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(2,2′-Biquinoline)tetracarbonylmolybdenum(0)

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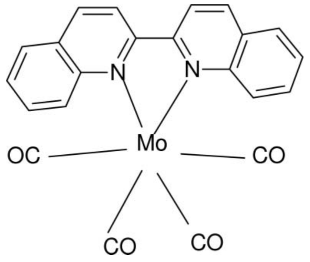
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.079; data-to-parameter ratio = 19.8.

In the title compound, $[Mo(C_{18}H_{12}N_2)(CO)_4]$, the differences in the Mo—C and C—O bond lengths may be interpreted in terms of a classical back-bonding model of electronic structure. In the crystal structure, an acute C—H···O interaction may help to establish the packing.

Related literature

For a related structure, see: Braga *et al.* (2007). For background, see: Cotton & Wilkinson (1966). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Mo(C_{18}H_{12}N_2)(CO)_4]$
M_r = 464.28
Triclinic, $P\overline{1}$
a = 7.7365 (4) Å
b = 9.8294 (5) Å
c = 12.8060 (6) Å
α = 93.512 (1)°
β = 94.215 (1)°
γ = 109.394 (1)°
V = 912.29 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.75 mm^{-1}
T = 296 (2) K
0.42 × 0.18 × 0.12 mm

Data collection

Bruker SMART1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.743, T_{max} = 0.917
8669 measured reflections
5200 independent reflections
4267 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.079
S = 0.99
5200 reflections
262 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mo1—C1	1.946 (3)	Mo1—N1	2.3107 (17)
Mo1—C3	1.953 (3)	C1—O1	1.158 (3)
Mo1—C2	2.031 (3)	C2—O2	1.134 (3)
Mo1—C4	2.051 (3)	C3—O3	1.160 (3)
Mo1—N2	2.3020 (18)	C4—O4	1.136 (3)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···O1^{i}	0.93	2.45	3.122 (3)	129

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

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: BT2494).

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doi:10.1107/S1600536807042547

supplementary materials

Acta Cryst. (2007). E**63**, m2452 [**doi:10.1107/S1600536807042547**]

(2,2'-Biquinoline)tetracarbonylmolybdenum(0)

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

Comment

Although the substitution reactions of $Mo(CO)_6$ with amine bases have been intensively studied for many decades (Cotton & Wilkinson, 1966), the crystal structures of many of the resulting compounds remain to be studied. The structure of the simple compound $Mo(CO)_4(C_{10}H_8N_2)$, (I), (Braga *et al.*, 2007) has just been reported ($C_{10}H_8N_2$ = 2,2-bipyridine or bipy).

In the title compound, (II), $Mo(CO)_4(C_{18}H_{12}N_2)$, 2,2'-biquinoline (biquin) has replaced bipy. A distorted *cis*-MoN_2C_4 octahedron results for the metal (Fig. 1, Table 1). The N—Mo—N bite angle for the biquin molecule is 72.31 (6)°. The dihedral angle between the N1/C5/C10—C13 and N2/C14—C17/C22 ring systems of 16.57 (11)° in (II) indicates a significant degree of twisting about the linking C13—C14 bond. The quinoline fused rings are slightly distorted from planarity: the C5—C10 and N1/C5/C10—C13 rings make a dihedral angle of 2.15 (11)°; C17—C22 and N2/C14—C17/C22 are twisted by 3.46 (12)°. Mo1 is close to coplanar with N1/C5/C10—C15 [displacement = −0.030 (1) Å] but substantially displaced, by 0.715 (1) Å, from N2/C14—C17/C22. Otherwise, all the biquin bond lengths and angles may be regarded as normal (Allen *et al.*, 1995). The C2—Mo1—C4 bond angle of 169.31 (9)° indicates that these two carbonyl groups are bent away from the biquin molecule, perhaps for steric reasons.

The four Mo—C bond lengths in (II) fall into two groups of two. The shorter Mo1—C1 and Mo1—C3 bonds are *trans* to the diquin N atoms and the longer Mo1—C2 and Mo1—C4 bonds are *trans* to each other. The traditional explanation for this phenomenon assesses the π-acceptor propeties of the ligand *trans* to the carbon atom in question. If the *trans* atom has little or no π acceptor properties, then there is a greater tendency for the C atom to accept back bonded metal d electrons, and the Mo—C bond assumes a higher bond order and is shortened. Because the back bonded electrons are accommodated in the antibonding π* orbital of CO, the C—O bond length is expected to be lengthened as the Mo—C bond length decreases. This effect seems to be just visible in the present study, with the mean of C1—O1 and C3—O3 some 0.024Å longer than the mean of C2—O2 and C4—O4.

