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Tricarbonyl-1,10-phenanthroline-(triphenylphosphine)molybdenum(0)

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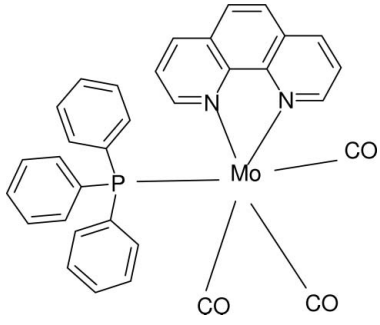
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.029; wR factor = 0.068; data-to-parameter ratio = 21.9.

In the title compound, $[Mo(CO)_3(C_{18}H_{15}P)(C_{12}H_8N_2)]$ or $C_{33}H_{23}MoN_2O_3P$, the carbonyl groups are attached to one face of the MoC_3N_2P octahedron. Slight differences in the Mo—C bond lengths may be interpreted in terms of back-bonding models of electronic structure. In the crystal structure, a short C—H···O interaction (H···O = 2.34 Å) may help to establish the packing.

Related literature

For a related structure, see: Muir *et al.* (2007). For background, see: Cotton & Wilkinson (1966); Howie & McQuillan (1986). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Mo(CO)_3(C_{18}H_{15}P)(C_{12}H_8N_2)]$
M_r = 622.44
Triclinic, $P\overline{1}$
a = 8.5179 (4) Å
b = 9.6376 (4) Å
c = 18.4119 (7) Å
α = 77.780 (1)°
β = 87.979 (1)°
γ = 70.723 (1)°
V = 1393.42 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.57 mm^{-1}
T = 293 (2) K
0.35 × 0.26 × 0.11 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.835, T_{max} = 0.946
12111 measured reflections
7912 independent reflections
6552 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.068
S = 0.95
7912 reflections
361 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mo1—C2	1.933 (2)	Mo1—N2	2.2304 (14)
Mo1—C3	1.9360 (18)	Mo1—N1	2.2589 (14)
Mo1—C1	1.9604 (18)	Mo1—P1	2.5965 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O2^{i}	0.93	2.34	3.058 (3)	134

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

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: LH2494).

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  doi:10.1107/S1600536807043176

supplementary materials

Acta Cryst. (2007). E**63**, m2492 [**doi:10.1107/S1600536807043176**]

Tricarbonyl-1,10-phenanthroline(triphenylphosphine)molybdenum(0)

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

Comment

The title compound, (I), $Mo(CO)_3(C_{18}H_{15}P)(C_{12}H_8N_2)$, is an example of a trisubstituted group-6 metal hexacarbonyl (Howie & McQuillan, 1986). The related tricarbonyl-triphenylphosphine-2,2-bipyridyl-molybdenum(0) is described in the next paper (Muir *et al.*, 2007).

The three remaining carbonyl groups atached to the Mo atom in (I) form one face of the distorted MoC_3N_2P octahedron. Otherwise, all the bond lengths and angles in (I) (Fig. 1) may be regarded as normal (Allen *et al.*, 1987). The diehdral angles for the phenyl rings for the triphenylphosphine molecule are C16—C21/C22—C27 = 83.94 (11)°, C16—C21/C28—C33 = 71.77 (12)°, and C22—C27/C28—C33 = 67.95 (12)°. The N—Mo—N bite angle for the 1,10-phenanthroline (phen) molecule is 73.48 (5)°.

There is a slight distinction between the shorter Mo1—C2 and Mo1—C3 bond lengths *trans* to N atoms and and the longer Mo1—C1 bond, which is *trans* to the P atom. The traditional explanation (Cotton & Wilkinson, 1966) for this phenomenon is that triphenylphosphine is a π-acceptor ligand and completes for metal d electrons with the carbonyl group *trans* to itself, hence the Mo—C bond has less double-bond character than a Mo—C bond *trans* to an atom with no π-acceptor properties such as N, and is therefore longer. The C1—Mo1—P1 bond angle is also closer to linear than the C—Mo—N angles.

In the crystal of (I), a rather short C—H···O interaction arising from a phen C—H grouping (Table 2) may help to establish the packing.

