45957 (8)	0.0268 (4)
O6	0.83117 (15)	0.58337 (12)	0.62954 (8)	0.0272 (5)
O13	0.72714 (14)	0.06971 (12)	0.30150 (8)	0.0248 (4)
O17	0.91457 (14)	0.13224 (12)	0.45641 (9)	0.0292 (5)
O14	0.60182 (14)	0.31598 (12)	0.44122 (9)	0.0271 (5)
O10	0.90167 (15)	0.37334 (13)	0.78715 (8)	0.0297 (5)
O9	0.55536 (15)	0.44298 (13)	0.67005 (9)	0.0318 (5)
O3	0.73539 (16)	0.81711 (14)	0.54428 (9)	0.0353 (5)
O8	0.58288 (16)	0.46437 (14)	0.79055 (9)	0.0358 (5)
O11	0.84774 (14)	0.30608 (12)	0.67638 (8)	0.0268 (5)
O2	0.61536 (15)	0.56935 (12)	0.47584 (9)	0.0277 (5)
O7	0.82496 (15)	0.64115 (13)	0.74359 (9)	0.0307 (5)
N1	0.73363 (17)	0.41607 (14)	0.59564 (10)	0.0241 (5)
N4	0.73917 (17)	0.01730 (14)	0.42392 (10)	0.0225 (5)
O4	0.59731 (18)	0.77912 (15)	0.34782 (12)	0.0501 (7)
O5	0.93195 (17)	0.58026 (14)	0.44560 (12)	0.0489 (7)
N2	0.7888 (2)	0.52186 (17)	0.83690 (11)	0.0325 (6)
N3	0.74427 (18)	0.38451 (14)	0.35748 (10)	0.0257 (5)
O1	0.92534 (17)	0.82770 (14)	0.38055 (11)	0.0462 (7)
C3	0.7446 (2)	0.77912 (17)	0.50344 (12)	0.0242 (6)
C1	0.8634 (2)	0.78785 (18)	0.40131 (13)	0.0266 (7)
C7	0.7739 (2)	0.56636 (19)	0.58056 (12)	0.0283 (7)
H7A	0.794915	0.603448	0.551617	0.034*
H7B	0.702664	0.575979	0.587040	0.034*
C6	0.7894 (2)	0.47771 (18)	0.56288 (12)	0.0266 (6)
H6A	0.768342	0.472358	0.524761	0.032*
H6B	0.861008	0.465023	0.565252	0.032*
C40	0.9224 (2)	0.04821 (18)	0.43908 (13)	0.0286 (7)
H40A	0.983464	0.023660	0.454531	0.034*
H40B	0.926443	0.045906	0.399442	0.034*
C37	0.9088 (2)	0.38705 (18)	0.41127 (13)	0.0309 (7)
H37A	0.971352	0.418182	0.414470	0.037*
H37B	0.869865	0.396845	0.443983	0.037*
C29	0.7392 (2)	−0.03248 (17)	0.37323 (13)	0.0270 (6)
H29A	0.715051	−0.087775	0.381451	0.032*
H29B	0.808115	−0.037411	0.360647	0.032*
C17	0.6251 (2)	0.41683 (19)	0.58094 (13)	0.0286 (7)
H17A	0.614361	0.383304	0.548374	0.034*
H17B	0.605060	0.473124	0.572095	0.034*
C2	0.6655 (2)	0.62352 (18)	0.46048 (11)	0.0220 (6)

C4	0.6559 (2)	0.75477 (19)	0.38106 (14)	0.0311 (7)
C41	0.8309 (2)	0.00013 (18)	0.45776 (13)	0.0268 (6)
H41A	0.845756	−0.058654	0.456221	0.032*
H41B	0.817507	0.014172	0.495611	0.032*
C26	0.7153 (2)	0.18464 (18)	0.23878 (13)	0.0299 (7)
H26A	0.788201	0.178293	0.237437	0.036*
H26B	0.690531	0.198122	0.202217	0.036*
C34	0.6165 (2)	0.07057 (18)	0.49218 (12)	0.0287 (7)
H34A	0.566082	0.051795	0.517782	0.034*
H34B	0.674802	0.090187	0.513080	0.034*
C30	0.6796 (2)	0.43092 (17)	0.39556 (13)	0.0279 (7)
H30A	0.664150	0.484523	0.379518	0.033*
H30B	0.717504	0.440571	0.429327	0.033*
C33	0.5368 (2)	0.20210 (19)	0.49248 (13)	0.0310 (7)
H33A	0.586708	0.218116	0.520082	0.037*