In the crystal of (II), an acute C—H···O interaction (Table 2) may help to establish the packing. There are also a number of π-π stacking contacts with centroid-centroid separations in the range 3.6623 (13)–3.8227 (13) Å.

Experimental

Equimolar quantities of $Mo(CO)_6$ and and 2,2'-biquinoline were refluxed in toluene under an N_2 atmosphere for six hours. After cooling, air-stable, dark orange, blocks of (II) were recovered by vacuum filtration and rinsing with light petroleum ether in 78% yield based on $Mo(CO)_6$.

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

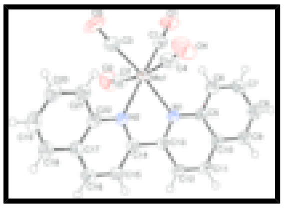


Fig. 1. View of the molecular structure of the title compound showing 50% displacement ellipsoids (arbitrary spheres for the H atoms).

(2,2'-Biquinoline)tetracarbonylmolybdenum(0)

Crystal data

$[Mo(C_{18}H_{12}N_2)(CO)_4]$

$M_r = 464.28$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.7365$ (4) Å

$b = 9.8294$ (5) Å

$c = 12.8060$ (6) Å

$\alpha = 93.512$ (1)°

$\beta = 94.215$ (1)°

$\gamma = 109.394$ (1)°

$V = 912.29$ (8) Å^3

$Z = 2$

$F_{000} = 464$

$D_x = 1.690$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 4201 reflections

$\theta = 2.6$–29.8°

$\mu = 0.75$ mm^{-1}

$T = 296$ (2) K

Block, very dark orange

0.42 × 0.18 × 0.12 mm

Data collection

Bruker SMART1000 CCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 296(2)$ K

ω scans

Absorption correction: multi-scan (SADABS; Bruker, 1999)

$T_{min} = 0.743$, $T_{max} = 0.917$

8669 measured reflections

5200 independent reflections

4267 reflections with $I > 2\sigma(I)$

$R_{int} = 0.021$

$\theta_{max} = 30.0$°

$\theta_{min} = 2.2$°

$h = -10 \rightarrow 10$

$k = -13 \rightarrow 12$

$l = -17 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.079$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0418P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$S = 0.99$	$(\Delta/\sigma)_{\max} = 0.001$
5200 reflections	$\Delta\rho_{\max} = 0.59$ e Å^{-3}
262 parameters	$\Delta\rho_{\min} = -0.66$ 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 $F^2 > 2\mathrm{sigma}(F^2)$ 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*	$U_{\rm iso}$*/$U_{\rm eq}$
Mo1	0.51011 (3)	0.182250 (18)	0.252976 (16)	0.03327 (7)
C1	0.4418 (3)	0.0088 (2)	0.1555 (2)	0.0449 (6)
C2	0.7505 (3)	0.2330 (3)	0.1855 (2)	0.0429 (5)
C3	0.6115 (4)	0.0645 (3)	0.3394 (2)	0.0480 (6)
C4	0.2617 (4)	0.0919 (3)	0.3117 (2)	0.0497 (6)
O1	0.4053 (3)	−0.0975 (2)	0.10119 (19)	0.0718 (6)
O2	0.8801 (3)	0.2432 (3)	0.14597 (19)	0.0728 (6)
O3	0.6716 (4)	−0.0104 (2)	0.3855 (2)	0.0820 (7)
O4	0.1260 (3)	0.0274 (3)	0.3410 (2)	0.0884 (8)
N1	0.4173 (2)	0.34601 (18)	0.16198 (14)	0.0305 (4)
N2	0.6003 (2)	0.39737 (18)	0.35795 (14)	0.0315 (4)
C5	0.3033 (3)	0.3170 (2)	0.06860 (17)	0.0318 (4)
C6	0.2348 (3)	0.1767 (2)	0.0164 (2)	0.0446 (6)
H6	0.2667	0.1025	0.0449	0.054*
C7	0.1222 (4)	0.1478 (3)	−0.0754 (2)	0.0514 (6)
H7	0.0809	0.0546	−0.1092	0.062*
C8	0.0679 (3)	0.2555 (3)	−0.1195 (2)	0.0487 (6)
H8	−0.0117	0.2335	−0.1810	0.058*
C9	0.1322 (3)	0.3924 (3)	−0.0720 (2)	0.0434 (5)
H9	0.0964	0.4643	−0.1015	0.052*
C10	0.2526 (3)	0.4278 (2)	0.02170 (18)	0.0339 (4)
C11	0.3256 (3)	0.5690 (2)	0.07031 (19)	0.0387 (5)
H11	0.2952	0.6435	0.0412	0.046*
C12	0.4409 (3)	0.5972 (2)	0.15997 (18)	0.0373 (5)
H12	0.4921	0.6913	0.1916	0.045*
C13	0.4835 (3)	0.4821 (2)	0.20574 (17)	0.0310 (4)
C14	0.5987 (3)	0.5123 (2)	0.30702 (17)	0.0324 (4)

