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Tricarbonyl-2,2-bipyridyl(triphenylphosphine)molybdenum(0)

Kathleen J. Muir, Geoffrey P. McQuillan and William T. A. Harrison*

Department of Chemistry, University of Aberdeen, Meston Walk, Aberdeen AB24 3UE, Scotland
Correspondence e-mail: w.harrison@abdn.ac.uk

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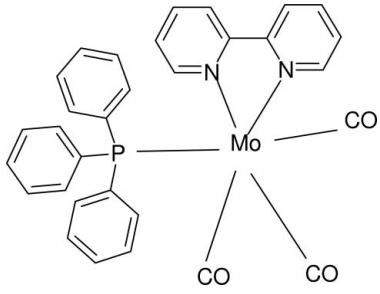
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.032; wR factor = 0.069; data-to-parameter ratio = 22.1.

In the title compound, $[Mo(CO)_3(C_{18}H_{15}P)(C_{10}H_8N_2)]$ or $C_{31}H_{23}MoN_2O_3P$, the carbonyl groups are attached to one face of the MoC_3N_2P octahedron. In the crystal structure, a short C—H···O interaction (H···O = 2.41 Å) may help to establish the packing.

Related literature

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



Experimental

Crystal data

$[Mo(CO)_3(C_{18}H_{15}P)(C_{10}H_8N_2)]$
M_r = 598.42
Triclinic, $P\overline{1}$
a = 8.5206 (4) Å
b = 9.3188 (4) Å
c = 18.4747 (8) Å
α = 91.986 (1)°
β = 102.425 (1)°
γ = 110.762 (1)°
V = 1329.62 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.59 mm^{-1}
T = 293 (2) K
0.33 × 0.30 × 0.14 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.829, T_{max} = 0.922
11901 measured reflections
7569 independent reflections
6055 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.069
S = 0.96
7569 reflections
343 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mo1—C1	1.936 (2)	Mo1—N2	2.2390 (16)
Mo1—C2	1.942 (2)	Mo1—N1	2.2491 (15)
Mo1—C3	1.961 (2)	Mo1—P1	2.6026 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O2^{i}	0.93	2.41	3.336 (4)	171

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: LH2495).

References

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supplementary materials

Acta Cryst. (2007). E**63**, m2493 [**doi:10.1107/S1600536807043164**]

Tricarbonyl-2,2-bipyridyl(triphenylphosphine)molybdenum(0)

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

Comment

The title compound,(I), $Mo(CO)_3(C_{18}H_{15}P)(C_{10}H_8N_2)$, is an example of a trisubstituted group-6 metal hexacarbonyl (Howie & McQuillan, 1986). The related tricarbonyl-triphenylphosphine-1,10-phenanthroline-molybdenum(0), (II), was described in the preceding 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 C14—C19/C20—C25 = 86.93 (11)°, C14—C19/C26—C31 = 77.16 (12)°, and C20—C25/C26—C31 = 63.38 (12)°. The N—Mo—N bite angle for the 2,2-bipyridyl (bipy) molecule is 71.89 (6)° and the twist angle of the N1/C4—C8 and N2/C9—C12 bipy rings is 6.57 (12)°.

There is a slight distinction between the shorter Mo1—C2 and Mo1—C3 bond lengths *trans* to the bipy N atoms and the longer Mo1—C1 bond, which is *trans* to the P atom. A similar pattern was seen in (II) and the possible origin of this effect is discussed in the previous paper (Muir *et al.*, 2007).

In the crystal of (I), a short, near linear, C—H···O interaction arising from a bipy C—H grouping may help to establish the packing.

Experimental

Equimolar quantities of $Mo(CO)_6$, triphenylphosphine and 2,2-bipyridine were refluxed in toluene under an N_2 atmosphere for seven hours. Air-stable black blocks of (I) were recovered by vacuum filtration and rinsing with light petroleum ether in 93% yield based on $Mo(CO)_6$. When the crystals of (I) are smeared on a glass slide, a very deep orange colour is apparent.

