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fac,*cis*-Bromidotricarbonylbis(tribenzylphosphine)-rhenium(I)

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.004 Å
R factor = 0.020
wR factor = 0.049
Data-to-parameter ratio = 14.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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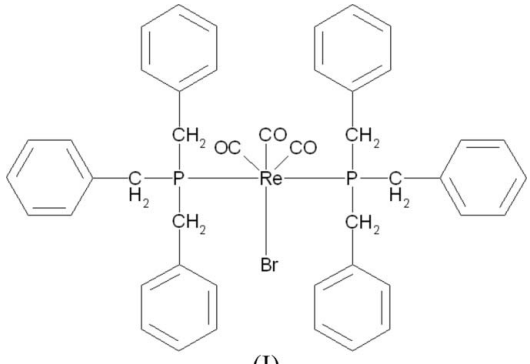
Crystals of the title compound, *fac*,*cis*-[ReBr($C_{21}H_{21}P$)$_2$-(CO)$_3$], were obtained by recrystallization of a sample from $CHCl_3$ layered with hexane. The geometry about the d^6 Re^I centre is (distorted) octahedral with the three CO ligands *fac* and the two tribenzylphosphine ligands *cis*. In accordance with the *trans* influence, the Re—C bond *trans* to Br is significantly shorter than those *trans* to the organophosphine ligands.

Comment

In recent reports, we have described the synthesis and spectroscopic characterization of a series of tricarbonylbis(triorganophosphine)halides of Mn^I and Re^I, together with structural studies on selected compounds: *mer*,*trans*-[MnBr(CO)$_3${P(C_6H_4Cl-4)$_3$}$_2$], *fac*,*cis*-[MnBr(CO)$_3$(dppe)], *fac*,*cis*-[MnBr(CO)$_3$(dppf)], *fac*,*cis*-[ReBr(CO)$_3${P(C_6H_4OMe-4)$_2$}$_2$] and *fac*,*cis*-[ReBr(CO)$_3$(dppf)] (Beckett *et al.*, 2003), and *fac*,*cis*-[$MnBr_{0.3}Cl_{0.7}$(CO)$_3$(dppp)] (Light *et al.*, 2004). The synthesis and spectroscopic characterization of *fac*,*cis*-[ReBr(CO)$_3${P($CH_2C_6H_5$)$_3$}$_2$], (I), was described in an earlier publication, but crystals suitable for X-ray diffraction were unavailable at the time. We can now report a crystallographic study of (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The overall *fac*,*cis* geometry about an octahedral d^6 Re^I centre, as was indicated by earlier spectroscopic (IR and NMR) evidence, is confirmed by this crystallographic study. The octahedral geometry is considerably distorted [*cis* angles range from 81.055 (14) to 98.32 (2)°, with P1—Re1—P2 the largest, and *trans* angles range from 169.03 (8) to 173.81 (8)°], but bond lengths and angles are well within previously reported ranges for related compounds (Beckett *et al.*, 2003; Carballo *et al.*, 2001; Gibson *et al.* 2001). The Re1—C1 bond *trans* to Br is significantly shorter than the Re1—C2 and Re1—C3 bonds *trans* to P.

Experimental

fac,*cis*-[ReBr(CO)$_3${P(CH$_2$C$_6$H$_5$)$_3$}$_2$], (I), was prepared by adapting a standard literature method (Angelici *et al.*, 1963) and its physical and spectroscopic properties have been reported previously (Beckett *et al.*, 2003). Orange single crystals suitable for X-ray diffraction studies were obtained by slow diffusion of hexane (layered) into a chloroform solution of (I) at 279 K.

Crystal data

[ReBr(C$_{21}$H$_{21}$P)$_2$(CO)$_3$]
M_r = 958.84
Triclinic, $P\overline{1}$
a = 10.158 (1) Å
b = 10.373 (1) Å
c = 19.289 (2) Å
α = 103.046 (5)°
β = 94.822 (6)°
γ = 92.164 (6)°
V = 1969.6 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 4.22 mm^{-1}
T = 150 (2) K
0.10 × 0.08 × 0.08 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.664, T_{max} = 0.714
32577 measured reflections
6638 independent reflections
6477 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.049
S = 1.07
6638 reflections
469 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −1.09 e Å^{-3}

Table 1
Selected bond angles (°).