H33B	0.476782	0.183225	0.511072	0.037*
C25	0.7381 (2)	0.32549 (18)	0.26203 (13)	0.0287 (7)
H25A	0.720240	0.340816	0.224668	0.034*
H25B	0.810995	0.319283	0.264625	0.034*
C27	0.6681 (2)	0.10553 (18)	0.25778 (12)	0.0289 (7)
H27A	0.600219	0.116496	0.270313	0.035*
H27B	0.663489	0.066803	0.227447	0.035*
C32	0.5110 (2)	0.27512 (19)	0.45714 (14)	0.0325 (7)
H32A	0.473607	0.256881	0.424783	0.039*
H32B	0.468679	0.313295	0.477177	0.039*
C28	0.6744 (2)	0.00361 (18)	0.32764 (13)	0.0271 (6)
H28A	0.658094	−0.039132	0.300994	0.032*
H28B	0.611659	0.024251	0.342466	0.032*
C35	0.6473 (2)	−0.00036 (18)	0.45569 (13)	0.0270 (6)
H35A	0.659294	−0.049068	0.478153	0.032*
H35B	0.591991	−0.012859	0.430419	0.032*
C36	0.8494 (2)	0.41556 (18)	0.36126 (13)	0.0297 (7)
H36A	0.847705	0.475637	0.361167	0.036*
H36B	0.884891	0.398028	0.328789	0.036*
C24	0.7038 (2)	0.39239 (18)	0.30122 (13)	0.0297 (7)
H24A	0.723738	0.445840	0.286798	0.036*
H24B	0.630521	0.391535	0.302431	0.036*
C38	0.9847 (2)	0.2695 (2)	0.45360 (14)	0.0339 (7)
H38A	0.945064	0.278299	0.486175	0.041*
H38B	1.048193	0.299020	0.458128	0.041*
C5	0.8676 (2)	0.62980 (19)	0.44144 (14)	0.0305 (7)
C31	0.5814 (2)	0.38854 (18)	0.40932 (13)	0.0297 (7)
H31A	0.539004	0.426104	0.429794	0.036*
H31B	0.545475	0.373383	0.375814	0.036*
C21	0.9350 (2)	0.2875 (2)	0.70928 (13)	0.0310 (7)
H21A	0.987760	0.327687	0.702161	0.037*
H21B	0.960359	0.233046	0.699827	0.037*
C23	0.7750 (2)	0.33246 (19)	0.58727 (13)	0.0315 (7)

H23A	0.788193	0.325213	0.548576	0.038*
H23B	0.724156	0.292171	0.597323	0.038*
C16	0.5584 (2)	0.3845 (2)	0.62611 (13)	0.0325 (7)
H16A	0.490530	0.375171	0.611711	0.039*
H16B	0.584707	0.332083	0.639572	0.039*
C11	0.8183 (3)	0.6100 (2)	0.83950 (14)	0.0376 (8)
H11A	0.854320	0.619694	0.873879	0.045*
H11B	0.757490	0.643509	0.839641	0.045*
C22	0.8711 (2)	0.3143 (2)	0.61944 (13)	0.0316 (7)
H22A	0.901273	0.263462	0.606258	0.038*
H22B	0.919150	0.358955	0.614572	0.038*
C39	1.0048 (2)	0.1785 (2)	0.44633 (15)	0.0351 (8)
H39A	1.027217	0.168091	0.409310	0.042*
H39B	1.058066	0.161074	0.471616	0.042*
C13	0.6017 (2)	0.5296 (2)	0.82879 (14)	0.0388 (8)
H13A	0.542849	0.537539	0.851370	0.047*
H13B	0.614249	0.580757	0.809216	0.047*
C10	0.8839 (3)	0.6386 (2)	0.79315 (14)	0.0393 (8)
H10A	0.910744	0.693277	0.801244	0.047*
H10B	0.940344	0.600886	0.788969	0.047*
C14	0.4937 (2)	0.4790 (2)	0.75821 (14)	0.0415 (9)
H14A	0.494811	0.535039	0.743909	0.050*
H14B	0.434550	0.473264	0.780886	0.050*
C18	0.8696 (3)	0.4684 (2)	0.86080 (14)	0.0392 (8)
H18A	0.864534	0.469820	0.900406	0.047*
H18B	0.934614	0.491834	0.851468	0.047*
