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cis-Bis(benzylmethylphenylphosphine-κ*P*)-tetracarbonylmolybdenum(0)

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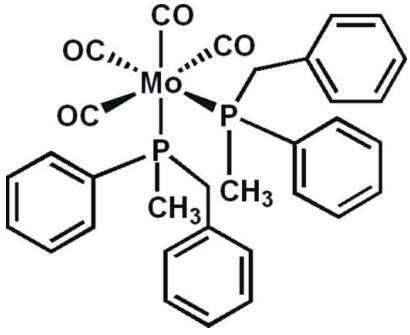
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.007 Å; disorder in main residue; R factor = 0.046; wR factor = 0.141; data-to-parameter ratio = 16.0.

In the title compound, $[Mo(CO)_4(C_{14}H_{15}P)_2]$, the molybdenum center has a slightly distorted *cis*-MoP_2C_4 octahedral geometry. One of the phosphine ligands is disordered over two orientations in a 0.686 (3):0.314 (3) ratio. The packing may be stabilized by weak C—H···O and C—H···π interactions.

Related literature

For related literature, see: Smith & Baird (1982).



Experimental

Crystal data

$[Mo(CO)_4(C_{14}H_{15}P)_2]$
M_r = 636.44
Triclinic, $P\overline{1}$
a = 9.9318 (4) Å
b = 10.6434 (5) Å
c = 14.9527 (7) Å
α = 88.643 (2)°
β = 77.279 (2)°
γ = 80.879 (2)°
V = 1522.23 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.57 mm^{-1}
T = 173 (2) K
0.20 × 0.18 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.895, T_{max} = 0.919
19662 measured reflections
6531 independent reflections
4924 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.141
S = 1.04
6531 reflections
408 parameters
4 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.97 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mo1—C1	2.021 (4)	Mo1—C4	1.973 (4)
Mo1—C2	2.000 (5)	Mo1—P2	2.5297 (10)
Mo1—C3	2.032 (5)	Mo1—P1	2.536 (3)

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

Cg is the centroid of the C20*A*–C25*A* aromatic ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12*A*···O4^{i}	0.96	2.53	3.424 (6)	154
C11—H11···*Cg*^{ii}	0.93	3.14	3.51	105

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2548).

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supplementary materials

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cis-Bis(benzylmethylphenylphosphine-*κP*)tetracarbonylmolybdenum(0)

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Comment

Tertiary phosphines, PR_3, have been used to modify both the solubility and stability aspects of metal carbonyl compounds (Smith & Baird, 1982). Herein, we report the synthesis and structure of the title compound, (I). It is observed that the Mo atom sits at the center of a distorted octahedron and the two phosphine ligands are *cis* to each other (Fig. 1, Table 1).

The Mo—P bond distances are almost the same with corresponding Mo—C$_{trans}$ bond distances of 1.973 (4) and 2.000 (5) Å respectively. The other two Mo—C bond distances are 2.021 (4) and 2.032 (5) Å. The relative shortening of the Mo—C$_{trans}$ bond can be attributed to the greater back donation from metal center to CO than phosphine, the former being a better π-acceptor.

In the packing of (I), a weak C—H···O bond (Fig. 2) may help to establish the packing, as does a C—H···π interaction between two phenyl rings of adjacent molecules with H···π = 2.85 Å.

Experimental

To a stirred solution of $Mo(CO)_6$ (0.18 g, 0.70 mmol) in toluene (20 ml) at room temperature was added dropwise, benzyl(methyl)(phenyl)phosphine (0.29 g, 1.40 mmol) in toluene (5 ml) over 10 minutes. After complete addition, the reaction mixture was refluxed for 5 h and the resultant blackish brown solution was pumped off completely to get a brown residue. This was extracted with hot hexane (5 × 5 ml) and the light brown hexane extract was concentrated to half of its volume and cooled in a deep freezer for two days to isolate pale yellow blocks of (I).

Refinement

One of the phosphine ligands is disordered over two orientations in a 0.686 (3):0.314 (3) ratio. The H atoms were geometrically placed (C—H = 0.93–0.97 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

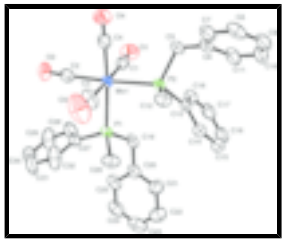


Figure 1. View of the molecular structure of (I) with displacement ellipsoids drawn with 50% probability for the non-H atoms. The minor disorder component of the phosphine ligand is not shown.
Figure 2. Packing diagram of (I) projected down the *b* axis with C—H···O interactions shown as dashed lines.

cis-Bis(benzylmethylphenylphosphine-kP)tetracarbonylmolybdenum(0)

Crystal data

$[Mo(CO)_4(C_{14}H_{15}P)_2]$	$Z = 2$
$M_r = 636.44$	$F_{000} = 652$
Triclinic, $P\overline{1}$	$D_x = 1.389$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.9318$ (4) Å	Cell parameters from 6018 reflections
$b = 10.6434$ (5) Å	$\theta = 2.4$–$25.0°$
$c = 14.9527$ (7) Å	$\mu = 0.57$ mm^{-1}
$\alpha = 88.643$ (2)°	$T = 173$ (2) K
$\beta = 77.279$ (2)°	Block, pale yellow
$\gamma = 80.879$ (2)°	0.20 × 0.18 × 0.15 mm
$V = 1522.23$ (12) Å^3	