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

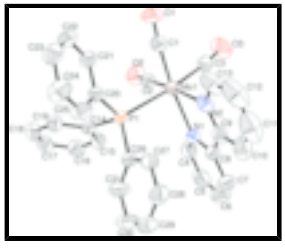


Fig. 1. View of the molecular structure of (I) showing 50% displacement ellipsoids (H atoms omitted for clarity).

Tricarbonyl-2,2-bipyridyl(triphenylphosphine)molybdenum(0)

Crystal data

$[Mo(CO)_3(C_{18}H_{15}P)(C_{10}H_8N_2)]$	$Z = 2$
$M_r = 598.42$	$F_{000} = 608$
Triclinic, $P\overline{1}$	$D_x = 1.495$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.5206$ (4) Å	Cell parameters from 5346 reflections
$b = 9.3188$ (4) Å	$\theta = 2.3$–29.8º
$c = 18.4747$ (8) Å	$\mu = 0.59$ mm^{-1}
$\alpha = 91.986$ (1)º	$T = 293$ (2) K
$\beta = 102.425$ (1)º	Block, black
$\gamma = 110.762$ (1)º	0.33 × 0.30 × 0.14 mm
$V = 1329.62$ (10) Å^3	

Data collection

Bruker SMART 1000 CCD diffractometer	7569 independent reflections
Radiation source: fine-focus sealed tube	6055 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.017$
$T = 293(2)$ K	$\theta_{max} = 30.0$º
ω scans	$\theta_{min} = 2.4$º
Absorption correction: multi-scan (SADABS; Bruker, 1999)	$h = -11 \rightarrow 11$
$T_{min} = 0.829$, $T_{max} = 0.922$	$k = -13 \rightarrow 13$
11901 measured reflections	$l = -25 \rightarrow 20$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.032$	H-atom parameters constrained
$wR(F^2) = 0.069$	$w = 1/[\sigma^2(F_o^2) + (0.0326P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.96$	$(\Delta/\sigma)_{max} = 0.002$
7569 reflections	$\Delta\rho_{max} = 0.39$ e Å^{-3}
343 parameters	$\Delta\rho_{min} = -0.40$ 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	0.54639 (2)	0.201182 (18)	0.340276 (9)	0.03355 (5)
C1	0.7158 (3)	0.1373 (3)	0.30803 (11)	0.0498 (5)
C2	0.4073 (3)	−0.0166 (2)	0.33589 (11)	0.0426 (4)
C3	0.6642 (3)	0.1705 (2)	0.43863 (12)	0.0459 (5)
O1	0.8222 (2)	0.0975 (2)	0.29381 (10)	0.0814 (6)
O2	0.3293 (2)	−0.14685 (17)	0.33732 (9)	0.0657 (4)
O3	0.7344 (2)	0.1385 (2)	0.49254 (9)	0.0794 (5)
P1	0.38541 (6)	0.21208 (5)	0.20506 (3)	0.03306 (10)
C4	0.2377 (3)	0.2269 (3)	0.40571 (12)	0.0553 (6)
H4	0.2012	0.1197	0.4007	0.066*
C5	0.1404 (3)	0.2959 (4)	0.43382 (13)	0.0729 (8)
H5	0.0407	0.2359	0.4475	0.088*
C6	0.1923 (4)	0.4526 (4)	0.44115 (14)	0.0800 (9)
H6	0.1280	0.5009	0.4596	0.096*
C7	0.3398 (4)	0.5385 (3)	0.42112 (13)	0.0671 (7)
H7	0.3761	0.6457	0.4257	0.080*
C8	0.4360 (3)	0.4648 (2)	0.39371 (10)	0.0458 (5)
C9	0.6016 (3)	0.5479 (2)	0.37634 (11)	0.0491 (5)
C10	0.6801 (4)	0.7096 (3)	0.38419 (14)	0.0729 (8)
H10	0.6236	0.7706	0.3987	0.087*
C11	0.8389 (5)	0.7766 (3)	0.37055 (18)	0.0955 (11)
H11	0.8924	0.8837	0.3766	0.115*
C12	0.9193 (4)	0.6879 (4)	0.34825 (18)	0.0913 (11)
H12	1.0284	0.7329	0.3391	0.110*
C13	0.8366 (3)	0.5293 (3)	0.33933 (14)	0.0655 (7)
H13	0.8914	0.4688	0.3229	0.079*
C14	0.1842 (2)	0.0461 (2)	0.16510 (10)	0.0349 (4)
C15	0.0669 (3)	−0.0116 (2)	0.20944 (11)	0.0451 (5)
H15	0.0935	0.0329	0.2585	0.054*
C16	−0.0870 (3)	−0.1329 (3)	0.18131 (13)	0.0541 (5)
H16	−0.1649	−0.1680	0.2111	0.065*
C17	−0.1271 (3)	−0.2033 (3)	0.10943 (13)	0.0559 (6)
H17	−0.2302	−0.2873	0.0911	0.067*