C12	0.6927 (3)	0.5085 (2)	0.86487 (14)	0.0382 (8)
H12A	0.691439	0.542422	0.897671	0.046*
H12B	0.688344	0.450963	0.876062	0.046*
C19	0.8671 (3)	0.3793 (2)	0.84241 (13)	0.0398 (8)
H19A	0.910065	0.346147	0.866398	0.048*
H19B	0.798618	0.358084	0.844452	0.048*
C8	0.8178 (3)	0.66710 (19)	0.64725 (13)	0.0341 (7)
H8A	0.746614	0.677990	0.652837	0.041*
H8B	0.841713	0.704848	0.619366	0.041*
C15	0.4875 (2)	0.4189 (2)	0.71187 (15)	0.0405 (9)
H15A	0.504761	0.363815	0.724921	0.049*
H15B	0.418913	0.417324	0.697108	0.049*
C20	0.9091 (2)	0.28955 (19)	0.76867 (13)	0.0328 (7)
H20A	0.845229	0.261398	0.774071	0.039*
H20B	0.960859	0.260792	0.789909	0.039*
C9	0.8759 (3)	0.6808 (2)	0.69973 (14)	0.0382 (8)
H9A	0.943586	0.658226	0.696627	0.046*
H9B	0.881655	0.739673	0.707024	0.046*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cs2	0.02092 (9)	0.01816 (9)	0.02251 (10)	0.00146 (7)	0.00008 (6)	0.00036 (7)
Cs1	0.02253 (9)	0.02529 (10)	0.02114 (10)	0.00046 (7)	−0.00109 (6)	−0.00001 (7)
Mo1	0.01902 (12)	0.01872 (12)	0.01932 (13)	0.00006 (9)	−0.00018 (9)	0.00094 (9)
O12	0.0384 (12)	0.0199 (10)	0.0203 (11)	0.0020 (9)	0.0018 (8)	−0.0013 (8)
O16	0.0294 (11)	0.0229 (11)	0.0330 (13)	−0.0012 (9)	−0.0057 (9)	0.0003 (9)
O15	0.0299 (11)	0.0251 (11)	0.0255 (12)	0.0008 (9)	0.0042 (8)	−0.0030 (9)
O6	0.0328 (11)	0.0253 (11)	0.0235 (11)	−0.0030 (9)	0.0009 (8)	−0.0020 (9)
O13	0.0276 (10)	0.0197 (10)	0.0268 (12)	0.0023 (8)	−0.0032 (8)	0.0013 (8)
O17	0.0224 (10)	0.0276 (11)	0.0374 (13)	−0.0012 (9)	−0.0032 (9)	0.0024 (9)
O14	0.0211 (10)	0.0222 (10)	0.0381 (13)	−0.0002 (8)	0.0044 (9)	−0.0028 (9)
O10	0.0347 (11)	0.0303 (11)	0.0239 (12)	0.0056 (9)	−0.0009 (9)	0.0023 (9)
O9	0.0241 (11)	0.0387 (12)	0.0325 (13)	−0.0076 (9)	0.0003 (9)	0.0060 (10)
O3	0.0398 (13)	0.0384 (13)	0.0278 (13)	0.0000 (10)	0.0046 (10)	−0.0097 (10)
O8	0.0283 (11)	0.0463 (14)	0.0330 (13)	0.0086 (10)	0.0030 (9)	0.0071 (11)
O11	0.0230 (10)	0.0303 (11)	0.0270 (12)	0.0026 (9)	−0.0014 (8)	0.0013 (9)
O2	0.0291 (11)	0.0210 (10)	0.0331 (13)	−0.0041 (9)	0.0038 (9)	−0.0012 (9)
O7	0.0334 (11)	0.0325 (12)	0.0262 (12)	−0.0072 (10)	−0.0006 (9)	−0.0054 (9)
N1	0.0258 (12)	0.0225 (12)	0.0238 (14)	−0.0006 (10)	−0.0027 (10)	0.0001 (10)
N4	0.0214 (12)	0.0196 (12)	0.0264 (14)	−0.0011 (10)	0.0002 (9)	0.0029 (10)
O4	0.0430 (14)	0.0448 (15)	0.0618 (19)	−0.0106 (12)	−0.0265 (13)	0.0213 (13)
O5	0.0341 (13)	0.0291 (13)	0.083 (2)	0.0085 (11)	0.0051 (12)	0.0028 (13)
N2	0.0372 (15)	0.0360 (15)	0.0242 (15)	0.0069 (12)	0.0008 (11)	−0.0004 (11)
N3	0.0288 (13)	0.0184 (12)	0.0297 (14)	0.0012 (10)	−0.0015 (10)	−0.0018 (10)