Data collection

Bruker APEX CCD diffractometer	6531 independent reflections
Radiation source: fine-focus sealed tube	4924 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.045$
$T = 298$(2) K	$\theta_{max} = 28.3°$
φ and ω scans	$\theta_{min} = 1.4°$
Absorption correction: multi-scan (SADABS; Bruker, 1999)	$h = -12 \rightarrow 13$
$T_{min} = 0.895$, $T_{max} = 0.919$	$k = -14 \rightarrow 14$
19662 measured reflections	$l = -16 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.046$	H-atom parameters constrained
$wR(F^2) = 0.141$	$w = 1/[\sigma^2(F_o^2) + (0.0864P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
6531 reflections	$\Delta\rho_{max} = 0.97$ e Å^{-3}
408 parameters	$\Delta\rho_{min} = -0.63$ e Å^{-3}
4 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	−0.1063 (4)	0.6468 (4)	0.8145 (3)	0.0384 (9)	
C2	−0.2223 (5)	0.8344 (4)	0.7017 (3)	0.0471 (10)	
C3	0.0285 (6)	0.8001 (4)	0.5665 (3)	0.0615 (13)	
C4	−0.1078 (5)	0.5936 (4)	0.6319 (3)	0.0481 (10)	
C5	0.1710 (4)	0.4053 (3)	0.6718 (3)	0.0441 (10)	
H5A	0.1343	0.3826	0.7347	0.053*	
H5B	0.1014	0.3962	0.6370	0.053*	
C6	0.3005 (4)	0.3117 (3)	0.6341 (3)	0.0405 (9)	
C7	0.3255 (5)	0.2625 (4)	0.5463 (3)	0.0485 (11)	
H7	0.2610	0.2874	0.5102	0.058*	
C8	0.4450 (5)	0.1767 (4)	0.5110 (3)	0.0533 (12)	
H8	0.4600	0.1448	0.4517	0.064*	
C9	0.5410 (5)	0.1387 (4)	0.5635 (3)	0.0542 (12)	
H9	0.6207	0.0805	0.5403	0.065*	
C10	0.5187 (5)	0.1875 (4)	0.6506 (4)	0.0587 (12)	
H10	0.5840	0.1628	0.6862	0.070*	
C11	0.3991 (5)	0.2735 (4)	0.6859 (3)	0.0516 (11)	
H11	0.3850	0.3058	0.7450	0.062*	
C12	0.3132 (4)	0.5864 (4)	0.5599 (3)	0.0440 (10)	
H12A	0.2636	0.5860	0.5116	0.066*	
H12B	0.3875	0.5152	0.5519	0.066*	
H12C	0.3515	0.6640	0.5580	0.066*	
C13	0.3038 (4)	0.5773 (3)	0.7537 (3)	0.0343 (8)	
C14	0.4370 (4)	0.6103 (3)	0.7307 (3)	0.0428 (9)	
H14	0.4745	0.6302	0.6704	0.051*	
C15	0.5145 (5)	0.6139 (4)	0.7972 (3)	0.0544 (12)	
H15	0.6039	0.6351	0.7813	0.065*	
C16	0.4592 (5)	0.5861 (4)	0.8861 (3)	0.0576 (12)	
H16	0.5112	0.5895	0.9305	0.069*	
C17	0.3276 (5)	0.5532 (4)	0.9109 (3)	0.0524 (11)	
H17	0.2909	0.5339	0.9715	0.063*	
C18	0.2503 (4)	0.5491 (3)	0.8445 (3)	0.0428 (9)	
H18	0.1612	0.5272	0.8611	0.051*	