C18	−0.0135 (3)	−0.1486 (3)	0.06497 (12)	0.0542 (5)
H18	−0.0401	−0.1951	0.0163	0.065*
C19	0.1399 (3)	−0.0247 (2)	0.09255 (11)	0.0449 (5)
H19	0.2151	0.0120	0.0618	0.054*
C20	0.5032 (2)	0.2250 (2)	0.13138 (10)	0.0364 (4)
C21	0.5974 (3)	0.1310 (2)	0.12924 (11)	0.0468 (5)
H21	0.6019	0.0647	0.1655	0.056*
C22	0.6851 (3)	0.1345 (3)	0.07362 (12)	0.0561 (6)
H22	0.7469	0.0701	0.0726	0.067*
C23	0.6810 (3)	0.2324 (3)	0.02036 (12)	0.0575 (6)
H23	0.7421	0.2363	−0.0161	0.069*
C24	0.5870 (3)	0.3242 (3)	0.02087 (13)	0.0634 (7)
H24	0.5829	0.3897	−0.0157	0.076*
C25	0.4971 (3)	0.3204 (3)	0.07585 (12)	0.0540 (6)
H25	0.4323	0.3825	0.0753	0.065*
C26	0.3143 (3)	0.3767 (2)	0.19348 (10)	0.0394 (4)
C27	0.4389 (3)	0.5245 (2)	0.20278 (11)	0.0466 (5)
H27	0.5553	0.5378	0.2130	0.056*
C28	0.3925 (4)	0.6529 (3)	0.19702 (13)	0.0599 (6)
H28	0.4774	0.7513	0.2028	0.072*
C29	0.2216 (4)	0.6345 (3)	0.18279 (15)	0.0721 (8)
H29	0.1903	0.7205	0.1789	0.087*
C30	0.0972 (4)	0.4900 (3)	0.17433 (17)	0.0800 (8)
H30	−0.0186	0.4783	0.1650	0.096*
C31	0.1417 (3)	0.3593 (3)	0.17956 (14)	0.0612 (6)
H31	0.0560	0.2614	0.1737	0.073*
N1	0.3831 (2)	0.30873 (19)	0.38523 (8)	0.0396 (3)
N2	0.6812 (2)	0.45842 (19)	0.35315 (9)	0.0450 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.03453 (9)	0.03719 (9)	0.03219 (9)	0.01658 (7)	0.00891 (6)	0.00554 (6)
C1	0.0499 (12)	0.0666 (14)	0.0390 (11)	0.0317 (11)	0.0060 (9)	0.0042 (10)
C2	0.0471 (12)	0.0456 (11)	0.0391 (11)	0.0232 (10)	0.0086 (9)	0.0053 (8)
C3	0.0483 (12)	0.0518 (12)	0.0403 (11)	0.0204 (10)	0.0128 (9)	0.0067 (9)
O1	0.0698 (12)	0.1285 (17)	0.0707 (12)	0.0680 (13)	0.0160 (9)	−0.0038 (11)
O2	0.0753 (12)	0.0396 (9)	0.0763 (12)	0.0147 (8)	0.0170 (9)	0.0097 (8)
O3	0.0828 (13)	0.1166 (16)	0.0461 (10)	0.0509 (12)	0.0045 (9)	0.0241 (10)
P1	0.0364 (3)	0.0349 (2)	0.0325 (2)	0.0181 (2)	0.00932 (19)	0.00561 (18)
C4	0.0414 (12)	0.0751 (16)	0.0453 (12)	0.0173 (11)	0.0118 (9)	−0.0063 (10)
C5	0.0466 (14)	0.130 (3)	0.0466 (14)	0.0390 (16)	0.0114 (10)	−0.0067 (14)
C6	0.089 (2)	0.132 (3)	0.0500 (15)	0.082 (2)	0.0119 (14)	−0.0012 (16)
C7	0.100 (2)	0.0775 (17)	0.0453 (13)	0.0639 (17)	0.0082 (13)	0.0024 (11)
C8	0.0598 (13)	0.0510 (12)	0.0309 (10)	0.0322 (11)	0.0004 (9)	0.0016 (8)
C9	0.0631 (14)	0.0377 (10)	0.0377 (11)	0.0185 (10)	−0.0054 (9)	0.0045 (8)
C10	0.096 (2)	0.0420 (13)	0.0619 (16)	0.0206 (14)	−0.0105 (14)	0.0049 (11)
C11	0.100 (3)	0.0490 (16)	0.091 (2)	−0.0051 (17)	−0.0167 (18)	0.0255 (15)

