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{2,2′-[(2,2-Dimethylpropane-1,3-diyl)bis(nitrilomethylidyne)]diphenolato}dioxidomolybdenum(VI)

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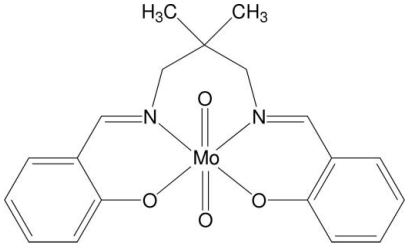
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.021; wR factor = 0.052; data-to-parameter ratio = 14.4.

In the structure of the title compound, $[Mo(C_{19}H_{20}N_2O_2)O_2]$, the Mo atom exhibits oxidation state +VI and is surrounded by two O atoms and the tetradentate Schiff base ligand 2,2′-[(2,2-dimethylpropane-1,3-diyl)bis(nitrilomethylidyne)]-diphenolate in a distorted octahedral configuration. An intramolecular C—H···O hydrogen bond between a methylene group and one O atom of the O=Mo^{VI}=O unit, as well as additional intermolecular hydrogen bonds between neighboring molecules, lead to a weakly bonded inversion-symmetric dimeric structure.

Related literature

For related structures with O=Mo^{VI}=O units and for synthesis, see: Arnaiz *et al.* (2000); Holm *et al.* (1996); Syamal & Maurya (1989). The crystal structure of the free ligand *N*,*N*′-bis(2-hydroxybenzylidene)-2,2-dimethyl-1,3-propanediamine was described by Corden *et al.* (1996).



Experimental

Crystal data

$[Mo(C_{19}H_{20}N_2O_2)O_2]$
M_r = 436.31
Triclinic, $P\overline{1}$
a = 9.3875 (10) Å
b = 9.5597 (10) Å
c = 11.0422 (11) Å
α = 104.6790 (17)°
β = 108.1939 (17)°
γ = 101.1218 (17)°
V = 869.87 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.78 mm^{-1}
T = 100 (2) K
0.18 × 0.12 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: none
8420 measured reflections
3413 independent reflections
3204 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.051
S = 1.07
3413 reflections
237 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mo1—O1	1.7072 (14)	Mo1—O3	2.0917 (14)
Mo1—O2	1.7120 (14)	Mo1—N2	2.1442 (16)
Mo1—O4	1.9373 (13)	Mo1—N1	2.3402 (16)

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4A···O2	0.97	2.49	2.986 (2)	112
C1—H1···O1^{i}	0.93	2.54	3.227 (2)	131
C4—H4B···O1^{i}	0.97	2.56	3.294 (2)	132
C7—H7···O2^{i}	0.93	2.55	3.315 (2)	140

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2183).

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{2,2′-[(2,2-Dimethylpropane-1,3-diyl)bis(nitrilomethylidyne)]diphenolato}dioxidomolybdenum(VI)

Alireza Abbasi, Iran Sheikhshoaie, Abbas Saghaei and Niaz Monadi

S1. Comment

Numerous chemical reactions are catalyzed by compounds containing complexes with the dioxidomolybdenum(VI) unit O═Mo^{VI}═O (Arnaiz *et al.* 2000). Moreover, Schiff base compounds containing molybdenum play a significant role in the chemistry of molybdoenzymes (Holm *et al.* 1996; Syamal & Maurya, 1989). Therefore we are interested in the structural chemistry of dioxidomolybdenum(VI) complexes and have synthesized and structurally characterized the title compound, $MoO_2(C_{19}H_{20}N_2O_2)$, (I).