C27	−0.0769 (4)	1.0486 (3)	0.7858 (3)	0.0443 (10)	
C28	−0.1767 (5)	1.0600 (5)	0.8649 (4)	0.0739 (16)	
H28	−0.1819	0.9912	0.9044	0.089*	
C29	−0.2703 (5)	1.1702 (5)	0.8885 (4)	0.0738 (15)	
H29	−0.3359	1.1756	0.9438	0.089*	
C30	−0.2674 (5)	1.2693 (4)	0.8323 (4)	0.0666 (14)	
H30	−0.3307	1.3438	0.8483	0.080*	
C31	−0.1726 (6)	1.2612 (6)	0.7523 (5)	0.095 (2)	
H31	−0.1723	1.3295	0.7124	0.114*	
C32	−0.0762 (6)	1.1530 (6)	0.7289 (4)	0.0801 (17)	
H32	−0.0097	1.1500	0.6741	0.096*	
Mo1	−0.03646 (3)	0.72449 (3)	0.69173 (2)	0.03031 (13)	
O3	0.0614 (5)	0.8413 (4)	0.4955 (3)	0.1113 (16)	
O1	−0.1525 (4)	0.5994 (3)	0.8822 (2)	0.0615 (9)	
O4	−0.1519 (4)	0.5186 (3)	0.5977 (3)	0.0780 (11)	
O2	−0.3300 (4)	0.8933 (3)	0.7044 (3)	0.0732 (10)	
P1A	0.0361 (6)	0.8890 (5)	0.7858 (4)	0.0307 (11)	0.314 (3)
C19A	0.2040 (12)	0.9480 (12)	0.7392 (8)	0.046 (3)	0.314 (3)
H19A	0.2753	0.8761	0.7157	0.056*	0.314 (3)
H19B	0.1929	1.0038	0.6882	0.056*	0.314 (3)
C20A	0.2545 (10)	1.0207 (8)	0.8106 (6)	0.041 (3)	0.314 (3)
C21A	0.3667 (11)	0.9626 (10)	0.8461 (10)	0.067 (8)	0.314 (3)
H21A	0.4119	0.8818	0.8257	0.080*	0.314 (3)
C22A	0.4113 (12)	1.0254 (16)	0.9120 (11)	0.065 (7)	0.314 (3)
H22A	0.4864	0.9866	0.9357	0.079*	0.314 (3)
C23A	0.3438 (15)	1.1463 (16)	0.9424 (9)	0.041 (5)	0.314 (3)
H23A	0.3737	1.1884	0.9865	0.049*	0.314 (3)
C24A	0.2316 (14)	1.2044 (10)	0.9069 (9)	0.052 (6)	0.314 (3)
H24A	0.1864	1.2853	0.9272	0.063*	0.314 (3)
C25A	0.1870 (9)	1.1416 (8)	0.8410 (7)	0.048 (3)	0.314 (3)
H25A	0.1119	1.1805	0.8173	0.058*	0.314 (3)
C26A	0.0523 (13)	0.8431 (11)	0.9012 (7)	0.032 (3)	0.314 (3)
H26A	−0.0300	0.8103	0.9323	0.049*	0.314 (3)
H26B	0.0628	0.9160	0.9341	0.049*	0.314 (3)
H26C	0.1327	0.7786	0.8982	0.049*	0.314 (3)
P1	0.0560 (3)	0.9086 (2)	0.74968 (17)	0.0304 (5)	0.686 (3)
C19	0.1234 (6)	0.8853 (5)	0.8552 (4)	0.0364 (13)	0.686 (3)
H19C	0.0456	0.8766	0.9059	0.044*	0.686 (3)
H19D	0.1875	0.8056	0.8492	0.044*	0.686 (3)
C20	0.1982 (4)	0.9895 (3)	0.8801 (3)	0.0381 (13)	0.686 (3)
C21	0.3430 (5)	0.9666 (5)	0.8660 (5)	0.052 (3)	0.686 (3)
H21	0.3926	0.8888	0.8419	0.063*	0.686 (3)
C22	0.4139 (5)	1.0601 (8)	0.8880 (6)	0.061 (3)	0.686 (3)
H22	0.5108	1.0448	0.8786	0.074*	0.686 (3)
C23	0.3399 (7)	1.1764 (7)	0.9241 (6)	0.066 (4)	0.686 (3)
H23	0.3873	1.2389	0.9389	0.080*	0.686 (3)
C24	0.1950 (7)	1.1992 (4)	0.9382 (4)	0.054 (3)	0.686 (3)
H24	0.1455	1.2770	0.9623	0.065*	0.686 (3)
C25	0.1242 (4)	1.1058 (4)	0.9162 (3)	0.0444 (15)	0.686 (3)