C12	0.0578 (18)	0.078 (2)	0.102 (2)	−0.0075 (16)	−0.0034 (16)	0.0469 (18)
C13	0.0440 (13)	0.0688 (16)	0.0720 (16)	0.0091 (12)	0.0066 (11)	0.0324 (13)
C14	0.0382 (10)	0.0347 (9)	0.0358 (10)	0.0189 (8)	0.0076 (7)	0.0066 (7)
C15	0.0415 (11)	0.0546 (12)	0.0397 (11)	0.0179 (10)	0.0108 (8)	0.0046 (9)
C16	0.0426 (12)	0.0646 (14)	0.0543 (14)	0.0164 (11)	0.0149 (10)	0.0135 (11)
C17	0.0424 (13)	0.0499 (13)	0.0620 (15)	0.0092 (11)	−0.0005 (10)	0.0030 (11)
C18	0.0549 (14)	0.0523 (13)	0.0463 (13)	0.0172 (11)	0.0007 (10)	−0.0072 (10)
C19	0.0495 (12)	0.0471 (11)	0.0386 (11)	0.0190 (10)	0.0103 (9)	0.0030 (8)
C20	0.0390 (10)	0.0384 (10)	0.0347 (10)	0.0170 (8)	0.0104 (8)	0.0059 (7)
C21	0.0574 (13)	0.0531 (12)	0.0409 (11)	0.0315 (11)	0.0147 (9)	0.0094 (9)
C22	0.0615 (14)	0.0738 (16)	0.0484 (13)	0.0417 (13)	0.0171 (11)	0.0036 (11)
C23	0.0613 (15)	0.0683 (15)	0.0510 (14)	0.0245 (13)	0.0296 (11)	0.0064 (11)
C24	0.094 (2)	0.0621 (14)	0.0551 (14)	0.0378 (14)	0.0419 (14)	0.0275 (11)
C25	0.0751 (16)	0.0580 (13)	0.0508 (13)	0.0417 (13)	0.0285 (11)	0.0224 (10)
C26	0.0496 (12)	0.0407 (10)	0.0345 (10)	0.0261 (9)	0.0079 (8)	0.0037 (8)
C27	0.0559 (13)	0.0407 (11)	0.0455 (12)	0.0236 (10)	0.0066 (9)	0.0081 (9)
C28	0.0847 (19)	0.0409 (12)	0.0539 (14)	0.0300 (12)	0.0051 (12)	0.0056 (10)
C29	0.094 (2)	0.0574 (15)	0.0753 (18)	0.0540 (16)	−0.0008 (14)	−0.0009 (12)
C30	0.0695 (18)	0.079 (2)	0.108 (2)	0.0565 (17)	0.0075 (16)	0.0021 (16)
C31	0.0497 (13)	0.0494 (13)	0.0879 (18)	0.0281 (11)	0.0078 (12)	0.0008 (12)
N1	0.0387 (9)	0.0464 (9)	0.0343 (8)	0.0182 (8)	0.0068 (7)	−0.0012 (7)
N2	0.0391 (9)	0.0441 (9)	0.0445 (10)	0.0105 (8)	0.0028 (7)	0.0137 (7)