The molecular structure of (I) and the atom-numbering scheme are shown in Fig. 1. The molybdenum(VI) atom is in a distorted octahedral coordination by two oxygen atoms and one tetradentate ligand *L*, where *L* is *N*,*N*′-bis(2-hydroxybenzylidene)-2,2-dimethyl-1,3-propanediamine. The Mo–O distances of the oxido ligands are significantly shorter (average 1.71 Å) than the corresponding distances to the O atoms of the tetradentate ligand (average 2.02 Å). The Mo–N distances are the longest (average 2.24 Å). An intramolecular hydrogen bond is present between the methylene group and one O atom from the O═Mo═O group (C4—H41···O2, 2.985 Å). Much weaker intermolecular hydrogen bonds exist between neighboring molecules, leading to an dimer structure (see hydrogen bond Table and Fig. 2). For a packing plot of the structure, see Fig. 3. Resulting from the coordination of the tetradentate *L* ligand to the molybdenum ion, the chelate ligand is more twisted than the free ligand, with a larger dihedral angle between two phenyl rings of 75.2 (1)° compared to the free ligand with 68.7 (1)° (Corden *et al.*, 1996).

S2. Experimental

The title compound was prepared by adding $MoO_2(acac)_2$ and the ligand H_2L (Corden *et al.*, 1996) in the molar ratio 1:1 to 30 mL dry methanol, followed by refluxing the solution for 1 h. Small prismatic, yellowish crystals precipitated which were filtered off and recrystallized from acetonitrile to get a better crystal quality.

S3. Refinement

All H atoms were placed in calculated positions with C—H = 0.93 Å for H atoms bonded to sp^2 C atoms, and C—H = 0.97 Å for H atoms bonded to sp^3 C atoms, and constrained to ride on their parent atoms with U_{iso}(H) = 1.2 and 1.5 U_{eq}(C), respectively.

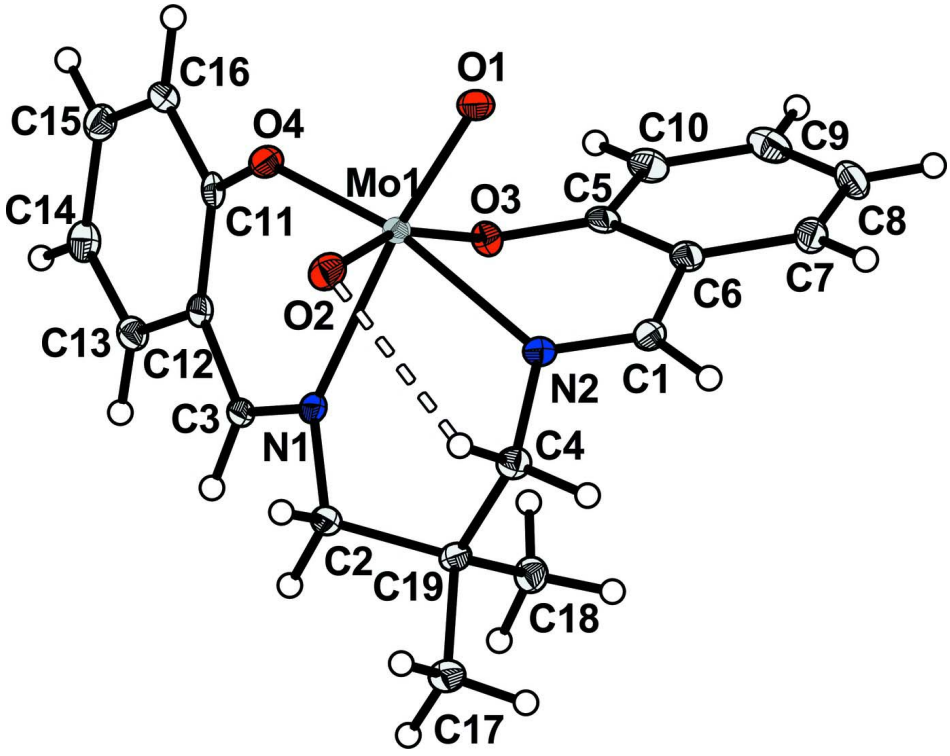

Figure 1

Molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as circles of arbitrary radius. Hydrogen bonds are represented as dotted lines.

