Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
Sn1	0.16618 (4)	0.51355 (4)	0.26968 (3)	0.0498 (2)
Sn2	−0.12148 (4)	0.52959 (4)	0.45381 (3)	0.04069 (15)
S1	0.6214 (2)	0.3932 (2)	0.24971 (15)	0.0574 (5)
S2	0.5663 (2)	0.1967 (2)	0.3130 (2)	0.0853 (7)
S3	−0.2731 (2)	0.6148 (2)	0.2180 (2)	0.0694 (6)
S4	−0.2112 (2)	0.8031 (2)	0.1428 (2)	0.1047 (10)
O1	0.3469 (5)	0.4643 (5)	0.3109 (4)	0.084 (2)
O2	0.3227 (4)	0.4551 (4)	0.4733 (4)	0.0633 (14)
O3	−0.0197 (4)	0.5547 (4)	0.2531 (3)	0.0514 (12)
O4	0.0779 (5)	0.5626 (4)	0.0948 (4)	0.0673 (15)
O5	0.0763 (4)	0.5051 (3)	0.4136 (3)	0.0404 (10)
N1	0.7249 (6)	0.2172 (5)	0.1461 (5)	0.065 (2)
N2	−0.4218 (7)	0.8033 (6)	0.2592 (7)	0.109 (3)
C1	0.1973 (7)	0.6583 (6)	0.2501 (6)	0.066 (2)
C2	0.0999 (8)	0.7507 (7)	0.2333 (7)	0.079 (3)
C3	0.1322 (9)	0.8498 (7)	0.2239 (7)	0.091 (3)
C4	0.0352 (11)	0.9377 (8)	0.1988 (10)	0.141 (5)
C5	0.2244 (8)	0.3652 (6)	0.1929 (6)	0.080 (3)
C6	0.3385 (13)	0.3319 (13)	0.1138 (10)	0.160 (6)
C7	0.3756 (13)	0.3949 (13)	0.0517 (11)	0.170 (7)
C8	0.4980 (10)	0.3545 (12)	−0.0349 (8)	0.158 (6)
C9	0.3857 (6)	0.4493 (5)	0.3859 (6)	0.050 (2)
C10	0.5232 (6)	0.4235 (6)	0.3734 (5)	0.061 (2)
C11	0.6438 (6)	0.2597 (6)	0.2305 (5)	0.054 (2)
C12	0.7953 (8)	0.2739 (7)	0.0761 (6)	0.077 (3)
C13	0.9186 (8)	0.2623 (8)	0.0961 (7)	0.097 (3)
C14	0.7569 (10)	0.1062 (7)	0.1198 (8)	0.096 (3)
C15	0.6812 (12)	0.0880 (8)	0.0542 (9)	0.134 (5)
C16	−0.0153 (6)	0.5626 (5)	0.1579 (5)	0.048 (2)
C17	−0.1308 (7)	0.5683 (7)	0.1279 (6)	0.070 (2)
C18	−0.3087 (7)	0.7493 (6)	0.2076 (6)	0.069 (2)
C19	−0.5313 (13)	0.7445 (10)	0.3019 (11)	0.150 (6)
C20	−0.5150 (13)	0.7381 (10)	0.3934 (10)	0.167 (6)
C21	−0.4686 (11)	0.9161 (8)	0.2603 (10)	0.124 (4)
C22	−0.5374 (12)	0.9511 (10)	0.1787 (13)	0.187 (7)
C23	−0.1725 (7)	0.6916 (5)	0.4463 (5)	0.060 (2)
C24	−0.2208 (9)	0.7526 (6)	0.5433 (7)	0.088 (3)
C25	−0.2362 (12)	0.8686 (9)	0.5342 (10)	0.128 (4)
C26	−0.3187 (16)	0.9184 (11)	0.4738 (13)	0.211 (8)
C27	−0.1139 (6)	0.3924 (5)	0.3813 (5)	0.051 (2)
C28	−0.1327 (7)	0.3069 (6)	0.4485 (6)	0.063 (2)
C29	−0.1139 (10)	0.2070 (7)	0.3932 (7)	0.093 (3)
C30	−0.1268 (11)	0.1207 (8)	0.4605 (9)	0.129 (4)

Table 2. *Selected geometric parameters* (Å, °)

