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Octacarbonyl-1 κ^4 C,2 κ^4 C- μ -dicyclohexylphosphido-1:2 κ^2 P:P-triphenylphosphine-2 κ P-silver-dirhenium(2 Re--Ag)

U. Flörke and H.-J. Haupt

Abstract

The title compound shows a nearly planar PRe₂Ag ring with significantly different Re—Ag single bond lengths of 2.7957 (7) and 2.8235 (7) Å.

Comment

The central molecular fragment of Re₂(AgPPh₃)(μ -PCy₂)(CO)₈ is a PRe₂Ag ring. Each rhenium atom is attached to four terminal carbonyl ligands and to the common bridging μ -PCy₂ group. With respect to these non-metal ligands and to the Re—Ag bonds, both Re atoms attain slightly distorted octahedral coordination, whereas the Ag atom is threefold coordinated through the two Re atoms and a terminal PPh₃ ligand. The carbonyl groups show almost eclipsed arrangement when viewed along the Re—Re vector with C—Re—Re—C torsion angles in the range from 0.8 to 9.9 (1)°. The four-membered central ring is nearly planar with a dihedral angle PRe₂/Re₂Ag of 4.3 (1)° and the Ag atom lies 0.173 (1)Å above the PRe₂ plane. The same ring geometry is valid for the related complex Mn₂(AuPPh₃)(μ -PPh₂)(CO)₈ (Haupt *et al.*, 1992). The Re—Re bond length of 3.1834 (6) Å is longer than that in the homologueous Cu compound with 3.102 (1) Å (Flörke & Haupt, 1992) but shorter than in the gold compound Re₂(AuPPh₃)(μ -PHCy)(CO)₈ with 3.261 (2)Å (Haupt *et al.*, 1995) and reflects the influence of the coin metal. The Re₂Ag ring is significantly distorted with two different Ag—Re single bond lengths of 2.7957 (7) (Re1) and 2.8235 (7)Å (Re2) but the μ -P bridge is nearly symmetrical with Re—P bond lengths of 2.4495 (18) and 2.4398 (18) Å, respectively. Connected with these different Ag—Re bond lengths are different exocyclic P—Ag—Re angles of 153.58 (5) (Re1) and 135.63 (5)° (Re2) with the smaller angle opposite to the shorter Ag—Re bond. There is only one other crystal structure known with Ag—Re bonding interactions and it provides a nearly linear Re—Ag—Re chain with one Ag—Re bond length of 2.838 (2) Å. The second Ag—Re bond of this example is rather uncertain and suffers from positional disorder of the other Re atom (Connelly *et al.*, 1984).

Experimental

Reaction of a thf solution of Re₂(μ -H)(μ -PCy₂)(CO)₈ and 1,8-diazabicyclo(5,4,0)undec-7-en with a thf solution of (PPh₃)₃AgCl and TIPF₆ at room temperature. After separation from TiCl₄ precipitate the solvent was removed *in vacuo* and the residue separated by TLC procedure. The solid yellow product was then recrystallized from CH₂Cl₂/hexane.

Computing details

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1995); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Octacarbonyl- μ -dicyclohexylphosphido-dirhenium-silver-triphenylphosphane

Crystal data

[Re ₂ Ag ₁ (C ₁₂ H ₂₂ P ₁)(C ₁₈ H ₁₅ P ₁)(C ₁ O ₁) ₈]	$V = 4037.1 (12) \text{ \AA}^3$
$M_r = 1163.89$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$
$a = 11.078 (2) \text{ \AA}$	$\mu = 6.59 \text{ mm}^{-1}$
$b = 12.869 (2) \text{ \AA}$	$T = 203 (2) \text{ K}$
$c = 28.770 (5) \text{ \AA}$	$0.52 \times 0.32 \times 0.17 \text{ mm}$
$\beta = 100.17 (1)^\circ$	

Data collection

Siemens P4 diffractometer	6526 reflections with $I > 2\sigma(I)$
Absorption correction: ψ scan (XPREP; Bruker, 1997)	$R_{\text{int}} = 0.037$
$T_{\text{min}} = 0.105$, $T_{\text{max}} = 0.326$	3 standard reflections
11625 measured reflections	every 397 reflections
9265 independent reflections	intensity decay: 4%