C2—Re1—C3	93.80 (11)	C1—Re1—P1	90.37 (9)
C2—Re1—C1	85.52 (11)	P2—Re1—P1	98.32 (2)
C3—Re1—C1	86.38 (12)	C2—Re1—Br1	173.81 (8)
C2—Re1—P2	92.78 (8)	C3—Re1—Br1	88.40 (8)
C3—Re1—P2	85.19 (8)	C1—Re1—Br1	88.85 (9)
C1—Re1—P2	171.28 (9)	P2—Re1—Br1	93.160 (18)
C2—Re1—P1	96.39 (8)	P1—Re1—Br1	81.055 (18)
C3—Re1—P1	169.03 (8)		

All H atoms were placed in idealized positions (C–H = 0.95–0.99 Å) and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C). The deepest residual electron-density hole is located 0.93 Å from atom Re1.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

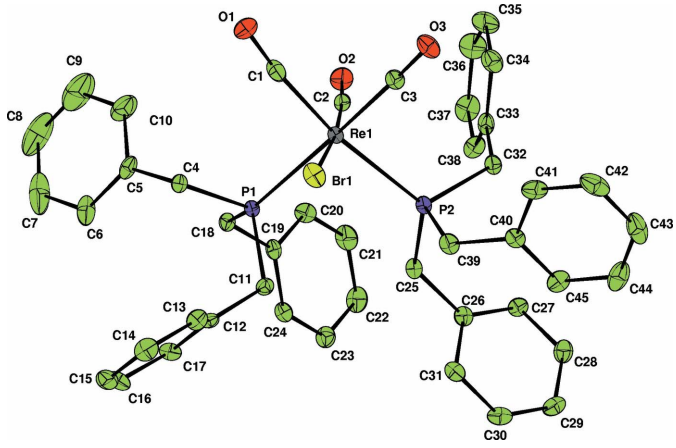


Figure 1
The molecular structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 35% probability level and H atoms have been omitted for clarity

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fac,*cis*-Bromidotricarbonylbis(tribenzylphosphine)rhenium(I)

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fac-Bromidootricarbonylbis(tribenzylphosphine-κ*P*)rhenium(I)

Crystal data

$[ReBr(C_{21}H_{21}P)_2(CO)_3]$
$M_r = 958.84$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 10.158$ (1) Å
$b = 10.373$ (1) Å
$c = 19.289$ (2) Å
$\alpha = 103.046$ (5)°
$\beta = 94.822$ (6)°
$\gamma = 92.164$ (6)°
$V = 1969.6$ (3) Å^3
$Z = 2$
$F(000) = 952$
$D_x = 1.617$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 6638 reflections
$\theta = 2.9$–25.0°
$\mu = 4.22$ mm^{-1}
$T = 150$ K
Block, colourless
0.10 × 0.08 × 0.08 mm