C15	0.7002 (3)	0.6559 (2)	0.34873 (19)	0.0413 (5)
H15	0.6994	0.7330	0.3103	0.050*
C16	0.7981 (3)	0.6816 (2)	0.4437 (2)	0.0436 (5)
H16	0.8690	0.7758	0.4694	0.052*
C17	0.7923 (3)	0.5647 (2)	0.50393 (19)	0.0381 (5)
C18	0.8853 (3)	0.5847 (3)	0.6060 (2)	0.0470 (6)
H18	0.9556	0.6774	0.6352	0.056*
C19	0.8721 (4)	0.4689 (3)	0.6615 (2)	0.0536 (7)
H19	0.9360	0.4825	0.7278	0.064*
C20	0.7634 (4)	0.3295 (3)	0.6195 (2)	0.0502 (6)
H20	0.7525	0.2515	0.6593	0.060*
C21	0.6725 (3)	0.3061 (3)	0.5205 (2)	0.0431 (5)
H21	0.6002	0.2127	0.4940	0.052*
C22	0.6881 (3)	0.4231 (2)	0.45865 (17)	0.0340 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.03857 (11)	0.02369 (9)	0.03904 (12)	0.01230 (7)	0.00274 (7)	0.00546 (7)
O1	0.0909 (16)	0.0349 (10)	0.0889 (17)	0.0275 (10)	−0.0093 (13)	−0.0141 (10)
O2	0.0544 (12)	0.0794 (15)	0.0858 (17)	0.0205 (11)	0.0272 (12)	0.0045 (12)
O3	0.114 (2)	0.0671 (14)	0.0856 (17)	0.0568 (14)	−0.0014 (14)	0.0281 (12)
O4	0.0646 (14)	0.0749 (16)	0.110 (2)	−0.0026 (12)	0.0359 (14)	0.0072 (14)
N1	0.0339 (9)	0.0258 (8)	0.0329 (10)	0.0116 (7)	0.0029 (7)	0.0040 (7)
N2	0.0342 (9)	0.0300 (8)	0.0321 (10)	0.0129 (7)	0.0029 (7)	0.0044 (7)
C1	0.0468 (13)	0.0303 (11)	0.0589 (16)	0.0156 (10)	−0.0004 (11)	0.0060 (10)
C2	0.0457 (13)	0.0359 (12)	0.0467 (14)	0.0141 (10)	0.0010 (11)	0.0034 (10)
C3	0.0590 (15)	0.0380 (12)	0.0519 (16)	0.0225 (11)	0.0034 (12)	0.0086 (11)
C4	0.0525 (15)	0.0379 (13)	0.0564 (17)	0.0124 (11)	0.0068 (12)	0.0013 (11)
C5	0.0333 (10)	0.0303 (10)	0.0329 (11)	0.0114 (8)	0.0052 (8)	0.0062 (8)
C6	0.0533 (14)	0.0295 (11)	0.0479 (14)	0.0122 (10)	−0.0062 (11)	0.0028 (10)
C7	0.0572 (15)	0.0369 (12)	0.0520 (16)	0.0086 (11)	−0.0083 (12)	−0.0002 (11)
C8	0.0447 (13)	0.0507 (14)	0.0439 (14)	0.0094 (11)	−0.0076 (11)	0.0064 (11)
C9	0.0433 (12)	0.0454 (13)	0.0438 (14)	0.0180 (10)	−0.0010 (10)	0.0108 (10)
C10	0.0343 (10)	0.0342 (10)	0.0361 (12)	0.0142 (8)	0.0046 (9)	0.0091 (9)
C11	0.0471 (13)	0.0326 (11)	0.0425 (13)	0.0201 (9)	0.0049 (10)	0.0106 (9)
C12	0.0488 (13)	0.0270 (10)	0.0393 (12)	0.0169 (9)	0.0035 (10)	0.0053 (8)
C13	0.0358 (10)	0.0258 (9)	0.0341 (11)	0.0138 (8)	0.0047 (8)	0.0023 (8)
C14	0.0379 (11)	0.0279 (9)	0.0333 (11)	0.0134 (8)	0.0048 (9)	0.0032 (8)
C15	0.0544 (14)	0.0278 (10)	0.0422 (13)	0.0158 (10)	0.0019 (11)	0.0016 (9)
C16	0.0487 (13)	0.0323 (11)	0.0458 (14)	0.0112 (10)	−0.0007 (11)	−0.0045 (10)
C17	0.0368 (11)	0.0427 (12)	0.0364 (12)	0.0165 (9)	0.0029 (9)	−0.0013 (9)
C18	0.0447 (13)	0.0547 (15)	0.0401 (14)	0.0179 (11)	−0.0020 (11)	−0.0048 (11)
C19	0.0498 (15)	0.0758 (19)	0.0369 (14)	0.0251 (14)	−0.0031 (11)	0.0058 (13)
C20	0.0535 (15)	0.0597 (16)	0.0415 (14)	0.0227 (13)	0.0037 (12)	0.0157 (12)
C21	0.0457 (13)	0.0445 (13)	0.0408 (14)	0.0161 (10)	0.0054 (10)	0.0111 (10)
C22	0.0337 (10)	0.0381 (11)	0.0332 (12)	0.0155 (9)	0.0047 (9)	0.0045 (9)

