cant differences exist between the four independent molecules.

Related literature. The structure of $Cp_2W_{1\cdot2}Mo_{0\cdot8}Fe(\mu_3\text{-}Te)_2(CO)_7$ is similar to that of $Cp_2Mo_2Fe(\mu_3\text{-}Te)_2(CO)_7$ (Bogan, Rauchfuss & Rheingold, 1985), in which the average Te···Te distances are also short. It may be significant that both clusters have strong Te···Te bonding interactions, which contribute to their stabilization.

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Heptacarbonyl-μ-(diphenylphosphanido)-μ-iodo-(triphenylphosphine)dirhenium(I)

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Abstract. $[Re_2I\{P(C_6H_5)_2\}(CO)_7\{P(C_6H_5)_3\}]$, $M_r = 1142\cdot8$, monoclinic, $P2_1/n$, $a = 10\cdot526\,(2)$, $b = 18\cdot381\,(6)$, $c = 19\cdot457\,(7)$ Å, $\beta = 100\cdot57\,(2)°$, $V = 3700\cdot6$ Å^3, $Z = 4$, $D_x = 2\cdot051$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 75\cdot8$ cm^{-1}, $F(000) = 2144$, $T = 298\,(1)$ K, $R = 0\cdot048$, $wR = 0\cdot043$ for 3538 unique observed intensities. The coordination polyhedra of the two Re atoms are distorted octahedra and share μ-I and μ-PPh_2 (Ph = phenyl) as common ligands. The terminal PPh_3 group is *trans* to the μ-PPh_2 bridge. There is no Re—Re bonding in this 36 valence electron cluster.

Experimental. The compound was prepared by reaction of $[Re_2(CO)_7(\mu\text{-}H)(\mu\text{-}PPh_2)(PPh_3)]$ (Haupt, Balsaa & Flörke, 1988) and iodine in $CHCl_3$ solution at 293 K for 6 h and recrystallized from $CHCl_3$. Yellow crystal, size 0·10 × 0·11 × 0·45 mm. Lattice parameters from 25 reflections $10 \leq 2\theta \leq 25°$. Nicolet *R3m/V* diffractometer, graphite monochromator, Mo $K\alpha$ radiation. ω–2θ scan; 5731 intensities $3 \leq 2\theta \leq 46°$; $0 \leq h \leq 11$, $0 \leq k \leq 20$, $-21 \leq l \leq 21$; three standard reflections monitored every 400 reflections, steady decrease of 10% in intensities scaled on standards, Lp correction, empirical absorption correction *via* ψ scans, min./max. transmission 0·141/0·163; 5177 unique intensities after merging, $R_{\rm int} = 0\cdot039$, 3538 with $F > 4\sigma(F)$. Structure solved by direct methods and subsequent ΔF maps; full-matrix least-squares refinement based on F and 383 parameters. All non-H atoms refined anisotropically, H atoms fixed from geometrical considerations with isotropic displacement parameters $U_{\rm iso} = 0\cdot09$ Å^2; phenyl groups treated as rigid bodies (C—C 1·395 Å); $R = 0\cdot0481$, $wR = 0\cdot0436$, $w^{-1} = \sigma^2(F) + 0\cdot000558F^2$, $S = 1\cdot148$; max. $(\Delta/\sigma) = 0\cdot001$; max. height in final ΔF map 1·1 e Å^{-3}, min. height in final ΔF map 1·0 e Å^{-3}. Scattering factors, structure solution and refinement: *SHELXTL-Plus*88 (Sheldrick, 1988). Atomic parameters are given in Table 1,

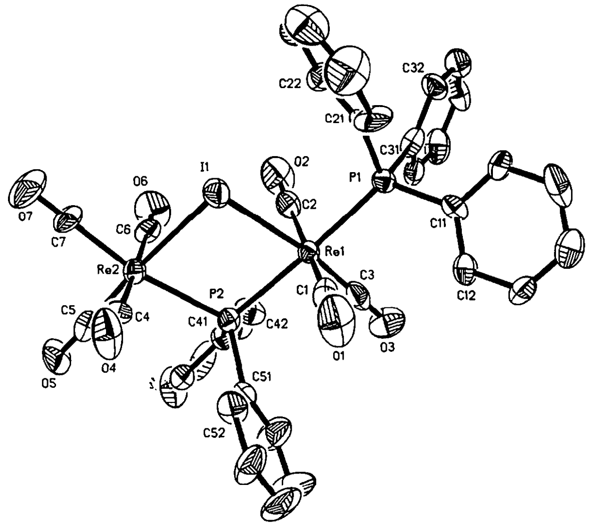

Fig. 1. Molecular structure of the title compound.