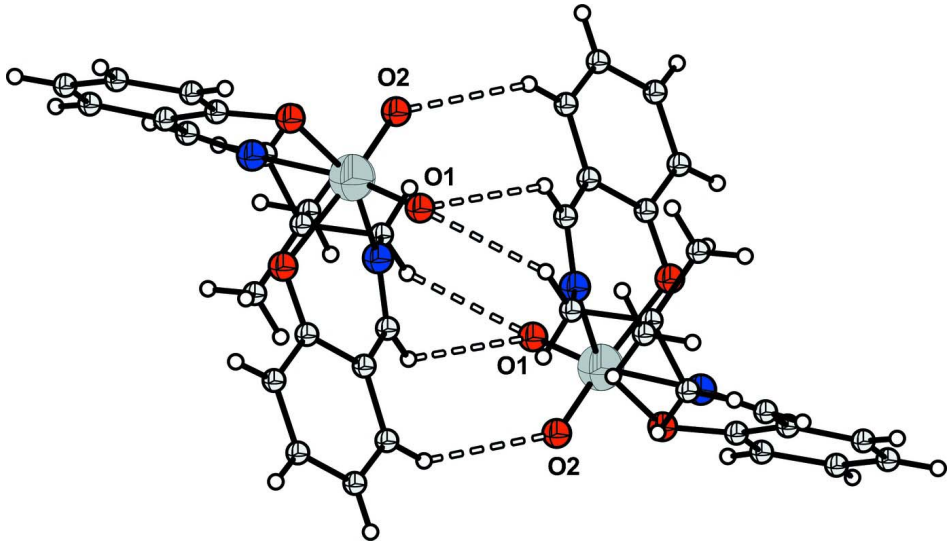

Figure 2

The inversion-symmetric dimeric structure of (I). Hydrogen bonds are represented as dotted lines.

