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catena-Poly[[tetrakis(μ-pentafluorobenzoato-κ²*O*:*O*′)dimolybdenum(II)]-μ-4,4′-bipyridine-κ²*N*:*N*′]

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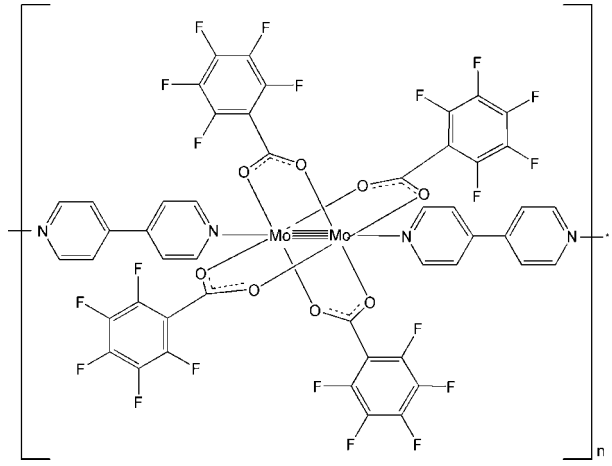
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.024; wR factor = 0.061; data-to-parameter ratio = 10.4.

In the title compound, $[Mo_2(C_7F_5O_2)_4(C_{10}H_8N_2)]_n$, the molecule forms a paddle-wheel-type structure. Each Mo_2^{4+} unit is equatorially coordinated by four pentafluorobenzoate groups, while the axial positions are occupied by two 4,4′-bipyridine molecules. The Mo—Mo bond length of 2.1227 (4) Å is representative of a dimolybdenum quadruple bond. An infinite linear chain parallel to [110] is formed by the Mo_2^{4+} unit coordinating axially to the two N atoms of the 4,4′-bipyridine ligand [Mo—N = 2.594 (2) Å]. The crystal packing shows molecules linked together into a three-dimensional network *via* Mo—N coordination interactions and weak π–π stacking interactions between perfluorophenyl rings [centroid–centroid distance = 3.7280 (3) Å and centroid-to-plane distance = 3.6103 (12) Å between two pentafluorophenyl rings].

Related literature

For background to coordination polymers, see: Batten (2002); Kumar *et al.* (2004). For torsion angles about the pentafluorobenzoate anion, see: Reddy *et al.* (2004); Bach *et al.* (2001); For Mo–Mo quadruple bond lengths, see: Cotton *et al.* (2005).



Experimental

Crystal data

$[Mo_2(C_7F_5O_2)_4(C_{10}H_8N_2)]$
M_r = 1192.34
Triclinic, $P\overline{1}$
a = 8.8858 (8) Å
b = 9.9311 (9) Å
c = 11.1978 (10) Å
α = 101.158 (1)°
β = 94.697 (1)°
γ = 99.092 (1)°
V = 950.83 (15) Å³
Z = 1
Mo $K\alpha$ radiation
μ = 0.82 mm⁻¹
T = 293 K
0.20 × 0.18 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.849, T_{max} = 0.884
4937 measured reflections
3294 independent reflections
3072 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.061
S = 1.01
3294 reflections
316 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å⁻³
$\Delta\rho_{min}$ = −0.47 e Å⁻³

Table 1
Selected bond lengths (Å).

Mo1—O1	2.1124 (17)	Mo1—O5	2.1427 (16)
Mo1—O6	2.1155 (16)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C55—H55*A*···F35	0.93	2.55	3.152 (2)	122
C51—H51*A*···F33^{ii}	0.93	2.78	2.987 (3)	94

Symmetry code: (ii) $-x+1, -y+1, -z+2$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2094).

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supporting information

Acta Cryst. (2011). E**67**, m1235–m1236 [doi:10.1107/S1600536811031734]

catena-Poly[[tetrakis(*μ*-pentafluorobenzoato-κ^2O:O')dimolybdenum(II)]-*μ*-4,4′-bipyridine-κ^2N:N']

Li-Juan Han

S1. Comment

The design and construction of coordination polymers are of great interest due to their structural topologies and potential application as functional materials (Batten, 2002; Kumar, *et al.*, 2004). Here, we report the synthesis and crystal structure of the coordination polymer $[Mo_2(OOCC_6F_5)_4(C_{10}H_8N_2)]_n$.

