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Dicarbonyl-bis(1,10-phenanthroline)-molybdenum(0)

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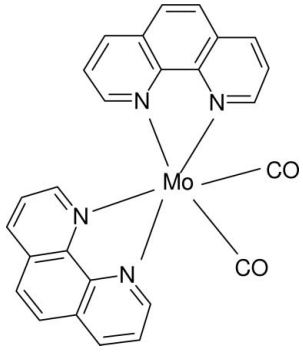
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.010 Å; R factor = 0.054; wR factor = 0.141; data-to-parameter ratio = 12.1.

In the title compound, $[Mo(CO)_2(phen)_2]$ (phen = $C_{12}H_8N_2$), the Mo atom adopts a *cis*-MoC_2N_4 geometry. The C—Mo—C angle of 88.0 (3)° is close to its ideal, undistorted value and the dihedral angle between the phen mean planes is 84.79 (9)°. A C—H···O bond and various π–π stacking interactions [centroid-centroid separation = 3.472 (3)–3.890 (4) Å] may help to establish the packing.

Related literature

For background, see: Behrens & Harder (1964); Cotton & Wing (1965); Chisholm *et al.* (1984); Kubácek & Hoffmann (1981).



Experimental

Crystal data

$[Mo(CO)_2(C_{12}H_8N_2)_2]$
M_r = 512.37
Monoclinic, $P2_1/c$
a = 9.7031 (6) Å
b = 14.5684 (10) Å
c = 14.7006 (9) Å
β = 101.142 (2)°
V = 2038.9 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.68 mm^{-1}
T = 296 (2) K
0.22 × 0.19 × 0.17 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.865, T_{max} = 0.896
11958 measured reflections
3603 independent reflections
2320 reflections with $I > 2\sigma(I)$
R_{int} = 0.069

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.141
S = 0.95
3603 reflections
298 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.58 e Å^{-3}
$\Delta\rho_{min}$ = −1.12 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mo1—C1	1.933 (7)	Mo1—N3	2.177 (5)
Mo1—C2	1.935 (6)	Mo1—N1	2.232 (5)
Mo1—N2	2.139 (5)	Mo1—N4	2.233 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11···O1^{i}	0.93	2.47	3.381 (8)	165

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2349).

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supplementary materials

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Dicarbonyl-bis(1,10-phenanthroline)molybdenum(0)

K. J. Muir, G. P. McQuillan and W. T. A. Harrison

Comment

The title compound, (I), $Mo(CO)_2(phen)_2$ (phen = 1,10-phenanthroline, $C_{12}H_8N_2$), was first reported over forty years ago by Behrens & Harder (1964). Chisholm *et al.* (1984) described the crystal structure of its close analogue $Mo(CO)_2(bipy)_2$ (bipy = 2,2'-bipyridine, $C_{10}H_8N_2$). Both compounds originate from $Mo(CO)_6$ by the replacement of four carbonyl groups by two N,*N*-bidentate aromatic ligands.

The asymmetric unit of compound (I) is built up around a distorted *cis*-MoC_2N_4 octahedron (Table 1; Fig. 1). The N1—Mo1—N2 and N3—Mo1—N4 phen bite angles are 74.43 (17)° and 73.97 (18)°, respectively, The *cis* C1—Mo1—C2 angle of 88.0 (3)° in (I) indicates a near ideal (90°) geometry for this grouping. The equivalent angle in $Mo(CO)_2(bipy)_2$ is compressed to 82.6 (3)°. Theoretical calculations (Kubácek & Hoffmann, 1981) have suggested an electronic origin for this type of distortion: it is not clear why it occurs in $Mo(CO)_2(bipy)_2$ but not in (I).

Both phen ligands in (I) are close to planar and show normal geometrical parameters. The dihedral angle between N1/N2/C3—C13 and N3/N4/C14—C22 is 84.74 (9)°, *i.e.* the phen molecules are close to perpendicular, and Mo1 is displaced from the N1 and N3-containing molecules by 0.262 (4)Å and 0.068 (4) Å, respectively.

The short Mo1—C1 and Mo1—C2 distances in (I) imply a substantial electron transfer from the Mo 5 d orbitals to the CO antibonding π* orbitals (Chisholm *et al.*, 1984). For comparison, the Mo—C separation in $Mo(CO)_6$, in which the Mo d electrons are "shared out" between six Mo—C bonds, is 2.06 (2)Å (Cotton & Wing, 1965). The difference in Mo—N bond lengths in (I) was also seen in the analagous $Mo(CO)_2(bipy)_2$ (Chisholm *et al.*, 1984), and related to models of possible Mo --> bipy(π*) back bonding.