O1	0.0343 (13)	0.0298 (12)	0.0753 (19)	0.0023 (10)	0.0252 (12)	0.0133 (12)
C3	0.0207 (14)	0.0246 (15)	0.0274 (17)	−0.0035 (12)	0.0007 (11)	0.0029 (12)
C1	0.0238 (15)	0.0217 (15)	0.0346 (18)	0.0056 (12)	0.0042 (12)	0.0021 (13)
C7	0.0316 (16)	0.0295 (16)	0.0237 (16)	−0.0046 (13)	−0.0010 (12)	0.0056 (13)
C6	0.0301 (15)	0.0320 (16)	0.0178 (15)	0.0020 (13)	0.0020 (11)	−0.0002 (12)
C40	0.0244 (15)	0.0306 (17)	0.0306 (17)	0.0074 (13)	−0.0026 (12)	0.0029 (13)
C37	0.0292 (16)	0.0259 (16)	0.0375 (19)	−0.0040 (13)	−0.0015 (13)	−0.0053 (14)
C29	0.0280 (15)	0.0186 (14)	0.0346 (18)	0.0033 (12)	0.0014 (12)	−0.0003 (12)
C17	0.0294 (16)	0.0278 (16)	0.0282 (17)	−0.0011 (13)	−0.0109 (12)	0.0013 (13)
C2	0.0201 (14)	0.0243 (15)	0.0216 (15)	0.0032 (12)	−0.0032 (11)	−0.0038 (12)
C4	0.0305 (16)	0.0258 (16)	0.0366 (19)	−0.0100 (13)	−0.0058 (14)	0.0067 (14)
C41	0.0281 (15)	0.0233 (15)	0.0288 (17)	0.0052 (12)	−0.0033 (12)	0.0063 (12)
C26	0.0376 (17)	0.0299 (16)	0.0221 (16)	0.0070 (14)	0.0028 (13)	0.0003 (13)
C34	0.0261 (15)	0.0324 (17)	0.0277 (17)	−0.0030 (13)	0.0042 (12)	0.0039 (13)
C30	0.0328 (16)	0.0178 (14)	0.0330 (18)	0.0025 (12)	0.0000 (13)	−0.0013 (12)
C33	0.0268 (15)	0.0335 (17)	0.0332 (18)	−0.0042 (13)	0.0107 (13)	−0.0112 (14)
C25	0.0383 (17)	0.0262 (16)	0.0215 (16)	−0.0018 (13)	0.0024 (12)	0.0057 (12)
C27	0.0374 (17)	0.0247 (16)	0.0245 (17)	0.0062 (13)	−0.0070 (13)	−0.0037 (12)
C32	0.0214 (15)	0.0300 (17)	0.046 (2)	−0.0010 (13)	0.0094 (13)	−0.0106 (14)
C28	0.0296 (16)	0.0219 (15)	0.0296 (17)	0.0002 (12)	−0.0013 (12)	−0.0031 (13)
C35	0.0294 (15)	0.0217 (15)	0.0301 (17)	−0.0021 (12)	0.0029 (12)	0.0058 (12)
C36	0.0329 (16)	0.0190 (15)	0.0373 (19)	−0.0040 (13)	0.0036 (13)	−0.0004 (13)

C24	0.0384 (17)	0.0203 (15)	0.0302 (18)	0.0010 (13)	−0.0034 (13)	0.0067 (13)
C38	0.0234 (15)	0.0391 (18)	0.039 (2)	−0.0072 (14)	−0.0094 (13)	0.0012 (15)
C5	0.0269 (16)	0.0234 (16)	0.041 (2)	−0.0042 (13)	0.0067 (13)	0.0011 (14)
C31	0.0282 (16)	0.0261 (16)	0.0347 (18)	0.0079 (13)	−0.0009 (13)	−0.0052 (13)
C21	0.0265 (15)	0.0307 (17)	0.0356 (19)	0.0059 (13)	−0.0032 (13)	0.0009 (14)
C23	0.0408 (18)	0.0281 (16)	0.0255 (17)	0.0039 (14)	−0.0047 (13)	−0.0040 (13)
C16	0.0281 (16)	0.0323 (17)	0.0369 (19)	−0.0055 (14)	−0.0094 (13)	0.0066 (14)
C11	0.0442 (19)	0.0409 (19)	0.0274 (18)	0.0034 (16)	−0.0058 (14)	−0.0072 (15)
C22	0.0322 (17)	0.0325 (17)	0.0304 (18)	0.0080 (14)	0.0030 (13)	−0.0030 (14)
C39	0.0191 (15)	0.0388 (19)	0.047 (2)	0.0003 (14)	−0.0076 (13)	0.0079 (16)
C13	0.0360 (18)	0.045 (2)	0.036 (2)	0.0102 (16)	0.0135 (14)	0.0069 (16)