Sn1—O1	2.264 (5)	Sn2—O2^i	2.291 (5)
Sn1—O3	2.179 (4)	Sn2—O5	2.192 (4)
Sn1—O5	2.020 (4)	Sn2—O5^i	2.043 (4)
Sn1—C1	2.112 (8)	Sn2—C23	2.114 (7)
Sn1—C5	2.139 (8)	Sn2—C27	2.107 (7)
O1—Sn1—O3	171.2 (2)	O5^i—Sn2—C23	107.8 (2)
O1—Sn1—O5	90.5 (2)	O5^i—Sn2—C27	108.6 (2)
O1—Sn1—C1	84.7 (3)	C23—Sn2—O2^i	88.2 (3)
O1—Sn1—C5	86.3 (3)	C23—Sn2—O5	96.1 (2)
O3—Sn1—O5	80.8 (2)	C27—Sn2—O2^i	86.3 (2)
O3—Sn1—C1	99.6 (2)	C27—Sn2—O5	96.4 (2)
O3—Sn1—C5	95.1 (3)	C27—Sn2—C23	143.3 (3)
O5—Sn1—C1	109.8 (2)	C9—O1—Sn1	139.4 (5)
O5—Sn1—C5	109.5 (3)	C9—O2—Sn2^i	134.7 (5)
C1—Sn1—C5	139.6 (3)	C16—O3—Sn1	108.6 (4)
O5—Sn2—O2^i	168.5 (2)	Sn1—O5—Sn2^i	136.6 (2)
O5^i—Sn2—O2^i	91.8 (2)	Sn1—O5—Sn2	120.0 (2)
O5^i—Sn2—O5	76.7 (2)	Sn2^i—O5—Sn2	103.3 (2)

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

H atoms were allowed to ride on their parent C atoms with displacement factors 1.5 times those of the C atoms.

Data collection: *CAD-4 VAX/PC Fortran System* (Enraf–Nonius, 1988). Cell refinement: *CAD-4 VAX/PC Fortran System*. Data reduction: *Xtal*3.0 (Hall & Stewart, 1990). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *SHELXL*93.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: TA1020). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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μ-Phenylphosphido-μ-[(pentacarbonylmanganese)phenylphosphido]-bis(tetracarbonylrhenium)

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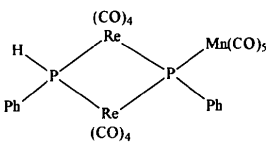
Abstract

A μ_3-phenylphosphido group bridges an Mn and two Re atoms in the title compound, $[Re_2(C_6H_5PH)\{C_6H_5PMn(CO)_5\}(CO)_8]$ (IUPAC name: tridecacarbonyl-1κ^5C,2κ^4C,3κ^4C-μ_3-phenylphosphanediido-1:2:3κ^3P-μ-phenylphosphanido-2:3κ^2P-manganesedirhenium). The Re atoms each have four carbonyl ligands and a common μ-

phosphido ligand. The resulting Re_2P_2 ring is not planar; this distortion is caused by inter- and intramolecular interactions.

Comment

The title compound, (I), belongs to the family of phosphido-bridged transition metal complexes with a central M_2P_2 ring (Flörke & Haupt, 1994, and references therein). There are two independent molecules per asymmetric unit with almost identical geometries (see Table 2). Four terminal carbonyl ligands and two bridging phosphido ligands at each Re atom of one molecule create two slightly distorted coordination octahedra that share one common edge.



(I)

The CO groups at the Re atoms have an eclipsed arrangement with torsion angles for the axial groups of average value 5.2°. One bridging P atom has a phenyl group and an H atom as terminal substituents, the other μ-P atom is linked to a phenyl and an $Mn(CO)_5$ group. The phenyl groups at both P atoms point to the same side of the Re_2P_2 ring; the orientations of their two planes are twisted by 81.5° (average value for both molecules).

The central M_2P_2 ring is not planar but folded along the P—P vector with a dihedral angle P_2Re1/P_2Re2 of 17.3°. With regard to the Re—P bond lengths the ring is asymmetric, having two bonds of average length 2.488 (4) Å (Re—P1) and two rather longer bonds of average length 2.594 (3) Å (Re—P2). This is associated with the different substituents at the P atoms, *i.e.* the sterically demanding $Mn(CO)_5$ group at P2. The enclosed ring angles of average values 74.9 (1)° for P—Re—P and 106.4 (1) and 100.3 (1)° for Re—P1—Re and Re—P2—Re, respectively, correspond well with those of other M_2P_2 complexes (Flörke & Haupt, 1994).