Geometric parameters (Å, °)

Mo1—C1	1.946 (3)	C9—H9	0.9300
Mo1—C3	1.953 (3)	C10—C11	1.399 (3)
Mo1—C2	2.031 (3)	C11—C12	1.355 (3)
Mo1—C4	2.051 (3)	C11—H11	0.9300
Mo1—N2	2.3020 (18)	C12—C13	1.425 (3)
Mo1—N1	2.3107 (17)	C12—H12	0.9300
C1—O1	1.158 (3)	C13—C14	1.474 (3)
C2—O2	1.134 (3)	C14—C15	1.416 (3)
C3—O3	1.160 (3)	C15—C16	1.347 (3)
C4—O4	1.136 (3)	C15—H15	0.9300
N1—C13	1.333 (3)	C16—C17	1.413 (3)
N1—C5	1.388 (3)	C16—H16	0.9300
N2—C14	1.342 (3)	C17—C18	1.415 (3)
N2—C22	1.381 (3)	C17—C22	1.418 (3)
C5—C6	1.406 (3)	C18—C19	1.357 (4)
C5—C10	1.425 (3)	C18—H18	0.9300
C6—C7	1.367 (4)	C19—C20	1.397 (4)
C6—H6	0.9300	C19—H19	0.9300
C7—C8	1.397 (4)	C20—C21	1.371 (4)
C7—H7	0.9300	C20—H20	0.9300
C8—C9	1.357 (4)	C21—C22	1.414 (3)
C8—H8	0.9300	C21—H21	0.9300
C9—C10	1.413 (3)		