C10	0.0406 (19)	0.0387 (19)	0.038 (2)	−0.0078 (16)	−0.0076 (15)	−0.0094 (16)
C14	0.0222 (16)	0.062 (2)	0.041 (2)	0.0089 (16)	0.0068 (14)	0.0126 (18)
C18	0.0442 (19)	0.052 (2)	0.0210 (17)	0.0117 (17)	−0.0087 (14)	−0.0053 (15)
C12	0.047 (2)	0.043 (2)	0.0243 (18)	0.0051 (16)	0.0043 (14)	0.0003 (15)
C19	0.050 (2)	0.046 (2)	0.0230 (18)	0.0152 (17)	−0.0017 (14)	0.0071 (15)
C8	0.0476 (19)	0.0229 (16)	0.0319 (19)	−0.0063 (14)	0.0068 (14)	0.0013 (13)
C15	0.0225 (16)	0.055 (2)	0.044 (2)	−0.0055 (15)	0.0011 (14)	0.0185 (17)
C20	0.0339 (17)	0.0289 (17)	0.0353 (19)	0.0073 (14)	−0.0044 (14)	0.0071 (14)
C9	0.0431 (19)	0.0334 (18)	0.038 (2)	−0.0141 (15)	0.0058 (15)	−0.0043 (15)

Geometric parameters (Å, º)

Cs2—O12	2.964 (2)	C17—H17A	0.9700
Cs2—O16	2.967 (2)	C17—H17B	0.9700
Cs2—O15	3.009 (2)	C17—C16	1.516 (4)
Cs2—O13	3.022 (2)	C41—H41A	0.9700
Cs2—O17	2.969 (2)	C41—H41B	0.9700
Cs2—O14	2.9457 (19)	C26—H26A	0.9700
Cs2—N4	3.076 (2)	C26—H26B	0.9700
Cs2—N3	3.070 (2)	C26—C27	1.498 (4)
Cs1—O6	2.956 (2)	C34—H34A	0.9700
Cs1—O10	2.954 (2)	C34—H34B	0.9700
Cs1—O9	2.956 (2)	C34—C35	1.511 (4)
Cs1—O8	3.021 (2)	C30—H30A	0.9700
Cs1—O11	3.010 (2)	C30—H30B	0.9700
Cs1—O7	2.994 (2)	C30—C31	1.510 (4)
Cs1—N1	3.053 (2)	C33—H33A	0.9700
Cs1—N2	3.107 (3)	C33—H33B	0.9700
Mo1—C3	1.961 (3)	C33—C32	1.497 (5)
Mo1—C1	2.016 (3)	C25—H25A	0.9700
Mo1—C2	2.017 (3)	C25—H25B	0.9700
Mo1—C4	1.989 (3)	C25—C24	1.517 (4)
Mo1—C5	2.000 (3)	C27—H27A	0.9700
O12—C26	1.426 (3)	C27—H27B	0.9700
O12—C25	1.422 (3)	C32—H32A	0.9700
O16—C37	1.436 (3)	C32—H32B	0.9700
O16—C38	1.433 (4)	C28—H28A	0.9700

O15—C34	1.422 (3)	C28—H28B	0.9700
O15—C33	1.437 (3)	C35—H35A	0.9700
O6—C7	1.431 (3)	C35—H35B	0.9700
O6—C8	1.431 (4)	C36—H36A	0.9700
O13—C27	1.433 (3)	C36—H36B	0.9700
O13—C28	1.430 (3)	C24—H24A	0.9700
O17—C40	1.425 (3)	C24—H24B	0.9700
O17—C39	1.433 (4)	C38—H38A	0.9700
O14—C32	1.430 (3)	C38—H38B	0.9700
O14—C31	1.429 (4)	C38—C39	1.503 (4)
O10—C19	1.434 (4)	C31—H31A	0.9700
O10—C20	1.430 (4)	C31—H31B	0.9700
O9—C16	1.430 (4)	C21—H21A	0.9700
O9—C15	1.424 (4)	C21—H21B	0.9700
O3—C3	1.178 (4)	C21—C20	1.495 (4)
O8—C13	1.425 (4)	C23—H23A	0.9700
O8—C14	1.428 (4)	C23—H23B	0.9700
O11—C21	1.427 (3)	C23—C22	1.511 (4)
O11—C22	1.434 (4)	C16—H16A	0.9700
O2—C2	1.164 (3)	C16—H16B	0.9700
O7—C10	1.428 (4)	C11—H11A	0.9700
O7—C9	1.426 (4)	C11—H11B	0.9700
N1—C6	1.481 (4)	C11—C10	1.509 (5)
N1—C17	1.473 (4)	C22—H22A	0.9700
N1—C23	1.472 (4)	C22—H22B	0.9700
N4—C29	1.475 (4)	C39—H39A	0.9700
N4—C41	1.482 (3)	C39—H39B	0.9700
N4—C35	1.479 (4)	C13—H13A	0.9700
O4—C4	1.180 (4)	C13—H13B	0.9700
O5—C5	1.171 (4)	C13—C12	1.518 (5)