Experimental

Equimolar quantities of $Mo(CO)_6$, triphenylphosphine and 1,10-phenanthroline were refluxed in toluene under an N_2 atmosphere for seven hours. After cooling, air-stable black slabs and blocks of (I) were recovered by vacuum filtration and rinsing with light petroleum ether in 79% yield based on $Mo(CO)_6$. The crystals of (I) smear to a deep orange colour on a glass slide.

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

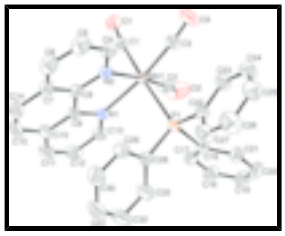


Fig. 1. View of the molecular structure of (I) showing 50% displacement ellipsoids (H atoms omitted for clarity).

Tricarbonyl-1,10-phenanthroline(triphenylphosphine)molybdenum(0)

Crystal data

$[Mo(CO)_3(C_{18}H_{15}P)(C_{12}H_8N_2)]$	$Z = 2$
$M_r = 622.44$	$F_{000} = 632$
Triclinic, $P\overline{1}$	$D_x = 1.484$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.5179$ (4) Å	Cell parameters from 6139 reflections
$b = 9.6376$ (4) Å	$\theta = 2.3$–30.0º
$c = 18.4119$ (7) Å	$\mu = 0.57$ mm^{-1}
$\alpha = 77.780$ (1)º	$T = 293$ (2) K
$\beta = 87.979$ (1)º	Slab, black
$\gamma = 70.723$ (1)º	0.35 × 0.26 × 0.11 mm
$V = 1393.42$ (10) Å^3	

Data collection

Bruker SMART 1000 CCD diffractometer	7912 independent reflections
Radiation source: fine-focus sealed tube	6552 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.015$
$T = 293$(2) K	$\theta_{max} = 30.0$º
ω scans	$\theta_{min} = 2.3$º
Absorption correction: multi-scan (SADABS; Bruker, 1999)	$h = -11 \rightarrow 11$
$T_{min} = 0.835$, $T_{max} = 0.946$	$k = -10 \rightarrow 13$
12111 measured reflections	$l = -25 \rightarrow 25$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.029$	H-atom parameters constrained
$wR(F^2) = 0.068$	$w = 1/[\sigma^2(F_o^2) + (0.036P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.95$	$(\Delta/\sigma)_{max} = 0.001$
7912 reflections	$\Delta\rho_{max} = 0.63$ e Å^{-3}
361 parameters	$\Delta\rho_{min} = -0.30$ 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	0.182959 (18)	−0.028421 (15)	0.334120 (8)	0.02732 (5)
C1	0.1241 (2)	−0.11580 (19)	0.43305 (10)	0.0338 (4)
C2	0.3428 (3)	−0.2261 (2)	0.33681 (12)	0.0483 (5)
C3	0.0106 (3)	−0.0987 (2)	0.30575 (10)	0.0417 (4)
O1	0.0855 (2)	−0.17694 (17)	0.48803 (8)	0.0563 (4)
O2	0.4411 (2)	−0.34549 (18)	0.34323 (14)	0.0988 (7)
O3	−0.0968 (2)	−0.1451 (2)	0.29626 (10)	0.0769 (6)
P1	0.25368 (6)	0.07815 (5)	0.20004 (2)	0.03263 (10)
C4	−0.1324 (2)	0.2719 (2)	0.32076 (11)	0.0409 (4)
H4	−0.1858	0.2202	0.2989	0.049*
C5	−0.2236 (3)	0.4158 (2)	0.33039 (13)	0.0560 (6)
H5	−0.3350	0.4586	0.3146	0.067*
C6	−0.1495 (3)	0.4932 (2)	0.36277 (13)	0.0565 (6)
H6	−0.2102	0.5888	0.3699	0.068*
C7	0.0191 (3)	0.4286 (2)	0.38543 (11)	0.0465 (5)
C8	0.1042 (2)	0.28319 (18)	0.37319 (9)	0.0341 (4)
C9	0.2773 (2)	0.2132 (2)	0.39245 (9)	0.0356 (4)
C10	0.3628 (3)	0.2892 (2)	0.42524 (11)	0.0483 (5)
C11	0.5331 (3)	0.2177 (3)	0.44151 (12)	0.0617 (7)
H11	0.5935	0.2640	0.4632	0.074*
C12	0.6104 (3)	0.0801 (3)	0.42563 (12)	0.0586 (6)
H12	0.7240	0.0324	0.4358	0.070*
C13	0.5168 (2)	0.0108 (2)	0.39374 (11)	0.0458 (5)
H13	0.5709	−0.0837	0.3836	0.055*
C14	0.1082 (4)	0.5014 (3)	0.41967 (13)	0.0616 (6)
H14	0.0528	0.5967	0.4285	0.074*