C1—Mo1—C3	81.52 (11)	C11—C10—C9	122.2 (2)
C1—Mo1—C2	83.18 (10)	C11—C10—C5	118.3 (2)
C3—Mo1—C2	85.46 (11)	C9—C10—C5	119.5 (2)
C1—Mo1—C4	86.98 (10)	C12—C11—C10	119.83 (19)
C3—Mo1—C4	88.99 (11)	C12—C11—H11	120.1
C2—Mo1—C4	169.31 (9)	C10—C11—H11	120.1
C1—Mo1—N2	175.64 (9)	C11—C12—C13	119.9 (2)
C3—Mo1—N2	101.26 (9)	C11—C12—H12	120.1
C2—Mo1—N2	93.66 (8)	C13—C12—H12	120.1
C4—Mo1—N2	96.38 (8)	N1—C13—C12	122.3 (2)
C1—Mo1—N1	104.72 (8)	N1—C13—C14	118.33 (17)
C3—Mo1—N1	172.97 (9)	C12—C13—C14	119.36 (18)
C2—Mo1—N1	92.03 (8)	N2—C14—C15	122.0 (2)
C4—Mo1—N1	94.50 (9)	N2—C14—C13	116.71 (18)
N2—Mo1—N1	72.31 (6)	C15—C14—C13	121.33 (19)
C13—N1—C5	118.22 (17)	C16—C15—C14	120.4 (2)
C13—N1—Mo1	114.78 (14)	C16—C15—H15	119.8
C5—N1—Mo1	127.00 (13)	C14—C15—H15	119.8
C14—N2—C22	117.79 (18)	C15—C16—C17	119.6 (2)
C14—N2—Mo1	114.41 (14)	C15—C16—H16	120.2
C22—N2—Mo1	126.38 (13)	C17—C16—H16	120.2
O1—C1—Mo1	176.5 (2)	C16—C17—C18	122.5 (2)
O2—C2—Mo1	171.4 (2)	C16—C17—C22	117.6 (2)

O3—C3—Mo1	176.1 (3)	C18—C17—C22	119.9 (2)
O4—C4—Mo1	172.3 (2)	C19—C18—C17	120.2 (2)
N1—C5—C6	120.94 (19)	C19—C18—H18	119.9
N1—C5—C10	121.43 (19)	C17—C18—H18	119.9
C6—C5—C10	117.6 (2)	C18—C19—C20	120.5 (2)
C7—C6—C5	121.1 (2)	C18—C19—H19	119.8
C7—C6—H6	119.5	C20—C19—H19	119.8
C5—C6—H6	119.5	C21—C20—C19	120.9 (2)
C6—C7—C8	121.2 (2)	C21—C20—H20	119.6
C6—C7—H7	119.4	C19—C20—H20	119.6
C8—C7—H7	119.4	C20—C21—C22	120.4 (2)
C9—C8—C7	119.4 (2)	C20—C21—H21	119.8
C9—C8—H8	120.3	C22—C21—H21	119.8
C7—C8—H8	120.3	N2—C22—C21	119.8 (2)
C8—C9—C10	121.1 (2)	N2—C22—C17	122.11 (19)
C8—C9—H9	119.4	C21—C22—C17	118.1 (2)
C10—C9—H9	119.4		

C1—Mo1—N1—C13	−167.03 (16)	C5—N1—C13—C12	0.1 (3)
C2—Mo1—N1—C13	−83.56 (16)	Mo1—N1—C13—C12	179.76 (16)
C4—Mo1—N1—C13	104.91 (16)	C5—N1—C13—C14	177.65 (18)
N2—Mo1—N1—C13	9.64 (14)	Mo1—N1—C13—C14	−2.7 (2)
C1—Mo1—N1—C5	12.61 (19)	C11—C12—C13—N1	1.7 (3)
C2—Mo1—N1—C5	96.09 (17)	C11—C12—C13—C14	−175.8 (2)
C4—Mo1—N1—C5	−75.44 (18)	C22—N2—C14—C15	7.0 (3)
N2—Mo1—N1—C5	−170.72 (18)	Mo1—N2—C14—C15	−160.21 (17)
C3—Mo1—N2—C14	160.90 (16)	C22—N2—C14—C13	−172.04 (18)
C2—Mo1—N2—C14	74.80 (16)	Mo1—N2—C14—C13	20.7 (2)
C4—Mo1—N2—C14	−108.86 (16)	N1—C13—C14—N2	−12.3 (3)
N1—Mo1—N2—C14	−16.16 (14)	C12—C13—C14—N2	165.3 (2)
C3—Mo1—N2—C22	−5.07 (19)	N1—C13—C14—C15	168.6 (2)
C2—Mo1—N2—C22	−91.17 (18)	C12—C13—C14—C15	−13.8 (3)
C4—Mo1—N2—C22	85.17 (18)	N2—C14—C15—C16	−2.1 (4)
N1—Mo1—N2—C22	177.87 (18)	C13—C14—C15—C16	176.9 (2)
C13—N1—C5—C6	177.5 (2)	C14—C15—C16—C17	−2.9 (4)
Mo1—N1—C5—C6	−2.1 (3)	C15—C16—C17—C18	−177.2 (2)
C13—N1—C5—C10	−2.0 (3)	C15—C16—C17—C22	2.7 (3)
Mo1—N1—C5—C10	178.40 (14)	C16—C17—C18—C19	178.6 (2)
N1—C5—C6—C7	179.9 (2)	C22—C17—C18—C19	−1.2 (4)
C10—C5—C6—C7	−0.6 (4)	C17—C18—C19—C20	−1.6 (4)
C5—C6—C7—C8	−1.4 (4)	C18—C19—C20—C21	2.0 (4)
C6—C7—C8—C9	1.9 (4)	C19—C20—C21—C22	0.4 (4)
C7—C8—C9—C10	−0.3 (4)	C14—N2—C22—C21	171.6 (2)
C8—C9—C10—C11	177.8 (2)	Mo1—N2—C22—C21	−22.9 (3)
C8—C9—C10—C5	−1.8 (4)	C14—N2—C22—C17	−7.2 (3)
N1—C5—C10—C11	2.1 (3)	Mo1—N2—C22—C17	158.32 (16)
C6—C5—C10—C11	−177.4 (2)	C20—C21—C22—N2	178.1 (2)
N1—C5—C10—C9	−178.3 (2)	C20—C21—C22—C17	−3.1 (3)
C6—C5—C10—C9	2.2 (3)	C16—C17—C22—N2	2.5 (3)
C9—C10—C11—C12	−179.8 (2)	C18—C17—C22—N2	−177.7 (2)