Geometric parameters (Å, °)

Mo1—C1	1.936 (2)	C14—C19	1.385 (3)
Mo1—C2	1.942 (2)	C14—C15	1.400 (2)
Mo1—C3	1.961 (2)	C15—C16	1.372 (3)
Mo1—N2	2.2390 (16)	C15—H15	0.9300
Mo1—N1	2.2491 (15)	C16—C17	1.377 (3)
Mo1—P1	2.6026 (5)	C16—H16	0.9300
C1—O1	1.167 (2)	C17—C18	1.376 (3)
C2—O2	1.163 (2)	C17—H17	0.9300
C3—O3	1.153 (2)	C18—C19	1.380 (3)
P1—C14	1.8364 (19)	C18—H18	0.9300
P1—C20	1.8409 (17)	C19—H19	0.9300
P1—C26	1.8413 (18)	C20—C25	1.385 (3)
C4—N1	1.346 (2)	C20—C21	1.387 (3)
C4—C5	1.382 (3)	C21—C22	1.390 (3)
C4—H4	0.9300	C21—H21	0.9300
C5—C6	1.360 (4)	C22—C23	1.368 (3)
C5—H5	0.9300	C22—H22	0.9300
C6—C7	1.365 (4)	C23—C24	1.365 (3)
C6—H6	0.9300	C23—H23	0.9300
C7—C8	1.398 (3)	C24—C25	1.392 (3)
C7—H7	0.9300	C24—H24	0.9300
C8—N1	1.354 (2)	C25—H25	0.9300
C8—C9	1.460 (3)	C26—C31	1.386 (3)
C9—N2	1.356 (3)	C26—C27	1.387 (3)