An acute C—H···O bond (Table 2) and various π-π stacking interactions [centroid-centroid separation = 3.472 (3)–3.890 (4) Å] may help to establish the packing for (I), which appears to be quite different to that for $Mo(CO)_2(bipy)_2$.

Experimental

$Mo(CO)_6$ and excess 1,10-phenanthroline were refluxed in toluene under an N_2 atmosphere for seven hours. After cooling, air-stable greenish-black chunks of (I) were recovered by vacuum filtration and rinsing with light petroleum ether.

Refinement

The hydrogen atoms were geometrically placed (C—H = 0.93 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

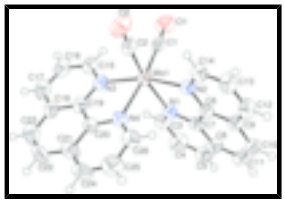


Fig. 1. View of the molecular structure of (I) showing 50% displacement ellipsoids (arbitrary spheres for the H atoms).

Dicarbonyl-bis(1,10-phenanthroline)molybdenum(0)

Crystal data

$[Mo(CO)_2(C_{12}H_8N_2)_2]$	F_{000} = 1032
M_r = 512.37	D_x = 1.669 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2524 reflections
a = 9.7031 (6) Å	θ = 2.6–24.6º
b = 14.5684 (10) Å	μ = 0.68 mm^{-1}
c = 14.7006 (9) Å	T = 296 (2) K
β = 101.142 (2)º	Chunk, green–black
V = 2038.9 (2) Å^3	0.22 × 0.19 × 0.17 mm
Z = 4	

Data collection

Bruker SMART 1000 CCD diffractometer	3603 independent reflections
Radiation source: fine-focus sealed tube	2320 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.069
T = 296(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Bruker, 1999)	h = −11→10
T_{min} = 0.865, T_{max} = 0.896	k = −17→17
11958 measured reflections	l = −11→17

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.054	H-atom parameters constrained
$wR(F^2)$ = 0.141	$w = 1/[\sigma^2(F_o^2) + (0.0827P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.95	$(\Delta/\sigma)_{max}$ = 0.001

3603 reflections	$\Delta\rho_{max}$ = 1.58 e Å^{-3}
298 parameters	$\Delta\rho_{min}$ = −1.12 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Mo1	0.75010 (5)	0.22662 (4)	0.54232 (3)	0.03397 (19)
C1	0.6848 (6)	0.1357 (5)	0.6200 (5)	0.0451 (16)
C2	0.5790 (7)	0.2066 (4)	0.4523 (4)	0.0416 (16)
O1	0.6409 (5)	0.0837 (4)	0.6684 (4)	0.0723 (16)
O2	0.4796 (5)	0.1909 (4)	0.3943 (3)	0.0636 (14)
C3	1.0121 (7)	0.2653 (4)	0.7098 (4)	0.0450 (15)
H3	0.9471	0.2952	0.7383	0.054*
C4	1.1505 (8)	0.2633 (5)	0.7554 (5)	0.0572 (19)
H4	1.1766	0.2906	0.8133	0.069*
C5	1.2489 (7)	0.2210 (5)	0.7151 (4)	0.0546 (18)
H5	1.3426	0.2206	0.7450	0.066*
C6	1.2089 (7)	0.1778 (5)	0.6280 (4)	0.0456 (16)
C7	1.0638 (6)	0.1824 (4)	0.5875 (4)	0.0359 (14)
C8	1.0123 (6)	0.1366 (4)	0.5012 (4)	0.0341 (13)
C9	1.1081 (6)	0.0892 (4)	0.4573 (4)	0.0393 (15)
C10	1.2543 (7)	0.0900 (5)	0.4978 (5)	0.0542 (19)
H10	1.3181	0.0611	0.4675	0.065*
C11	1.3007 (7)	0.1321 (5)	0.5797 (5)	0.0536 (18)
H11	1.3963	0.1310	0.6050	0.064*
C12	1.0530 (8)	0.0430 (5)	0.3735 (4)	0.0508 (18)
H12	1.1117	0.0122	0.3407	0.061*
C13	0.9112 (7)	0.0450 (5)	0.3422 (4)	0.0484 (17)
H13	0.8725	0.0146	0.2876	0.058*
C14	0.8251 (7)	0.0912 (4)	0.3903 (4)	0.0420 (16)
H14	0.7290	0.0900	0.3667	0.050*
C15	0.5923 (7)	0.3434 (5)	0.6732 (4)	0.0455 (16)
H15	0.5796	0.2874	0.7008	0.055*
C16	0.5330 (7)	0.4205 (5)	0.7049 (5)	0.0544 (19)