C15	0.2699 (4)	0.4352 (3)	0.43927 (13)	0.0639 (7)
H15	0.3237	0.4847	0.4625	0.077*
C16	0.4248 (2)	−0.0531 (2)	0.15991 (10)	0.0363 (4)
C17	0.5718 (2)	−0.1331 (2)	0.20295 (11)	0.0457 (5)
H17	0.5813	−0.1162	0.2503	0.055*
C18	0.7025 (3)	−0.2362 (3)	0.17655 (12)	0.0535 (5)
H18	0.8000	−0.2863	0.2055	0.064*
C19	0.6887 (3)	−0.2653 (3)	0.10715 (13)	0.0569 (6)
H19	0.7755	−0.3369	0.0898	0.068*
C20	0.5452 (3)	−0.1874 (3)	0.06374 (12)	0.0569 (6)
H20	0.5363	−0.2054	0.0167	0.068*
C21	0.4150 (3)	−0.0829 (2)	0.08978 (11)	0.0462 (5)
H21	0.3190	−0.0314	0.0599	0.055*
C22	0.0873 (2)	0.1417 (2)	0.12703 (10)	0.0371 (4)
C23	−0.0135 (3)	0.0546 (2)	0.12557 (11)	0.0500 (5)
H23	0.0013	−0.0320	0.1622	0.060*
C24	−0.1362 (3)	0.0959 (3)	0.06987 (12)	0.0617 (6)
H24	−0.2015	0.0356	0.0689	0.074*
C25	−0.1617 (3)	0.2246 (3)	0.01642 (13)	0.0614 (6)
H25	−0.2463	0.2534	−0.0199	0.074*
C26	−0.0620 (3)	0.3109 (3)	0.01664 (13)	0.0671 (7)
H26	−0.0776	0.3974	−0.0201	0.081*
C27	0.0625 (3)	0.2694 (2)	0.07173 (12)	0.0552 (6)
H27	0.1299	0.3283	0.0713	0.066*
C28	0.3183 (3)	0.2461 (2)	0.19056 (10)	0.0397 (4)
C29	0.2019 (3)	0.3773 (2)	0.20503 (11)	0.0495 (5)
H29	0.0940	0.3794	0.2163	0.059*
C30	0.2460 (4)	0.5050 (3)	0.20269 (13)	0.0658 (7)
H30	0.1678	0.5915	0.2129	0.079*
C31	0.4042 (4)	0.5037 (3)	0.18538 (15)	0.0754 (8)
H31	0.4334	0.5891	0.1838	0.091*
C32	0.5193 (4)	0.3760 (3)	0.17038 (17)	0.0797 (8)
H32	0.6264	0.3754	0.1583	0.096*
C33	0.4770 (3)	0.2459 (3)	0.17305 (14)	0.0604 (6)
H33	0.5561	0.1597	0.1630	0.072*
N1	0.35406 (18)	0.07416 (16)	0.37739 (8)	0.0339 (3)
N2	0.02783 (17)	0.20492 (15)	0.34142 (8)	0.0314 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.02579 (7)	0.02575 (7)	0.02999 (7)	−0.00736 (5)	0.00105 (5)	−0.00686 (5)
C1	0.0333 (9)	0.0311 (9)	0.0374 (9)	−0.0099 (7)	−0.0007 (7)	−0.0092 (7)
C2	0.0411 (11)	0.0354 (10)	0.0634 (13)	−0.0091 (8)	0.0159 (9)	−0.0079 (9)
C3	0.0471 (11)	0.0447 (11)	0.0368 (9)	−0.0210 (9)	−0.0025 (8)	−0.0061 (8)
O1	0.0755 (11)	0.0585 (9)	0.0408 (8)	−0.0333 (8)	0.0109 (7)	−0.0066 (7)
O2	0.0744 (13)	0.0388 (10)	0.155 (2)	0.0073 (8)	0.0483 (13)	−0.0085 (11)
O3	0.0799 (13)	0.1001 (14)	0.0739 (12)	−0.0637 (12)	−0.0134 (10)	−0.0101 (10)