Data collection

Bruker–Nonius CCD camera on κ-goniostat diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans to fill the asymmetric unit
Absorption correction: multi-scan (SORTAV; Blessing, 1995)
$T_{min} = 0.664$, $T_{max} = 0.714$
6638 measured reflections
6638 independent reflections
6477 reflections with $I > 2\sigma(I)$
$R_{int} = 0.000$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.9°$
$h = 0 \rightarrow 12$
$k = -12 \rightarrow 12$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.020$
$wR(F^2) = 0.049$
$S = 1.07$
6638 reflections
469 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0155P)^2 + 2.6094P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.005$
$\Delta\rho_{max} = 0.69$ e Å^{-3}
$\Delta\rho_{min} = -1.09$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.0450 (3)	−0.0953 (3)	0.87704 (16)	0.0255 (6)
C2	1.0029 (3)	0.1519 (3)	0.87778 (14)	0.0198 (6)
C3	1.2052 (3)	0.0217 (3)	0.80536 (14)	0.0207 (6)
C4	0.7497 (3)	−0.2293 (2)	0.81734 (14)	0.0183 (5)
H4A	0.7059	−0.2979	0.7769	0.022*
H4B	0.8376	−0.2600	0.8302	0.022*
C5	0.6690 (3)	−0.2190 (3)	0.88019 (14)	0.0227 (6)
C6	0.5342 (3)	−0.2461 (3)	0.87048 (19)	0.0349 (7)
H6	0.4901	−0.2736	0.8237	0.042*
C7	0.4621 (4)	−0.2324 (4)	0.9311 (3)	0.0591 (12)
H7	0.3689	−0.2505	0.9256	0.071*
C8	0.5298 (6)	−0.1919 (5)	0.9989 (2)	0.0699 (15)
H8	0.4815	−0.1801	1.0398	0.084*
C9	0.6626 (6)	−0.1692 (5)	1.0079 (2)	0.0679 (14)
H9	0.7072	−0.1450	1.0547	0.081*
C10	0.7327 (4)	−0.1811 (3)	0.94939 (16)	0.0419 (8)
H10	0.8259	−0.1633	0.9559	0.050*
C11	0.7020 (3)	−0.1151 (3)	0.69143 (13)	0.0178 (5)
H11A	0.6616	−0.0355	0.6808	0.021*
H11B	0.7750	−0.1356	0.6605	0.021*
C12	0.5990 (3)	−0.2295 (2)	0.67042 (13)	0.0166 (5)
C13	0.6381 (3)	−0.3553 (3)	0.63834 (14)	0.0231 (6)
H13	0.7280	−0.3668	0.6296	0.028*
C14	0.5470 (3)	−0.4631 (3)	0.61921 (15)	0.0283 (7)
H14	0.5745	−0.5476	0.5966	0.034*
C15	0.4164 (3)	−0.4482 (3)	0.63291 (16)	0.0304 (7)
H15	0.3544	−0.5225	0.6204	0.036*
C16	0.3762 (3)	−0.3245 (3)	0.66499 (16)	0.0282 (7)
H16	0.2866	−0.3139	0.6747	0.034*
C17	0.4675 (3)	−0.2158 (3)	0.68306 (14)	0.0224 (6)
H17	0.4391	−0.1309	0.7044	0.027*
C18	0.6525 (3)	0.0344 (2)	0.83373 (13)	0.0166 (5)
H18A	0.5655	−0.0156	0.8242	0.020*
H18B	0.6785	0.0503	0.8857	0.020*
C19	0.6353 (3)	0.1670 (2)	0.81524 (13)	0.0169 (5)
C20	0.6965 (3)	0.2821 (3)	0.85946 (14)	0.0227 (6)
H20	0.7524	0.2762	0.9005	0.027*
C21	0.6775 (3)	0.4054 (3)	0.84466 (16)	0.0293 (7)
H21	0.7192	0.4830	0.8758	0.035*
C22	0.5979 (3)	0.4151 (3)	0.78459 (16)	0.0282 (7)

