attached to the same Hg would be in different tautomeric forms. In this case the twist of the amide group at C(8)C(9) may be due to intermolecular interactions.

In addition to the covalent Hg—N bonds, there are intermolecular contacts from Hg to O(2), one of 2·67 (2) Å to O(2′) of a *c*-glide-related molecule, and the other of 2·83 (3) Å to O(2″) of a centrosymmetrically related molecule. The effective coordination of Hg is thus of an irregular fourfold type similar to that found in (chloromercurio)acetaldehyde (Halfpenny & Small, 1979). The angles around Hg are given in Table 2. There are no short contacts from O(1) to neighbouring Hg atoms; instead, there is an intermolecular distance of 3·03 (5) Å to N(2) of a *c*-glide-related molecule; an H atom bonded with normal distances and angles to either O(1) or N(2) would be close to the O(1′)···N(2) direction. This contact must therefore be regarded as a weak hydrogen bond, either N—H···O or N···H—O depending upon whether the amide group at C(8) is in the keto or enol form. The presence, in this structure, of a balance between intermolecular Hg···O bonding and hydrogen bonds suggest that there is a similarity in the energies of the two types of bond. The molecules are arranged with their longest directions parallel to *b*; *c*-glide-related molecules are bound by Hg···O bonds and hydrogen bonds into strips one molecule wide. Pairs of adjacent centrosymmetrically related strips are bonded by Hg···O bonds.

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(2-Benzoylphenyl)tricarbonyl(triphenylphosphine)rhenium

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Abstract. $[\mathrm{Re(C_{13}H_9O)(C_{18}H_{15}P)(CO)_3}]$, $\mathrm{C_{34}H_{24}O_4PRe}$, $M_r = 713{\cdot}7$, triclinic, $a = 11{\cdot}708\,(2)$, $b = 12{\cdot}371\,(2)$, $c = 9{\cdot}922\,(2)$ Å, $\alpha = 88{\cdot}60\,(7)$, $\beta = 77{\cdot}45\,(7)$, $\gamma = 89{\cdot}58\,(7)°$, $U = 1402$ Å^3; $Z = 2$, $D_c = 1{\cdot}691$ Mg m^{-3}; $F(000) = 350$; Mo $K\alpha$ radiation, $\lambda = 0{\cdot}71069$ Å, μ(Mo $K\alpha$) = 2·11 mm^{-1}. Space group $P\bar{1}$. Final $R = 0{\cdot}08$ for 5780 unique X-ray diffractometer data. The molecular structure has been elucidated.

Introduction. The title compound is a metallation product of benzophenone and $[\mathrm{Re(C_6H_5)(CO)_5}]$ reacted with phosphine (Schwab, 1975). The following is a structural characterization of this Re metallated benzophenone. The structure was solved by Patterson and Fourier methods and refined by blocked full-matrix least squares with isotropic temperature factors for C(1), O(1), C(2), O(2), C(3), O(3), C(4) and O(4), a common isotropic temperature factor for H [0·05 (1) Å^2] and anisotropic temperature factors for the remaining atoms. The phenyl rings were treated as rigid groups (C—C—C = 120, C—C—H = 120°, C—C = 1·395, C—H = 1·08 Å). Refinement converged with unit weights to $R = 0{\cdot}08$.*

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* Lists of structure factors and thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35065 (36 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Data were collected with a crystal 0·17 × 0·40 × 0·44 mm. Cell parameters were determined by least squares from the angles of 17 reflexions measured with a Hilger & Watts Y290 automatic four-circle diffractometer, graphite-monochromated Mo $K\alpha$ radiation and a scintillation counter. The intensities of 6614 reflexions ($I > 3\sigma$) with $2 \leq \theta \leq 30{\cdot}0°$ were measured by the $\omega/2\theta$ scan technique, with a scan width $\Delta 2\theta = 1{\cdot}34° + 0{\cdot}34° \tan\theta$ from background to background and a scan speed of 0·02° s^{-1} in 2θ. Backgrounds were measured at either end of the scan range for 7 s. Five standards were measured every fifty reflexions, and showed only random deviations from their mean intensities. Lp and absorption corrections were applied, and after averaging the equivalent reflexions the data set contained 5780 independent reflexions.