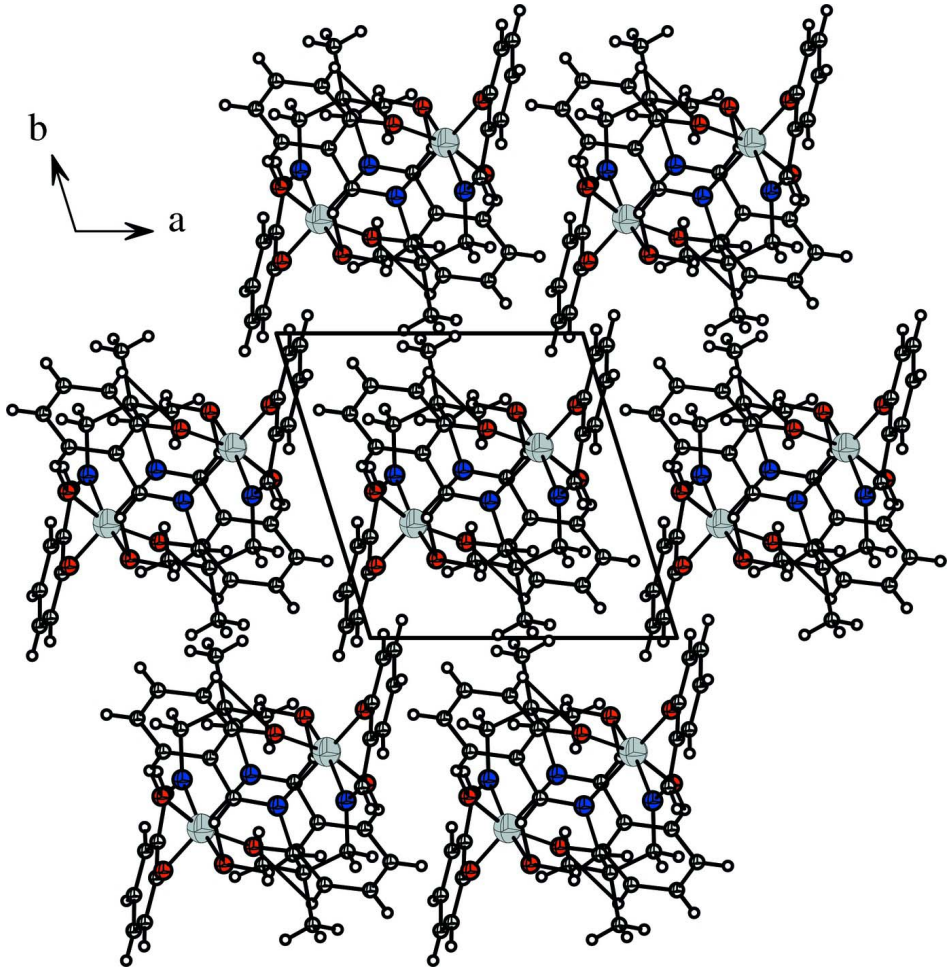

Figure 3

Packing plot of (I) along [001].

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Crystal data

$[Mo(C_{19}H_{20}N_2O_2)O_2]$
$M_r = 436.31$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.3875$ (10) Å
$b = 9.5597$ (10) Å
$c = 11.0422$ (11) Å
$\alpha = 104.6790$ (17)°
$\beta = 108.1939$ (17)°
$\gamma = 101.1218$ (17)°
$V = 869.87$ (16) Å^3
$Z = 2$
$F(000) = 444$
$D_x = 1.666$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8420 reflections
$\theta = 2.5$–26.0°
$\mu = 0.78$ mm^{-1}
$T = 100$ K
Prism, light yellow
0.18 × 0.12 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
8420 measured reflections
3413 independent reflections
3204 reflections with $I > 2\sigma(I)$

R_{int} = 0.020
θ_{max} = 26.0°, θ_{min} = 2.1°
h = −11→11
k = −11→11
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.051
S = 1.07
3413 reflections
237 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
$w = 1/[\sigma^2(F_o^2) + (0.0184P)^2 + 0.8169P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 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	0.742950 (19)	0.625366 (18)	0.282813 (16)	0.01031 (6)
O1	0.70502 (16)	0.74204 (15)	0.19043 (14)	0.0161 (3)
O2	0.84039 (16)	0.52119 (16)	0.20730 (14)	0.0167 (3)
O3	0.59172 (16)	0.68583 (15)	0.37734 (13)	0.0135 (3)
O4	0.90918 (16)	0.76348 (15)	0.44982 (13)	0.0146 (3)
N1	0.75678 (18)	0.46531 (18)	0.41243 (16)	0.0115 (3)
N2	0.52861 (19)	0.44879 (18)	0.15515 (16)	0.0112 (3)
C1	0.3927 (2)	0.4737 (2)	0.11735 (19)	0.0127 (4)
H1	0.3111	0.3981	0.0443	0.015*
C2	0.7108 (2)	0.3002 (2)	0.34369 (19)	0.0122 (4)
H2A	0.7190	0.2512	0.4115	0.015*
H2B	0.7855	0.2782	0.3032	0.015*
C3	0.8231 (2)	0.5116 (2)	0.5423 (2)	0.0121 (4)
H3	0.8229	0.4382	0.5838	0.014*
C4	0.5301 (2)	0.2902 (2)	0.11404 (19)	0.0131 (4)
H4A	0.6177	0.2836	0.0863	0.016*
H4B	0.4339	0.2289	0.0375	0.016*
C5	0.4553 (2)	0.7013 (2)	0.3131 (2)	0.0127 (4)
C6	0.3575 (2)	0.6066 (2)	0.1779 (2)	0.0132 (4)
C7	0.2101 (2)	0.6264 (2)	0.1145 (2)	0.0156 (4)
H7	0.1467	0.5643	0.0262	0.019*
C8	0.1596 (2)	0.7357 (2)	0.1811 (2)	0.0188 (4)