In the title compound, $Mo_2(C_7F_5O_2)_4(C_{10}H_8N_2)$, (**I**), the molecule forms a paddle-wheel-type structure. Each quadruply bonded Mo_2^{4+} unit is equatorially coordinated by four pertafluoro-benzoate ($OOCC_6F_5$) groups and the axial positions have associated with them two 4, 4-bipyridine molecules (Fig. 1). The Mo–Mo bond length of 2.1227 (4) Å is representative for dimolybdenum quadruple bonds (Cotton *et al.*, 2005). The torsion angles between the C_6F_5 group and the connected chelating ring (Mo_2OCO) are 72.081 (3)°, 75.537 (3)°, 22.059 (3)° and 22.422 (3)°, respectively, and relate to the O···F repulsion within the pentafluoro-benzonate anion (Reddy *et al.*, 2004; Bach *et al.*, 2001). Weak *π*–*π* stacking interactions between perfluorophenyl rings also affect the 72.081 (3)° and 75.537 (3)° torsion angles.

An infinite, linear chain coordination polymer is formed by the Mo_2^{4+} unit coordinating axially to the two N atoms of the 4, 4-bipyridine ligand [Mo–N distance = 2.5938 (2) Å] (Fig. 2). A one-dimensional linear chain is generated by the *π*-*π* stacking between perfluorophenyl rings as viewed along the equatorial position of the Mo–Mo quadruple bonds (Fig. 3), [the center-to-center distance = 3.7280 (3) Å and center-to-plane distance = 3.6103 (0) Å between two pentafluoro-phenyl rings]. Crystal packing shows molecules linked together into a three-dimensional network (Fig. 4) *via* Mo–N coordination interactions and perfluorophenyl rings via weak *π*–*π* stacking interactions. Weak C–H···F intermolecular interactions further stabilize the crystal structure [(F···H distances = 2.7879 (15) Å].

S2. Experimental

4, 4-bipyridine (0.312 g, 2 mmol) was dissolved in dichloromethane (30 ml), and the solution was filtered to a Schelenk tube. $Mo_2(OOCC_6F_5)_4$ (0.207 g, 0.2 mmol) was dissolved in ethanol (10 ml), resulting in a clear yellow solution. The yellow solution was carefully layered on the top of the Schelenk tube. Solution diffusion at low temperature (in refrigetator) afforded yellow X-ray quality crystals after three days. Yield: 0.190 g (80%). Anal. Calcd. for $C_{38}H_8N_2O_8F_{20}Mo_2$: C, 38.28; H, 0.68; N, 2.35. Found: C, 38.13; H, 0.53; N, 2.37.

S3. Refinement

The H atoms were positioned geometrically and refined using the riding model with C–H = 0.93 Å for aromatic H, 0.96 Å for methyl H atoms. The U_{iso} parameters for H atoms were constrained to be $1.5U_{eq}$ of the carrier atom for the methyl H atoms and $1.2U_{eq}$ of the carrier atom for the remaining H atoms.

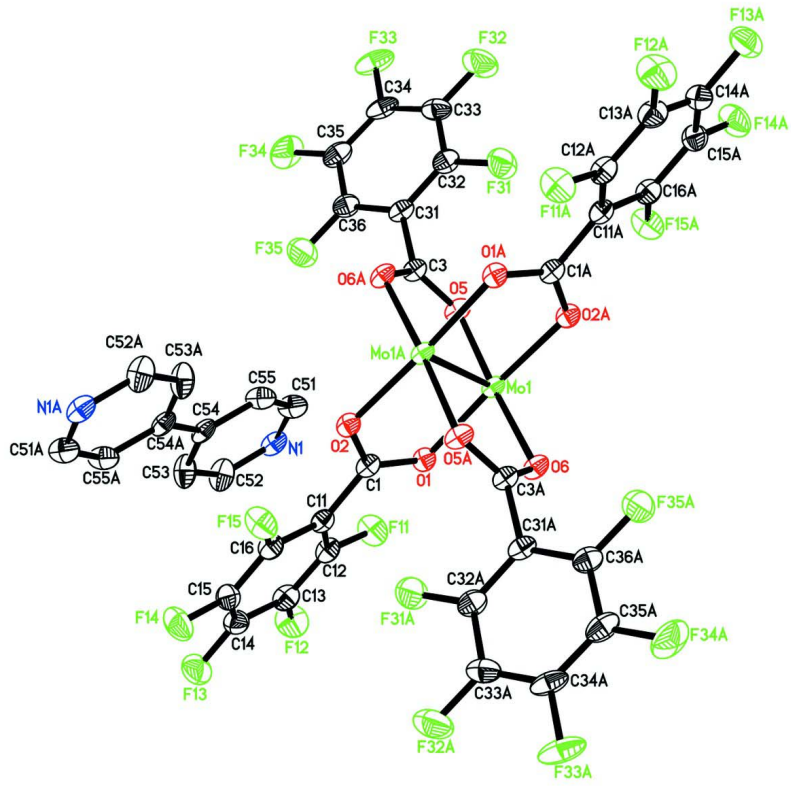

Figure 1

Molecular structure of the title compound drawn with displacement ellipsoids at the 30% probability level. All hydrogen atoms have been omitted for clarity.