The $Mn(CO)_5$ group displays nearly undistorted octahedral coordination with average angles of 90.5 (7)°, but the carbonyl ligand C10—O10 with a P2—Mn—C10 angle of 83.7 (5)° is considerably bent, which is obviously caused by intermolecular repulsions: O10···O12($-x$, $y - \frac{1}{2}$, $\frac{1}{2} - z$) 3.047 (18) and O10···O3($-x$, $y - \frac{1}{2}$, $\frac{1}{2} - z$) 3.137 (16) Å. As a consequence, this ligand forms short non-bonding intramolecular contacts of 3.009 (17) (O10···O7) and 3.018 (19) Å (O10···O1) with CO ligands attached to the Re atoms. The Re—CO coordinations are not influenced by this interaction and show common geometries (average 89.0° for C—Re—C, average 175.9° for Re—C—O). However, the axial ligands on the $Mn(CO)_5$ side of the M_2P_2 ring are forced apart [O1···O7 5.512 (19) Å] and those on the phenyl side come as close as 3.023 (16) Å to each other (O2···O5) which, as a result, leads to the described distortion of the M_2P_2 ring. Corresponding relations hold for the second molecule.

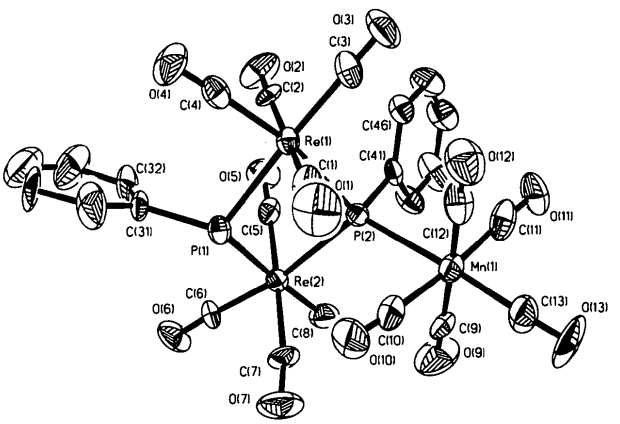


Fig. 1. Molecular structure of the title compound with H atoms omitted. Displacement ellipsoids are plotted at the 50% probability level. Only one of the two independent molecules is shown.

Experimental

The title compound was prepared by reaction of $Re_2(CO)_8(\mu$-$PHPh)_2$ with $BrMn(CO)_5$ and 1,8-diazabicyclo[5.4.0]undec-7-ene in thf solution at room temperature for 1 h. Recrystallization from methanol/hexane yielded suitable crystals for structure determination.

Crystal data

$[MnRe_2(C_6H_5P)(C_6H_6P)(CO)_{13}]$
M_r = 1008.64
Monoclinic
$P2_1/c$
a = 14.460 (1) Å
b = 13.158 (2) Å
c = 31.733 (5) Å
β = 94.130 (10)°
V = 6021.9 (14) Å^3
Z = 8
D_x = 2.225 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 40 reflections
θ = 7–18°
μ = 8.69 mm^{-1}
T = 293 (2) K
Prism
0.42 × 0.33 × 0.21 mm
Yellow

Data collection

Siemens *R3m* diffractometer
ω–2θ scans
Absorption correction: ψ scans
T_{min} = 0.476, T_{max} = 0.988
10742 measured reflections
10522 independent reflections
6476 observed reflections [$I > 2\sigma(I)$]
R_{int} = 0.0346
θ_{max} = 25.06°
h = −17 → 17
k = −15 → 15
l = 0 → 37
3 standard reflections monitored every 400 reflections
intensity decay: 3%