H8	0.0631	0.7486	0.1380	0.023*
C9	0.2546 (3)	0.8278 (2)	0.3146 (2)	0.0189 (4)
H9	0.2204	0.9020	0.3600	0.023*
C10	0.3979 (2)	0.8102 (2)	0.3795 (2)	0.0161 (4)
H10	0.4579	0.8713	0.4688	0.019*
C11	0.9390 (2)	0.7870 (2)	0.58181 (19)	0.0122 (4)
C12	0.8984 (2)	0.6685 (2)	0.62999 (19)	0.0120 (4)
C13	0.9480 (2)	0.6997 (2)	0.7706 (2)	0.0139 (4)
H13	0.9255	0.6212	0.8035	0.017*
C14	1.0294 (2)	0.8440 (2)	0.8609 (2)	0.0154 (4)
H14	1.0595	0.8633	0.9536	0.019*
C15	1.0658 (2)	0.9608 (2)	0.8110 (2)	0.0156 (4)
H15	1.1204	1.0585	0.8712	0.019*
C16	1.0218 (2)	0.9330 (2)	0.6732 (2)	0.0143 (4)
H16	1.0473	1.0118	0.6414	0.017*
C17	0.5230 (2)	0.0591 (2)	0.1785 (2)	0.0166 (4)
H17A	0.5356	0.0183	0.2509	0.025*
H17B	0.5999	0.0428	0.1404	0.025*
H17C	0.4197	0.0095	0.1098	0.025*
C18	0.4199 (2)	0.2557 (2)	0.2899 (2)	0.0156 (4)
H18A	0.3185	0.2163	0.2174	0.023*
H18B	0.4408	0.3623	0.3329	0.023*
H18C	0.4216	0.2051	0.3549	0.023*
C19	0.5451 (2)	0.2294 (2)	0.23343 (19)	0.0119 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.01067 (9)	0.01016 (9)	0.00976 (9)	0.00212 (6)	0.00322 (6)	0.00433 (6)
O1	0.0185 (7)	0.0120 (7)	0.0142 (7)	0.0015 (6)	0.0028 (6)	0.0051 (6)
O2	0.0143 (7)	0.0182 (7)	0.0193 (7)	0.0037 (6)	0.0090 (6)	0.0064 (6)
O3	0.0135 (7)	0.0145 (7)	0.0121 (7)	0.0054 (6)	0.0038 (5)	0.0046 (5)
O4	0.0148 (7)	0.0147 (7)	0.0117 (7)	0.0006 (6)	0.0026 (6)	0.0058 (6)
N1	0.0081 (8)	0.0116 (8)	0.0149 (8)	0.0030 (6)	0.0043 (6)	0.0046 (7)
N2	0.0139 (8)	0.0106 (8)	0.0093 (8)	0.0031 (6)	0.0052 (6)	0.0032 (6)
C1	0.0132 (10)	0.0134 (9)	0.0099 (9)	0.0013 (8)	0.0031 (7)	0.0047 (7)
C2	0.0116 (9)	0.0116 (9)	0.0150 (10)	0.0042 (8)	0.0053 (8)	0.0059 (8)
C3	0.0086 (9)	0.0135 (9)	0.0167 (10)	0.0037 (7)	0.0048 (8)	0.0090 (8)
C4	0.0152 (10)	0.0106 (9)	0.0114 (9)	0.0030 (8)	0.0045 (8)	0.0014 (7)
C5	0.0145 (10)	0.0123 (9)	0.0150 (10)	0.0036 (8)	0.0069 (8)	0.0088 (8)
C6	0.0137 (10)	0.0142 (9)	0.0148 (10)	0.0041 (8)	0.0070 (8)	0.0082 (8)
C7	0.0133 (10)	0.0184 (10)	0.0157 (10)	0.0035 (8)	0.0047 (8)	0.0083 (8)
C8	0.0161 (10)	0.0238 (11)	0.0253 (11)	0.0111 (9)	0.0100 (9)	0.0163 (9)
C9	0.0248 (12)	0.0181 (10)	0.0244 (11)	0.0123 (9)	0.0156 (9)	0.0121 (9)
C10	0.0220 (11)	0.0143 (10)	0.0141 (10)	0.0066 (8)	0.0084 (8)	0.0058 (8)
C11	0.0075 (9)	0.0169 (10)	0.0124 (9)	0.0052 (8)	0.0023 (7)	0.0059 (8)
C12	0.0078 (9)	0.0142 (9)	0.0148 (10)	0.0044 (7)	0.0041 (7)	0.0056 (8)
C13	0.0119 (10)	0.0173 (10)	0.0163 (10)	0.0060 (8)	0.0068 (8)	0.0091 (8)