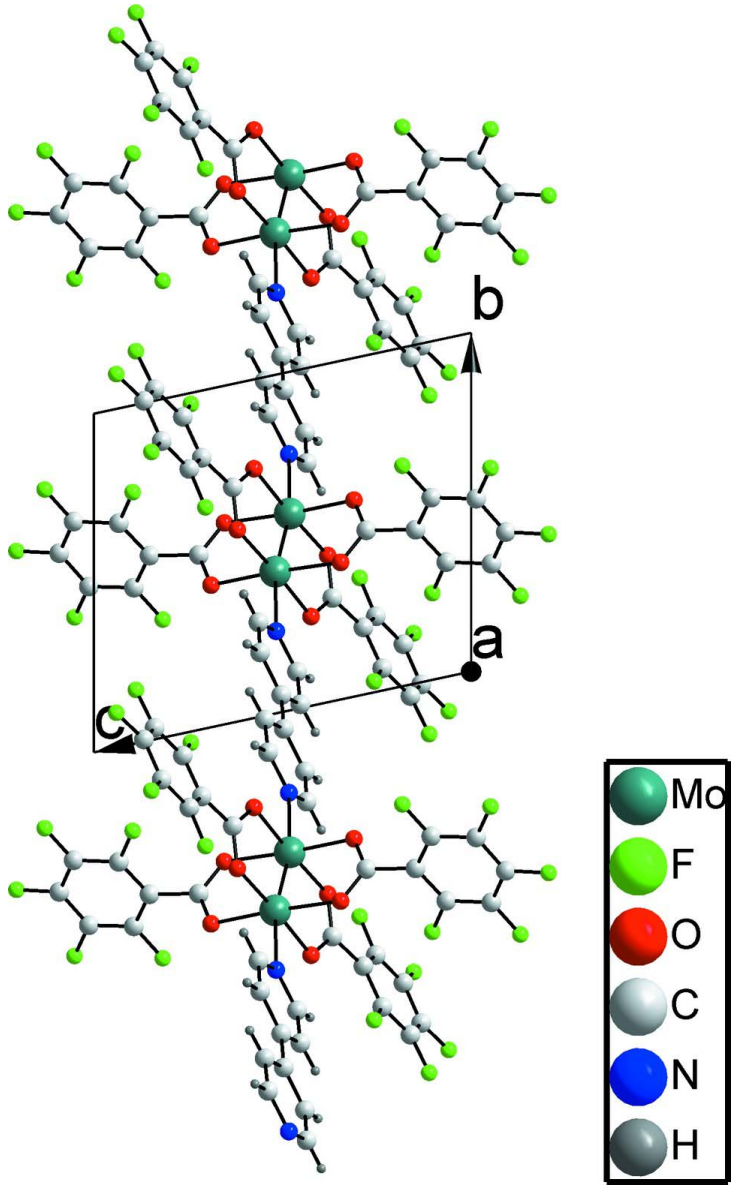

Figure 2

Part of a one-dimensional linear chain formed by a Mo–N coordination bond viewed along the *a* axis.