P1	0.0331 (2)	0.0361 (2)	0.0309 (2)	−0.01468 (18)	0.00072 (17)	−0.00656 (18)
C4	0.0322 (9)	0.0352 (9)	0.0498 (11)	−0.0053 (7)	0.0011 (8)	−0.0066 (8)
C5	0.0441 (12)	0.0420 (12)	0.0666 (14)	0.0031 (9)	0.0037 (10)	−0.0074 (10)
C6	0.0643 (15)	0.0306 (10)	0.0620 (14)	−0.0002 (9)	0.0122 (11)	−0.0099 (9)
C7	0.0686 (14)	0.0304 (9)	0.0411 (10)	−0.0174 (9)	0.0122 (10)	−0.0089 (8)
C8	0.0445 (10)	0.0279 (8)	0.0313 (8)	−0.0144 (7)	0.0065 (7)	−0.0061 (6)
C9	0.0437 (10)	0.0385 (9)	0.0299 (8)	−0.0218 (8)	0.0019 (7)	−0.0057 (7)
C10	0.0642 (14)	0.0552 (12)	0.0393 (10)	−0.0386 (11)	0.0007 (9)	−0.0088 (9)
C11	0.0700 (17)	0.0840 (18)	0.0513 (13)	−0.0525 (15)	−0.0044 (11)	−0.0127 (12)
C12	0.0388 (12)	0.0898 (18)	0.0516 (13)	−0.0317 (12)	−0.0075 (10)	−0.0062 (12)
C13	0.0334 (10)	0.0623 (13)	0.0408 (10)	−0.0166 (9)	−0.0018 (8)	−0.0073 (9)
C14	0.098 (2)	0.0388 (12)	0.0598 (14)	−0.0322 (12)	0.0120 (13)	−0.0201 (10)
C15	0.104 (2)	0.0557 (14)	0.0555 (14)	−0.0526 (15)	0.0049 (14)	−0.0204 (11)
C16	0.0338 (9)	0.0425 (10)	0.0366 (9)	−0.0184 (8)	0.0059 (7)	−0.0086 (7)
C17	0.0380 (11)	0.0622 (13)	0.0377 (10)	−0.0164 (9)	0.0031 (8)	−0.0127 (9)
C18	0.0363 (11)	0.0648 (14)	0.0537 (13)	−0.0115 (9)	0.0047 (9)	−0.0097 (10)
C19	0.0478 (13)	0.0612 (14)	0.0623 (14)	−0.0143 (10)	0.0175 (11)	−0.0229 (11)
C20	0.0595 (15)	0.0702 (15)	0.0460 (12)	−0.0197 (12)	0.0117 (10)	−0.0274 (11)
C21	0.0482 (12)	0.0553 (12)	0.0371 (10)	−0.0177 (10)	0.0018 (8)	−0.0131 (9)
C22	0.0352 (10)	0.0430 (10)	0.0331 (9)	−0.0142 (8)	−0.0003 (7)	−0.0059 (7)
C23	0.0584 (14)	0.0593 (13)	0.0389 (10)	−0.0318 (11)	−0.0049 (9)	−0.0031 (9)
C24	0.0593 (15)	0.0878 (18)	0.0500 (13)	−0.0416 (14)	−0.0090 (11)	−0.0102 (12)
C25	0.0494 (14)	0.0791 (17)	0.0519 (13)	−0.0184 (12)	−0.0175 (10)	−0.0069 (12)
C26	0.0755 (18)	0.0570 (14)	0.0594 (14)	−0.0207 (12)	−0.0278 (13)	0.0106 (11)
C27	0.0574 (14)	0.0531 (13)	0.0543 (13)	−0.0255 (10)	−0.0145 (11)	0.0049 (10)
C28	0.0496 (11)	0.0428 (10)	0.0330 (9)	−0.0250 (9)	0.0003 (8)	−0.0056 (7)
C29	0.0644 (14)	0.0451 (11)	0.0436 (11)	−0.0267 (10)	0.0081 (10)	−0.0066 (9)
C30	0.101 (2)	0.0432 (12)	0.0599 (14)	−0.0341 (13)	0.0065 (13)	−0.0087 (10)
C31	0.103 (2)	0.0654 (17)	0.0790 (18)	−0.0579 (17)	0.0007 (16)	−0.0122 (14)
C32	0.0749 (19)	0.088 (2)	0.099 (2)	−0.0591 (17)	0.0076 (16)	−0.0172 (17)
C33	0.0570 (15)	0.0611 (14)	0.0736 (16)	−0.0326 (12)	0.0038 (12)	−0.0159 (12)
N1	0.0314 (8)	0.0402 (8)	0.0312 (7)	−0.0145 (6)	0.0001 (6)	−0.0053 (6)
N2	0.0310 (7)	0.0266 (7)	0.0340 (7)	−0.0074 (5)	0.0034 (6)	−0.0049 (5)