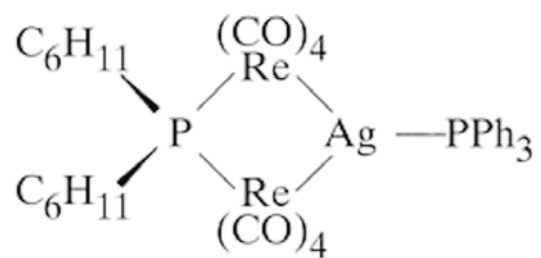
Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$	765 restraints
$wR(F^2) = 0.077$	H-atom parameters constrained
$S = 1.17$	$\Delta\rho_{\text{max}} = 0.97 \text{ e \AA}^{-3}$
9265 reflections	$\Delta\rho_{\text{min}} = -0.87 \text{ e \AA}^{-3}$
461 parameters	

References

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Scheme 1



supplementary materials

Octacarbonyl- μ -dicyclohexylphosphido-dirhenium-silver-triphenylphosphane

Crystal data

$[\text{Re}_2\text{Ag}_1(\text{C}_{12}\text{H}_{22}\text{P}_1)(\text{C}_{18}\text{H}_{15}\text{P}_1)(\text{C}_1\text{O}_1)_8]$	$F_{000} = 2224$
$M_r = 1163.89$	$D_x = 1.915 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 11.078 (2) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 12.869 (2) \text{ \AA}$	Cell parameters from 35 reflections
$c = 28.770 (5) \text{ \AA}$	$\theta = 15.8\text{--}45.5^\circ$
$\beta = 100.17 (1)^\circ$	$\mu = 6.59 \text{ mm}^{-1}$
$V = 4037.1 (12) \text{ \AA}^3$	$T = 203 (2) \text{ K}$
$Z = 4$	Block, colorless
	$0.52 \times 0.32 \times 0.17 \text{ mm}$

Data collection

Siemens P4 diffractometer	$R_{\text{int}} = 0.037$
Radiation source: fine-focus sealed tube	$\theta_{\text{max}} = 27.5^\circ$
Monochromator: graphite	$\theta_{\text{min}} = 2.1^\circ$
$T = 203(2) \text{ K}$	$h = -1 \rightarrow 14$
ω scans	$k = -16 \rightarrow 1$
Absorption correction: ψ scan (XPREP; Bruker, 1997)	$l = -37 \rightarrow 37$
$T_{\text{min}} = 0.105$, $T_{\text{max}} = 0.326$	3 standard reflections
11625 measured reflections	every 397 reflections
9265 independent reflections	intensity decay: 4%
6526 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.048$	H-atom parameters constrained
$wR(F^2) = 0.077$	$w = 1/[\sigma^2(F_o^2) + (0.0175P)^2 + 4.5283P]$
$S = 1.17$	where $P = (F_o^2 + 2F_c^2)/3$
9265 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
461 parameters	$\Delta\rho_{\text{max}} = 0.97 \text{ e \AA}^{-3}$
765 restraints	$\Delta\rho_{\text{min}} = -0.87 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL, $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.00068 (3)