H25	0.0272	1.1211	0.9256	0.053*	0.686 (3)
C26	0.2017 (6)	0.9632 (6)	0.6689 (4)	0.0465 (16)	0.686 (3)
H26D	0.2737	0.8920	0.6484	0.070*	0.686 (3)
H26E	0.2386	1.0245	0.6988	0.070*	0.686 (3)
H26F	0.1693	1.0017	0.6172	0.070*	0.686 (3)
P2	0.19348 (10)	0.57500 (8)	0.67027 (7)	0.0320 (2)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.036 (2)	0.041 (2)	0.039 (2)	−0.0035 (16)	−0.0104 (17)	−0.0065 (17)
C2	0.057 (3)	0.034 (2)	0.056 (3)	−0.0087 (19)	−0.022 (2)	0.0012 (18)
C3	0.083 (4)	0.045 (3)	0.051 (3)	0.002 (2)	−0.011 (2)	0.010 (2)
C4	0.065 (3)	0.038 (2)	0.049 (3)	−0.0033 (19)	−0.033 (2)	0.0013 (18)
C5	0.046 (2)	0.0250 (18)	0.063 (3)	−0.0071 (16)	−0.014 (2)	0.0022 (17)
C6	0.048 (2)	0.0238 (17)	0.051 (3)	−0.0062 (16)	−0.0122 (19)	0.0006 (16)
C7	0.071 (3)	0.030 (2)	0.050 (3)	−0.0055 (19)	−0.027 (2)	−0.0006 (18)
C8	0.079 (3)	0.029 (2)	0.047 (3)	−0.009 (2)	−0.001 (2)	−0.0077 (18)
C9	0.055 (3)	0.028 (2)	0.073 (3)	0.0008 (18)	−0.005 (2)	−0.003 (2)
C10	0.062 (3)	0.039 (2)	0.077 (4)	0.007 (2)	−0.028 (3)	−0.004 (2)
C11	0.070 (3)	0.034 (2)	0.049 (3)	0.004 (2)	−0.019 (2)	−0.0047 (18)
C12	0.049 (2)	0.041 (2)	0.039 (2)	−0.0111 (18)	−0.0008 (18)	−0.0059 (17)
C13	0.038 (2)	0.0193 (16)	0.045 (2)	0.0006 (14)	−0.0123 (16)	−0.0009 (14)
C14	0.042 (2)	0.034 (2)	0.055 (3)	−0.0063 (16)	−0.0152 (19)	0.0045 (17)
C15	0.048 (2)	0.044 (2)	0.080 (4)	−0.0100 (19)	−0.032 (2)	0.009 (2)
C16	0.074 (3)	0.037 (2)	0.072 (4)	−0.001 (2)	−0.043 (3)	0.005 (2)
C17	0.074 (3)	0.038 (2)	0.045 (3)	0.000 (2)	−0.022 (2)	0.0053 (18)
C18	0.045 (2)	0.035 (2)	0.046 (3)	−0.0019 (17)	−0.0097 (19)	−0.0004 (17)
C27	0.043 (2)	0.0289 (19)	0.067 (3)	−0.0020 (16)	−0.026 (2)	−0.0148 (18)
C28	0.044 (3)	0.055 (3)	0.109 (4)	0.005 (2)	0.003 (3)	0.034 (3)
C29	0.052 (3)	0.082 (4)	0.072 (4)	0.021 (3)	−0.003 (3)	0.001 (3)
C30	0.054 (3)	0.036 (2)	0.110 (5)	0.009 (2)	−0.029 (3)	−0.010 (3)
C31	0.080 (4)	0.074 (4)	0.124 (5)	0.012 (3)	−0.030 (4)	0.054 (4)
C32	0.081 (4)	0.095 (4)	0.051 (3)	0.026 (3)	−0.017 (3)	0.015 (3)
Mo1	0.03718 (19)	0.02467 (17)	0.0308 (2)	−0.00361 (12)	−0.01183 (13)	−0.00042 (12)
O3	0.149 (4)	0.109 (3)	0.059 (3)	0.000 (3)	−0.007 (3)	0.045 (2)
O1	0.074 (2)	0.073 (2)	0.0398 (18)	−0.0291 (18)	−0.0062 (16)	0.0109 (16)
O4	0.113 (3)	0.0510 (19)	0.095 (3)	−0.0215 (19)	−0.071 (2)	−0.0036 (18)
O2	0.055 (2)	0.053 (2)	0.112 (3)	0.0126 (16)	−0.035 (2)	0.0015 (19)
P1A	0.033 (2)	0.029 (2)	0.030 (3)	−0.0027 (15)	−0.009 (2)	−0.002 (2)
C19A	0.040 (7)	0.044 (7)	0.048 (9)	−0.007 (6)	0.006 (6)	0.001 (6)
C20A	0.042 (7)	0.036 (6)	0.040 (8)	−0.015 (5)	0.008 (6)	−0.008 (5)
C21A	0.052 (11)	0.057 (15)	0.092 (17)	0.000 (10)	−0.024 (12)	0.006 (11)
C22A	0.042 (10)	0.082 (16)	0.073 (16)	−0.002 (9)	−0.020 (9)	0.009 (13)
C23A	0.043 (9)	0.060 (11)	0.031 (9)	−0.029 (8)	−0.015 (7)	−0.010 (9)
C24A	0.051 (10)	0.044 (9)	0.061 (14)	−0.013 (7)	−0.004 (10)	−0.008 (8)
C25A	0.052 (8)	0.035 (7)	0.057 (9)	−0.009 (6)	−0.007 (7)	0.008 (6)
C26A	0.054 (7)	0.033 (6)	0.015 (6)	−0.012 (5)	−0.013 (5)	−0.003 (4)

P1	0.0377 (10)	0.0243 (9)	0.0286 (14)	−0.0061 (7)	−0.0048 (10)	−0.0010 (9)
C19	0.048 (3)	0.026 (3)	0.034 (3)	0.001 (2)	−0.010 (3)	0.003 (2)
C20	0.053 (3)	0.035 (3)	0.027 (3)	−0.005 (2)	−0.012 (3)	0.000 (2)
C21	0.050 (5)	0.048 (6)	0.064 (5)	−0.007 (4)	−0.020 (5)	−0.019 (4)
C22	0.066 (6)	0.064 (6)	0.064 (6)	−0.019 (4)	−0.028 (5)	−0.008 (5)
C23	0.102 (9)	0.049 (5)	0.057 (6)	−0.032 (5)	−0.022 (6)	0.003 (5)
C24	0.087 (7)	0.036 (4)	0.042 (5)	−0.008 (4)	−0.018 (5)	−0.007 (3)
C25	0.065 (4)	0.034 (3)	0.032 (3)	−0.002 (3)	−0.010 (3)	−0.002 (2)
C26	0.056 (4)	0.047 (3)	0.036 (4)	−0.022 (3)	0.003 (3)	−0.005 (3)
P2	0.0352 (5)	0.0237 (4)	0.0367 (6)	−0.0047 (4)	−0.0066 (4)	−0.0024 (4)