H16	0.4791	0.4151	0.7505	0.065*
C17	0.5542 (8)	0.5049 (6)	0.6686 (5)	0.061 (2)
H17	0.5154	0.5574	0.6895	0.073*
C18	0.6350 (7)	0.5108 (5)	0.6000 (5)	0.0477 (17)
C19	0.6890 (6)	0.4298 (4)	0.5716 (4)	0.0392 (15)
C20	0.7682 (6)	0.4315 (4)	0.4978 (4)	0.0392 (15)
C21	0.7944 (8)	0.5157 (5)	0.4583 (5)	0.054 (2)
C22	0.7413 (8)	0.5977 (5)	0.4908 (6)	0.067 (2)
H22	0.7598	0.6538	0.4655	0.080*
C23	0.6639 (9)	0.5951 (5)	0.5583 (6)	0.066 (2)
H23	0.6289	0.6495	0.5778	0.079*
C24	0.8739 (8)	0.5126 (6)	0.3866 (5)	0.062 (2)
H24	0.8949	0.5664	0.3582	0.075*
C25	0.9182 (9)	0.4314 (6)	0.3605 (5)	0.068 (2)
H25	0.9707	0.4288	0.3139	0.081*
C26	0.8862 (7)	0.3515 (5)	0.4027 (4)	0.0522 (18)
H26	0.9175	0.2960	0.3829	0.063*
N1	0.9670 (5)	0.2270 (3)	0.6277 (3)	0.0366 (11)
N2	0.8708 (5)	0.1393 (3)	0.4707 (3)	0.0347 (12)
N3	0.6669 (5)	0.3443 (4)	0.6053 (3)	0.0367 (12)
N4	0.8127 (5)	0.3502 (3)	0.4701 (3)	0.0373 (12)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.0355 (3)	0.0410 (3)	0.0249 (3)	0.0045 (3)	0.00437 (18)	0.0041 (2)
C1	0.032 (4)	0.049 (4)	0.052 (4)	0.011 (3)	0.004 (3)	0.009 (3)
C2	0.043 (4)	0.045 (4)	0.038 (4)	0.011 (3)	0.010 (3)	0.005 (3)
O1	0.060 (4)	0.083 (4)	0.079 (4)	0.002 (3)	0.026 (3)	0.039 (3)
O2	0.045 (3)	0.094 (4)	0.044 (3)	0.007 (3)	−0.010 (2)	−0.006 (3)
C3	0.054 (4)	0.051 (4)	0.030 (3)	−0.003 (3)	0.010 (3)	0.002 (3)
C4	0.066 (5)	0.067 (5)	0.032 (4)	−0.004 (4)	−0.007 (3)	−0.003 (3)
C5	0.047 (4)	0.068 (5)	0.042 (4)	−0.007 (4)	−0.010 (3)	0.007 (3)
C6	0.040 (4)	0.056 (4)	0.038 (4)	−0.002 (3)	−0.001 (3)	0.009 (3)
C7	0.037 (4)	0.038 (3)	0.032 (3)	−0.002 (3)	0.007 (3)	0.007 (3)
C8	0.043 (4)	0.033 (3)	0.026 (3)	−0.001 (3)	0.007 (3)	0.006 (2)
C9	0.039 (4)	0.043 (4)	0.037 (4)	0.002 (3)	0.011 (3)	0.008 (3)
C10	0.044 (4)	0.061 (5)	0.062 (5)	0.006 (3)	0.020 (3)	0.002 (4)
C11	0.032 (4)	0.071 (5)	0.057 (5)	0.003 (3)	0.005 (3)	0.006 (4)
C12	0.066 (5)	0.055 (4)	0.035 (4)	0.014 (4)	0.018 (3)	0.008 (3)
C13	0.057 (5)	0.057 (4)	0.027 (3)	0.007 (4)	0.000 (3)	−0.006 (3)
C14	0.051 (4)	0.043 (4)	0.027 (3)	0.003 (3)	−0.004 (3)	0.001 (3)
C15	0.046 (4)	0.061 (5)	0.030 (3)	0.006 (3)	0.009 (3)	0.003 (3)
C16	0.050 (4)	0.079 (6)	0.034 (4)	0.011 (4)	0.008 (3)	−0.014 (3)
C17	0.057 (5)	0.068 (5)	0.051 (5)	0.018 (4)	−0.004 (4)	−0.021 (4)
C18	0.045 (4)	0.046 (4)	0.044 (4)	0.004 (3)	−0.010 (3)	−0.007 (3)
C19	0.039 (4)	0.048 (4)	0.025 (3)	0.001 (3)	−0.008 (3)	−0.002 (3)
C20	0.036 (4)	0.044 (4)	0.033 (3)	0.001 (3)	−0.005 (3)	0.008 (3)