The data were processed on an IBM 370/158 computer with *SHELX* (Sheldrick, 1976). The scattering factors were taken from Cromer & Mann (1968) and Cromer & Liberman (1970) for Re, P, O and C and from Cromer (personal communication to G. M. Sheldrick) for H. The figures were drawn with *PLUTO*, written by Drs W. D. S. Motherwell and W. Clegg, and *POP*1 written by B. W. van de Waal.

Discussion. The molecular structure of the title compound is shown in Fig. 1; a stereoview of the two molecules in the unit cell is given in Fig. 2. The final

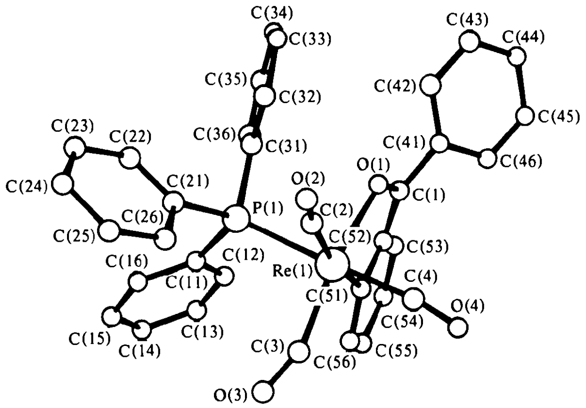

Fig. 1. General view of the molecule.

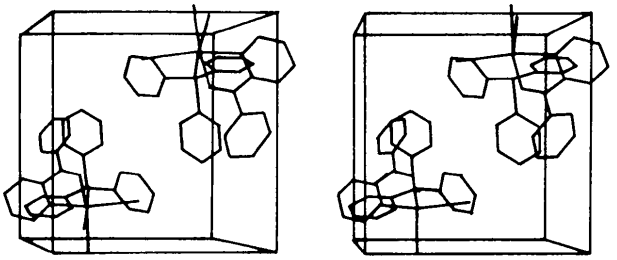

Fig. 2. Stereoscopic view of the molecules in the unit cell.