N2—C11	1.476 (4)	C10—H10A	0.9700
N2—C18	1.485 (4)	C10—H10B	0.9700
N2—C12	1.468 (4)	C14—H14A	0.9700
N3—C30	1.478 (4)	C14—H14B	0.9700
N3—C36	1.479 (4)	C14—C15	1.491 (5)
N3—C24	1.470 (4)	C18—H18A	0.9700
O1—C1	1.165 (3)	C18—H18B	0.9700
C7—H7A	0.9700	C18—C19	1.508 (5)
C7—H7B	0.9700	C12—H12A	0.9700
C7—C6	1.510 (4)	C12—H12B	0.9700
C6—H6A	0.9700	C19—H19A	0.9700
C6—H6B	0.9700	C19—H19B	0.9700
C40—H40A	0.9700	C8—H8A	0.9700
C40—H40B	0.9700	C8—H8B	0.9700
C40—C41	1.515 (4)	C8—C9	1.498 (5)
C37—H37A	0.9700	C15—H15A	0.9700
C37—H37B	0.9700	C15—H15B	0.9700
C37—C36	1.512 (4)	C20—H20A	0.9700

C29—H29A	0.9700	C20—H20B	0.9700
C29—H29B	0.9700	C9—H9A	0.9700
C29—C28	1.509 (4)	C9—H9B	0.9700
O12—Cs2—O16	99.83 (6)	O12—C26—C27	109.2 (2)
O12—Cs2—O15	117.06 (6)	H26A—C26—H26B	108.3
O12—Cs2—O13	60.32 (5)	C27—C26—H26A	109.8
O12—Cs2—O17	141.38 (6)	C27—C26—H26B	109.8
O12—Cs2—N4	120.31 (6)	O15—C34—H34A	109.7
O12—Cs2—N3	60.23 (6)	O15—C34—H34B	109.7
O16—Cs2—O15	136.88 (6)	O15—C34—C35	109.7 (2)
O16—Cs2—O13	121.97 (6)	H34A—C34—H34B	108.2
O16—Cs2—O17	60.36 (5)	C35—C34—H34A	109.7
O16—Cs2—N4	120.43 (6)	C35—C34—H34B	109.7
O16—Cs2—N3	60.50 (6)	N3—C30—H30A	108.6
O15—Cs2—O13	96.53 (5)	N3—C30—H30B	108.6
O15—Cs2—N4	59.55 (6)	N3—C30—C31	114.8 (2)
O15—Cs2—N3	118.86 (6)	H30A—C30—H30B	107.5
O13—Cs2—N4	61.22 (6)	C31—C30—H30A	108.6
O13—Cs2—N3	119.62 (6)	C31—C30—H30B	108.6
O17—Cs2—O15	96.95 (6)	O15—C33—H33A	109.6
O17—Cs2—O13	100.22 (5)	O15—C33—H33B	109.6
O17—Cs2—N4	60.88 (6)	O15—C33—C32	110.1 (3)
O17—Cs2—N3	119.79 (6)	H33A—C33—H33B	108.2
O14—Cs2—O12	94.93 (6)	C32—C33—H33A	109.6
O14—Cs2—O16	97.75 (5)	C32—C33—H33B	109.6
O14—Cs2—O15	59.56 (5)	O12—C25—H25A	109.9
O14—Cs2—O13	134.82 (5)	O12—C25—H25B	109.9
O14—Cs2—O17	119.07 (6)	O12—C25—C24	109.0 (2)
O14—Cs2—N4	118.36 (6)	H25A—C25—H25B	108.3
O14—Cs2—N3	60.06 (6)	C24—C25—H25A	109.9
N3—Cs2—N4	178.41 (6)	C24—C25—H25B	109.9
O6—Cs1—O8	134.25 (6)	O13—C27—C26	110.5 (2)
O6—Cs1—O11	101.60 (5)	O13—C27—H27A	109.6
O6—Cs1—O7	59.15 (6)	O13—C27—H27B	109.6
O6—Cs1—N1	62.07 (6)	C26—C27—H27A	109.6
O6—Cs1—N2	117.89 (6)	C26—C27—H27B	109.6
O10—Cs1—O6	123.21 (6)	H27A—C27—H27B	108.1
O10—Cs1—O9	135.70 (6)	O14—C32—C33	109.6 (2)
O10—Cs1—O8	96.75 (6)	O14—C32—H32A	109.8
O10—Cs1—O11	60.12 (6)	O14—C32—H32B	109.8
O10—Cs1—O7	100.19 (6)	C33—C32—H32A	109.8
O10—Cs1—N1	119.38 (6)	C33—C32—H32B	109.8
O10—Cs1—N2	61.11 (6)	H32A—C32—H32B	108.2
O9—Cs1—O6	96.77 (6)	O13—C28—C29	110.0 (2)
O9—Cs1—O8	59.71 (6)	O13—C28—H28A	109.7
O9—Cs1—O11	96.57 (6)	O13—C28—H28B	109.7
O9—Cs1—O7	117.78 (6)	C29—C28—H28A	109.7

O9—Cs1—N1	60.55 (6)	C29—C28—H28B	109.7
O9—Cs1—N2	119.00 (6)	H28A—C28—H28B	108.2