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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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Re1	0.44357 (3)	1.17647 (2)	-0.176356 (10)	0.02989 (9)
Re2	0.54372 (3)	1.03292 (2)	-0.087817 (9)	0.02477 (8)
Ag1	0.61559 (5)	1.24077 (4)	-0.098593 (19)	0.03197 (14)
P1	0.40523 (17)	0.99306 (14)	-0.16142 (6)	0.0272 (4)
P2	0.77629 (18)	1.35412 (15)	-0.05870 (7)	0.0324 (5)
O1	0.3007 (5)	1.1634 (5)	-0.27750 (19)	0.0562 (17)
C1	0.3524 (7)	1.1700 (6)	-0.2393 (3)	0.0404 (19)
O2	0.6870 (6)	1.1357 (6)	-0.2137 (2)	0.077 (2)
C2	0.5969 (8)	1.1485 (7)	-0.1996 (3)	0.046 (2)
O3	0.2161 (6)	1.2389 (5)	-0.1320 (2)	0.0628 (18)
C3	0.2988 (8)	1.2128 (6)	-0.1476 (3)	0.0397 (18)
O4	0.4854 (7)	1.4147 (5)	-0.1833 (2)	0.085 (2)
C4	0.4797 (9)	1.3263 (7)	-0.1798 (3)	0.058 (2)
O5	0.3205 (5)	1.1144 (5)	-0.04549 (18)	0.0489 (15)
C5	0.4025 (7)	1.0824 (6)	-0.0612 (2)	0.0326 (16)
O6	0.7119 (5)	1.1041 (4)	0.00476 (17)	0.0472 (15)
C6	0.6506 (7)	1.0826 (5)	-0.0303 (2)	0.0320 (16)
O7	0.5325 (5)	0.8118 (4)	-0.04813 (19)	0.0542 (16)
C7	0.5359 (7)	0.8947 (6)	-0.0621 (2)	0.0403 (19)
O8	0.7786 (5)	0.9809 (5)	-0.1290 (2)	0.0664 (19)
C8	0.6912 (7)	0.9995 (6)	-0.1153 (3)	0.0377 (17)
C11	0.4459 (8)	0.8884 (6)	-0.2005 (2)	0.049 (2)
H11	0.3644	0.8625	-0.2158	0.058*
C12	0.5024 (8)	0.7932 (6)	-0.1742 (3)	0.062 (2)
H12A	0.5809	0.8127	-0.1548	0.074*
H12B	0.4483	0.7691	-0.1529	0.074*
C13	0.5237 (10)	0.7052 (7)	-0.2062 (4)	0.086 (3)
H13A	0.5748	0.6524	-0.1876	0.104*
H13B	0.4448	0.6731	-0.2192	0.104*
C14	0.5831 (11)	0.7387 (8)	-0.2448 (4)	0.109 (4)
H14A	0.5850	0.6799	-0.2663	0.130*
H14B	0.6682	0.7572	-0.2318	0.130*
C15	0.5239 (10)	0.8293 (7)	-0.2729 (3)	0.084 (3)