Geometric parameters (Å, °)

Mo1—C2	1.933 (2)	C15—H15	0.9300
Mo1—C3	1.9360 (18)	C16—C21	1.392 (2)
Mo1—C1	1.9604 (18)	C16—C17	1.401 (3)
Mo1—N2	2.2304 (14)	C17—C18	1.378 (3)
Mo1—N1	2.2589 (14)	C17—H17	0.9300
Mo1—P1	2.5965 (5)	C18—C19	1.382 (3)
C1—O1	1.154 (2)	C18—H18	0.9300
C2—O2	1.163 (2)	C19—C20	1.380 (3)
C3—O3	1.175 (2)	C19—H19	0.9300
P1—C16	1.8368 (19)	C20—C21	1.380 (3)
P1—C22	1.8449 (18)	C20—H20	0.9300
P1—C28	1.8483 (17)	C21—H21	0.9300
C4—N2	1.332 (2)	C22—C27	1.382 (3)

C4—C5	1.393 (3)	C22—C23	1.389 (2)
C4—H4	0.9300	C23—C24	1.390 (3)
C5—C6	1.355 (3)	C23—H23	0.9300
C5—H5	0.9300	C24—C25	1.369 (3)
C6—C7	1.402 (3)	C24—H24	0.9300
C6—H6	0.9300	C25—C26	1.372 (3)
C7—C8	1.411 (3)	C25—H25	0.9300
C7—C14	1.428 (3)	C26—C27	1.392 (3)
C8—N2	1.369 (2)	C26—H26	0.9300
C8—C9	1.426 (3)	C27—H27	0.9300
C9—N1	1.366 (2)	C28—C33	1.379 (3)
C9—C10	1.415 (2)	C28—C29	1.395 (3)
C10—C11	1.397 (3)	C29—C30	1.393 (3)
C10—C15	1.441 (3)	C29—H29	0.9300
C11—C12	1.360 (3)	C30—C31	1.370 (4)
C11—H11	0.9300	C30—H30	0.9300
C12—C13	1.407 (3)	C31—C32	1.372 (4)
C12—H12	0.9300	C31—H31	0.9300
C13—N1	1.333 (2)	C32—C33	1.405 (3)
C13—H13	0.9300	C32—H32	0.9300
C14—C15	1.339 (3)	C33—H33	0.9300
C14—H14	0.9300		
C2—Mo1—C3	89.07 (9)	C21—C16—C17	117.52 (18)
C2—Mo1—C1	85.59 (8)	C21—C16—P1	123.70 (15)
C3—Mo1—C1	80.56 (7)	C17—C16—P1	118.73 (14)
C2—Mo1—N2	171.18 (7)	C18—C17—C16	121.27 (19)
C3—Mo1—N2	99.32 (7)	C18—C17—H17	119.4
C1—Mo1—N2	93.09 (6)	C16—C17—H17	119.4
C2—Mo1—N1	97.92 (7)	C17—C18—C19	120.1 (2)
C3—Mo1—N1	171.27 (7)	C17—C18—H18	120.0
C1—Mo1—N1	94.70 (6)	C19—C18—H18	120.0
N2—Mo1—N1	73.48 (5)	C20—C19—C18	119.6 (2)
C2—Mo1—P1	93.28 (6)	C20—C19—H19	120.2
C3—Mo1—P1	96.47 (6)	C18—C19—H19	120.2
C1—Mo1—P1	176.82 (5)	C21—C20—C19	120.4 (2)
N2—Mo1—P1	88.48 (4)	C21—C20—H20	119.8
N1—Mo1—P1	88.40 (4)	C19—C20—H20	119.8
O1—C1—Mo1	173.32 (15)	C20—C21—C16	121.15 (19)
O2—C2—Mo1	175.6 (2)	C20—C21—H21	119.4
O3—C3—Mo1	173.06 (17)	C16—C21—H21	119.4
C16—P1—C22	102.43 (8)	C27—C22—C23	118.30 (17)
C16—P1—C28	103.58 (9)	C27—C22—P1	122.83 (14)
C22—P1—C28	101.84 (8)	C23—C22—P1	118.82 (14)
C16—P1—Mo1	114.85 (6)	C22—C23—C24	120.53 (19)
C22—P1—Mo1	117.58 (6)	C22—C23—H23	119.7
C28—P1—Mo1	114.60 (6)	C24—C23—H23	119.7
N2—C4—C5	123.04 (18)	C25—C24—C23	120.5 (2)
N2—C4—H4	118.5	C25—C24—H24	119.8
C5—C4—H4	118.5	C23—C24—H24	119.8