Table 1. *Positional parameters* ($\times 10^4$) *with e.s.d.'s in parentheses*

	x	y	z
Re(1)	3323 (0)	1603 (0)	679 (1)
P(1)	2915 (3)	2578 (3)	2889 (4)
C(11)	1612 (9)	2174 (10)	4206 (11)
C(12)	507 (9)	2224 (10)	3895 (11)
C(13)	−471 (9)	1856 (10)	4862 (11)
C(14)	−342 (9)	1438 (10)	6139 (11)
C(15)	763 (9)	1388 (10)	6450 (11)
C(16)	1741 (9)	1756 (10)	5483 (11)
H(12)	408 (9)	2548 (10)	2906 (11)
H(13)	−1327 (9)	1894 (10)	4620 (11)
H(14)	−1100 (9)	1152 (10)	6887 (11)
H(15)	862 (9)	1064 (10)	7439 (11)
H(16)	2596 (9)	1717 (10)	5724 (11)
C(21)	4047 (9)	2516 (7)	3901 (11)
C(22)	4103 (9)	3330 (7)	4833 (11)
C(23)	4865 (9)	3228 (7)	5731 (11)
C(24)	5571 (9)	2311 (7)	5698 (11)
C(25)	5515 (9)	1497 (7)	4766 (11)
C(26)	4753 (9)	1600 (7)	3867 (11)
H(22)	3557 (9)	4040 (7)	4858 (11)
H(23)	4908 (9)	3858 (7)	6453 (11)
H(24)	6161 (9)	2232 (7)	6395 (11)
H(25)	6061 (9)	788 (7)	4741 (11)
H(26)	4710 (9)	970 (7)	3146 (11)
C(31)	2803 (6)	4038 (7)	2549 (11)
C(32)	3841 (6)	4572 (7)	1951 (11)
C(33)	3830 (6)	5682 (7)	1670 (11)
C(34)	2781 (6)	6258 (7)	1989 (11)
C(35)	1743 (6)	5724 (7)	2588 (11)
C(36)	1754 (6)	4614 (7)	2868 (11)
H(32)	4654 (6)	4126 (7)	1704 (11)
H(33)	4634 (6)	6096 (7)	1206 (11)
H(34)	2772 (6)	7117 (7)	1771 (11)
H(35)	930 (6)	6170 (7)	2834 (11)
H(36)	950 (6)	4200 (7)	3332 (11)
C(41)	2153 (9)	4312 (8)	−1593 (11)
C(42)	2892 (9)	5189 (8)	−1578 (11)
C(43)	2950 (9)	6030 (8)	−2553 (11)
C(44)	2269 (9)	5993 (8)	−3544 (11)
C(45)	1530 (9)	5116 (8)	−3559 (11)
C(46)	1472 (9)	4276 (8)	−2584 (11)
H(42)	3419 (9)	5217 (8)	−811 (11)
H(43)	3522 (9)	6709 (8)	−2542 (11)
H(44)	2314 (9)	6644 (8)	−4299 (11)
H(45)	1003 (9)	5088 (8)	−4326 (11)
H(46)	900 (9)	3597 (8)	−2595 (11)
C(51)	1471 (8)	1733 (7)	572 (13)
C(52)	1216 (8)	2705 (7)	−44 (13)
C(53)	66 (8)	2945 (7)	−126 (13)
C(54)	−828 (8)	2213 (7)	408 (13)
C(55)	−572 (8)	1241 (7)	1023 (13)
C(56)	577 (8)	1001 (7)	1105 (13)
H(53)	−131 (8)	3698 (7)	−602 (13)
H(54)	−1718 (8)	2399 (7)	345 (13)
H(55)	−1265 (8)	674 (7)	1437 (13)
H(56)	775 (8)	249 (7)	1582 (13)
C(1)	2198 (11)	3369 (11)	−631 (14)
O(1)	3174 (8)	3116 (7)	−430 (10)
C(2)	5010 (12)	1743 (13)	494 (17)
O(2)	5980 (11)	1870 (11)	423 (15)
C(3)	3242 (14)	194 (12)	1625 (17)
O(3)	3143 (12)	−580 (11)	2269 (16)
C(4)	3592 (17)	902 (16)	−1089 (19)
O(4)	3668 (13)	419 (13)	−2060 (18)

Table 2. *Bond lengths* (Å) *and angles* (°)