H15A	0.4459	0.8071	-0.2918	0.101*
H15B	0.5772	0.8533	-0.2945	0.101*
C16	0.5006 (12)	0.9189 (7)	-0.2408 (3)	0.106 (4)
H16A	0.5787	0.9538	-0.2292	0.127*
H16B	0.4465	0.9694	-0.2596	0.127*
C21	0.2444 (6)	0.9637 (5)	-0.1558 (2)	0.0335 (16)
H21	0.2229	1.0156	-0.1332	0.040*
C22	0.1526 (6)	0.9801 (6)	-0.2010 (3)	0.045 (2)
H22A	0.1706	0.9317	-0.2252	0.054*
H22B	0.1606	1.0510	-0.2125	0.054*
C23	0.0220 (6)	0.9629 (7)	-0.1932 (3)	0.055 (2)
H23A	0.0008	1.0168	-0.1719	0.066*
H23B	-0.0342	0.9696	-0.2234	0.066*
C24	0.0052 (7)	0.8580 (6)	-0.1725 (3)	0.052 (2)
H24A	0.0171	0.8040	-0.1952	0.062*
H24B	-0.0786	0.8520	-0.1662	0.062*
C25	0.0956 (7)	0.8419 (7)	-0.1270 (3)	0.053 (2)
H25A	0.0869	0.7711	-0.1154	0.063*
H25B	0.0768	0.8904	-0.1030	0.063*
C26	0.2275 (6)	0.8586 (6)	-0.1339 (3)	0.0404 (19)
H26A	0.2824	0.8536	-0.1033	0.048*
H26B	0.2502	0.8038	-0.1544	0.048*
C31	0.7281 (6)	1.4343 (6)	-0.0131 (3)	0.0356 (17)
C32	0.6614 (7)	1.3866 (7)	0.0184 (3)	0.050 (2)
H32	0.6466	1.3147	0.0167	0.060*
C33	0.6185 (8)	1.4448 (7)	0.0513 (3)	0.063 (3)
H33	0.5734	1.4123	0.0720	0.076*
C34	0.6389 (9)	1.5482 (8)	0.0551 (3)	0.064 (3)
H34	0.6096	1.5865	0.0786	0.077*
C35	0.7018 (8)	1.5968 (7)	0.0248 (3)	0.061 (2)
H35	0.7139	1.6691	0.0268	0.074*
C36	0.7483 (7)	1.5395 (6)	-0.0091 (3)	0.0455 (19)
H36	0.7939	1.5730	-0.0294	0.055*
C41	0.8483 (7)	1.4415 (5)	-0.0956 (2)	0.0349 (16)
C42	0.9727 (7)	1.4540 (6)	-0.0905 (3)	0.046 (2)
H42	1.0246	1.4176	-0.0666	0.055*
C43	1.0226 (8)	1.5194 (7)	-0.1201 (3)	0.058 (2)
H43	1.1082	1.5269	-0.1163	0.070*
C44	0.9504 (10)	1.5723 (7)	-0.1541 (3)	0.063 (3)
H44	0.9852	1.6175	-0.1737	0.076*
C45	0.8268 (10)	1.5608 (8)	-0.1603 (3)	0.071 (3)
H45	0.7761	1.5977	-0.1844	0.086*
C46	0.7762 (8)	1.4958 (6)	-0.1317 (3)	0.058 (2)
H46	0.6906	1.4877	-0.1366	0.069*
C51	0.9020 (6)	1.2746 (6)	-0.0293 (2)	0.0313 (16)
C52	0.9654 (6)	1.2943 (6)	0.0154 (2)	0.0355 (17)
H52	0.9436	1.3517	0.0324	0.043*
C53	1.0615 (7)	1.2305 (7)	0.0357 (3)	0.049 (2)
H53	1.1023	1.2438	0.0667	0.059*