C6—C5—C4	119.8 (2)	C24—C25—C26	119.7 (2)
C6—C5—H5	120.1	C24—C25—H25	120.2
C4—C5—H5	120.1	C26—C25—H25	120.2
C5—C6—C7	119.67 (19)	C25—C26—C27	120.2 (2)
C5—C6—H6	120.2	C25—C26—H26	119.9
C7—C6—H6	120.2	C27—C26—H26	119.9
C6—C7—C8	117.46 (18)	C22—C27—C26	120.8 (2)
C6—C7—C14	123.8 (2)	C22—C27—H27	119.6
C8—C7—C14	118.7 (2)	C26—C27—H27	119.6
N2—C8—C7	122.48 (18)	C33—C28—C29	118.79 (18)
N2—C8—C9	117.20 (15)	C33—C28—P1	123.17 (16)
C7—C8—C9	120.30 (16)	C29—C28—P1	117.98 (15)
N1—C9—C10	122.71 (18)	C30—C29—C28	120.6 (2)
N1—C9—C8	117.67 (14)	C30—C29—H29	119.7
C10—C9—C8	119.62 (18)	C28—C29—H29	119.7
C11—C10—C9	117.5 (2)	C31—C30—C29	120.2 (3)
C11—C10—C15	124.1 (2)	C31—C30—H30	119.9
C9—C10—C15	118.3 (2)	C29—C30—H30	119.9
C12—C11—C10	119.91 (19)	C30—C31—C32	119.8 (2)
C12—C11—H11	120.0	C30—C31—H31	120.1
C10—C11—H11	120.0	C32—C31—H31	120.1
C11—C12—C13	119.3 (2)	C31—C32—C33	120.7 (3)
C11—C12—H12	120.3	C31—C32—H32	119.7
C13—C12—H12	120.3	C33—C32—H32	119.7
N1—C13—C12	123.0 (2)	C28—C33—C32	120.0 (2)
N1—C13—H13	118.5	C28—C33—H33	120.0
C12—C13—H13	118.5	C32—C33—H33	120.0
C15—C14—C7	121.3 (2)	C13—N1—C9	117.47 (16)
C15—C14—H14	119.4	C13—N1—Mo1	127.39 (13)
C7—C14—H14	119.4	C9—N1—Mo1	115.00 (11)
C14—C15—C10	121.7 (2)	C4—N2—C8	117.53 (15)
C14—C15—H15	119.2	C4—N2—Mo1	126.27 (12)
C10—C15—H15	119.2	C8—N2—Mo1	116.14 (11)
C2—Mo1—P1—C16	−3.87 (9)	C16—P1—C22—C23	84.52 (18)
C3—Mo1—P1—C16	−93.31 (9)	C28—P1—C22—C23	−168.51 (17)
N2—Mo1—P1—C16	167.49 (7)	Mo1—P1—C22—C23	−42.39 (19)
N1—Mo1—P1—C16	93.97 (7)	C27—C22—C23—C24	−0.2 (3)
C2—Mo1—P1—C22	116.76 (10)	P1—C22—C23—C24	−177.66 (18)
C3—Mo1—P1—C22	27.33 (9)	C22—C23—C24—C25	−1.3 (4)
N2—Mo1—P1—C22	−71.88 (8)	C23—C24—C25—C26	2.0 (4)
N1—Mo1—P1—C22	−145.40 (8)	C24—C25—C26—C27	−1.2 (4)
C2—Mo1—P1—C28	−123.64 (10)	C23—C22—C27—C26	1.0 (4)
C3—Mo1—P1—C28	146.92 (9)	P1—C22—C27—C26	178.3 (2)
N2—Mo1—P1—C28	47.71 (8)	C25—C26—C27—C22	−0.3 (4)
N1—Mo1—P1—C28	−25.80 (8)	C16—P1—C28—C33	−13.0 (2)
N2—C4—C5—C6	−0.7 (3)	C22—P1—C28—C33	−119.11 (18)
C4—C5—C6—C7	0.8 (3)	Mo1—P1—C28—C33	112.84 (17)
C5—C6—C7—C8	−0.1 (3)	C16—P1—C28—C29	169.78 (15)
C5—C6—C7—C14	179.7 (2)	C22—P1—C28—C29	63.70 (16)

