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## Key indicators

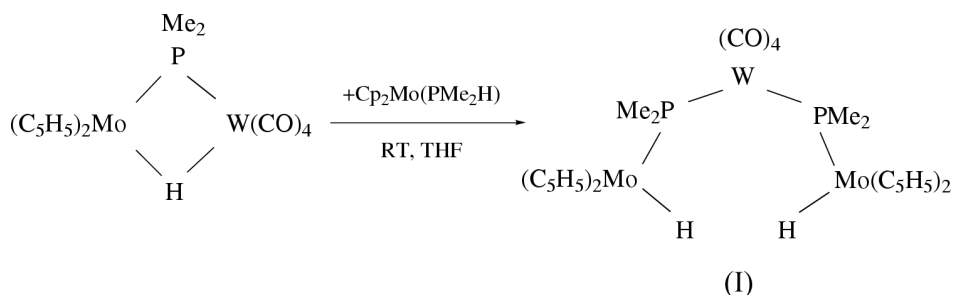
Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.019\text{ \AA}$   
 $R$  factor = 0.042  
 $wR$  factor = 0.084  
Data-to-parameter ratio = 16.6For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Tetracarbonyltungsten(0)-bis( $\mu$ -dimethylphosphido)-bis[dicyclopentadienyldihydromolybdenum(IV)]

The title trinuclear  $\text{WMo}_2$  compound,  $[\text{Mo}_2\text{WH}_2(\text{C}_5\text{H}_5)_4(\text{C}_2\text{H}_6\text{P})_2(\text{CO})_4]$ , was obtained by opening of the hydride bridge in the dinuclear dibridged ( $\mu$ - $\text{PMe}_2\text{H}$ ){( $\text{C}_5\text{H}_5$ )<sub>2</sub>Mo}{ $\text{W}(\text{CO})_4$ } complex ( $\text{Mo}^{\text{IV}}$ ) upon the action of ( $\text{C}_5\text{H}_5$ )<sub>2</sub>Mo( $\text{PMe}_2\text{H}$ ) ( $\text{Mo}^{\text{II}}$ ) in THF solution. This involves the formal conversion of  $\text{Mo}^{\text{II}}$  to  $\text{Mo}^{\text{IV}}$ .

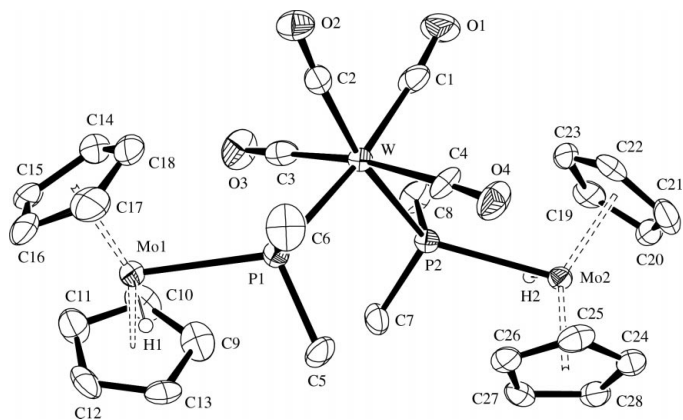
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## Comment

In the course of our research on phosphido–hydrido dibridged bimetallics containing group 5 and 6 (Nb, Ta, Mo, W) metallocene and group 6 (Cr, Mo, W) metal–carbonyl fragments, we expected to open the hydride bridge with two electron-donor ligands. Effectively, these reactions work very well with different phosphines (Boni *et al.*, 1999). The use of complexes containing secondary phosphine  $M(\text{PR}_2\text{H})$  for this type of reactivity is less evident. However, we have shown (Barré *et al.*, 1993) that these metal–secondary phosphine species easily undergo the tautomeric rearrangement from ( $\text{C}_5\text{H}_5$ )<sub>2</sub>Mo( $\text{PR}_2\text{H}$ ) ( $\text{Mo}^{\text{II}}$ ) to ( $\text{C}_5\text{H}_5$ )<sub>2</sub>Mo( $\text{PR}_2$ )H ( $\text{Mo}^{\text{IV}}$ ) and so may be considered as metallophosphines  $M\text{PR}_2$ . Thus, the reaction of dibridged bimetallic ( $\mu$ - $\text{PMe}_2\text{H}$ ){( $\text{C}_5\text{H}_5$ )<sub>2</sub>Mo}{ $\text{W}(\text{CO})_4$ } with ( $\text{C}_5\text{H}_5$ )<sub>2</sub>Mo( $\text{PMe}_2\text{H}$ ) gives the trimetallic title complex, (I)



The trimetallic molecule has a pseudo-twofold molecular axis which is not a crystallographic axis. It is built of distorted *cis*- $\text{W}(\text{CO})_4\text{P}_2$  octahedral and of bent metallocene fragments (Fig. 1). The  $\text{W}$ –carbonyl bonds *trans* to the  $\text{P}$  atoms [C1 and C2, mean 1.956 (14) Å] are shorter than those involving mutually *trans* C3 and C4 [mean 2.017 (14) Å]. This indicates an effective operation of the donor *trans* influence and electron-rich nature of metallophosphines. The dihedral angles between the cyclopentadienyl planes are 141.3 (5) and 139.5 (5)° for fragments based on Mo1 and Mo2, respectively. The ring centroid to molybdenum distances of 1.958 Å (mean) and the centroid–molybdenum–centroid angles, 142.6° (mean), are normal. Other metric parameters, in particular the non-bonding  $\text{Mo}\cdots\text{W}$  distances and  $\text{Mo}-\text{P}-\text{W}$  angles



**Figure 1**  
ORTEP-3 (Farrugia, 1997) drawing, showing 30% probability displacement ellipsoids. H atoms, except for the hydrides H1 and H2, have been omitted for clarity.