H22	0.5862	0.4992	0.7739	0.034*
C23	0.5354 (3)	0.3023 (3)	0.74003 (15)	0.0241 (6)
H23	0.4807	0.3087	0.6987	0.029*
C24	0.5529 (3)	0.1797 (3)	0.75586 (14)	0.0191 (5)
H24	0.5078	0.1029	0.7256	0.023*
C25	0.8579 (3)	0.2131 (3)	0.69043 (14)	0.0195 (6)
H25A	0.7844	0.1445	0.6826	0.023*
H25B	0.8426	0.2813	0.7335	0.023*
C26	0.8495 (3)	0.2773 (3)	0.62743 (14)	0.0195 (6)
C27	0.9074 (3)	0.4030 (3)	0.63119 (14)	0.0200 (6)
H27	0.9521	0.4518	0.6750	0.024*
C28	0.9006 (3)	0.4578 (3)	0.57154 (15)	0.0247 (6)
H28	0.9425	0.5426	0.5745	0.030*
C29	0.8326 (3)	0.3891 (3)	0.50777 (15)	0.0264 (6)
H29	0.8273	0.4266	0.4671	0.032*
C30	0.7728 (3)	0.2654 (3)	0.50383 (15)	0.0284 (7)
H30	0.7253	0.2183	0.4604	0.034*
C31	0.7814 (3)	0.2095 (3)	0.56274 (15)	0.0236 (6)
H31	0.7405	0.1241	0.5591	0.028*
C32	1.1414 (3)	0.2737 (3)	0.73241 (13)	0.0189 (5)
H32A	1.2289	0.2357	0.7274	0.023*
H32B	1.1284	0.3283	0.6967	0.023*
C33	1.1447 (3)	0.3643 (3)	0.80622 (14)	0.0217 (6)
C34	1.2524 (3)	0.3653 (3)	0.85597 (15)	0.0274 (6)
H34	1.3228	0.3096	0.8432	0.033*
C35	1.2580 (3)	0.4472 (3)	0.92417 (17)	0.0368 (8)
H35	1.3321	0.4470	0.9576	0.044*
C36	1.1566 (4)	0.5286 (3)	0.94344 (16)	0.0359 (8)
H36	1.1602	0.5833	0.9903	0.043*
C37	1.0501 (3)	0.5304 (3)	0.89464 (16)	0.0318 (7)
H37	0.9805	0.5870	0.9077	0.038*
C38	1.0446 (3)	0.4490 (3)	0.82605 (15)	0.0258 (6)
H38	0.9714	0.4515	0.7924	0.031*
C39	1.0502 (3)	0.0409 (3)	0.62038 (14)	0.0218 (6)
H39A	1.0709	−0.0498	0.6245	0.026*
H39B	0.9686	0.0326	0.5875	0.026*
C40	1.1609 (3)	0.0950 (3)	0.58586 (13)	0.0193 (6)
C41	1.2900 (3)	0.0610 (3)	0.59931 (14)	0.0273 (6)
H41	1.3084	0.0059	0.6317	0.033*
C42	1.3923 (3)	0.1064 (4)	0.56616 (17)	0.0385 (8)
H42	1.4798	0.0812	0.5755	0.046*
C43	1.3676 (4)	0.1882 (3)	0.51945 (17)	0.0397 (9)
H43	1.4377	0.2197	0.4968	0.048*
C44	1.2404 (4)	0.2234 (3)	0.50620 (16)	0.0352 (8)
H44	1.2226	0.2798	0.4744	0.042*
C45	1.1380 (3)	0.1773 (3)	0.53878 (14)	0.0248 (6)
H45	1.0506	0.2023	0.5289	0.030*
O1	1.0737 (2)	−0.1429 (2)	0.92452 (12)	0.0407 (6)