C9—C10	1.403 (3)	C27—C28	1.387 (3)
C10—C11	1.358 (4)	C27—H27	0.9300
C10—H10	0.9300	C28—C29	1.369 (4)
C11—C12	1.349 (5)	C28—H28	0.9300
C11—H11	0.9300	C29—C30	1.365 (4)
C12—C13	1.379 (4)	C29—H29	0.9300
C12—H12	0.9300	C30—C31	1.398 (3)
C13—N2	1.339 (3)	C30—H30	0.9300
C13—H13	0.9300	C31—H31	0.9300
C1—Mo1—C2	87.51 (9)	C16—C15—C14	120.81 (19)
C1—Mo1—C3	82.55 (8)	C16—C15—H15	119.6
C2—Mo1—C3	83.16 (8)	C14—C15—H15	119.6
C1—Mo1—N2	100.21 (8)	C15—C16—C17	120.59 (19)
C2—Mo1—N2	172.16 (7)	C15—C16—H16	119.7
C3—Mo1—N2	96.37 (7)	C17—C16—H16	119.7
C1—Mo1—N1	171.38 (8)	C18—C17—C16	119.5 (2)
C2—Mo1—N1	100.33 (7)	C18—C17—H17	120.3
C3—Mo1—N1	94.73 (7)	C16—C17—H17	120.3
N2—Mo1—N1	71.89 (6)	C17—C18—C19	120.1 (2)
C1—Mo1—P1	93.91 (6)	C17—C18—H18	119.9
C2—Mo1—P1	91.80 (6)	C19—C18—H18	120.0
C3—Mo1—P1	173.94 (6)	C18—C19—C14	121.35 (19)
N2—Mo1—P1	89.09 (4)	C18—C19—H19	119.3
N1—Mo1—P1	89.47 (4)	C14—C19—H19	119.3
O1—C1—Mo1	175.20 (18)	C25—C20—C21	118.05 (17)
O2—C2—Mo1	176.14 (18)	C25—C20—P1	123.02 (14)
O3—C3—Mo1	172.57 (19)	C21—C20—P1	118.89 (14)
C14—P1—C20	101.81 (8)	C20—C21—C22	120.79 (19)
C14—P1—C26	102.34 (9)	C20—C21—H21	119.6
C20—P1—C26	102.08 (8)	C22—C21—H21	119.6
C14—P1—Mo1	115.77 (6)	C23—C22—C21	120.3 (2)
C20—P1—Mo1	117.49 (6)	C23—C22—H22	119.9
C26—P1—Mo1	115.11 (6)	C21—C22—H22	119.9
N1—C4—C5	122.6 (2)	C24—C23—C22	119.82 (19)
N1—C4—H4	118.7	C24—C23—H23	120.1
C5—C4—H4	118.7	C22—C23—H23	120.1
C6—C5—C4	119.2 (2)	C23—C24—C25	120.4 (2)
C6—C5—H5	120.4	C23—C24—H24	119.8
C4—C5—H5	120.4	C25—C24—H24	119.8
C5—C6—C7	119.4 (2)	C20—C25—C24	120.6 (2)
C5—C6—H6	120.3	C20—C25—H25	119.7
C7—C6—H6	120.3	C24—C25—H25	119.7
C6—C7—C8	119.8 (2)	C31—C26—C27	118.67 (18)
C6—C7—H7	120.1	C31—C26—P1	122.59 (16)
C8—C7—H7	120.1	C27—C26—P1	118.66 (15)
N1—C8—C7	120.9 (2)	C26—C27—C28	121.0 (2)
N1—C8—C9	115.68 (17)	C26—C27—H27	119.5
C7—C8—C9	123.4 (2)	C28—C27—H27	119.5
N2—C9—C10	120.4 (2)	C29—C28—C27	119.9 (2)