Refinement

Refinement on F^2
$R(F) = 0.0548$
$wR(F^2) = 0.1044$
$S = 1.172$
10522 reflections
776 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.0531P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.767$ e Å^{-3}
$\Delta\rho_{min} = -1.368$ e Å^{-3}
Extinction correction: *SHELXL*93 (Sheldrick, 1993)
Extinction coefficient: 0.00011 (2)
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
Re1	0.33183 (4)	0.93495 (4)	0.15990 (2)	0.02779 (15)
Re2	0.35153 (4)	0.67330 (4)	0.09806 (2)	0.0283 (2)
Mn1	0.57918 (14)	0.7552 (2)	0.19245 (7)	0.0381 (6)
P1	0.2445 (2)	0.7785 (3)	0.13783 (11)	0.0296 (8)
P2	0.4565 (2)	0.8099 (2)	0.13688 (11)	0.0259 (8)
C1	0.3421 (10)	0.8907 (13)	0.2206 (5)	0.045 (4)
O1	0.3442 (9)	0.8727 (11)	0.2550 (4)	0.082 (4)
C2	0.3173 (9)	0.9875 (10)	0.0997 (6)	0.041 (4)
O2	0.3102 (8)	1.0186 (9)	0.0678 (4)	0.065 (4)
C3	0.4072 (10)	1.0556 (12)	0.1767 (5)	0.042 (4)
O3	0.4479 (8)	1.1226 (8)	0.1885 (4)	0.063 (3)
C4	0.2191 (10)	1.0084 (11)	0.1700 (5)	0.038 (4)
O4	0.1509 (7)	1.0493 (9)	0.1776 (4)	0.064 (3)
C5	0.3474 (9)	0.7688 (11)	0.0491 (5)	0.034 (3)
O5	0.3423 (8)	0.8228 (8)	0.0211 (3)	0.056 (3)
C6	0.2572 (9)	0.5919 (11)	0.0677 (5)	0.041 (4)
O6	0.2025 (8)	0.5404 (8)	0.0510 (4)	0.059 (3)
C7	0.3542 (10)	0.5718 (11)	0.1452 (5)	0.044 (4)
O7	0.3455 (9)	0.5094 (9)	0.1686 (4)	0.080 (4)
C8	0.4447 (11)	0.5934 (11)	0.0692 (5)	0.045 (4)
O8	0.4937 (8)	0.5449 (9)	0.0522 (4)	0.075 (4)
C9	0.5940 (10)	0.6387 (12)	0.1600 (5)	0.046 (4)
O9	0.6027 (10)	0.5715 (10)	0.1390 (5)	0.091 (5)
C10	0.4796 (10)	0.6974 (12)	0.2178 (5)	0.052 (4)
O10	0.4161 (8)	0.6662 (9)	0.2320 (4)	0.073 (4)
C11	0.6715 (11)	0.8214 (14)	0.1640 (5)	0.050 (4)
O11	0.7303 (8)	0.8600 (10)	0.1482 (4)	0.068 (4)
C12	0.5623 (10)	0.8744 (14)	0.2220 (5)	0.049 (4)
O12	0.5530 (8)	0.9451 (10)	0.2421 (4)	0.073 (4)
C13	0.6674 (11)	0.7088 (14)	0.2334 (6)	0.056 (5)
O13	0.7223 (8)	0.6824 (12)	0.2567 (4)	0.103 (6)
C31	0.1263 (8)	0.8029 (10)	0.1142 (4)	0.032 (3)
C32	0.1112 (10)	0.8173 (11)	0.0712 (5)	0.054 (5)
C33	0.0241 (13)	0.8362 (15)	0.0521 (7)	0.086 (7)
C34	−0.0494 (16)	0.8437 (16)	0.0778 (7)	0.099 (9)
C35	−0.0346 (10)	0.8274 (14)	0.1207 (8)	0.086 (8)
C36	0.0528 (11)	0.8129 (14)	0.1398 (7)	0.086 (7)
C41	0.5284 (8)	0.8670 (8)	0.0977 (4)	0.029 (3)
C42	0.5747 (9)	0.8074 (11)	0.0690 (4)	0.041 (4)
C43	0.6289 (10)	0.8462 (13)	0.0396 (5)	0.060 (5)
C44	0.6371 (11)	0.9494 (10)	0.0355 (5)	0.053 (4)
C45	0.5915 (11)	1.0128 (12)	0.0613 (6)	0.063 (5)
C46	0.5364 (9)	0.9724 (10)	0.0905 (4)	0.035 (3)
Re3	0.17028 (4)	0.69585 (4)	0.34468 (2)	0.0303 (2)
Re4	0.15000 (4)	0.95426 (4)	0.40875 (2)	0.0333 (2)
Mn2	−0.07376 (15)	0.8798 (2)	0.31053 (7)	0.0400 (6)
P3	0.2576 (2)	0.8506 (3)	0.36861 (12)	0.0323 (9)
P4	0.0454 (2)	0.8210 (2)	0.36727 (11)	0.0268 (8)
C14	0.2832 (11)	0.6216 (12)	0.3322 (5)	0.047 (4)
O14	0.3482 (8)	0.5809 (10)	0.3255 (4)	0.074 (4)
C15	0.1796 (8)	0.6405 (10)	0.4022 (5)	0.031 (3)
O15	0.1855 (8)	0.6042 (9)	0.4352 (4)	0.067 (3)
C16	0.1632 (11)	0.7434 (11)	0.2856 (5)	0.043 (4)
O16	0.1622 (9)	0.7658 (11)	0.2518 (4)	0.078 (4)
C17	0.0917 (10)	0.5833 (11)	0.3246 (5)	0.047 (4)
O17	0.0506 (8)	0.5144 (9)	0.3107 (4)	0.067 (4)
C18	0.1514 (10)	0.8513 (13)	0.4551 (5)	0.046 (4)
O18	0.1528 (8)	0.7983 (9)	0.4820 (4)	0.064 (3)
C19	0.0574 (11)	1.0294 (12)	0.4370 (6)	0.053 (5)
O19	0.0095 (9)	1.0768 (9)	0.4569 (5)	0.087 (5)
C20	0.2440 (11)	1.0327 (11)	0.4406 (5)	0.045 (4)
O20	0.3005 (9)	1.0795 (9)	0.4600 (4)	0.082 (4)
C21	0.1511 (12)	1.0552 (12)	0.3649 (6)	0.061 (5)
O21	0.1570 (10)	1.1164 (9)	0.3392 (4)	0.085 (4)
C22	−0.0586 (10)	0.7633 (13)	0.2806 (5)	0.045 (4)
O22	−0.0478 (8)	0.6944 (10)	0.2592 (4)	0.070 (4)
C23	−0.0863 (10)	0.9916 (13)	0.3448 (6)	0.056 (5)
O23	−0.0952 (9)	1.0612 (9)	0.3647 (4)	0.080 (4)
C24	0.0261 (12)	0.9382 (13)	0.2859 (5)	0.054 (4)
O24	0.0874 (8)	0.9733 (10)	0.2712 (4)	0.076 (4)
C25	−0.1669 (10)	0.8151 (12)	0.3376 (6)	0.050 (4)
O25	−0.2254 (8)	0.7756 (10)	0.3525 (4)	0.075 (4)
C26	−0.1565 (13)	0.9278 (14)	0.2715 (6)	0.066 (5)
O26	−0.2121 (9)	0.9579 (12)	0.2461 (4)	0.088 (5)
C51	0.3757 (9)	0.8292 (9)	0.3922 (4)	0.035 (3)
C52	0.4468 (9)	0.8207 (12)	0.3657 (5)	0.058 (5)
C53	0.5353 (11)	0.7988 (14)	0.3817 (6)	0.070 (6)
C54	0.5547 (10)	0.7909 (14)	0.4243 (5)	0.063 (5)
C55	0.4841 (11)	0.7970 (16)	0.4501 (6)	0.081 (7)
C56	0.3952 (10)	0.8151 (12)	0.4342 (5)	0.050 (4)
C61	−0.0290 (8)	0.7617 (8)	0.4057 (4)	0.025 (3)
C62	−0.0417 (8)	0.6567 (10)	0.4072 (4)	0.040 (4)
C63	−0.0998 (10)	0.6152 (11)	0.4351 (5)	0.051 (4)
C64	−0.1467 (11)	0.6758 (11)	0.4611 (5)	0.059 (5)
C65	−0.1364 (10)	0.7790 (12)	0.4611 (5)	0.051 (4)
C66	−0.0783 (10)	0.8213 (11)	0.4326 (4)	0.046 (4)