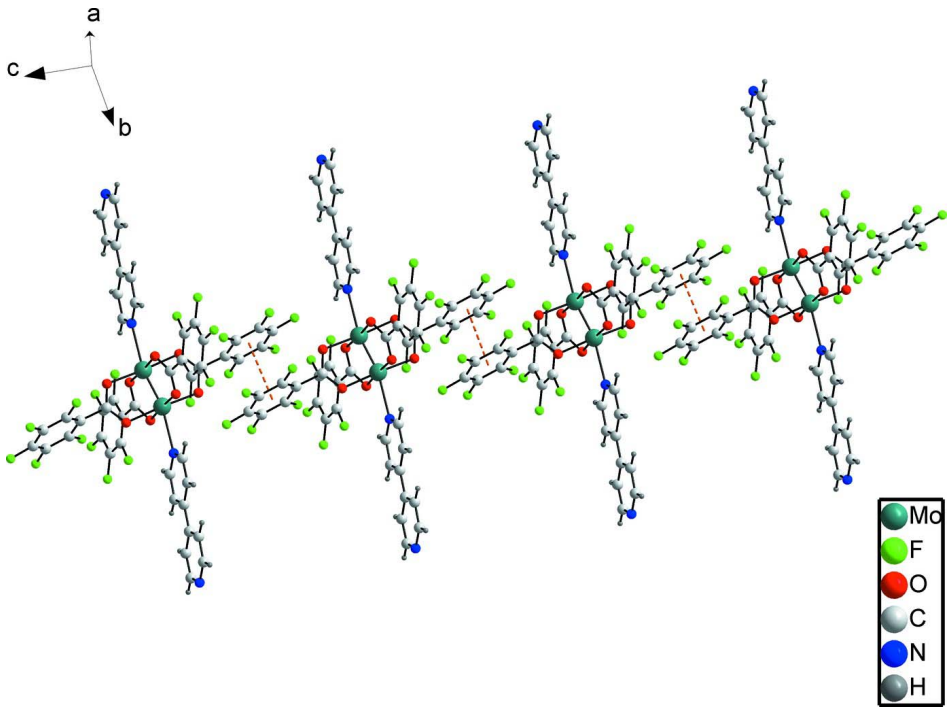

Figure 3

Part of a one-dimensional linear chain formed by the π–π intermolecular stacking interactions.

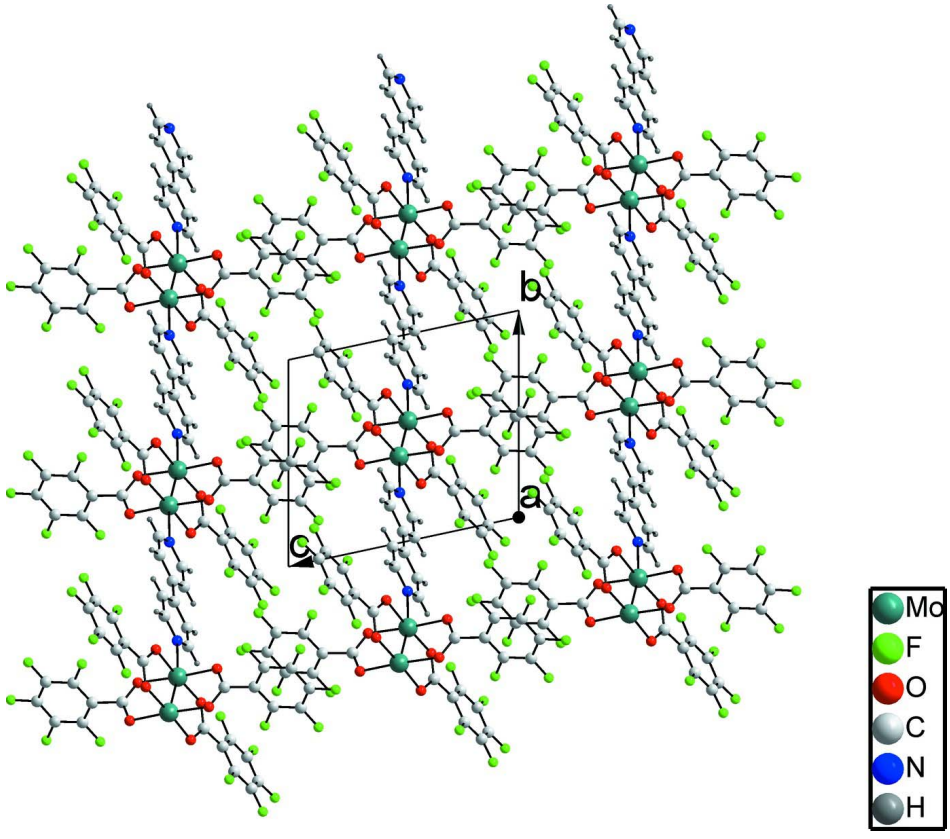

Figure 4

Molecular packing diagram of (**I**) with a view along the *a* axis.

catena-Poly[[tetrakis(μ-pentafluorobenzoato- κ²O:O′)dimolybdenum(II)]-μ-4,4′-bipyridine- κ²N:N′]

Crystal data

$[Mo_2(C_7F_5O_2)_4(C_{10}H_8N_2)]$
M_r = 1192.34
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 8.8858 (8) Å
b = 9.9311 (9) Å
c = 11.1978 (10) Å
α = 101.158 (1)°
β = 94.697 (1)°
γ = 99.092 (1)°
V = 950.83 (15) Å^3
Z = 1
F(000) = 578
D_x = 2.082 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4122 reflections
θ = 2.5–27.6°
μ = 0.82 mm^{-1}
T = 293 K
Block, yellow
0.20 × 0.18 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.849, T_{max} = 0.884
4937 measured reflections
3294 independent reflections
3072 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 25.0°, θ_{min} = 2.1°
h = −8→10
k = −11→11
l = −13→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.061$
$S = 1.01$
3294 reflections
316 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0323P)^2 + 0.6373P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.47$ e Å^{-3}