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C54	1.0970 (8)	1.1487 (7)	0.0112 (3)	0.056 (2)
H54	1.1633	1.1068	0.0248	0.067*
C55	1.0353 (8)	1.1281 (7)	-0.0334 (3)	0.059 (2)
H55	1.0593	1.0717	-0.0504	0.071*
C56	0.9379 (7)	1.1900 (6)	-0.0535 (3)	0.048 (2)
H56	0.8955	1.1746	-0.0840	0.058*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Re1	0.03397 (18)	0.02579 (15)	0.02803 (15)	-0.00534 (15)	0.00033 (13)	0.00434 (13)
Re2	0.02610 (16)	0.02228 (14)	0.02545 (14)	-0.00191 (14)	0.00322 (11)	0.00123 (13)
Ag1	0.0325 (3)	0.0261 (3)	0.0354 (3)	-0.0083 (3)	0.0007 (3)	-0.0002 (2)
P1	0.0288 (10)	0.0236 (9)	0.0290 (9)	-0.0034 (8)	0.0047 (8)	-0.0003 (8)
P2	0.0302 (11)	0.0266 (10)	0.0399 (11)	-0.0082 (9)	0.0044 (9)	-0.0024 (8)
O1	0.056 (4)	0.065 (4)	0.043 (3)	-0.002 (3)	-0.006 (3)	0.014 (3)
C1	0.050 (5)	0.036 (4)	0.033 (3)	-0.006 (4)	0.003 (3)	0.008 (3)
O2	0.049 (4)	0.107 (6)	0.081 (5)	-0.022 (4)	0.032 (4)	0.005 (4)
C2	0.044 (4)	0.064 (6)	0.029 (4)	-0.024 (4)	0.004 (3)	-0.001 (4)
O3	0.063 (4)	0.059 (4)	0.068 (4)	0.026 (4)	0.017 (3)	-0.002 (3)
C3	0.047 (4)	0.035 (4)	0.034 (4)	0.005 (4)	-0.001 (3)	-0.007 (3)
O4	0.123 (6)	0.031 (3)	0.082 (5)	-0.016 (4)	-0.031 (4)	0.020 (3)
C4	0.081 (7)	0.038 (4)	0.046 (5)	-0.021 (4)	-0.016 (4)	0.016 (4)
O5	0.040 (3)	0.066 (4)	0.042 (3)	0.014 (3)	0.012 (3)	-0.001 (3)
C5	0.040 (4)	0.034 (4)	0.020 (3)	-0.003 (3)	-0.004 (3)	0.003 (3)
O6	0.050 (4)	0.056 (4)	0.031 (3)	-0.018 (3)	-0.005 (3)	0.001 (3)
C6	0.037 (4)	0.026 (4)	0.032 (3)	0.000 (3)	0.003 (3)	0.002 (3)
O7	0.074 (4)	0.029 (3)	0.054 (4)	-0.004 (3)	-0.002 (3)	0.013 (3)
C7	0.055 (5)	0.033 (4)	0.031 (4)	-0.007 (4)	0.001 (4)	0.005 (3)
O8	0.046 (4)	0.085 (5)	0.074 (4)	0.011 (4)	0.026 (3)	-0.016 (4)
C8	0.036 (4)	0.036 (4)	0.039 (4)	0.002 (3)	0.002 (3)	-0.006 (3)
C11	0.077 (6)	0.039 (4)	0.030 (4)	0.015 (4)	0.008 (4)	-0.010 (3)
C12	0.053 (6)	0.037 (5)	0.097 (7)	0.008 (4)	0.017 (5)	-0.002 (4)
C13	0.098 (9)	0.049 (6)	0.111 (8)	0.016 (6)	0.015 (7)	-0.019 (5)
C14	0.120 (10)	0.054 (6)	0.175 (11)	0.021 (7)	0.091 (8)	-0.018 (7)
C15	0.119 (9)	0.071 (7)	0.075 (7)	0.001 (7)	0.052 (6)	-0.032 (5)
C16	0.191 (12)	0.048 (6)	0.109 (8)	0.014 (7)	0.110 (8)	-0.008 (5)
C21	0.032 (3)	0.032 (4)	0.038 (4)	-0.007 (3)	0.009 (3)	-0.003 (3)
C22	0.029 (4)	0.049 (5)	0.054 (5)	-0.009 (4)	0.000 (3)	0.009 (4)
C23	0.032 (4)	0.065 (5)	0.066 (6)	-0.009 (5)	0.007 (4)	-0.003 (5)
C24	0.038 (4)	0.043 (5)	0.080 (6)	-0.010 (4)	0.028 (4)	-0.017 (4)
C25	0.059 (5)	0.047 (5)	0.059 (5)	-0.022 (4)	0.029 (4)	-0.009 (4)
C26	0.046 (4)	0.038 (4)	0.040 (4)	-0.007 (4)	0.013 (4)	0.003 (3)
C31	0.026 (4)	0.034 (4)	0.045 (4)	-0.005 (3)	0.003 (3)	-0.008 (3)
C32	0.050 (5)	0.046 (5)	0.061 (5)	0.001 (4)	0.027 (4)	-0.009 (4)
C33	0.057 (6)	0.063 (6)	0.078 (6)	-0.006 (5)	0.035 (5)	-0.018 (5)
C34	0.063 (6)	0.062 (6)	0.069 (6)	0.014 (5)	0.019 (5)	-0.023 (5)
C35	0.062 (6)	0.038 (5)	0.084 (7)	0.006 (5)	0.012 (5)	-0.016 (4)