(Table 1) are also typical for monophosphido-bridged bimetallic structures (Boni *et al.*, 1999).

## Experimental

A mixture of 100 mg (0.17 mmol) of  $(\mu\text{-PMe}_2\text{H})\{(\text{C}_5\text{H}_5)_2\text{Mo}\}\text{-}\{\text{W}(\text{CO})_4\}$  in 10 ml of anhydrous THF and a stoichiometric amount of  $(\text{C}_5\text{H}_5)_2\text{Mo}(\text{PMe}_2\text{H})$  in 10 ml of THF was stirred at room temperature. The progress of the reaction was monitored by IR and  $^1\text{H}$  NMR (hydride resonances). After 1 h of stirring, there were neither the high field resonance of the hydride bridge nor the  $\nu(\text{CO})$  vibrations of the starting dinuclear complex. The solvent was evaporated off and the crude product dissolved in toluene. Crystallization, assisted by an addition of pentane, gave the title trimetallic complex in 70% yield.

### Crystal data

$[\text{Mo}_2\text{WH}_2(\text{C}_5\text{H}_5)_4(\text{C}_2\text{H}_6\text{P})_2(\text{CO})_4]$	$D_x = 1.993 \text{ Mg m}^{-3}$
$M_r = 872.21$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 25 reflections
$a = 15.342 (5) \text{ \AA}$	$\theta = 7.8\text{--}14.2^\circ$
$b = 17.087 (2) \text{ \AA}$	$\mu = 4.94 \text{ mm}^{-1}$
$c = 11.274 (2) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 100.40 (2)^\circ$	Irregular, yellow
$V = 2907.0 (11) \text{ \AA}^3$	$0.20 \times 0.10 \times 0.08 \text{ mm}$
$Z = 4$	

### Data collection

Enraf–Nonius CAD-4 diffractometer	2986 reflections with $I > 2\sigma(I)$
$\omega$ scans	$R_{\text{int}} = 0.049$
Absorption correction: refined from $\Delta F$ (DIFABS; Walker & Stuart, 1983)	$\theta_{\text{max}} = 26.0^\circ$
$T_{\text{min}} = 0.595$ , $T_{\text{max}} = 0.674$	$h = 0 \rightarrow 18$
5899 measured reflections	$k = 0 \rightarrow 21$
5683 independent reflections	$l = -13 \rightarrow 13$
	3 standard reflections
	frequency: 120 min
	intensity decay: $-4.1\%$

### Refinement

Refinement on $F^2$	H atoms refined by a mixture of constrained and independent refinement
$R[F^2 > 2\sigma(F^2)] = 0.042$	$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2]$
$wR(F^2) = 0.084$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{\text{max}} = 0.001$
5683 reflections	$\Delta\rho_{\text{max}} = 1.43 \text{ e \AA}^{-3}$
342 parameters	$\Delta\rho_{\text{min}} = -1.46 \text{ e \AA}^{-3}$

**Table 1**  
Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

W–C2	1.946 (13)	Mo1–P1	2.589 (3)
W–C1	1.967 (14)	Mo1–H1	1.62 (8)
W–C3	2.015 (14)	Mo2–P2	2.583 (3)
W–C4	2.020 (12)	Mo2–H2	1.56 (13)
W–P1	2.614 (3)	P1–C5	1.857 (11)
W–P2	2.617 (3)	P1–C6	1.859 (12)
W–Mo2	4.5474 (12)	P2–C7	1.845 (12)
W–Mo1	4.5749 (14)	P2–C8	1.852 (10)
P1–W–P2	105.11 (9)	C6–P1–W	106.0 (5)
Mo2–W–Mo1	124.79 (2)	Mo1–P1–W	123.08 (11)
P1–Mo1–H1	73 (3)	C7–P2–C8	93.6 (6)
P2–Mo2–H2	67 (5)	C7–P2–Mo2	107.7 (4)
C5–P1–C6	94.1 (6)	C8–P2–Mo2	108.4 (4)
C5–P1–Mo1	107.4 (4)	C7–P2–W	114.3 (4)
C6–P1–Mo1	108.1 (4)	C8–P2–W	106.9 (4)
C5–P1–W	114.1 (4)	Mo2–P2–W	121.97 (12)

H atoms (except hydrides) were included in calculated positions and treated as riding, with isotropic displacement parameters set to 1.3 times those of the C atoms bearing them. The two hydride atoms bound to the Mo atoms were located from a difference Fourier map and isotropically refined.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1992); cell refinement: *CAD-4 EXPRESS*; data reduction: *PROCESS* in *MolEN* (Fair, 1990); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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