C21	0.064 (5)	0.046 (4)	0.041 (4)	−0.008 (3)	−0.012 (4)	0.012 (3)
C22	0.075 (6)	0.037 (4)	0.075 (6)	−0.004 (4)	−0.016 (5)	0.013 (4)
C23	0.078 (6)	0.049 (5)	0.059 (5)	0.010 (4)	−0.013 (4)	−0.017 (4)
C24	0.066 (5)	0.058 (5)	0.057 (5)	−0.013 (4)	−0.002 (4)	0.031 (4)
C25	0.078 (6)	0.085 (7)	0.043 (5)	0.001 (5)	0.017 (4)	0.024 (4)
C26	0.062 (5)	0.059 (5)	0.037 (4)	0.002 (4)	0.013 (3)	0.009 (3)
N1	0.044 (3)	0.035 (3)	0.029 (3)	−0.002 (3)	0.001 (2)	0.003 (2)
N2	0.036 (3)	0.042 (3)	0.024 (3)	0.000 (2)	0.001 (2)	0.004 (2)
N3	0.030 (3)	0.054 (3)	0.024 (3)	0.004 (2)	0.001 (2)	0.002 (2)
N4	0.046 (3)	0.039 (3)	0.026 (3)	0.001 (2)	0.005 (2)	0.005 (2)

Geometric parameters (Å, °)

Mo1—C1	1.933 (7)	C13—C14	1.371 (9)
Mo1—C2	1.935 (6)	C13—H13	0.9300
Mo1—N2	2.139 (5)	C14—N2	1.372 (7)
Mo1—N3	2.177 (5)	C14—H14	0.9300
Mo1—N1	2.232 (5)	C15—N3	1.343 (7)
Mo1—N4	2.233 (5)	C15—C16	1.382 (9)
C1—O1	1.174 (8)	C15—H15	0.9300
C2—O2	1.180 (7)	C16—C17	1.371 (10)
C3—N1	1.326 (7)	C16—H16	0.9300
C3—C4	1.380 (9)	C17—C18	1.396 (10)
C3—H3	0.9300	C17—H17	0.9300
C4—C5	1.364 (9)	C18—C19	1.388 (9)
C4—H4	0.9300	C18—C23	1.423 (10)
C5—C6	1.412 (9)	C19—N3	1.372 (7)
C5—H5	0.9300	C19—C20	1.446 (9)
C6—C11	1.410 (9)	C20—N4	1.350 (8)
C6—C7	1.420 (8)	C20—C21	1.401 (9)
C7—N1	1.367 (7)	C21—C22	1.419 (11)
C7—C8	1.434 (8)	C21—C24	1.421 (11)
C8—N2	1.360 (7)	C22—C23	1.355 (11)
C8—C9	1.411 (8)	C22—H22	0.9300
C9—C12	1.415 (9)	C23—H23	0.9300
C9—C10	1.429 (8)	C24—C25	1.340 (10)
C10—C11	1.348 (10)	C24—H24	0.9300
C10—H10	0.9300	C25—C26	1.382 (9)
C11—H11	0.9300	C25—H25	0.9300
C12—C13	1.364 (9)	C26—N4	1.329 (8)
C12—H12	0.9300	C26—H26	0.9300
C1—Mo1—C2	88.0 (3)	C13—C14—H14	117.7
C1—Mo1—N2	99.0 (2)	N2—C14—H14	117.7
C2—Mo1—N2	93.0 (2)	N3—C15—C16	124.2 (7)
C1—Mo1—N3	95.6 (2)	N3—C15—H15	117.9
C2—Mo1—N3	94.0 (2)	C16—C15—H15	117.9
N2—Mo1—N3	163.99 (19)	C17—C16—C15	119.6 (7)
C1—Mo1—N1	92.9 (2)	C17—C16—H16	120.2
C2—Mo1—N1	167.4 (2)	C15—C16—H16	120.2