C36	0.045 (5)	0.034 (4)	0.058 (5)	-0.003 (4)	0.011 (4)	-0.004 (4)
C41	0.040 (4)	0.024 (4)	0.041 (4)	-0.006 (3)	0.007 (3)	-0.005 (3)
C42	0.042 (4)	0.050 (5)	0.044 (4)	-0.022 (4)	0.005 (4)	0.000 (4)
C43	0.056 (5)	0.058 (6)	0.064 (6)	-0.028 (5)	0.020 (4)	0.000 (4)
C44	0.088 (6)	0.050 (6)	0.055 (5)	-0.027 (5)	0.020 (5)	0.003 (4)
C45	0.079 (6)	0.061 (6)	0.075 (7)	-0.002 (6)	0.017 (6)	0.033 (5)
C46	0.050 (5)	0.049 (6)	0.072 (6)	-0.002 (4)	0.005 (4)	0.026 (4)
C51	0.025 (4)	0.031 (4)	0.037 (4)	-0.010 (3)	0.005 (3)	0.002 (3)
C52	0.035 (4)	0.039 (4)	0.036 (4)	-0.003 (3)	0.014 (3)	0.007 (3)
C53	0.037 (5)	0.067 (6)	0.041 (4)	0.001 (4)	0.004 (4)	0.014 (4)
C54	0.038 (5)	0.054 (6)	0.079 (6)	0.008 (4)	0.022 (4)	0.020 (5)
C55	0.038 (5)	0.051 (5)	0.092 (6)	0.005 (4)	0.022 (5)	-0.013 (5)
C56	0.041 (5)	0.040 (5)	0.064 (5)	-0.007 (4)	0.011 (4)	-0.015 (4)

Geometric parameters (Å, °)

Re1—C1	1.913 (7)	C12—C13	1.503 (9)
Re1—C2	1.965 (9)	C13—C14	1.453 (10)
Re1—C4	1.975 (9)	C14—C15	1.501 (10)
Re1—C3	1.985 (9)	C15—C16	1.526 (9)
Re1—P1	2.4495 (18)	C21—C22	1.517 (8)
Re1—Ag1	2.7957 (7)	C21—C26	1.517 (8)
Re1—Re2	3.1834 (6)	C22—C23	1.519 (8)
Re2—C7	1.934 (8)	C23—C24	1.500 (9)
Re2—C6	1.964 (7)	C24—C25	1.516 (9)
Re2—C5	1.965 (8)	C25—C26	1.525 (8)
Re2—C8	1.985 (8)	C31—C36	1.374 (10)
Re2—P1	2.4398 (18)	C31—C32	1.409 (10)
Re2—Ag1	2.8235 (7)	C32—C33	1.357 (11)
Ag1—P2	2.4274 (19)	C33—C34	1.351 (13)
P1—C21	1.856 (7)	C34—C35	1.360 (12)
P1—C11	1.860 (7)	C35—C36	1.393 (11)
P2—C51	1.812 (7)	C41—C42	1.369 (10)
P2—C31	1.820 (8)	C41—C46	1.383 (10)
P2—C41	1.825 (8)	C42—C43	1.381 (10)
O1—C1	1.150 (8)	C43—C44	1.334 (12)
O2—C2	1.153 (9)	C44—C45	1.358 (12)
O3—C3	1.141 (9)	C45—C46	1.362 (11)
O4—C4	1.146 (9)	C51—C52	1.376 (9)
O5—C5	1.160 (8)	C51—C56	1.388 (10)
O6—C6	1.146 (7)	C52—C53	1.389 (10)
O7—C7	1.143 (8)	C53—C54	1.362 (11)
O8—C8	1.132 (9)	C54—C55	1.370 (11)
C11—C16	1.454 (9)	C55—C56	1.383 (11)
C11—C12	1.517 (9)		
C1—Re1—C2	90.8 (3)	C31—P2—C41	106.5 (3)
C1—Re1—C4	94.2 (3)	C51—P2—Ag1	108.7 (2)
C2—Re1—C4	88.1 (4)	C31—P2—Ag1	113.4 (2)
C1—Re1—C3	94.2 (3)	C41—P2—Ag1	117.0 (2)