Re(1)–P(1)	2·481 (4)	O(1)–Re(1)–C(3)	171·9 (5)
Re(1)–O(1)	2·174 (9)	O(1)–Re(1)–C(4)	87·4 (6)
Re(1)–C(2)	1·951 (15)	O(1)–Re(1)–C(51)	74·4 (4)
Re(1)–C(3)	1·952 (15)	C(2)–Re(1)–C(3)	94·1 (7)
Re(1)–C(4)	1·938 (18)	C(2)–Re(1)–C(4)	89·8 (7)
Re(1)–C(51)	2·199 (10)	C(2)–Re(1)–C(51)	167·9 (5)
P(1)–C(11)	1·843 (11)	C(3)–Re(1)–C(4)	90·2 (7)
P(1)–C(21)	1·829 (12)	C(3)–Re(1)–C(51)	97·8 (5)
P(1)–C(31)	1·838 (9)	C(4)–Re(1)–C(51)	87·4 (6)
C(1)–O(1)	1·240 (17)	Re(1)–O(1)–C(1)	117·7 (9)
C(1)–C(41)	1·497 (17)	Re(1)–C(2)–O(2)	176·6 (14)
C(1)–C(52)	1·427 (17)	Re(1)–C(3)–O(3)	174·2 (15)
C(2)–O(2)	1·134 (20)	Re(1)–C(4)–O(4)	173·1 (18)
C(3)–O(3)	1·130 (21)	Re(1)–C(51)–C(52)	112·6 (7)
C(4)–O(4)	1·134 (25)	Re(1)–C(51)–C(56)	127·3 (8)
		O(1)–C(1)–C(52)	119·1 (12)
Re(1)–P(1)–C(11)	117·7 (4)	O(1)–C(1)–C(41)	116·7 (11)
Re(1)–P(1)–C(21)	116·7 (4)	C(41)–C(1)–C(52)	124·1 (11)
Re(1)–P(1)–C(31)	110·0 (3)	C(1)–C(52)–C(51)	115·7 (10)
C(11)–P(1)–C(21)	101·1 (5)	C(1)–C(52)–C(53)	124·2 (10)
C(11)–P(1)–C(31)	107·6 (5)	P(1)–C(11)–C(12)	120·0 (9)
C(21)–P(1)–C(31)	102·2 (5)	P(1)–C(11)–C(16)	119·9 (9)
P(1)–Re(1)–O(1)	89·8 (3)	P(1)–C(21)–C(22)	119·4 (8)
P(1)–Re(1)–C(2)	91·9 (5)	P(1)–C(21)–C(26)	120·1 (8)
P(1)–Re(1)–C(3)	92·4 (5)	P(1)–C(31)–C(32)	116·5 (7)
P(1)–Re(1)–C(4)	176·8 (6)	P(1)–C(31)–C(36)	123·5 (7)
P(1)–Re(1)–C(51)	90·4 (3)	C(1)–C(41)–C(42)	118·9 (10)
O(1)–Re(1)–C(2)	93·6 (5)	C(1)–C(41)–C(46)	120·8 (10)

atomic coordinates, bond distances and angles are given in Tables 1 and 2.

Of special interest in the molecule is the heterocyclic five-membered ring containing Re(1), O(1), C(1), C(52) and C(51), the geometry of which, apart from the angle at the metal atom, agrees with the corresponding ring in $[Mn(CH_3COC_6H_4)(CO)_4]$ (Knobler, Crawford & Kaesz, 1975): C–Mn–O 79·4 (1), C(51)–Re(1)–O(1) 74·4 (4)°. The maximum distance of the atoms of the five-membered ring from the least-squares plane of the phenyl ring, atoms C(51) to C(56), is 0·125 (1) Å.

The coordination around the Re atom is a distorted octahedron. Each of the three CO ligands at the Re atom is *trans* to a different atom.

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Dichlorooxobis(triphenylphosphine oxide)vanadium(IV)

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Abstract. $C_{36}H_{30}Cl_2O_3P_2V$, $[V(C_{18}H_{15}OP)_2Cl_2O]$, monoclinic, $P2_1/c$, a = 17·19 (1), b = 18·34 (1), c = 11·15 (1) Å, β = 98·67 (5)°, V = 3473·3 Å^3, M_r = 694·4, Z = 4, D_c = 1·328, D_m = 1·33 Mg m^{-3} (by flotation); μ(Mo $K\alpha$) = 0·51 mm^{-1}. The V atom is pentacoordinate with the triphenylphosphine oxide ligands in a *trans* arrangement; the O atoms from these ligands and two Cl atoms comprise the base of a square pyramid which is completed by an apical double-bonded O atom.

Introduction. Complexes of oxovanadium(IV) have been studied extensively (Kepert, 1972) and, in particular, complexes of the type $VOCl_2.2L$ (du Preez & Gibson, 1970). However, despite the large number of compounds studied, not much reliable spectroscopic information has become available which is of use for making stereochemical predictions by comparison with compounds of known structure. Usually only infrared measurements are reported, and assignments on the basis of these alone are only tentative. In an investigation of the vibrational spectra of some oxovanadium(IV) complexes (Gellatly & Caira, 1979), a strong band at 384 cm^{-1} in the infrared spectrum of

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