O2	0.9960 (2)	0.23532 (19)	0.92824 (10)	0.0272 (4)
O3	1.3187 (2)	0.0273 (2)	0.80676 (11)	0.0312 (5)
P1	0.77483 (7)	−0.07233 (6)	0.78622 (3)	0.01423 (13)
P2	1.01289 (7)	0.13525 (6)	0.71007 (3)	0.01552 (14)
Br1	1.02464 (3)	−0.22602 (3)	0.706163 (15)	0.02625 (7)
Re1	1.015147 (9)	0.000364 (9)	0.801968 (5)	0.01501 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0182 (16)	0.0228 (15)	0.0348 (17)	−0.0033 (11)	0.0009 (12)	0.0063 (13)
C2	0.0154 (15)	0.0258 (15)	0.0205 (14)	−0.0002 (11)	0.0021 (10)	0.0107 (12)
C3	0.0209 (18)	0.0200 (14)	0.0196 (14)	−0.0002 (11)	0.0027 (11)	0.0012 (11)
C4	0.0195 (15)	0.0160 (13)	0.0202 (13)	−0.0008 (10)	0.0016 (10)	0.0062 (10)
C5	0.0369 (18)	0.0135 (13)	0.0194 (14)	0.0009 (11)	0.0074 (12)	0.0057 (10)
C6	0.032 (2)	0.0286 (17)	0.052 (2)	0.0045 (13)	0.0171 (15)	0.0198 (15)
C7	0.046 (3)	0.046 (2)	0.103 (4)	0.0124 (18)	0.041 (2)	0.039 (2)
C8	0.111 (5)	0.067 (3)	0.046 (3)	0.027 (3)	0.051 (3)	0.023 (2)
C9	0.108 (4)	0.067 (3)	0.033 (2)	0.006 (3)	0.025 (2)	0.013 (2)
C10	0.061 (3)	0.043 (2)	0.0220 (16)	−0.0019 (17)	0.0030 (15)	0.0094 (14)
C11	0.0187 (15)	0.0200 (13)	0.0152 (13)	0.0020 (10)	0.0026 (10)	0.0046 (10)
C12	0.0199 (15)	0.0185 (13)	0.0106 (12)	0.0010 (10)	−0.0010 (10)	0.0026 (10)
C13	0.0272 (17)	0.0224 (14)	0.0196 (14)	0.0043 (11)	0.0049 (11)	0.0031 (11)
C14	0.040 (2)	0.0175 (14)	0.0252 (15)	0.0038 (12)	0.0013 (13)	0.0008 (11)
C15	0.0329 (19)	0.0254 (16)	0.0298 (16)	−0.0099 (13)	−0.0093 (13)	0.0063 (13)
C16	0.0164 (16)	0.0333 (17)	0.0325 (16)	−0.0015 (12)	−0.0039 (12)	0.0057 (13)
C17	0.0205 (16)	0.0219 (14)	0.0227 (14)	0.0028 (11)	−0.0028 (11)	0.0022 (11)
C18	0.0149 (14)	0.0183 (13)	0.0175 (13)	0.0026 (10)	0.0054 (10)	0.0044 (10)
C19	0.0145 (14)	0.0182 (13)	0.0181 (13)	0.0012 (10)	0.0082 (10)	0.0021 (10)
C20	0.0228 (16)	0.0230 (14)	0.0203 (14)	0.0031 (11)	0.0025 (11)	0.0006 (11)
C21	0.0357 (19)	0.0171 (14)	0.0306 (16)	−0.0035 (12)	0.0041 (13)	−0.0034 (12)
C22	0.0330 (18)	0.0172 (14)	0.0360 (17)	0.0047 (12)	0.0085 (13)	0.0067 (12)
C23	0.0228 (16)	0.0230 (15)	0.0281 (15)	0.0029 (11)	0.0044 (11)	0.0086 (12)
C24	0.0179 (15)	0.0169 (13)	0.0215 (13)	0.0002 (10)	0.0035 (10)	0.0017 (10)
C25	0.0196 (15)	0.0179 (13)	0.0216 (13)	−0.0007 (10)	0.0048 (10)	0.0048 (11)
C26	0.0162 (15)	0.0225 (14)	0.0202 (13)	0.0047 (10)	0.0063 (10)	0.0033 (11)
C27	0.0235 (16)	0.0185 (13)	0.0175 (13)	0.0028 (11)	0.0018 (10)	0.0026 (10)
C28	0.0270 (17)	0.0193 (14)	0.0293 (15)	0.0023 (11)	0.0064 (12)	0.0074 (12)
C29	0.0297 (17)	0.0324 (16)	0.0192 (14)	0.0071 (13)	0.0023 (11)	0.0093 (12)
C30	0.0275 (17)	0.0333 (17)	0.0218 (15)	0.0024 (13)	−0.0048 (12)	0.0033 (12)
C31	0.0196 (16)	0.0225 (14)	0.0274 (15)	−0.0005 (11)	−0.0001 (11)	0.0038 (11)
C32	0.0208 (15)	0.0183 (13)	0.0159 (13)	−0.0033 (10)	0.0040 (10)	0.0003 (10)
C33	0.0292 (16)	0.0154 (13)	0.0188 (13)	−0.0069 (11)	0.0045 (11)	0.0007 (11)
C34	0.0268 (17)	0.0243 (15)	0.0270 (15)	−0.0041 (12)	0.0033 (12)	−0.0018 (12)
C35	0.039 (2)	0.0364 (18)	0.0265 (16)	−0.0094 (15)	−0.0077 (13)	−0.0040 (13)
C36	0.049 (2)	0.0271 (16)	0.0223 (15)	−0.0048 (14)	0.0017 (14)	−0.0110 (12)
C37	0.047 (2)	0.0201 (15)	0.0250 (15)	0.0025 (13)	0.0090 (14)	−0.0042 (12)
C38	0.0378 (18)	0.0189 (14)	0.0196 (14)	0.0001 (12)	0.0027 (12)	0.0023 (11)