Geometric parameters (Å, °)

Mo1—C1	2.021 (4)	C28—H28	0.9300
Mo1—C2	2.000 (5)	C29—C30	1.333 (7)
Mo1—C3	2.032 (5)	C29—H29	0.9300
Mo1—C4	1.973 (4)	C30—C31	1.343 (8)
Mo1—P2	2.5297 (10)	C30—H30	0.9300
Mo1—P1	2.536 (3)	C31—C32	1.373 (8)
Mo1—P1A	2.555 (6)	C31—H31	0.9300
C1—O1	1.155 (5)	C32—H32	0.9300
C2—O2	1.144 (5)	P1A—C26A	1.816 (12)
C3—O3	1.139 (6)	P1A—C19A	1.860 (11)
C4—O4	1.149 (5)	C19A—C20A	1.546 (9)
C5—C6	1.505 (5)	C19A—H19A	0.9700
C5—P2	1.853 (3)	C19A—H19B	0.9700
C5—H5A	0.9700	C20A—C21A	1.3900
C5—H5B	0.9700	C20A—C25A	1.3900
C6—C7	1.380 (6)	C21A—C22A	1.3900
C6—C11	1.384 (6)	C21A—H21A	0.9300
C7—C8	1.387 (6)	C22A—C23A	1.3900
C7—H7	0.9300	C22A—H22A	0.9300
C8—C9	1.372 (7)	C23A—C24A	1.3900
C8—H8	0.9300	C23A—H23A	0.9300
C9—C10	1.371 (6)	C24A—C25A	1.3900
C9—H9	0.9300	C24A—H24A	0.9300
C10—C11	1.389 (6)	C25A—H25A	0.9300
C10—H10	0.9300	C26A—H26A	0.9600
C11—H11	0.9300	C26A—H26B	0.9600
C12—P2	1.823 (4)	C26A—H26C	0.9600
C12—H12A	0.9600	P1—C26	1.832 (6)
C12—H12B	0.9600	P1—C19	1.842 (6)
C12—H12C	0.9600	C19—C20	1.524 (6)
C13—C18	1.389 (5)	C19—H19C	0.9700
C13—C14	1.391 (5)	C19—H19D	0.9700
C13—P2	1.835 (4)	C20—C21	1.3900
C14—C15	1.389 (6)	C20—C25	1.3900
C14—H14	0.9300	C21—C22	1.3900
C15—C16	1.366 (6)	C21—H21	0.9300

C15—H15	0.9300	C22—C23	1.3900
C16—C17	1.377 (6)	C22—H22	0.9300
C16—H16	0.9300	C23—C24	1.3900
C17—C18	1.387 (6)	C23—H23	0.9300
C17—H17	0.9300	C24—C25	1.3900
C18—H18	0.9300	C24—H24	0.9300
C27—C28	1.361 (6)	C25—H25	0.9300
C27—C32	1.383 (7)	C26—H26D	0.9600
C27—P1	1.832 (4)	C26—H26E	0.9600
C27—P1A	1.882 (6)	C26—H26F	0.9600
C28—C29	1.376 (7)		
O1—C1—Mo1	175.6 (3)	C3—Mo1—P1	84.01 (15)
O2—C2—Mo1	176.6 (4)	P2—Mo1—P1	94.45 (6)
O3—C3—Mo1	177.8 (5)	C4—Mo1—P1A	173.46 (17)
O4—C4—Mo1	178.7 (4)	C2—Mo1—P1A	89.50 (17)
C6—C5—P2	116.0 (3)	C1—Mo1—P1A	84.76 (16)
C6—C5—H5A	108.3	C3—Mo1—P1A	97.06 (19)
P2—C5—H5A	108.3	P2—Mo1—P1A	94.86 (12)
C6—C5—H5B	108.3	P1—Mo1—P1A	13.06 (9)
P2—C5—H5B	108.3	C26A—P1A—C19A	102.2 (6)
H5A—C5—H5B	107.4	C26A—P1A—C27	111.3 (5)
C7—C6—C11	117.9 (4)	C19A—P1A—C27	95.3 (5)
C7—C6—C5	121.0 (4)	C26A—P1A—Mo1	116.3 (4)
C11—C6—C5	121.1 (4)	C19A—P1A—Mo1	118.3 (4)
C6—C7—C8	121.3 (4)	C27—P1A—Mo1	111.4 (3)
C6—C7—H7	119.4	C20A—C19A—P1A	113.6 (8)
C8—C7—H7	119.4	C20A—C19A—H19A	108.8
C9—C8—C7	120.1 (4)	P1A—C19A—H19A	108.8
C9—C8—H8	119.9	C20A—C19A—H19B	108.8
C7—C8—H8	119.9	P1A—C19A—H19B	108.8
C10—C9—C8	119.5 (4)	H19A—C19A—H19B	107.7
C10—C9—H9	120.3	C21A—C20A—C25A	120.0
C8—C9—H9	120.3	C21A—C20A—C19A	119.2 (9)
C9—C10—C11	120.4 (5)	C25A—C20A—C19A	120.8 (9)
C9—C10—H10	119.8	C20A—C21A—C22A	120.0
C11—C10—H10	119.8	C20A—C21A—H21A	120.0
C6—C11—C10	120.8 (4)	C22A—C21A—H21A	120.0
C6—C11—H11	119.6	C23A—C22A—C21A	120.0
C10—C11—H11	119.6	C23A—C22A—H22A	120.0
P2—C12—H12A	109.5	C21A—C22A—H22A	120.0
P2—C12—H12B	109.5	C22A—C23A—C24A	120.0
H12A—C12—H12B	109.5	C22A—C23A—H23A	120.0
P2—C12—H12C	109.5	C24A—C23A—H23A	120.0
H12A—C12—H12C	109.5	C25A—C24A—C23A	120.0
H12B—C12—H12C	109.5	C25A—C24A—H24A	120.0
C18—C13—C14	118.3 (4)	C23A—C24A—H24A	120.0
C18—C13—P2	118.7 (3)	C24A—C25A—C20A	120.0
C14—C13—P2	122.9 (3)	C24A—C25A—H25A	120.0
C15—C14—C13	120.5 (4)	C20A—C25A—H25A	120.0