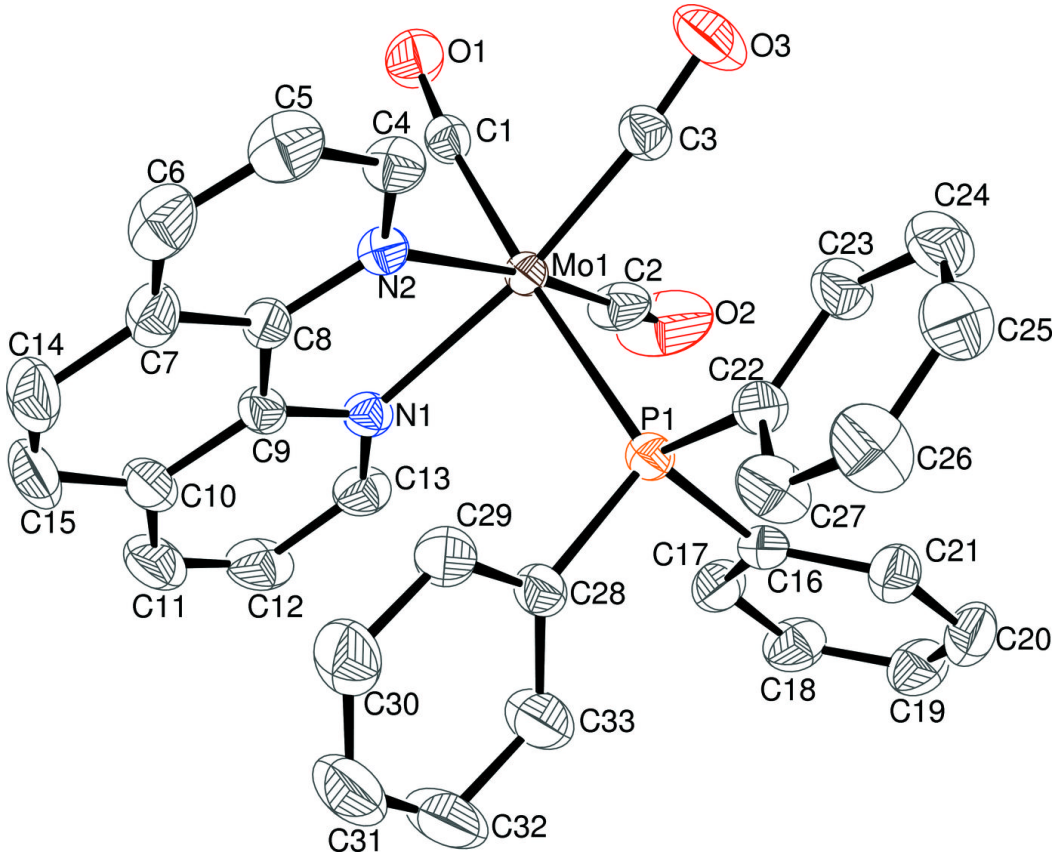
C6—C7—C8—N2	−0.8 (3)	Mo1—P1—C28—C29	−64.35 (16)
C14—C7—C8—N2	179.33 (17)	C33—C28—C29—C30	−0.8 (3)
C6—C7—C8—C9	177.72 (17)	P1—C28—C29—C30	176.55 (17)
C14—C7—C8—C9	−2.1 (3)	C28—C29—C30—C31	0.7 (3)
N2—C8—C9—N1	0.4 (2)	C29—C30—C31—C32	−0.1 (4)
C7—C8—C9—N1	−178.20 (15)	C30—C31—C32—C33	−0.4 (4)
N2—C8—C9—C10	179.80 (15)	C29—C28—C33—C32	0.3 (3)
C7—C8—C9—C10	1.2 (2)	P1—C28—C33—C32	−176.86 (19)
N1—C9—C10—C11	0.8 (3)	C31—C32—C33—C28	0.3 (4)
C8—C9—C10—C11	−178.51 (17)	C12—C13—N1—C9	0.3 (3)
N1—C9—C10—C15	−179.60 (17)	C12—C13—N1—Mo1	−175.18 (14)
C8—C9—C10—C15	1.1 (3)	C10—C9—N1—C13	−1.0 (2)
C9—C10—C11—C12	0.1 (3)	C8—C9—N1—C13	178.33 (15)
C15—C10—C11—C12	−179.4 (2)	C10—C9—N1—Mo1	175.01 (13)
C10—C11—C12—C13	−0.8 (3)	C8—C9—N1—Mo1	−5.63 (19)
C11—C12—C13—N1	0.6 (3)	C2—Mo1—N1—C13	3.59 (16)
C6—C7—C14—C15	−179.0 (2)	C1—Mo1—N1—C13	89.77 (15)
C8—C7—C14—C15	0.8 (3)	N2—Mo1—N1—C13	−178.39 (16)
C7—C14—C15—C10	1.5 (4)	P1—Mo1—N1—C13	−89.50 (14)
C11—C10—C15—C14	177.1 (2)	C2—Mo1—N1—C9	−171.98 (12)
C9—C10—C15—C14	−2.4 (3)	C1—Mo1—N1—C9	−85.79 (12)
C22—P1—C16—C21	1.63 (18)	N2—Mo1—N1—C9	6.04 (11)