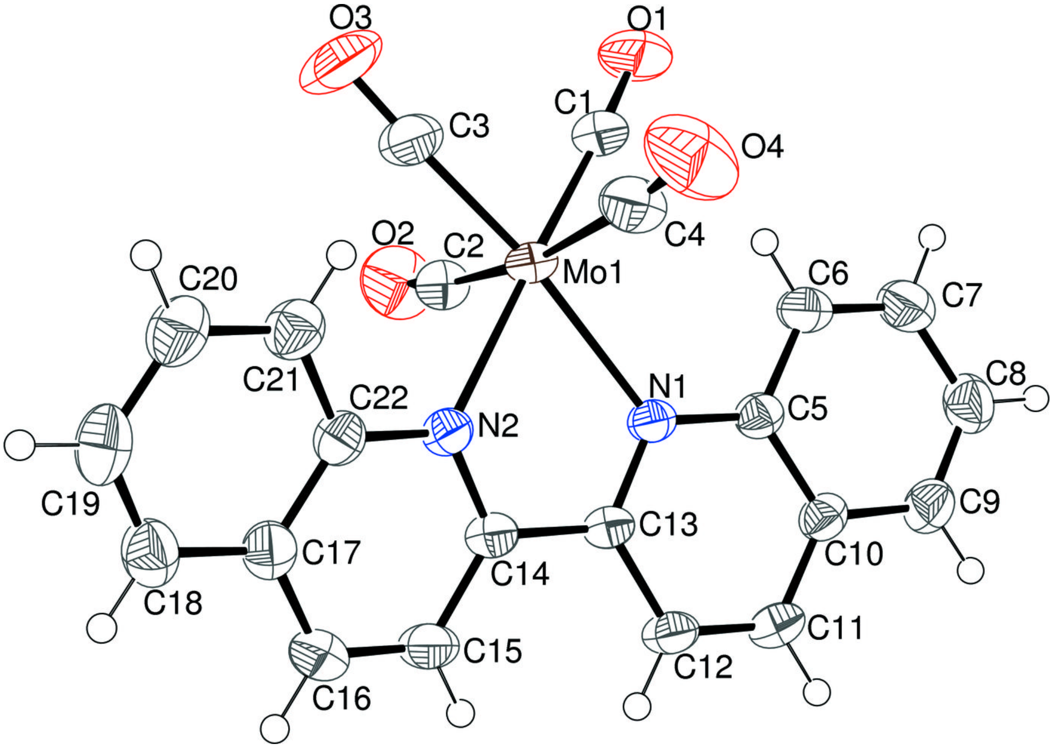
C5—C10—C11—C12	−0.2 (3)	C16—C17—C22—C21	−176.4 (2)
C10—C11—C12—C13	−1.6 (3)	C18—C17—C22—C21	3.5 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···O1[i]	0.93	2.45	3.122 (3)	129

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

Fig. 1


O3
O1
C1
C3
O4
C4
O2
C2
Mo1
C20
C6
C7
C21
C22
N2
N1
C5
C8
C19
C13
C9
C17
C14
C10
C18
C11
C15
C12
C16