C15—C14—H14	119.8	P1A—C26A—H26A	109.5
C13—C14—H14	119.8	P1A—C26A—H26B	109.5
C16—C15—C14	120.0 (4)	H26A—C26A—H26B	109.5
C16—C15—H15	120.0	P1A—C26A—H26C	109.5
C14—C15—H15	120.0	H26A—C26A—H26C	109.5
C15—C16—C17	120.8 (4)	H26B—C26A—H26C	109.5
C15—C16—H16	119.6	C27—P1—C26	107.1 (3)
C17—C16—H16	119.6	C27—P1—C19	98.8 (2)
C16—C17—C18	119.3 (4)	C26—P1—C19	102.4 (3)
C16—C17—H17	120.4	C27—P1—Mo1	114.09 (17)
C18—C17—H17	120.4	C26—P1—Mo1	114.7 (2)
C17—C18—C13	121.1 (4)	C19—P1—Mo1	117.85 (19)
C17—C18—H18	119.5	C20—C19—P1	116.4 (4)
C13—C18—H18	119.5	C20—C19—H19C	108.2
C28—C27—C32	116.4 (4)	P1—C19—H19C	108.2
C28—C27—P1	125.6 (3)	C20—C19—H19D	108.2
C32—C27—P1	118.0 (4)	P1—C19—H19D	108.2
C28—C27—P1A	107.8 (4)	H19C—C19—H19D	107.3
C32—C27—P1A	135.7 (4)	C21—C20—C25	120.0
P1—C27—P1A	17.87 (13)	C21—C20—C19	118.8 (4)
C27—C28—C29	122.1 (4)	C25—C20—C19	121.2 (4)
C27—C28—H28	119.0	C20—C21—C22	120.0
C29—C28—H28	119.0	C20—C21—H21	120.0
C30—C29—C28	120.2 (5)	C22—C21—H21	120.0
C30—C29—H29	119.9	C23—C22—C21	120.0
C28—C29—H29	119.9	C23—C22—H22	120.0
C29—C30—C31	119.7 (5)	C21—C22—H22	120.0
C29—C30—H30	120.1	C22—C23—C24	120.0
C31—C30—H30	120.1	C22—C23—H23	120.0
C30—C31—C32	120.8 (5)	C24—C23—H23	120.0
C30—C31—H31	119.6	C25—C24—C23	120.0
C32—C31—H31	119.6	C25—C24—H24	120.0
C31—C32—C27	120.8 (5)	C23—C24—H24	120.0
C31—C32—H32	119.6	C24—C25—C20	120.0
C27—C32—H32	119.6	C24—C25—H25	120.0
C4—Mo1—C2	88.07 (17)	C20—C25—H25	120.0
C4—Mo1—C1	89.19 (16)	P1—C26—H26D	109.5
C2—Mo1—C1	90.28 (16)	P1—C26—H26E	109.5
C4—Mo1—C3	88.95 (19)	H26D—C26—H26E	109.5
C2—Mo1—C3	88.77 (19)	P1—C26—H26F	109.5
C1—Mo1—C3	177.94 (18)	H26D—C26—H26F	109.5
C4—Mo1—P2	87.67 (13)	H26E—C26—H26F	109.5
C2—Mo1—P2	175.58 (12)	C12—P2—C13	103.78 (18)
C1—Mo1—P2	90.82 (11)	C12—P2—C5	102.11 (18)
C3—Mo1—P2	89.99 (14)	C13—P2—C5	101.58 (18)
C4—Mo1—P1	172.65 (13)	C12—P2—Mo1	114.92 (15)
C2—Mo1—P1	89.64 (13)	C13—P2—Mo1	119.66 (11)
C1—Mo1—P1	97.81 (12)	C5—P2—Mo1	112.57 (13)
P2—C5—C6—C7	−100.2 (4)	C28—C27—P1—C26	−156.6 (5)