N2—Mo1—N1	74.43 (17)	C16—C17—C18	119.0 (7)
N3—Mo1—N1	98.39 (17)	C16—C17—H17	120.5
C1—Mo1—N4	169.5 (2)	C18—C17—H17	120.5
C2—Mo1—N4	94.2 (2)	C19—C18—C17	117.5 (7)
N2—Mo1—N4	91.20 (19)	C19—C18—C23	119.2 (7)
N3—Mo1—N4	73.97 (18)	C17—C18—C23	123.3 (7)
N1—Mo1—N4	87.24 (17)	N3—C19—C18	124.7 (7)
O1—C1—Mo1	176.7 (6)	N3—C19—C20	115.4 (6)
O2—C2—Mo1	175.7 (6)	C18—C19—C20	119.8 (6)
N1—C3—C4	123.5 (6)	N4—C20—C21	123.3 (7)
N1—C3—H3	118.3	N4—C20—C19	117.2 (6)
C4—C3—H3	118.3	C21—C20—C19	119.4 (6)
C5—C4—C3	119.8 (6)	C20—C21—C22	119.4 (8)
C5—C4—H4	120.1	C20—C21—C24	116.5 (7)
C3—C4—H4	120.1	C22—C21—C24	124.1 (7)
C4—C5—C6	120.1 (6)	C23—C22—C21	120.8 (7)
C4—C5—H5	119.9	C23—C22—H22	119.6
C6—C5—H5	119.9	C21—C22—H22	119.6
C11—C6—C5	125.2 (6)	C22—C23—C18	121.5 (7)
C11—C6—C7	118.9 (6)	C22—C23—H23	119.3
C5—C6—C7	115.9 (6)	C18—C23—H23	119.3
N1—C7—C6	123.3 (5)	C25—C24—C21	119.4 (7)
N1—C7—C8	116.9 (5)	C25—C24—H24	120.3
C6—C7—C8	119.8 (6)	C21—C24—H24	120.3
N2—C8—C9	125.1 (5)	C24—C25—C26	120.1 (8)
N2—C8—C7	115.8 (5)	C24—C25—H25	119.9
C9—C8—C7	119.0 (5)	C26—C25—H25	119.9
C8—C9—C12	117.4 (6)	N4—C26—C25	123.2 (7)
C8—C9—C10	119.6 (6)	N4—C26—H26	118.4
C12—C9—C10	123.0 (6)	C25—C26—H26	118.4
C11—C10—C9	120.6 (7)	C3—N1—C7	117.4 (5)
C11—C10—H10	119.7	C3—N1—Mo1	128.5 (4)
C9—C10—H10	119.7	C7—N1—Mo1	114.1 (3)
C10—C11—C6	122.0 (6)	C8—N2—C14	114.0 (5)
C10—C11—H11	119.0	C8—N2—Mo1	118.0 (4)
C6—C11—H11	119.0	C14—N2—Mo1	127.7 (4)
C13—C12—C9	118.1 (6)	C15—N3—C19	114.9 (6)
C13—C12—H12	121.0	C15—N3—Mo1	127.3 (5)
C9—C12—H12	121.0	C19—N3—Mo1	117.7 (4)
C12—C13—C14	120.8 (6)	C26—N4—C20	117.5 (6)
C12—C13—H13	119.6	C26—N4—Mo1	126.9 (4)
C14—C13—H13	119.6	C20—N4—Mo1	115.6 (4)
C13—C14—N2	124.6 (6)		

N1—C3—C4—C5	0.8 (11)	C2—Mo1—N1—C3	−169.4 (9)
C3—C4—C5—C6	−1.3 (11)	N2—Mo1—N1—C3	−174.3 (5)
C4—C5—C6—C11	180.0 (7)	N3—Mo1—N1—C3	20.4 (5)
C4—C5—C6—C7	0.3 (10)	N4—Mo1—N1—C3	93.7 (5)
C11—C6—C7—N1	−178.3 (6)	C1—Mo1—N1—C7	105.3 (4)
C5—C6—C7—N1	1.4 (9)	C2—Mo1—N1—C7	11.6 (12)