N2—C9—C8	115.70 (17)	C29—C28—H28	120.0
C10—C9—C8	123.8 (2)	C27—C28—H28	120.0
C11—C10—C9	119.6 (3)	C30—C29—C28	120.0 (2)
C11—C10—H10	120.2	C30—C29—H29	120.0
C9—C10—H10	120.2	C28—C29—H29	120.0
C12—C11—C10	120.1 (3)	C29—C30—C31	120.8 (2)
C12—C11—H11	119.9	C29—C30—H30	119.6
C10—C11—H11	119.9	C31—C30—H30	119.6
C11—C12—C13	118.7 (3)	C26—C31—C30	119.6 (2)
C11—C12—H12	120.6	C26—C31—H31	120.2
C13—C12—H12	120.6	C30—C31—H31	120.2
N2—C13—C12	123.2 (3)	C4—N1—C8	118.09 (18)
N2—C13—H13	118.4	C4—N1—Mo1	123.74 (14)
C12—C13—H13	118.4	C8—N1—Mo1	118.15 (13)
C19—C14—C15	117.63 (18)	C13—N2—C9	117.9 (2)
C19—C14—P1	123.55 (14)	C13—N2—Mo1	123.65 (17)
C15—C14—P1	118.82 (14)	C9—N2—Mo1	118.43 (13)
C1—Mo1—P1—C14	101.14 (9)	C20—C21—C22—C23	0.6 (4)
C2—Mo1—P1—C14	13.52 (8)	C21—C22—C23—C24	−1.5 (4)
N2—Mo1—P1—C14	−158.69 (8)	C22—C23—C24—C25	0.9 (4)
N1—Mo1—P1—C14	−86.79 (7)	C21—C20—C25—C24	−1.7 (3)
C1—Mo1—P1—C20	−19.34 (10)	P1—C20—C25—C24	−179.15 (19)
C2—Mo1—P1—C20	−106.96 (9)	C23—C24—C25—C20	0.8 (4)
N2—Mo1—P1—C20	80.83 (8)	C14—P1—C26—C31	17.05 (19)
N1—Mo1—P1—C20	152.72 (8)	C20—P1—C26—C31	122.18 (18)
C1—Mo1—P1—C26	−139.63 (10)	Mo1—P1—C26—C31	−109.39 (18)
C2—Mo1—P1—C26	132.75 (9)	C14—P1—C26—C27	−166.29 (15)
N2—Mo1—P1—C26	−39.46 (8)	C20—P1—C26—C27	−61.16 (16)
N1—Mo1—P1—C26	32.43 (8)	Mo1—P1—C26—C27	67.27 (15)
N1—C4—C5—C6	0.1 (4)	C31—C26—C27—C28	−1.1 (3)
C4—C5—C6—C7	−0.4 (4)	P1—C26—C27—C28	−177.93 (16)
C5—C6—C7—C8	−0.3 (4)	C26—C27—C28—C29	0.7 (3)
C6—C7—C8—N1	1.4 (3)	C27—C28—C29—C30	0.0 (4)
C6—C7—C8—C9	−175.2 (2)	C28—C29—C30—C31	−0.4 (4)
N1—C8—C9—N2	0.6 (3)	C27—C26—C31—C30	0.8 (3)
C7—C8—C9—N2	177.40 (18)	P1—C26—C31—C30	177.4 (2)
N1—C8—C9—C10	−177.78 (19)	C29—C30—C31—C26	0.0 (4)
C7—C8—C9—C10	−1.0 (3)	C5—C4—N1—C8	0.9 (3)
N2—C9—C10—C11	−1.9 (3)	C5—C4—N1—Mo1	179.41 (17)
C8—C9—C10—C11	176.4 (2)	C7—C8—N1—C4	−1.7 (3)
C9—C10—C11—C12	1.2 (4)	C9—C8—N1—C4	175.21 (17)
C10—C11—C12—C13	0.4 (5)	C7—C8—N1—Mo1	179.76 (15)
C11—C12—C13—N2	−1.3 (4)	C9—C8—N1—Mo1	−3.4 (2)
C20—P1—C14—C19	−8.21 (18)	C2—Mo1—N1—C4	3.97 (17)
C26—P1—C14—C19	97.13 (17)	C3—Mo1—N1—C4	−79.92 (17)
Mo1—P1—C14—C19	−136.86 (14)	N2—Mo1—N1—C4	−175.09 (17)
C20—P1—C14—C15	172.80 (15)	P1—Mo1—N1—C4	95.70 (16)
C26—P1—C14—C15	−81.86 (16)	C2—Mo1—N1—C8	−177.54 (14)
Mo1—P1—C14—C15	44.15 (16)	C3—Mo1—N1—C8	98.57 (15)