P2—C5—C6—C11	78.9 (4)	C32—C27—P1—C26	22.7 (5)
C11—C6—C7—C8	0.5 (6)	P1A—C27—P1—C26	−148.9 (10)
C5—C6—C7—C8	179.7 (3)	C28—C27—P1—C19	−50.6 (5)
C6—C7—C8—C9	0.2 (6)	C32—C27—P1—C19	128.6 (4)
C7—C8—C9—C10	−0.8 (6)	P1A—C27—P1—C19	−42.9 (8)
C8—C9—C10—C11	0.7 (7)	C28—C27—P1—Mo1	75.3 (5)
C7—C6—C11—C10	−0.5 (6)	C32—C27—P1—Mo1	−105.4 (4)
C5—C6—C11—C10	−179.7 (4)	P1A—C27—P1—Mo1	83.0 (8)
C9—C10—C11—C6	−0.1 (7)	C4—Mo1—P1—C27	77.6 (11)
C18—C13—C14—C15	0.5 (5)	C2—Mo1—P1—C27	5.8 (2)
P2—C13—C14—C15	178.2 (3)	C1—Mo1—P1—C27	−84.4 (2)
C13—C14—C15—C16	−0.7 (6)	C3—Mo1—P1—C27	94.6 (2)
C14—C15—C16—C17	0.7 (6)	P2—Mo1—P1—C27	−175.86 (19)
C15—C16—C17—C18	−0.4 (6)	P1A—Mo1—P1—C27	−83.5 (7)
C16—C17—C18—C13	0.2 (6)	C4—Mo1—P1—C26	−46.5 (12)
C14—C13—C18—C17	−0.2 (5)	C2—Mo1—P1—C26	−118.3 (3)
P2—C13—C18—C17	−178.1 (3)	C1—Mo1—P1—C26	151.5 (3)
C32—C27—C28—C29	−1.4 (8)	C3—Mo1—P1—C26	−29.5 (3)
P1—C27—C28—C29	177.9 (5)	P2—Mo1—P1—C26	60.0 (3)
P1A—C27—C28—C29	175.4 (5)	P1A—Mo1—P1—C26	152.4 (9)
C27—C28—C29—C30	1.6 (9)	C4—Mo1—P1—C19	−167.1 (11)
C28—C29—C30—C31	0.0 (9)	C2—Mo1—P1—C19	121.1 (3)
C29—C30—C31—C32	−1.7 (10)	C1—Mo1—P1—C19	30.8 (3)
C30—C31—C32—C27	1.8 (10)	C3—Mo1—P1—C19	−150.1 (3)
C28—C27—C32—C31	−0.3 (9)	P2—Mo1—P1—C19	−60.6 (2)
P1—C27—C32—C31	−179.6 (5)	P1A—Mo1—P1—C19	31.7 (7)
P1A—C27—C32—C31	−175.9 (5)	C27—P1—C19—C20	−65.7 (4)
C28—C27—P1A—C26A	−33.2 (6)	C26—P1—C19—C20	44.1 (5)
C32—C27—P1A—C26A	142.7 (7)	Mo1—P1—C19—C20	171.0 (3)
P1—C27—P1A—C26A	153.4 (11)	P1—C19—C20—C21	−105.0 (4)
C28—C27—P1A—C19A	−138.5 (5)	P1—C19—C20—C25	74.9 (5)
C32—C27—P1A—C19A	37.4 (7)	C25—C20—C21—C22	0.0
P1—C27—P1A—C19A	48.1 (8)	C19—C20—C21—C22	180.0 (5)
C28—C27—P1A—Mo1	98.4 (4)	C20—C21—C22—C23	0.0
C32—C27—P1A—Mo1	−85.7 (6)	C21—C22—C23—C24	0.0
P1—C27—P1A—Mo1	−75.1 (8)	C22—C23—C24—C25	0.0
C4—Mo1—P1A—C26A	41.6 (17)	C23—C24—C25—C20	0.0
C2—Mo1—P1A—C26A	109.8 (5)	C21—C20—C25—C24	0.0
C1—Mo1—P1A—C26A	19.4 (5)	C19—C20—C25—C24	−180.0 (5)
C3—Mo1—P1A—C26A	−161.5 (5)	C18—C13—P2—C12	−169.6 (3)
P2—Mo1—P1A—C26A	−70.9 (5)	C14—C13—P2—C12	12.7 (3)
P1—Mo1—P1A—C26A	−159.6 (10)	C18—C13—P2—C5	−63.9 (3)
C4—Mo1—P1A—C19A	163.9 (14)	C14—C13—P2—C5	118.4 (3)
C2—Mo1—P1A—C19A	−128.0 (6)	C18—C13—P2—Mo1	60.7 (3)
C1—Mo1—P1A—C19A	141.7 (6)	C14—C13—P2—Mo1	−117.0 (3)
C3—Mo1—P1A—C19A	−39.3 (6)	C6—C5—P2—C12	39.8 (4)
P2—Mo1—P1A—C19A	51.3 (6)	C6—C5—P2—C13	−67.2 (3)
P1—Mo1—P1A—C19A	−37.4 (7)	C6—C5—P2—Mo1	163.6 (3)
C4—Mo1—P1A—C27	−87.3 (15)	C4—Mo1—P2—C12	86.45 (19)