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Mo1	0.94356 (2)	0.58128 (2)	0.480838 (17)	0.02757 (8)
F11	0.46291 (19)	0.34697 (17)	0.29542 (17)	0.0569 (4)
F12	0.2509 (2)	0.1493 (2)	0.1523 (2)	0.0712 (5)
F13	0.3174 (2)	−0.10294 (19)	0.05942 (18)	0.0682 (5)
F14	0.6015 (2)	−0.15799 (17)	0.11139 (18)	0.0662 (5)
F15	0.81465 (19)	0.03236 (17)	0.25713 (17)	0.0568 (4)
F31	1.0522 (2)	0.7439 (2)	0.89717 (17)	0.0701 (5)
F32	0.9848 (3)	0.8073 (2)	1.13037 (18)	0.0825 (6)
F33	0.7539 (2)	0.6435 (2)	1.20533 (14)	0.0708 (6)
F34	0.5986 (3)	0.4110 (2)	1.05142 (19)	0.0823 (6)
F35	0.6643 (2)	0.3488 (2)	0.81764 (17)	0.0770 (6)
O1	0.75702 (18)	0.43333 (16)	0.38004 (15)	0.0332 (4)
O2	0.87528 (19)	0.26377 (17)	0.42436 (15)	0.0345 (4)
O5	0.85431 (19)	0.59500 (18)	0.65400 (15)	0.0355 (4)
O6	1.03083 (19)	0.58024 (17)	0.31053 (15)	0.0352 (4)
C1	0.7665 (3)	0.3051 (3)	0.3681 (2)	0.0330 (5)
C3	0.8955 (3)	0.5167 (3)	0.7219 (2)	0.0325 (5)
C11	0.6483 (3)	0.1984 (3)	0.2857 (2)	0.0341 (5)
C12	0.5018 (3)	0.2234 (3)	0.2528 (2)	0.0391 (6)
C13	0.3913 (3)	0.1235 (3)	0.1796 (3)	0.0456 (7)
C14	0.4231 (3)	−0.0065 (3)	0.1325 (3)	0.0467 (7)
C15	0.5677 (3)	−0.0340 (3)	0.1609 (2)	0.0437 (6)
C16	0.6762 (3)	0.0656 (3)	0.2357 (2)	0.0382 (6)
C31	0.8594 (3)	0.5460 (3)	0.8527 (2)	0.0346 (5)
C32	0.9392 (3)	0.6610 (3)	0.9340 (2)	0.0428 (6)