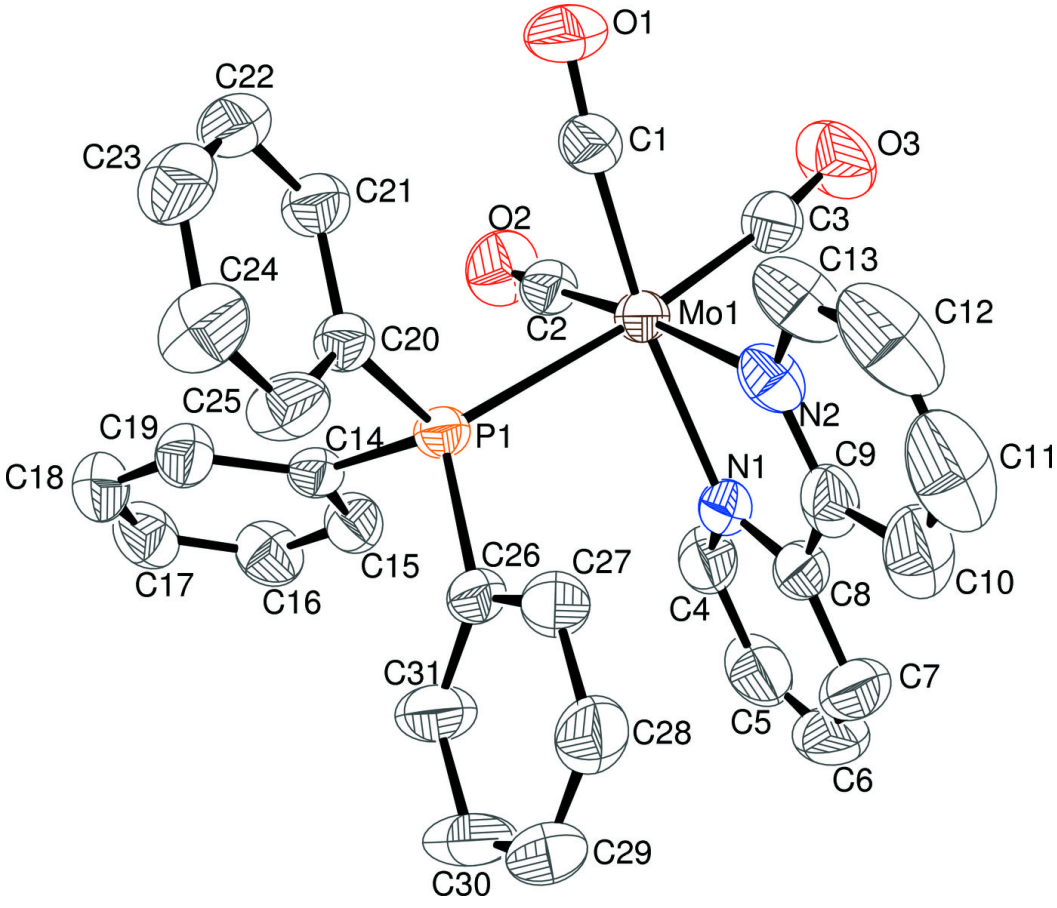
C19—C14—C15—C16	−0.7 (3)	N2—Mo1—N1—C8	3.41 (13)
P1—C14—C15—C16	178.40 (16)	P1—Mo1—N1—C8	−85.81 (13)
C14—C15—C16—C17	1.8 (3)	C12—C13—N2—C9	0.6 (3)
C15—C16—C17—C18	−1.7 (3)	C12—C13—N2—Mo1	−179.26 (19)
C16—C17—C18—C19	0.4 (3)	C10—C9—N2—C13	1.0 (3)
C17—C18—C19—C14	0.7 (3)	C8—C9—N2—C13	−177.45 (18)
C15—C14—C19—C18	−0.6 (3)	C10—C9—N2—Mo1	−179.10 (16)
P1—C14—C19—C18	−179.59 (16)	C8—C9—N2—Mo1	2.4 (2)
C14—P1—C20—C25	94.16 (19)	C1—Mo1—N2—C13	0.37 (18)
C26—P1—C20—C25	−11.4 (2)	C3—Mo1—N2—C13	83.91 (17)
Mo1—P1—C20—C25	−138.29 (17)	N1—Mo1—N2—C13	176.82 (18)
C14—P1—C20—C21	−83.26 (17)	P1—Mo1—N2—C13	−93.44 (16)
C26—P1—C20—C21	171.20 (17)	C1—Mo1—N2—C9	−179.51 (14)
Mo1—P1—C20—C21	44.29 (18)	C3—Mo1—N2—C9	−95.97 (15)
C25—C20—C21—C22	1.0 (3)	N1—Mo1—N2—C9	−3.06 (13)
P1—C20—C21—C22	178.58 (17)	P1—Mo1—N2—C9	86.68 (14)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···O2^{i}	0.93	2.41	3.336 (4)	171

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

Fig. 1


O1
C22
C1
O3
C23
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C3
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C13
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Mo1
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C25
C19
C14
P1
C9
C11
C18
N1
C15
C26
C27
C17
C16
C4
C8
C10
C31
C7
C28
C5
C6
C29
C30