supplementary materials

C2—Re1—C3	174.2 (3)	O1—C1—Re1	177.5 (8)
C4—Re1—C3	88.7 (4)	O2—C2—Re1	177.6 (8)
C1—Re1—P1	92.6 (2)	O3—C3—Re1	176.3 (7)
C2—Re1—P1	94.0 (3)	O4—C4—Re1	171.6 (9)
C4—Re1—P1	172.9 (2)	O5—C5—Re2	178.1 (7)
C3—Re1—P1	88.6 (2)	O6—C6—Re2	174.6 (6)
C1—Re1—Ag1	160.3 (2)	O7—C7—Re2	177.8 (7)
C2—Re1—Ag1	79.5 (2)	O8—C8—Re2	176.8 (7)
C4—Re1—Ag1	68.7 (2)	C16—C11—C12	115.0 (7)
C3—Re1—Ag1	94.8 (2)	C16—C11—P1	117.8 (6)
P1—Re1—Ag1	105.05 (4)	C12—C11—P1	114.0 (5)
C1—Re1—Re2	141.6 (2)	C13—C12—C11	113.5 (7)
C2—Re1—Re2	88.0 (2)	C14—C13—C12	112.7 (8)
C4—Re1—Re2	124.2 (2)	C13—C14—C15	115.4 (9)
C3—Re1—Re2	89.8 (2)	C14—C15—C16	111.5 (8)
P1—Re1—Re2	49.24 (4)	C11—C16—C15	114.6 (7)
Ag1—Re1—Re2	55.906 (16)	C22—C21—C26	111.5 (6)
C7—Re2—C6	92.2 (3)	C22—C21—P1	113.9 (5)
C7—Re2—C5	93.2 (3)	C26—C21—P1	114.1 (5)
C6—Re2—C5	88.3 (3)	C21—C22—C23	111.4 (6)
C7—Re2—C8	92.8 (3)	C24—C23—C22	112.2 (7)
C6—Re2—C8	89.4 (3)	C23—C24—C25	110.9 (6)
C5—Re2—C8	173.6 (3)	C24—C25—C26	111.7 (6)
C7—Re2—P1	94.3 (2)	C21—C26—C25	111.8 (6)
C6—Re2—P1	173.1 (2)	C36—C31—C32	118.1 (8)
C5—Re2—P1	89.11 (19)	C36—C31—P2	123.7 (7)
C8—Re2—P1	92.5 (2)	C32—C31—P2	118.1 (6)
C7—Re2—Ag1	161.0 (2)	C33—C32—C31	119.8 (9)
C6—Re2—Ag1	69.2 (2)	C34—C33—C32	121.7 (10)
C5—Re2—Ag1	89.7 (2)	C33—C34—C35	120.0 (9)
C8—Re2—Ag1	83.9 (2)	C34—C35—C36	120.0 (9)
P1—Re2—Ag1	104.49 (5)	C31—C36—C35	120.4 (8)
C7—Re2—Re1	143.8 (2)	C42—C41—C46	117.3 (8)
C6—Re2—Re1	123.9 (2)	C42—C41—P2	123.0 (6)
C5—Re2—Re1	86.26 (19)	C46—C41—P2	119.7 (6)
C8—Re2—Re1	90.1 (2)	C41—C42—C43	120.6 (8)
P1—Re2—Re1	49.51 (4)	C44—C43—C42	120.6 (9)
Ag1—Re2—Re1	55.081 (14)	C43—C44—C45	120.2 (9)
P2—Ag1—Re1	153.58 (5)	C44—C45—C46	120.0 (9)
P2—Ag1—Re2	135.63 (5)	C45—C46—C41	121.3 (9)
Re1—Ag1—Re2	69.013 (15)	C52—C51—C56	118.0 (7)
C21—P1—C11	104.1 (4)	C52—C51—P2	123.7 (6)
C21—P1—Re2	115.7 (2)	C56—C51—P2	118.3 (6)
C11—P1—Re2	119.6 (3)	C51—C52—C53	120.7 (8)
C21—P1—Re1	114.2 (2)	C54—C53—C52	120.6 (8)
C11—P1—Re1	121.6 (3)	C53—C54—C55	119.6 (8)
Re2—P1—Re1	81.25 (6)	C54—C55—C56	120.2 (9)
C51—P2—C31	106.4 (3)	C55—C56—C51	120.9 (8)
C51—P2—C41	103.9 (3)		