C33	0.9070 (4)	0.6945 (3)	1.0538 (2)	0.0497 (7)
C34	0.7909 (3)	0.6100 (3)	1.0917 (2)	0.0480 (7)
C35	0.7115 (3)	0.4929 (3)	1.0133 (3)	0.0502 (7)
C36	0.7458 (3)	0.4611 (3)	0.8941 (2)	0.0437 (6)
N1	0.2434 (3)	0.2426 (2)	0.5169 (2)	0.0434 (5)
C51	0.3883 (4)	0.2800 (3)	0.5640 (2)	0.0498 (7)
H51A	0.4226	0.3727	0.6027	0.060*
C52	0.1981 (3)	0.1097 (3)	0.4617 (3)	0.0555 (8)
H52A	0.0966	0.0810	0.4270	0.067*
C53	0.2934 (3)	0.0113 (3)	0.4527 (3)	0.0540 (8)
H53A	0.2554	−0.0805	0.4130	0.065*
C54	0.4463 (3)	0.0507 (3)	0.5034 (2)	0.0377 (6)
C55	0.4927 (3)	0.1900 (3)	0.5594 (2)	0.0467 (7)
H55A	0.5938	0.2230	0.5938	0.056*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.03074 (12)	0.03149 (12)	0.02725 (12)	0.01909 (8)	0.00822 (8)	0.00964 (8)
F11	0.0419 (9)	0.0543 (10)	0.0761 (12)	0.0260 (8)	0.0033 (8)	0.0049 (9)
F12	0.0397 (9)	0.0805 (13)	0.0925 (14)	0.0211 (9)	−0.0114 (9)	0.0154 (11)
F13	0.0585 (11)	0.0614 (11)	0.0735 (12)	−0.0033 (9)	−0.0153 (10)	0.0079 (9)
F14	0.0698 (12)	0.0416 (9)	0.0795 (13)	0.0163 (9)	−0.0058 (10)	−0.0049 (9)
F15	0.0458 (9)	0.0479 (9)	0.0739 (12)	0.0251 (8)	−0.0035 (8)	−0.0034 (8)
F31	0.0668 (12)	0.0753 (13)	0.0585 (11)	−0.0139 (10)	0.0155 (9)	0.0085 (9)
F32	0.1018 (17)	0.0801 (14)	0.0504 (11)	0.0059 (12)	0.0050 (11)	−0.0135 (10)
F33	0.0872 (14)	0.1141 (16)	0.0306 (8)	0.0598 (12)	0.0245 (9)	0.0213 (9)
F34	0.0797 (14)	0.1097 (17)	0.0669 (12)	0.0041 (12)	0.0374 (11)	0.0393 (12)
F35	0.0870 (15)	0.0773 (13)	0.0534 (11)	−0.0205 (11)	0.0149 (10)	0.0069 (10)
O1	0.0319 (9)	0.0335 (9)	0.0390 (9)	0.0169 (7)	0.0043 (7)	0.0098 (7)
O2	0.0357 (9)	0.0349 (9)	0.0375 (9)	0.0162 (7)	0.0044 (7)	0.0108 (7)
O5	0.0391 (9)	0.0449 (10)	0.0318 (9)	0.0260 (8)	0.0126 (7)	0.0124 (7)
O6	0.0403 (10)	0.0412 (9)	0.0334 (9)	0.0225 (8)	0.0121 (7)	0.0153 (7)
C1	0.0331 (13)	0.0395 (13)	0.0328 (12)	0.0160 (11)	0.0105 (10)	0.0123 (10)
C3	0.0317 (12)	0.0401 (13)	0.0312 (12)	0.0150 (11)	0.0092 (10)	0.0116 (10)
C11	0.0344 (13)	0.0394 (13)	0.0339 (12)	0.0131 (11)	0.0097 (10)	0.0131 (10)
C12	0.0380 (14)	0.0440 (14)	0.0426 (14)	0.0178 (12)	0.0109 (11)	0.0162 (12)
C13	0.0342 (14)	0.0573 (17)	0.0504 (16)	0.0141 (13)	0.0022 (12)	0.0196 (14)
C14	0.0457 (16)	0.0500 (16)	0.0420 (15)	0.0011 (13)	−0.0020 (13)	0.0126 (13)
C15	0.0505 (16)	0.0375 (14)	0.0441 (15)	0.0117 (12)	0.0056 (13)	0.0079 (12)
C16	0.0351 (13)	0.0423 (14)	0.0419 (14)	0.0151 (11)	0.0053 (11)	0.0132 (11)
C31	0.0365 (13)	0.0452 (14)	0.0298 (12)	0.0206 (11)	0.0109 (10)	0.0128 (11)
C32	0.0408 (15)	0.0538 (16)	0.0387 (14)	0.0140 (13)	0.0112 (12)	0.0141 (12)
C33	0.0576 (18)	0.0579 (17)	0.0334 (14)	0.0234 (15)	0.0003 (13)	0.0008 (13)
C34	0.0540 (17)	0.076 (2)	0.0283 (13)	0.0404 (16)	0.0159 (12)	0.0177 (14)
C35	0.0463 (16)	0.073 (2)	0.0427 (16)	0.0201 (15)	0.0188 (13)	0.0262 (15)
C36	0.0443 (15)	0.0543 (16)	0.0357 (14)	0.0124 (13)	0.0101 (12)	0.0117 (12)
N1	0.0503 (14)	0.0533 (14)	0.0405 (12)	0.0343 (11)	0.0176 (11)	0.0187 (10)

C51	0.0609 (19)	0.0551 (17)	0.0396 (15)	0.0382 (15)	0.0052 (13)	0.0025 (13)
C52	0.0399 (16)	0.0552 (18)	0.084 (2)	0.0259 (14)	0.0165 (15)	0.0281 (17)
C53	0.0416 (16)	0.0402 (15)	0.090 (2)	0.0202 (13)	0.0163 (15)	0.0234 (15)
C54	0.0446 (15)	0.0458 (14)	0.0363 (13)	0.0264 (12)	0.0179 (11)	0.0211 (11)
C55	0.0491 (16)	0.0586 (17)	0.0360 (14)	0.0320 (14)	0.0019 (12)	0.0018 (12)

Geometric parameters (Å, º)