C39	0.0242 (16)	0.0194 (14)	0.0185 (13)	−0.0016 (11)	0.0039 (11)	−0.0028 (11)
C40	0.0216 (16)	0.0186 (13)	0.0141 (12)	0.0002 (11)	0.0038 (10)	−0.0042 (10)
C41	0.0283 (18)	0.0347 (17)	0.0150 (13)	0.0065 (13)	0.0011 (11)	−0.0025 (12)
C42	0.0213 (18)	0.057 (2)	0.0281 (17)	0.0009 (15)	0.0031 (12)	−0.0088 (15)
C43	0.039 (2)	0.044 (2)	0.0294 (17)	−0.0156 (16)	0.0185 (14)	−0.0081 (15)
C44	0.054 (2)	0.0288 (17)	0.0244 (16)	0.0009 (15)	0.0169 (14)	0.0052 (13)
C45	0.0310 (17)	0.0242 (15)	0.0189 (14)	0.0070 (12)	0.0061 (11)	0.0021 (11)
O1	0.0386 (15)	0.0463 (14)	0.0442 (14)	−0.0032 (11)	−0.0086 (10)	0.0306 (12)
O2	0.0327 (13)	0.0262 (11)	0.0205 (10)	0.0014 (9)	0.0050 (8)	−0.0002 (9)
O3	0.0179 (13)	0.0366 (12)	0.0378 (12)	0.0005 (9)	0.0044 (9)	0.0051 (9)
P1	0.0137 (4)	0.0140 (3)	0.0148 (3)	−0.0002 (2)	0.0021 (2)	0.0029 (2)
P2	0.0172 (4)	0.0147 (3)	0.0133 (3)	−0.0016 (3)	0.0038 (2)	−0.0001 (2)
Br1	0.02517 (17)	0.01728 (14)	0.03362 (16)	0.00298 (11)	0.00645 (12)	−0.00132 (11)
Re1	0.01352 (7)	0.01471 (7)	0.01646 (6)	−0.00017 (4)	0.00179 (4)	0.00291 (4)

Geometric parameters (Å, º)

C1—O1	1.156 (4)	C24—H24	0.9500
C1—Re1	1.942 (3)	C25—C26	1.510 (4)
C2—O2	1.156 (3)	C25—P2	1.846 (3)
C2—Re1	1.906 (3)	C25—H25A	0.9900
C3—O3	1.149 (3)	C25—H25B	0.9900
C3—Re1	1.929 (3)	C26—C27	1.393 (4)
C4—C5	1.507 (4)	C26—C31	1.397 (4)
C4—P1	1.874 (2)	C27—C28	1.392 (4)
C4—H4A	0.9900	C27—H27	0.9500
C4—H4B	0.9900	C28—C29	1.386 (4)
C5—C6	1.376 (5)	C28—H28	0.9500
C5—C10	1.398 (4)	C29—C30	1.382 (4)
C6—C7	1.414 (5)	C29—H29	0.9500
C6—H6	0.9500	C30—C31	1.385 (4)
C7—C8	1.393 (7)	C30—H30	0.9500
C7—H7	0.9500	C31—H31	0.9500
C8—C9	1.350 (7)	C32—C33	1.515 (3)
C8—H8	0.9500	C32—P2	1.854 (3)
C9—C10	1.369 (5)	C32—H32A	0.9900
C9—H9	0.9500	C32—H32B	0.9900
C10—H10	0.9500	C33—C38	1.391 (4)
C11—C12	1.512 (4)	C33—C34	1.391 (4)
C11—P1	1.862 (3)	C34—C35	1.391 (4)
C11—H11A	0.9900	C34—H34	0.9500
C11—H11B	0.9900	C35—C36	1.378 (5)
C12—C17	1.385 (4)	C35—H35	0.9500
C12—C13	1.399 (4)	C36—C37	1.377 (5)
C13—C14	1.386 (4)	C36—H36	0.9500
C13—H13	0.9500	C37—C38	1.395 (4)
C14—C15	1.382 (5)	C37—H37	0.9500
C14—H14	0.9500	C38—H38	0.9500