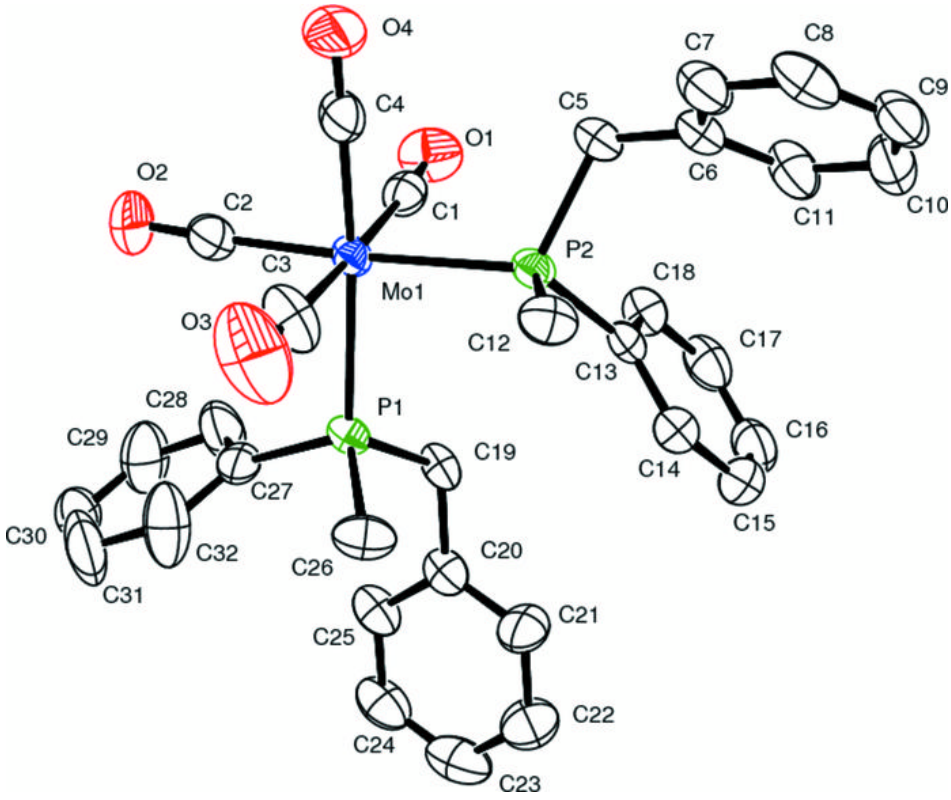
C2—Mo1—P1A—C27	−19.1 (3)	C2—Mo1—P2—C12	71.2 (16)
C1—Mo1—P1A—C27	−109.5 (3)	C1—Mo1—P2—C12	175.61 (17)
C3—Mo1—P1A—C27	69.6 (3)	C3—Mo1—P2—C12	−2.5 (2)
P2—Mo1—P1A—C27	160.2 (3)	P1—Mo1—P2—C12	−86.49 (15)
P1—Mo1—P1A—C27	71.4 (7)	P1A—Mo1—P2—C12	−99.58 (18)
C26A—P1A—C19A—C20A	−37.0 (10)	C4—Mo1—P2—C13	−149.02 (18)
C27—P1A—C19A—C20A	76.1 (9)	C2—Mo1—P2—C13	−164.3 (16)
Mo1—P1A—C19A—C20A	−166.1 (7)	C1—Mo1—P2—C13	−59.87 (17)
P1A—C19A—C20A—C21A	106.4 (9)	C3—Mo1—P2—C13	122.0 (2)
P1A—C19A—C20A—C25A	−72.0 (11)	P1—Mo1—P2—C13	38.03 (14)
C25A—C20A—C21A—C22A	0.0	P1A—Mo1—P2—C13	24.94 (17)
C19A—C20A—C21A—C22A	−178.4 (9)	C4—Mo1—P2—C5	−29.9 (2)
C20A—C21A—C22A—C23A	0.0	C2—Mo1—P2—C5	−45.1 (16)
C21A—C22A—C23A—C24A	0.0	C1—Mo1—P2—C5	59.27 (19)
C22A—C23A—C24A—C25A	0.0	C3—Mo1—P2—C5	−118.8 (2)
C23A—C24A—C25A—C20A	0.0	P1—Mo1—P2—C5	157.17 (17)
C21A—C20A—C25A—C24A	0.0	P1A—Mo1—P2—C5	144.1 (2)
C19A—C20A—C25A—C24A	178.4 (9)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12A···O4^{i}	0.96	2.53	3.424 (6)	154

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

Fig. 1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