Mo1—O2^{i}	2.0955 (17)	C11—C12	1.397 (3)
Mo1—O1	2.1124 (17)	C11—C16	1.398 (3)
Mo1—O6	2.1155 (16)	C12—C13	1.366 (4)
Mo1—Mo1^{i}	2.1227 (4)	C13—C14	1.379 (4)
Mo1—O5	2.1427 (16)	C14—C15	1.379 (4)
Mo1—N1^{ii}	2.594 (2)	C15—C16	1.362 (4)
F11—C12	1.337 (3)	C31—C32	1.368 (4)
F12—C13	1.335 (3)	C31—C36	1.379 (4)
F13—C14	1.325 (3)	C32—C33	1.383 (4)
F14—C15	1.340 (3)	C33—C34	1.373 (4)
F15—C16	1.338 (3)	C34—C35	1.365 (4)
F31—C32	1.338 (3)	C35—C36	1.381 (4)
F32—C33	1.325 (3)	N1—C51	1.318 (4)
F33—C34	1.333 (3)	N1—C52	1.327 (4)
F34—C35	1.341 (3)	C51—C55	1.383 (4)
F35—C36	1.333 (3)	C51—H51A	0.9300
O1—C1	1.272 (3)	C52—C53	1.385 (4)
O2—C1	1.274 (3)	C52—H52A	0.9300
O2—Mo1^{i}	2.0955 (17)	C53—C54	1.393 (4)
O5—C3	1.261 (3)	C53—H53A	0.9300
O6—C3^{i}	1.261 (3)	C54—C55	1.385 (4)
C1—C11	1.480 (3)	C54—C54^{iii}	1.489 (5)
C3—O6^{i}	1.261 (3)	C55—H55A	0.9300
C3—C31	1.508 (3)		
O2^{i}—Mo1—O1	176.82 (6)	F15—C16—C11	120.6 (2)
O2^{i}—Mo1—O6	92.90 (7)	C15—C16—C11	122.5 (2)
O1—Mo1—O6	85.79 (7)	C32—C31—C36	118.0 (2)
O2^{i}—Mo1—Mo1^{i}	92.41 (4)	C32—C31—C3	119.8 (2)
O1—Mo1—Mo1^{i}	90.57 (4)	C36—C31—C3	122.2 (2)
O6—Mo1—Mo1^{i}	93.70 (4)	F31—C32—C31	119.4 (2)
O2^{i}—Mo1—O5	85.43 (7)	F31—C32—C33	118.7 (3)
O1—Mo1—O5	95.73 (7)	C31—C32—C33	121.9 (3)
O6—Mo1—O5	176.63 (6)	F32—C33—C34	120.4 (3)
Mo1^{i}—Mo1—O5	89.29 (4)	F32—C33—C32	120.8 (3)
C1—O1—Mo1	117.52 (15)	C34—C33—C32	118.9 (3)
C1—O2—Mo1^{i}	116.51 (15)	F33—C34—C35	119.8 (3)
C3—O5—Mo1	117.24 (14)	F33—C34—C33	119.8 (3)
C3^{i}—O6—Mo1	114.32 (14)	C35—C34—C33	120.5 (2)
O1—C1—O2	122.5 (2)	F34—C35—C34	119.9 (3)

O1—C1—C11	119.5 (2)	F34—C35—C36	120.3 (3)
O2—C1—C11	118.0 (2)	C34—C35—C36	119.8 (3)
O5—C3—O6^{i}	124.7 (2)	F35—C36—C31	119.9 (2)
O5—C3—C31	117.2 (2)	F35—C36—C35	119.0 (3)
O6^{i}—C3—C31	118.1 (2)	C31—C36—C35	121.0 (3)
C12—C11—C16	115.6 (2)	C51—N1—C52	116.5 (2)
C12—C11—C1	122.4 (2)	N1—C51—C55	124.1 (3)
C16—C11—C1	122.0 (2)	N1—C51—H51A	117.9
F11—C12—C13	117.1 (2)	C55—C51—H51A	117.9
F11—C12—C11	120.6 (2)	N1—C52—C53	123.8 (3)
C13—C12—C11	122.3 (2)	N1—C52—H52A	118.1
F12—C13—C12	121.0 (3)	C53—C52—H52A	118.1
F12—C13—C14	118.7 (3)	C52—C53—C54	119.7 (3)
C12—C13—C14	120.3 (2)	C52—C53—H53A	120.2
F13—C14—C15	120.5 (3)	C54—C53—H53A	120.2
F13—C14—C13	120.6 (3)	C55—C54—C53	116.0 (2)
C15—C14—C13	119.0 (3)	C55—C54—C54^{iii}	122.0 (3)
F14—C15—C16	120.4 (2)	C53—C54—C54^{iii}	122.0 (3)
F14—C15—C14	119.3 (3)	C51—C55—C54	119.9 (3)
C16—C15—C14	120.3 (2)	C51—C55—H55A	120.1
F15—C16—C15	116.8 (2)	C54—C55—H55A	120.1