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Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic displacement parameters* ($Å^2 \times 10^3$)

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Re(1)	1664 (1)	9153 (1)	3547 (1)	28 (1)
Re(2)	1734 (1)	9819 (1)	1571 (1)	33 (1)
I(1)	3441 (1)	9053 (1)	2611 (1)	45 (1)
P(1)	2885 (4)	8361 (2)	4424 (2)	30 (1)
P(2)	619 (4)	9991 (2)	2611 (2)	30 (1)
C(1)	2753 (19)	9986 (11)	3967 (9)	52 (7)
O(1)	3387 (17)	10449 (9)	4209 (8)	93 (7)
C(2)	814 (16)	8278 (11)	3081 (8)	43 (7)
O(2)	384 (16)	7754 (8)	2819 (7)	80 (6)
C(4)	2910 (19)	10681 (10)	1732 (9)	42 (7)
O(4)	3644 (15)	11149 (8)	1800 (6)	73 (6)
C(3)	361 (20)	9299 (9)	4068 (9)	47 (7)
O(3)	−470 (12)	9395 (7)	4381 (7)	63 (6)
C(5)	529 (17)	10376 (10)	915 (9)	44 (7)
O(5)	−174 (12)	10694 (8)	506 (6)	62 (5)
C(6)	625 (17)	8936 (9)	1405 (8)	37 (6)
O(6)	−17 (15)	8443 (8)	1280 (7)	76 (6)
C(7)	2601 (16)	9490 (10)	824 (9)	42 (6)
O(7)	3133 (14)	9324 (9)	395 (8)	81 (7)
C(11)	3333 (11)	8714 (5)	5319 (4)	29 (5)
C(12)	2881	9388	5501	47 (7)
C(13)	3213	9639	6187	52 (7)
C(14)	3996	9217	6691	54 (7)
C(15)	4448	8544	6509	70 (9)
C(16)	4117	8292	5823	53 (7)
C(21)	4421 (10)	8077 (6)	4198 (6)	37 (6)
C(22)	4408	7551	3679	46 (7)
C(23)	5550	7369	3452	56 (8)
C(24)	6705	7712	3745	74 (10)
C(25)	6719	8237	4263	92 (12)
C(26)	5577	8420	4490	58 (8)
C(31)	2100 (10)	7495 (5)	4601 (5)	34 (6)
C(32)	2833	6881	4836	43 (6)
C(33)	2226	6254	5020	46 (7)
C(34)	887	6241	4968	57 (8)
C(35)	154	6855	4732	56 (8)
C(36)	761	7481	4549	41 (6)
C(41)	−1138 (7)	9841 (6)	2291 (5)	36 (6)
C(42)	−1784	9233	2483	54 (7)
C(43)	−3078	9116	2186	52 (7)
C(44)	−3726	9607	1698	58 (8)
C(45)	−3080	10216	1506	75 (9)
C(46)	−1786	10333	1803	41 (6)
C(51)	595 (12)	10931 (5)	2970 (6)	43 (6)
C(52)	1688	11369	3013	51 (7)
C(53)	1731	12046	3341	72 (9)
C(54)	680	12285	3624	85 (11)
C(55)	−414	11846	3581	92 (12)
C(56)	−457	11169	3254	67 (9)

Table 2. *Selected bond lengths* (Å) *and angles* (°)

Re(1)—I(1)	2·846 (1)	Re(1)—P(1)	2·425 (4)
Re(1)—P(2)	2·482 (4)	Re(2)—I(1)	2·823 (1)
Re(2)—P(2)	2·538 (4)		
I(1)—Re(1)—P(1)	94·9 (1)	I(1)—Re(1)—P(2)	80·0 (1)
P(1)—Re(1)—P(2)	174·3 (1)	I(1)—Re(2)—P(2)	79·5 (1)
Re(1)—I(1)—Re(2)	91·1 (1)	Re(1)—P(2)—Re(2)	107·5 (2)

selected bond lengths and angles in Table 2.* Fig. 1 shows the molecular structure.

Related literature. The structural parameters can be compared with those of $[Re_2(CO)_8(\mu\text{-}PPh_2)_2]$ (Flörke, Woyciechowski & Haupt, 1988), $[Re_2(CO)_8(\mu\text{-}H)(\mu\text{-}PPh_2)]$ (Haupt, Balsaa & Flörke, 1987) and $[Re_2(CO)_7(\mu\text{-}H)(\mu\text{-}PPh_2)(PPh_3)]$ (Haupt, Balsaa & Flörke, 1988). The related compounds $[Mn_2(CO)_8(\mu\text{-}I)(\mu\text{-}PPh_2)]$ and $[Re_2(CO)_8(\mu\text{-}Br)(\mu\text{-}PPh_2)]$ have been reported without structural data (Manning, Peterson, Wada & Dhami, 1986).

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* Lists of structure factors, anisotropic displacement parameters, H-atom parameters and bond lengths and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53742 (24 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of 3-Hydroxy-17-oxoestra-1,3,5(10)-trien-11β-yl Acetate

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Abstract. $C_{20}H_{24}O_4$, $M_r = 328{\cdot}41$, orthorhombic, $P2_12_12_1$, $a = 11{\cdot}688\,(3)$, $b = 15{\cdot}377\,(5)$, $c = 9{\cdot}466\,(2)$ Å, $V = 1701\,(1)$ Å^3, $Z = 4$, $D_x = 1{\cdot}282$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71073$ Å, $\mu = 0{\cdot}823$ cm^{-1}, $F(000) = 704$, $T = 298$ K, $R = 0{\cdot}063$ for 1921 reflections with $F > 2\sigma(F)$. The structure was determined to observe the effect of the 11β-acetate substituent on the conformation of the molecule. The 3-hydroxy is hydrogen bonded to O19 at 2·86 Å. The *B* ring has a 7α,8β-half chair conformation, the most commonly observed *B* ring conformation in estrogen analogues.

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