C15—C16	1.385 (4)	C39—C40	1.506 (4)
C15—H15	0.9500	C39—P2	1.862 (3)
C16—C17	1.394 (4)	C39—H39A	0.9900
C16—H16	0.9500	C39—H39B	0.9900
C17—H17	0.9500	C40—C41	1.389 (4)
C18—C19	1.510 (4)	C40—C45	1.392 (4)
C18—P1	1.856 (3)	C41—C42	1.386 (5)
C18—H18A	0.9900	C41—H41	0.9500
C18—H18B	0.9900	C42—C43	1.385 (5)
C19—C20	1.391 (4)	C42—H42	0.9500
C19—C24	1.395 (4)	C43—C44	1.375 (5)
C20—C21	1.389 (4)	C43—H43	0.9500
C20—H20	0.9500	C44—C45	1.383 (4)
C21—C22	1.381 (4)	C44—H44	0.9500
C21—H21	0.9500	C45—H45	0.9500
C22—C23	1.381 (4)	P1—Re1	2.5005 (7)
C22—H22	0.9500	P2—Re1	2.4931 (7)
C23—C24	1.388 (4)	Br1—Re1	2.6508 (4)
C23—H23	0.9500		

O1—C1—Re1	172.9 (2)	C29—C28—C27	120.2 (3)
O2—C2—Re1	173.2 (2)	C29—C28—H28	119.9
O3—C3—Re1	176.4 (2)	C27—C28—H28	119.9
C5—C4—P1	115.43 (18)	C30—C29—C28	119.5 (3)
C5—C4—H4A	108.4	C30—C29—H29	120.3
P1—C4—H4A	108.4	C28—C29—H29	120.3
C5—C4—H4B	108.4	C29—C30—C31	120.5 (3)
P1—C4—H4B	108.4	C29—C30—H30	119.7
H4A—C4—H4B	107.5	C31—C30—H30	119.7
C6—C5—C10	119.8 (3)	C30—C31—C26	120.8 (3)
C6—C5—C4	121.1 (3)	C30—C31—H31	119.6
C10—C5—C4	119.1 (3)	C26—C31—H31	119.6
C5—C6—C7	119.1 (4)	C33—C32—P2	116.41 (18)
C5—C6—H6	120.4	C33—C32—H32A	108.2
C7—C6—H6	120.4	P2—C32—H32A	108.2
C8—C7—C6	119.0 (4)	C33—C32—H32B	108.2
C8—C7—H7	120.5	P2—C32—H32B	108.2
C6—C7—H7	120.5	H32A—C32—H32B	107.3
C9—C8—C7	121.4 (4)	C38—C33—C34	118.3 (3)
C9—C8—H8	119.3	C38—C33—C32	122.3 (3)
C7—C8—H8	119.3	C34—C33—C32	119.4 (3)
C8—C9—C10	119.8 (4)	C35—C34—C33	120.6 (3)
C8—C9—H9	120.1	C35—C34—H34	119.7
C10—C9—H9	120.1	C33—C34—H34	119.7
C9—C10—C5	120.9 (4)	C36—C35—C34	120.4 (3)
C9—C10—H10	119.6	C36—C35—H35	119.8
C5—C10—H10	119.6	C34—C35—H35	119.8
C12—C11—P1	116.92 (17)	C37—C36—C35	119.9 (3)