C11—C6—C7—C8	3.3 (9)	N2—Mo1—N1—C7	6.8 (4)
C5—C6—C7—C8	−177.0 (6)	N3—Mo1—N1—C7	−158.6 (4)
N1—C7—C8—N2	−2.8 (8)	N4—Mo1—N1—C7	−85.3 (4)
C6—C7—C8—N2	175.6 (5)	C9—C8—N2—C14	−0.6 (8)
N1—C7—C8—C9	−179.6 (5)	C7—C8—N2—C14	−177.2 (5)
C6—C7—C8—C9	−1.2 (8)	C9—C8—N2—Mo1	−174.2 (4)
N2—C8—C9—C12	2.0 (9)	C7—C8—N2—Mo1	9.2 (6)
C7—C8—C9—C12	178.5 (5)	C13—C14—N2—C8	−0.9 (9)
N2—C8—C9—C10	−178.4 (6)	C13—C14—N2—Mo1	172.0 (5)
C7—C8—C9—C10	−1.9 (9)	C1—Mo1—N2—C8	−99.1 (4)
C8—C9—C10—C11	3.0 (10)	C2—Mo1—N2—C8	172.5 (4)
C12—C9—C10—C11	−177.5 (7)	N3—Mo1—N2—C8	56.5 (8)
C9—C10—C11—C6	−0.8 (11)	N1—Mo1—N2—C8	−8.6 (4)
C5—C6—C11—C10	177.9 (7)	N4—Mo1—N2—C8	78.2 (4)
C7—C6—C11—C10	−2.3 (11)	C1—Mo1—N2—C14	88.3 (5)
C8—C9—C12—C13	−2.0 (9)	C2—Mo1—N2—C14	−0.2 (5)
C10—C9—C12—C13	178.5 (6)	N3—Mo1—N2—C14	−116.2 (7)
C9—C12—C13—C14	0.7 (10)	N1—Mo1—N2—C14	178.8 (5)
C12—C13—C14—N2	0.8 (10)	N4—Mo1—N2—C14	−94.4 (5)
N3—C15—C16—C17	−2.7 (10)	C16—C15—N3—C19	3.8 (8)
C15—C16—C17—C18	0.3 (10)	C16—C15—N3—Mo1	−174.6 (5)
C16—C17—C18—C19	0.5 (9)	C18—C19—N3—C15	−3.0 (8)
C16—C17—C18—C23	−179.6 (6)	C20—C19—N3—C15	−179.5 (5)
C17—C18—C19—N3	0.9 (9)	C18—C19—N3—Mo1	175.6 (4)
C23—C18—C19—N3	−179.0 (5)	C20—C19—N3—Mo1	−0.9 (6)
C17—C18—C19—C20	177.3 (6)	C1—Mo1—N3—C15	−2.0 (5)
C23—C18—C19—C20	−2.6 (8)	C2—Mo1—N3—C15	86.4 (5)
N3—C19—C20—N4	−0.4 (8)	N2—Mo1—N3—C15	−157.7 (6)
C18—C19—C20—N4	−177.1 (5)	N1—Mo1—N3—C15	−95.8 (5)
N3—C19—C20—C21	179.2 (5)	N4—Mo1—N3—C15	179.6 (5)
C18—C19—C20—C21	2.5 (8)	C1—Mo1—N3—C19	179.7 (4)
N4—C20—C21—C22	178.9 (6)	C2—Mo1—N3—C19	−92.0 (4)
C19—C20—C21—C22	−0.7 (9)	N2—Mo1—N3—C19	23.9 (8)
N4—C20—C21—C24	−0.9 (9)	N1—Mo1—N3—C19	85.9 (4)
C19—C20—C21—C24	179.5 (6)	N4—Mo1—N3—C19	1.2 (4)
C20—C21—C22—C23	−1.1 (10)	C25—C26—N4—C20	0.0 (10)
C24—C21—C22—C23	178.7 (7)	C25—C26—N4—Mo1	178.8 (5)
C21—C22—C23—C18	1.0 (11)	C21—C20—N4—C26	0.8 (9)
C19—C18—C23—C22	0.9 (10)	C19—C20—N4—C26	−179.7 (5)
C17—C18—C23—C22	−179.0 (7)	C21—C20—N4—Mo1	−178.2 (4)
C20—C21—C24—C25	0.4 (10)	C19—C20—N4—Mo1	1.4 (6)
C22—C21—C24—C25	−179.4 (7)	C1—Mo1—N4—C26	171.2 (11)
C21—C24—C25—C26	0.3 (11)	C2—Mo1—N4—C26	−87.2 (5)
C24—C25—C26—N4	−0.5 (11)	N2—Mo1—N4—C26	5.9 (5)
C4—C3—N1—C7	0.8 (9)	N3—Mo1—N4—C26	179.8 (6)
C4—C3—N1—Mo1	−178.1 (5)	N1—Mo1—N4—C26	80.3 (5)
C6—C7—N1—C3	−1.9 (9)	C1—Mo1—N4—C20	−10.0 (14)
C8—C7—N1—C3	176.5 (5)	C2—Mo1—N4—C20	91.6 (4)
C6—C7—N1—Mo1	177.2 (5)	N2—Mo1—N4—C20	−175.3 (4)