O8—Cs1—N1	119.42 (6)	N4—C35—C34	113.2 (2)
O8—Cs1—N2	60.20 (7)	N4—C35—H35A	108.9
O11—Cs1—O8	118.55 (6)	N4—C35—H35B	108.9
O11—Cs1—N1	60.06 (6)	C34—C35—H35A	108.9
O11—Cs1—N2	120.39 (6)	C34—C35—H35B	108.9
O7—Cs1—O8	95.51 (6)	H35A—C35—H35B	107.7
O7—Cs1—O11	141.12 (5)	N3—C36—C37	115.0 (2)
O7—Cs1—N1	120.43 (6)	N3—C36—H36A	108.5
O7—Cs1—N2	59.44 (6)	N3—C36—H36B	108.5
N1—Cs1—N2	179.48 (7)	C37—C36—H36A	108.5
C3—Mo1—C1	96.68 (12)	C37—C36—H36B	108.5
C3—Mo1—C2	93.98 (11)	H36A—C36—H36B	107.5
C3—Mo1—C4	108.89 (13)	N3—C24—C25	114.7 (2)
C3—Mo1—C5	112.35 (13)	N3—C24—H24A	108.6
C1—Mo1—C2	168.11 (11)	N3—C24—H24B	108.6
C4—Mo1—C1	89.93 (12)	C25—C24—H24A	108.6
C4—Mo1—C2	91.60 (11)	C25—C24—H24B	108.6
C4—Mo1—C5	138.76 (14)	H24A—C24—H24B	107.6
C5—Mo1—C1	85.78 (11)	O16—C38—H38A	109.8
C5—Mo1—C2	85.30 (11)	O16—C38—H38B	109.8
C26—O12—Cs2	110.09 (16)	O16—C38—C39	109.3 (3)
C25—O12—Cs2	110.52 (16)	H38A—C38—H38B	108.3
C25—O12—C26	112.1 (2)	C39—C38—H38A	109.8
C37—O16—Cs2	111.78 (16)	C39—C38—H38B	109.8
C38—O16—Cs2	108.87 (16)	O5—C5—Mo1	179.0 (3)
C38—O16—C37	111.8 (2)	O14—C31—C30	109.7 (2)
C34—O15—Cs2	107.55 (15)	O14—C31—H31A	109.7
C34—O15—C33	112.0 (2)	O14—C31—H31B	109.7
C33—O15—Cs2	109.78 (15)	C30—C31—H31A	109.7
C7—O6—Cs1	107.69 (15)	C30—C31—H31B	109.7
C7—O6—C8	111.5 (2)	H31A—C31—H31B	108.2
C8—O6—Cs1	109.88 (16)	O11—C21—H21A	109.6
C27—O13—Cs2	106.33 (15)	O11—C21—H21B	109.6
C28—O13—Cs2	103.63 (16)	O11—C21—C20	110.1 (2)
C28—O13—C27	111.7 (2)	H21A—C21—H21B	108.2
C40—O17—Cs2	104.45 (16)	C20—C21—H21A	109.6
C40—O17—C39	112.4 (2)	C20—C21—H21B	109.6
C39—O17—Cs2	109.77 (16)	N1—C23—H23A	108.6
C32—O14—Cs2	111.76 (15)	N1—C23—H23B	108.6
C31—O14—Cs2	113.70 (16)	N1—C23—C22	114.7 (3)
C31—O14—C32	112.0 (2)	H23A—C23—H23B	107.6
C19—O10—Cs1	108.50 (17)	C22—C23—H23A	108.6
C20—O10—Cs1	110.37 (17)	C22—C23—H23B	108.6
C20—O10—C19	112.6 (2)	O9—C16—C17	110.0 (2)
C16—O9—Cs1	109.44 (16)	O9—C16—H16A	109.7
C15—O9—Cs1	111.09 (18)	O9—C16—H16B	109.7

C15—O9—C16	112.5 (2)	C17—C16—H16A	109.7
C13—O8—Cs1	104.66 (17)	C17—C16—H16B	109.7
C13—O8—C14	111.9 (2)	H16A—C16—H16B	108.2
C14—O8—Cs1	108.00 (17)	N2—C11—H11A	108.6
C21—O11—Cs1	108.13 (16)	N2—C11—H11B	108.6
C21—O11—C22	112.3 (2)	N2—C11—C10	114.7 (3)
C22—O11—Cs1	108.25 (16)	H11A—C11—H11B	107.6
C10—O7—Cs1	108.36 (18)	C10—C11—H11A	108.6
C9—O7—Cs1	112.26 (17)	C10—C11—H11B	108.6
C9—O7—C10	113.0 (2)	O11—C22—C23	109.2 (2)
C6—N1—Cs1	106.09 (16)	O11—C22—H22A	109.8
C17—N1—Cs1	109.48 (17)	O11—C22—H22B	109.8
C17—N1—C6	110.8 (2)	C23—C22—H22A	109.8
C23—N1—Cs1	110.17 (17)	C23—C22—H22B	109.8
C23—N1—C6	110.6 (2)	H22A—C22—H22B	108.3