Table 2. *Selected geometric parameters* (Å, °)

Re1—P1	2.489 (4)	Re3—P3	2.486 (4)
Re1—P2	2.584 (3)	Re3—P4	2.582 (3)
Re2—P1	2.487 (3)	Re4—P3	2.488 (4)
Re2—P2	2.604 (3)	Re4—P4	2.609 (4)
Mn1—P2	2.515 (4)	Mn2—P4	2.523 (4)
P1—C31	1.844 (13)	P3—C51	1.836 (14)
P2—C41	1.840 (12)	P4—C61	1.855 (12)
P1—Re1—P2	75.15 (11)	P3—Re3—P4	75.10 (11)
P1—Re2—P2	74.82 (11)	P3—Re4—P4	74.60 (11)
C31—P1—Re2	118.9 (4)	C51—P3—Re3	115.8 (4)
C31—P1—Re1	114.0 (4)	C51—P3—Re4	118.3 (4)
Re2—P1—Re1	106.37 (12)	Re3—P3—Re4	106.42 (13)
C41—P2—Mn1	100.7 (4)	C61—P4—Mn2	101.5 (4)
C41—P2—Re1	111.8 (4)	C61—P4—Re3	111.4 (4)
Mn1—P2—Re1	117.07 (14)	Mn2—P4—Re3	116.93 (14)
C41—P2—Re2	107.5 (4)	C61—P4—Re4	107.1 (4)
Mn1—P2—Re2	119.46 (14)	Mn2—P4—Re4	119.66 (14)
Re1—P2—Re2	100.30 (11)	Re3—P4—Re4	100.21 (11)

The presence H atom bonded to P1 was ascertained by ^{1}H NMR measurements, but not located crystallographically.

Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993).

Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: JZ1040). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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