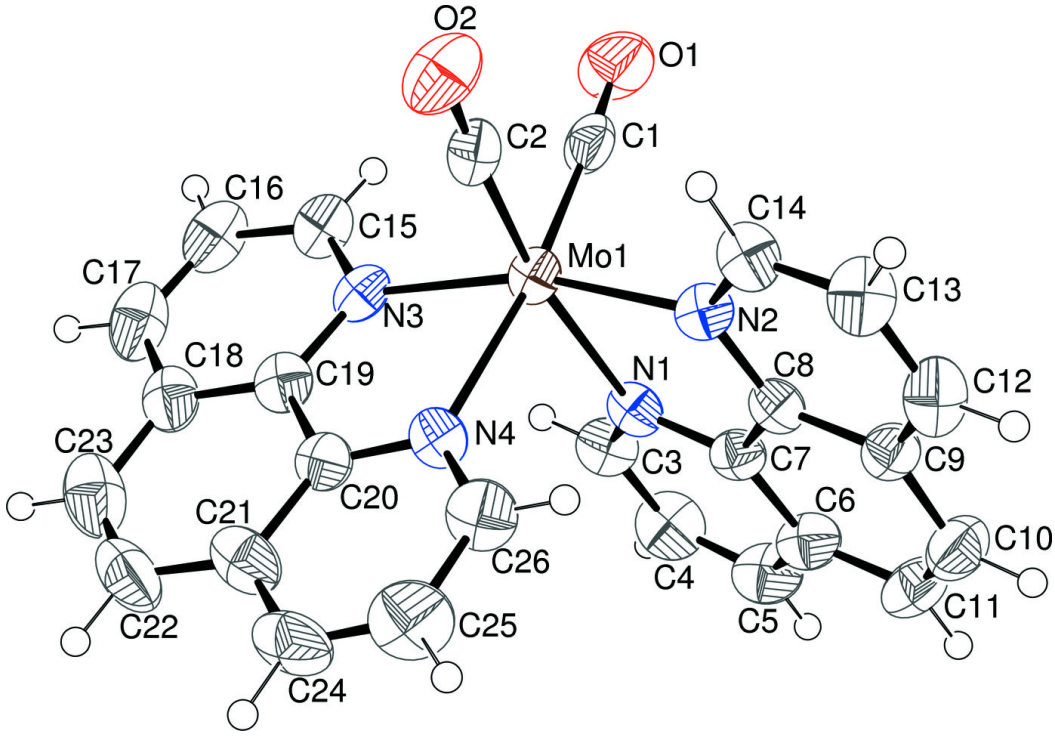
C8—C7—N1—Mo1	−4.4 (6)	N3—Mo1—N4—C20	−1.4 (4)
C1—Mo1—N1—C3	−75.8 (5)	N1—Mo1—N4—C20	−100.9 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···O1^{i}	0.93	2.47	3.381 (8)	165

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

Fig. 1


O2
O1
C2
C1
C16
C15
C14
Mo1
C17
N3
N2
C13
C18
C19
N1
C8
C12
N4
C23
C3
C7
C9
C20
C6
C21
C26
C10
C4
C22
C25
C5
C11
C24