



Figure 1. Structure of complex **5**. The heavy atom ellipsoids are scaled to enclose 50% of the electron density; hydrogen atoms are omitted. Principal bond distances (Å): W₁-C₂₁, 2.46 (1); W₁-P, 2.607 (4); P-C₂₁, 1.78 (1); P-C₂₄, 1.81 (2); C₂₁-C₂₂, 1.49 (2); C₂₂-C₂₃, 1.21 (2); C₂₃-C₂₄, 1.54 (2); P-W₂, 2.490 (4). Selected bond angles (deg): W₁-P-W₂, 125.3 (1); W₁-P-C₂₁, 65.2 (4); W₁-C₂₁-P, 73.8 (5); C₂₁-P-C₂₄, 93.2 (8); P-C₂₁-C₂₂, 105 (1); C₂₁-C₂₂-C₂₃, 121 (2); C₂₂-C₂₃-C₂₄, 113 (1); P-C₂₄-C₂₃, 106 (1); W₂-P-C₂₁, 128.3 (5); W₂-P-C₂₄, 108.6 (6).

$a = 15.063$ (6) Å, $b = 7.306$ (3) Å, $c = 19.903$ (8) Å, $\beta = 104.56$ (2)°, $U = 2120$ Å³, $d_{\text{obsd}} = 2.33 \pm 0.03$ g cm⁻³, $d_{\text{calcd}} = 2.381$ g cm⁻³, $Z = 4$, space group $P2_1/C$ ($N^\circ 14$); because of very low diffraction power and very bad crystals, CuK α (1.5418 Å) radiation was used for cell dimension determination and intensity measurements; $\mu = 212.0$ cm⁻¹ $F_{000} = 1392$.

Diffraction data were collected in the $\theta/2\theta$ flying step-scan mode using a Philips PW 1100/16 automatic diffractometer, graphite monochromated CuK α radiation, and a crystal of dimensions $0.018 \times 0.025 \times 0.080$ cm. Absorption corrections were applied using the numerical integration method (transmission coefficients 0.03–0.26). The structure was solved by the heavy-atom method using the Enraf-Nonius SDP/V + 1¹⁴ package on

a PDP 11/60 computer. Full matrix refinement using 2074 reflections having $I > 3\sigma(I)$ converged to conventional agreement factors R_1 and R_2 of 0.089 and 0.109 with anisotropic temperature factors for the two tungsten atoms and the phosphorus atom and isotropic ones for all other atoms. Hydrogen atoms were introduced by their computed coordinates but not refined.

The structure (Figure 1)¹⁵ consists of discrete molecules linked only by Van der Waals contacts and hydrogen bonds. Selected geometrical details are given in the caption of Figure 1.

As already stated, the P-C₂₁ double bond acts as a 4-electron donor towards two W(CO)₅ units in that complex.

Within experimental error, the P-C₂₁ bond length (1.78 (1) Å) agrees with the only other value reported for an η^2 -phosphaalkene (1.773 (8) Å in ref 13). The P-C₂₄ single bond is logically longer (1.81 (2) Å) than the P-C₂₁ double bond but the difference is perhaps not significant in view of the poor data.

The C=C double bond is well localized between C₂₂ and C₂₃ and, quite predictably, C₂₁-C₂₂ is slightly shortened with respect to the normal C-C bond found between C₂₃ and C₂₄.

Registry No. 1, 88296-54-2; **2**, 83576-94-7; **3**, 88296-55-3; **4**, 88296-56-4; **5**, 88296-57-5; Cr(CO)₅(THF), 15038-41-2; W(CO)₅(THF), 36477-75-5; (3,4-dimethylphospholy)lithium, 67918-40-5.

Supplementary Material Available: Listings of the atomic coordinates and B_{eqv} (Table I) and the observed and calculated structure factors ($\times 10$) for all observed reflections (Table II) (11 pages). Ordering information is given on any current masthead page.

(14) Frenz, B. A. "The Enraf-Nonius CAD4-SDP. Computing in Crystallography"; Schenk, H., Olthof-Hazekamp, R., Van Koningsveld, H., Bassi, G. C., Ed.; Delft University Press: Delft, Holland, 1978; p 64.

(15) Drawing performed by using program ORTEP: Johnson, C. K.; Report ORNL 3794; Oak Ridge, TN, 1965.

Additions and Corrections

Radiation-Induced Reduction of Thymidine in Aqueous Solution: Isolation and Characterization of a Novel Dimeric Product [*J. Am. Chem. Soc.* **1983**, *105*, 6740]. SEI-ICHI NISHIMOTO, HIROSHI IDE, KIKUMI NAKAMICHI, and TSUTOMU KAGIYA*

Page 6740, the caption to Figure 1 should read: ¹³C NMR (25 MHz) spectra of 5,5'-bi-5,6-dihydrothymidine (**2**) with (a) complete decoupling and (b) off-resonance decoupling in D₂O at 20 °C. CD₃CN (δ_{CN} 119.5 ppm,*) was used as an internal standard and the signal of the CD₃ (δ 1.7 ppm) is omitted in a and b.