C14	0.0140 (10)	0.0207 (10)	0.0110 (9)	0.0054 (8)	0.0045 (8)	0.0046 (8)
C15	0.0129 (10)	0.0139 (10)	0.0160 (10)	0.0035 (8)	0.0032 (8)	0.0019 (8)
C16	0.0127 (10)	0.0131 (10)	0.0181 (10)	0.0044 (8)	0.0043 (8)	0.0083 (8)
C17	0.0173 (10)	0.0122 (10)	0.0175 (10)	0.0026 (8)	0.0047 (8)	0.0042 (8)
C18	0.0131 (10)	0.0190 (10)	0.0168 (10)	0.0049 (8)	0.0067 (8)	0.0083 (8)
C19	0.0117 (9)	0.0098 (9)	0.0139 (9)	0.0021 (7)	0.0054 (8)	0.0035 (8)

Geometric parameters (Å, º)

Mo1—O1	1.7072 (14)	C7—C8	1.370 (3)
Mo1—O2	1.7120 (14)	C7—H7	0.9300
Mo1—O4	1.9373 (13)	C8—C9	1.401 (3)
Mo1—O3	2.0917 (14)	C8—H8	0.9300
Mo1—N2	2.1442 (16)	C9—C10	1.378 (3)
Mo1—N1	2.3402 (16)	C9—H9	0.9300
O3—C5	1.313 (2)	C10—H10	0.9300
O4—C11	1.345 (2)	C11—C16	1.395 (3)
N1—C3	1.286 (2)	C11—C12	1.407 (3)
N1—C2	1.477 (2)	C12—C13	1.406 (3)
N2—C1	1.301 (3)	C13—C14	1.379 (3)
N2—C4	1.472 (2)	C13—H13	0.9300
C1—C6	1.428 (3)	C14—C15	1.395 (3)
C1—H1	0.9300	C14—H14	0.9300
C2—C19	1.534 (3)	C15—C16	1.385 (3)
C2—H2A	0.9700	C15—H15	0.9300
C2—H2B	0.9700	C16—H16	0.9300
C3—C12	1.454 (3)	C17—C19	1.534 (3)
C3—H3	0.9300	C17—H17A	0.9600
C4—C19	1.549 (3)	C17—H17B	0.9600
C4—H4A	0.9700	C17—H17C	0.9600
C4—H4B	0.9700	C18—C19	1.525 (3)
C5—C10	1.410 (3)	C18—H18A	0.9600
C5—C6	1.425 (3)	C18—H18B	0.9600
C6—C7	1.415 (3)	C18—H18C	0.9600
O1—Mo1—O2	103.33 (7)	C8—C7—H7	119.5
O1—Mo1—O4	101.99 (6)	C6—C7—H7	119.5
O2—Mo1—O4	102.79 (6)	C7—C8—C9	119.36 (19)
O1—Mo1—O3	90.82 (6)	C7—C8—H8	120.3
O2—Mo1—O3	161.79 (6)	C9—C8—H8	120.3
O4—Mo1—O3	85.05 (6)	C10—C9—C8	120.94 (19)
O1—Mo1—N2	93.87 (6)	C10—C9—H9	119.5
O2—Mo1—N2	88.54 (6)	C8—C9—H9	119.5
O4—Mo1—N2	157.64 (6)	C9—C10—C5	121.24 (19)
O3—Mo1—N2	79.01 (6)	C9—C10—H10	119.4
O1—Mo1—N1	170.94 (6)	C5—C10—H10	119.4
O2—Mo1—N1	84.17 (6)	O4—C11—C16	117.93 (17)
O4—Mo1—N1	80.95 (6)	O4—C11—C12	122.15 (17)