C28—P1—C16—C21	−104.00 (16)	P1—Mo1—N1—C9	94.93 (11)
Mo1—P1—C16—C21	130.28 (15)	C5—C4—N2—C8	−0.3 (3)
C22—P1—C16—C17	−175.63 (14)	C5—C4—N2—Mo1	176.72 (15)
C28—P1—C16—C17	78.74 (16)	C7—C8—N2—C4	1.0 (2)
Mo1—P1—C16—C17	−46.98 (16)	C9—C8—N2—C4	−177.56 (15)
C21—C16—C17—C18	0.7 (3)	C7—C8—N2—Mo1	−176.28 (13)
P1—C16—C17—C18	178.11 (16)	C9—C8—N2—Mo1	5.13 (18)
C16—C17—C18—C19	−1.6 (3)	C3—Mo1—N2—C4	−8.00 (15)
C17—C18—C19—C20	1.8 (4)	C1—Mo1—N2—C4	−88.93 (15)
C18—C19—C20—C21	−1.1 (4)	N1—Mo1—N2—C4	177.08 (15)
C19—C20—C21—C16	0.2 (3)	P1—Mo1—N2—C4	88.30 (14)
C17—C16—C21—C20	0.1 (3)	C3—Mo1—N2—C8	169.03 (12)
P1—C16—C21—C20	−177.23 (17)	C1—Mo1—N2—C8	88.10 (12)
C16—P1—C22—C27	−92.80 (19)	N1—Mo1—N2—C8	−5.88 (11)
C28—P1—C22—C27	14.2 (2)	P1—Mo1—N2—C8	−94.66 (11)
Mo1—P1—C22—C27	140.29 (17)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O2^{i}	0.93	2.34	3.058 (3)	134

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

Fig. 1


O1
O3
C5
C4
C1
C3
C6
C24
C23
N2
Mo1
C2
O2
C25
C14
C7
C8
C22
N1
P1
C9
C26
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C10
C27
C15
C29
C17
C21
C16
C28
C11
C12
C20
C18
C30
C33
C19
C31
C32