C12—C11—H11A	108.1	C37—C36—H36	120.1
P1—C11—H11A	108.1	C35—C36—H36	120.1
C12—C11—H11B	108.1	C36—C37—C38	119.9 (3)
P1—C11—H11B	108.1	C36—C37—H37	120.1
H11A—C11—H11B	107.3	C38—C37—H37	120.1
C17—C12—C13	118.4 (2)	C33—C38—C37	120.9 (3)
C17—C12—C11	122.7 (2)	C33—C38—H38	119.5
C13—C12—C11	118.9 (2)	C37—C38—H38	119.5
C14—C13—C12	120.7 (3)	C40—C39—P2	118.06 (18)
C14—C13—H13	119.6	C40—C39—H39A	107.8
C12—C13—H13	119.6	P2—C39—H39A	107.8
C15—C14—C13	120.2 (3)	C40—C39—H39B	107.8
C15—C14—H14	119.9	P2—C39—H39B	107.8
C13—C14—H14	119.9	H39A—C39—H39B	107.1
C14—C15—C16	119.8 (3)	C41—C40—C45	117.9 (3)
C14—C15—H15	120.1	C41—C40—C39	120.2 (3)
C16—C15—H15	120.1	C45—C40—C39	121.9 (3)
C15—C16—C17	119.9 (3)	C42—C41—C40	121.0 (3)
C15—C16—H16	120.1	C42—C41—H41	119.5
C17—C16—H16	120.1	C40—C41—H41	119.5
C12—C17—C16	121.0 (3)	C43—C42—C41	120.3 (3)
C12—C17—H17	119.5	C43—C42—H42	119.8
C16—C17—H17	119.5	C41—C42—H42	119.8
C19—C18—P1	116.85 (17)	C44—C43—C42	119.2 (3)
C19—C18—H18A	108.1	C44—C43—H43	120.4
P1—C18—H18A	108.1	C42—C43—H43	120.4
C19—C18—H18B	108.1	C43—C44—C45	120.5 (3)
P1—C18—H18B	108.1	C43—C44—H44	119.7
H18A—C18—H18B	107.3	C45—C44—H44	119.7
C20—C19—C24	117.7 (2)	C44—C45—C40	121.1 (3)
C20—C19—C18	120.5 (2)	C44—C45—H45	119.5
C24—C19—C18	121.7 (2)	C40—C45—H45	119.5
C21—C20—C19	121.2 (3)	C18—P1—C11	103.78 (12)
C21—C20—H20	119.4	C18—P1—C4	102.14 (12)
C19—C20—H20	119.4	C11—P1—C4	104.09 (12)
C22—C21—C20	120.0 (3)	C18—P1—Re1	120.77 (9)
C22—C21—H21	120.0	C11—P1—Re1	114.05 (9)
C20—C21—H21	120.0	C4—P1—Re1	110.19 (9)
C21—C22—C23	119.9 (3)	C25—P2—C32	104.72 (13)
C21—C22—H22	120.0	C25—P2—C39	103.24 (13)
C23—C22—H22	120.0	C32—P2—C39	103.34 (12)
C22—C23—C24	119.8 (3)	C25—P2—Re1	117.55 (8)
C22—C23—H23	120.1	C32—P2—Re1	112.68 (9)
C24—C23—H23	120.1	C39—P2—Re1	113.82 (9)
C23—C24—C19	121.3 (2)	C2—Re1—C3	93.80 (11)
C23—C24—H24	119.3	C2—Re1—C1	85.52 (11)
C19—C24—H24	119.3	C3—Re1—C1	86.38 (12)
C26—C25—P2	117.58 (18)	C2—Re1—P2	92.78 (8)

C26—C25—H25A	107.9	C3—Re1—P2	85.19 (8)
P2—C25—H25A	107.9	C1—Re1—P2	171.28 (9)
C26—C25—H25B	107.9	C2—Re1—P1	96.39 (8)
P2—C25—H25B	107.9	C3—Re1—P1	169.03 (8)
H25A—C25—H25B	107.2	C1—Re1—P1	90.37 (9)
C27—C26—C31	118.2 (2)	P2—Re1—P1	98.32 (2)
C27—C26—C25	122.4 (2)	C2—Re1—Br1	173.81 (8)
C31—C26—C25	119.4 (2)	C3—Re1—Br1	88.40 (8)
C28—C27—C26	120.8 (3)	C1—Re1—Br1	88.85 (9)
C28—C27—H27	119.6	P2—Re1—Br1	93.160 (18)
C26—C27—H27	119.6	P1—Re1—Br1	81.055 (18)