O3—Mo1—N1	80.84 (5)	C16—C11—C12	119.80 (18)
N2—Mo1—N1	81.12 (6)	C13—C12—C11	118.62 (18)
C5—O3—Mo1	123.46 (12)	C13—C12—C3	117.94 (17)
C11—O4—Mo1	134.29 (12)	C11—C12—C3	123.05 (17)
C3—N1—C2	115.90 (16)	C14—C13—C12	121.52 (18)
C3—N1—Mo1	124.12 (13)	C14—C13—H13	119.2
C2—N1—Mo1	119.23 (12)	C12—C13—H13	119.2
C1—N2—C4	117.18 (16)	C13—C14—C15	118.99 (18)
C1—N2—Mo1	122.83 (13)	C13—C14—H14	120.5
C4—N2—Mo1	119.87 (12)	C15—C14—H14	120.5
N2—C1—C6	125.94 (18)	C16—C15—C14	120.85 (19)
N2—C1—H1	117.0	C16—C15—H15	119.6
C6—C1—H1	117.0	C14—C15—H15	119.6
N1—C2—C19	115.73 (15)	C15—C16—C11	120.17 (18)
N1—C2—H2A	108.3	C15—C16—H16	119.9
C19—C2—H2A	108.3	C11—C16—H16	119.9
N1—C2—H2B	108.3	C19—C17—H17A	109.5
C19—C2—H2B	108.3	C19—C17—H17B	109.5
H2A—C2—H2B	107.4	H17A—C17—H17B	109.5
N1—C3—C12	125.78 (17)	C19—C17—H17C	109.5
N1—C3—H3	117.1	H17A—C17—H17C	109.5
C12—C3—H3	117.1	H17B—C17—H17C	109.5
N2—C4—C19	110.04 (15)	C19—C18—H18A	109.5
N2—C4—H4A	109.7	C19—C18—H18B	109.5
C19—C4—H4A	109.7	H18A—C18—H18B	109.5
N2—C4—H4B	109.7	C19—C18—H18C	109.5
C19—C4—H4B	109.7	H18A—C18—H18C	109.5
H4A—C4—H4B	108.2	H18B—C18—H18C	109.5
O3—C5—C10	120.15 (18)	C18—C19—C2	111.61 (16)
O3—C5—C6	122.19 (18)	C18—C19—C17	109.71 (16)
C10—C5—C6	117.62 (18)	C2—C19—C17	106.47 (16)
C7—C6—C5	119.77 (18)	C18—C19—C4	110.70 (16)
C7—C6—C1	119.37 (18)	C2—C19—C4	110.88 (15)
C5—C6—C1	119.60 (17)	C17—C19—C4	107.29 (15)
C8—C7—C6	121.04 (19)		