C23—N1—C17	109.7 (2)	O17—C39—C38	109.9 (2)
C29—N4—Cs2	107.23 (16)	O17—C39—H39A	109.7
C29—N4—C41	110.7 (2)	O17—C39—H39B	109.7
C29—N4—C35	110.2 (2)	C38—C39—H39A	109.7
C41—N4—Cs2	108.03 (16)	C38—C39—H39B	109.7
C35—N4—Cs2	110.47 (16)	H39A—C39—H39B	108.2
C35—N4—C41	110.1 (2)	O8—C13—H13A	109.7
C11—N2—Cs1	109.65 (18)	O8—C13—H13B	109.7
C11—N2—C18	110.8 (3)	O8—C13—C12	110.0 (3)
C18—N2—Cs1	106.43 (18)	H13A—C13—H13B	108.2
C12—N2—Cs1	108.47 (19)	C12—C13—H13A	109.7
C12—N2—C11	110.6 (3)	C12—C13—H13B	109.7
C12—N2—C18	110.8 (3)	O7—C10—C11	109.3 (3)
C30—N3—Cs2	109.07 (16)	O7—C10—H10A	109.8
C30—N3—C36	110.0 (2)	O7—C10—H10B	109.8
C36—N3—Cs2	108.40 (16)	C11—C10—H10A	109.8
C24—N3—Cs2	108.73 (16)	C11—C10—H10B	109.8
C24—N3—C30	109.7 (2)	H10A—C10—H10B	108.3
C24—N3—C36	110.9 (2)	O8—C14—H14A	109.6
O3—C3—Mo1	179.2 (3)	O8—C14—H14B	109.6
O1—C1—Mo1	177.8 (3)	O8—C14—C15	110.3 (3)
O6—C7—H7A	109.6	H14A—C14—H14B	108.1
O6—C7—H7B	109.6	C15—C14—H14A	109.6
O6—C7—C6	110.4 (2)	C15—C14—H14B	109.6
H7A—C7—H7B	108.1	N2—C18—H18A	108.5
C6—C7—H7A	109.6	N2—C18—H18B	108.5
C6—C7—H7B	109.6	N2—C18—C19	115.2 (3)
N1—C6—C7	114.3 (2)	H18A—C18—H18B	107.5
N1—C6—H6A	108.7	C19—C18—H18A	108.5
N1—C6—H6B	108.7	C19—C18—H18B	108.5
C7—C6—H6A	108.7	N2—C12—C13	112.4 (3)
C7—C6—H6B	108.7	N2—C12—H12A	109.1
H6A—C6—H6B	107.6	N2—C12—H12B	109.1

O17—C40—H40A	109.7	C13—C12—H12A	109.1
O17—C40—H40B	109.7	C13—C12—H12B	109.1
O17—C40—C41	109.6 (2)	H12A—C12—H12B	107.9
H40A—C40—H40B	108.2	O10—C19—C18	109.8 (3)
C41—C40—H40A	109.7	O10—C19—H19A	109.7
C41—C40—H40B	109.7	O10—C19—H19B	109.7
O16—C37—H37A	109.8	C18—C19—H19A	109.7
O16—C37—H37B	109.8	C18—C19—H19B	109.7
O16—C37—C36	109.5 (2)	H19A—C19—H19B	108.2
H37A—C37—H37B	108.2	O6—C8—H8A	109.8
C36—C37—H37A	109.8	O6—C8—H8B	109.8
C36—C37—H37B	109.8	O6—C8—C9	109.5 (3)
N4—C29—H29A	108.9	H8A—C8—H8B	108.2
N4—C29—H29B	108.9	C9—C8—H8A	109.8
N4—C29—C28	113.5 (2)	C9—C8—H8B	109.8
H29A—C29—H29B	107.7	O9—C15—C14	109.7 (3)
C28—C29—H29A	108.9	O9—C15—H15A	109.7
C28—C29—H29B	108.9	O9—C15—H15B	109.7
N1—C17—H17A	108.9	C14—C15—H15A	109.7
N1—C17—H17B	108.9	C14—C15—H15B	109.7
N1—C17—C16	113.4 (2)	H15A—C15—H15B	108.2
H17A—C17—H17B	107.7	O10—C20—C21	110.2 (3)
C16—C17—H17A	108.9	O10—C20—H20A	109.6
C16—C17—H17B	108.9	O10—C20—H20B	109.6
O2—C2—Mo1	177.3 (2)	C21—C20—H20A	109.6
O4—C4—Mo1	178.3 (3)	C21—C20—H20B	109.6
N4—C41—C40	112.8 (2)	H20A—C20—H20B	108.1
N4—C41—H41A	109.0	O7—C9—C8	109.5 (3)
N4—C41—H41B	109.0	O7—C9—H9A	109.8
C40—C41—H41A	109.0	O7—C9—H9B	109.8
C40—C41—H41B	109.0	C8—C9—H9A	109.8
H41A—C41—H41B	107.8	C8—C9—H9B	109.8
O12—C26—H26A	109.8	H9A—C9—H9B	108.2
O12—C26—H26B	109.8		