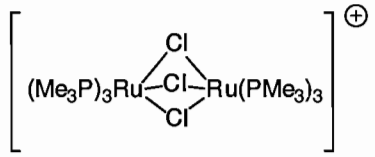
Massachusetts Institute of Technology

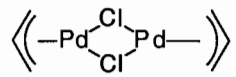
5.44: Organometallic Chemistry — *Problem Set 1*

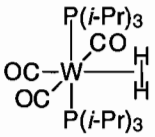
Due: Tuesday, November 9, 2004

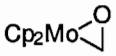
(1) For the following compounds, please provide for each metal:
- (a) the total electron count
- (b) the formal oxidation state of the metal
- (c) the d^n electron count (i.e., give n)
- (d) the ML_aX_b assignment (i.e., give a and b)

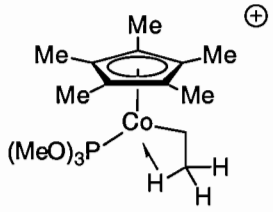
(1.1) $(t\text{-Bu})_3P\text{–Pd–}P(t\text{-Bu})_3$

(1.2) 

(1.3) 

(1.4) 

(1.5) 

(1.6) 

(2) Provide an explanation for the following data:

	IR stretching frequency of CO (cm^{-1})
$(\eta^5\text{-}C_5H_5)_2Ti(CO)_2$	1899
$(\eta^5\text{-}C_5Me_5)_2Ti(CO)_2$	1858

(3) Ferrocene reacts with the acylium ion, $Me\text{–}C{\equiv}\overset{\oplus}{O}$, to give complex **X**, which is a cation. A base then abstracts a proton from **X** to give **Y**, which has the formula $C_{12}H_{12}FeO$. **Y** reacts further with the acylium ion, followed by base, to give **Z**. Provide structures for **X**, **Y**, and **Z**.

(4) N_2 has molecular orbitals slightly different than those of CO. Draw a π^* orbital of N_2 and a π^* orbital of CO, and compare the two orbitals. Would you expect N_2 to be a stronger or a weaker π-acceptor than CO? Briefly explain your reasoning.

(5) Suggest the structure of $Os_3(CO)_{12}$, based on the information that it obeys the 18-electron rule for each osmium.