O1—Mo1—O3—C5	41.55 (15)	Mo1—O3—C5—C10	−146.68 (14)
O2—Mo1—O3—C5	−99.9 (2)	Mo1—O3—C5—C6	35.9 (2)
O4—Mo1—O3—C5	143.51 (15)	O3—C5—C6—C7	178.78 (17)
N2—Mo1—O3—C5	−52.23 (14)	C10—C5—C6—C7	1.3 (3)
N1—Mo1—O3—C5	−134.88 (15)	O3—C5—C6—C1	11.6 (3)
O1—Mo1—O4—C11	135.68 (17)	C10—C5—C6—C1	−165.83 (18)
O2—Mo1—O4—C11	−117.46 (17)	N2—C1—C6—C7	171.47 (18)
O3—Mo1—O4—C11	45.89 (17)	N2—C1—C6—C5	−21.3 (3)
N2—Mo1—O4—C11	1.4 (3)	C5—C6—C7—C8	0.1 (3)
N1—Mo1—O4—C11	−35.61 (17)	C1—C6—C7—C8	167.25 (19)
O2—Mo1—N1—C3	121.32 (16)	C6—C7—C8—C9	−0.8 (3)
O4—Mo1—N1—C3	17.34 (15)	C7—C8—C9—C10	0.1 (3)

O3—Mo1—N1—C3	−69.06 (15)	C8—C9—C10—C5	1.3 (3)
N2—Mo1—N1—C3	−149.25 (16)	O3—C5—C10—C9	−179.54 (18)
O2—Mo1—N1—C2	−48.30 (13)	C6—C5—C10—C9	−2.0 (3)
O4—Mo1—N1—C2	−152.29 (13)	Mo1—O4—C11—C16	−150.25 (15)
O3—Mo1—N1—C2	121.32 (13)	Mo1—O4—C11—C12	33.8 (3)
N2—Mo1—N1—C2	41.12 (13)	O4—C11—C12—C13	173.48 (17)
O1—Mo1—N2—C1	−48.07 (15)	C16—C11—C12—C13	−2.4 (3)
O2—Mo1—N2—C1	−151.34 (15)	O4—C11—C12—C3	0.8 (3)
O4—Mo1—N2—C1	87.3 (2)	C16—C11—C12—C3	−175.13 (18)
O3—Mo1—N2—C1	42.02 (15)	N1—C3—C12—C13	172.40 (18)
N1—Mo1—N2—C1	124.33 (15)	N1—C3—C12—C11	−14.9 (3)
O1—Mo1—N2—C4	136.02 (13)	C11—C12—C13—C14	2.7 (3)
O2—Mo1—N2—C4	32.75 (14)	C3—C12—C13—C14	175.75 (18)
O4—Mo1—N2—C4	−88.6 (2)	C12—C13—C14—C15	−1.4 (3)
O3—Mo1—N2—C4	−133.89 (14)	C13—C14—C15—C16	−0.2 (3)
N1—Mo1—N2—C4	−51.57 (13)	C14—C15—C16—C11	0.4 (3)
C4—N2—C1—C6	159.34 (18)	O4—C11—C16—C15	−175.12 (17)
Mo1—N2—C1—C6	−16.7 (3)	C12—C11—C16—C15	1.0 (3)
C3—N1—C2—C19	133.97 (18)	N1—C2—C19—C18	−59.5 (2)
Mo1—N1—C2—C19	−55.57 (19)	N1—C2—C19—C17	−179.21 (16)
C2—N1—C3—C12	170.57 (17)	N1—C2—C19—C4	64.4 (2)
Mo1—N1—C3—C12	0.6 (3)	N2—C4—C19—C18	52.6 (2)
C1—N2—C4—C19	−100.26 (19)	N2—C4—C19—C2	−71.82 (19)
Mo1—N2—C4—C19	75.87 (17)	N2—C4—C19—C17	172.30 (15)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4*A*···O2	0.97	2.49	2.986 (2)	112
C1—H1···O1^{i}	0.93	2.54	3.227 (2)	131
C4—H4*B*···O1^{i}	0.97	2.56	3.294 (2)	132
C7—H7···O2^{i}	0.93	2.55	3.315 (2)	140

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