O6—Mo1—O1—C1	91.22 (16)	C1—C11—C16—F15	−2.7 (4)
Mo1^{i}—Mo1—O1—C1	−2.45 (16)	C12—C11—C16—C15	−0.8 (4)
O5—Mo1—O1—C1	−91.80 (16)	C1—C11—C16—C15	179.2 (2)
O2^{i}—Mo1—O5—C3	−89.66 (18)	O5—C3—C31—C32	−72.1 (3)
O1—Mo1—O5—C3	93.32 (18)	O6^{i}—C3—C31—C32	105.4 (3)
Mo1^{i}—Mo1—O5—C3	2.82 (18)	O5—C3—C31—C36	107.0 (3)
O2^{i}—Mo1—O6—C3^{i}	98.99 (17)	O6^{i}—C3—C31—C36	−75.6 (3)
O1—Mo1—O6—C3^{i}	−83.91 (17)	C36—C31—C32—F31	178.7 (2)
Mo1^{i}—Mo1—O6—C3^{i}	6.38 (17)	C3—C31—C32—F31	−2.2 (4)
Mo1—O1—C1—O2	7.3 (3)	C36—C31—C32—C33	−1.2 (4)
Mo1—O1—C1—C11	−172.39 (15)	C3—C31—C32—C33	177.9 (2)
Mo1^{i}—O2—C1—O1	−8.4 (3)	F31—C32—C33—F32	0.9 (4)
Mo1^{i}—O2—C1—C11	171.27 (15)	C31—C32—C33—F32	−179.3 (3)
Mo1—O5—C3—O6^{i}	−9.2 (3)	F31—C32—C33—C34	179.8 (2)
Mo1—O5—C3—C31	168.03 (16)	C31—C32—C33—C34	−0.3 (4)
O1—C1—C11—C12	−22.4 (3)	F32—C33—C34—F33	1.7 (4)
O2—C1—C11—C12	157.9 (2)	C32—C33—C34—F33	−177.3 (2)
O1—C1—C11—C16	157.6 (2)	F32—C33—C34—C35	−179.4 (3)
O2—C1—C11—C16	−22.1 (3)	C32—C33—C34—C35	1.7 (4)
C16—C11—C12—F11	−179.9 (2)	F33—C34—C35—F34	−1.1 (4)
C1—C11—C12—F11	0.0 (4)	C33—C34—C35—F34	179.9 (3)
C16—C11—C12—C13	2.0 (4)	F33—C34—C35—C36	177.4 (3)
C1—C11—C12—C13	−178.1 (2)	C33—C34—C35—C36	−1.5 (4)
F11—C12—C13—F12	0.0 (4)	C32—C31—C36—F35	179.4 (2)
C11—C12—C13—F12	178.2 (2)	C3—C31—C36—F35	0.3 (4)
F11—C12—C13—C14	−179.9 (2)	C32—C31—C36—C35	1.3 (4)

C11—C12—C13—C14	−1.8 (4)	C3—C31—C36—C35	−177.8 (2)
F12—C13—C14—F13	1.4 (4)	F34—C35—C36—F35	0.5 (4)
C12—C13—C14—F13	−178.6 (2)	C34—C35—C36—F35	−178.0 (3)
F12—C13—C14—C15	−179.6 (3)	F34—C35—C36—C31	178.6 (3)
C12—C13—C14—C15	0.3 (4)	C34—C35—C36—C31	0.0 (4)
F13—C14—C15—F14	1.7 (4)	C52—N1—C51—C55	−0.3 (4)
C13—C14—C15—F14	−177.2 (3)	C51—N1—C52—C53	0.6 (4)
F13—C14—C15—C16	179.7 (2)	N1—C52—C53—C54	−0.1 (5)
C13—C14—C15—C16	0.8 (4)	C52—C53—C54—C55	−0.7 (4)
F14—C15—C16—F15	−0.7 (4)	C52—C53—C54—C54^{iii}	179.9 (3)
C14—C15—C16—F15	−178.7 (2)	N1—C51—C55—C54	−0.5 (4)
F14—C15—C16—C11	177.5 (2)	C53—C54—C55—C51	1.0 (4)
C14—C15—C16—C11	−0.5 (4)	C54^{iii}—C54—C55—C51	−179.6 (3)
C12—C11—C16—F15	177.3 (2)		

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*+1, −*y*, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C55—H55*A*···F35	0.93	2.55	3.152 (2)	122
C51—H51*A*···F33^{iv}	0.93	2.78	2.987 (3)	94

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