IR Spectroscopy of CO Ligands

How much electron density is on the central metal?

- CO stretching frequency (can also use NO^+, CN^-, NCR, alkene, alkyne *etc.*)
- ν(CO)(cm^{-1}) → Free CO (2143), terminal M–CO (2120-1850 unless highly reduced CO), μ_2-CO (1850-1700), μ_3-CO (1700-1600), non-classical M–CO (>2143)

$[Ni(CO)_4]$ = 2060 cm^{-1}

$[Co(CO)_4]^-$ = 1890 cm^{-1}

$[Fe(CO)_4]^{2-}$ = 1790 cm^{-1}

$(F_3C)_3B$-CO = 2267 cm^{-1} (Helge Willner, 02)

$[Ag(CO)][B(OTeF_5)_4]$ = 2204 cm^{-1} (Steven Strauss, 91)

$[Rh(CO)_4][Al_2Cl_7]$ = 2167 cm^{-1} (Helge Willner, 03)

Redox potentials by cyclic voltammetry

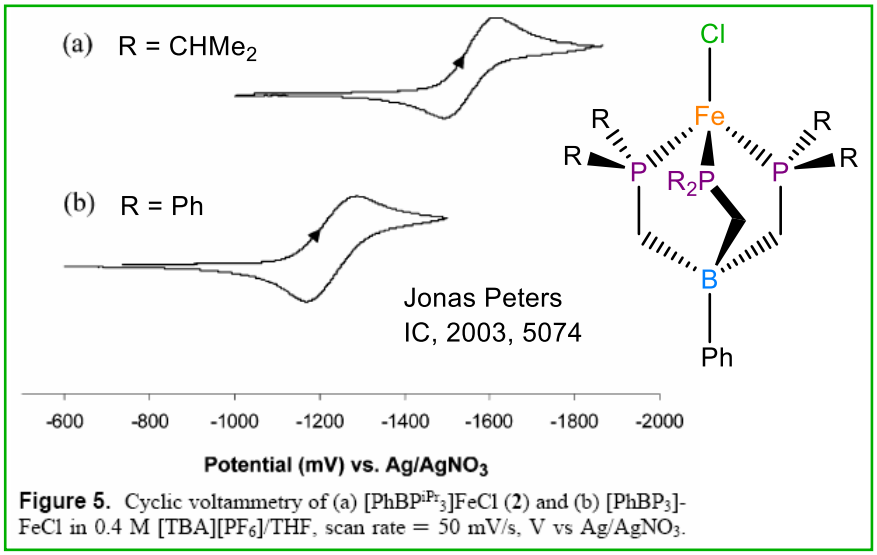
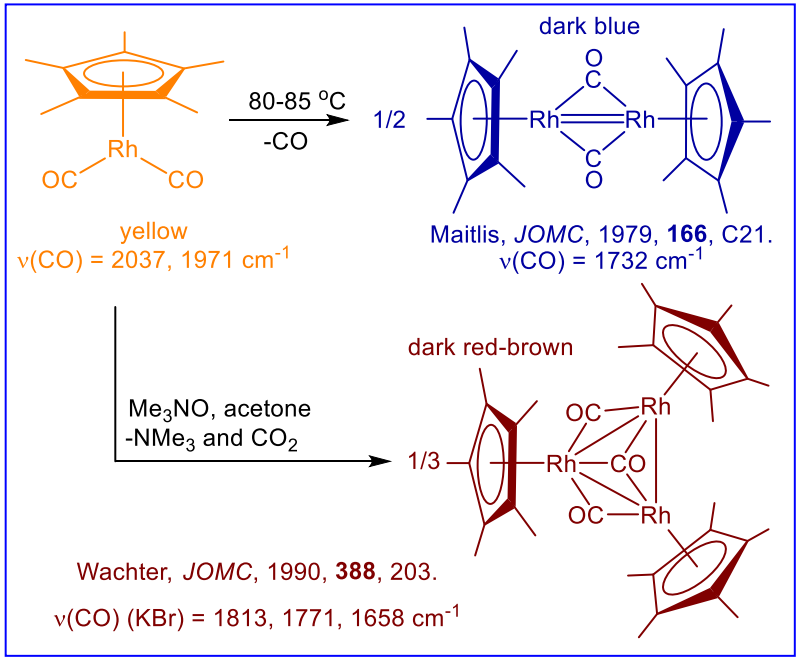
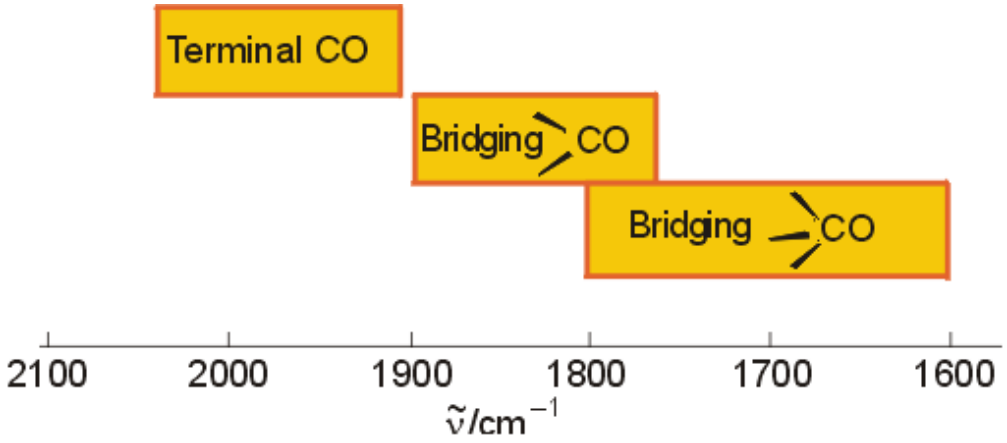
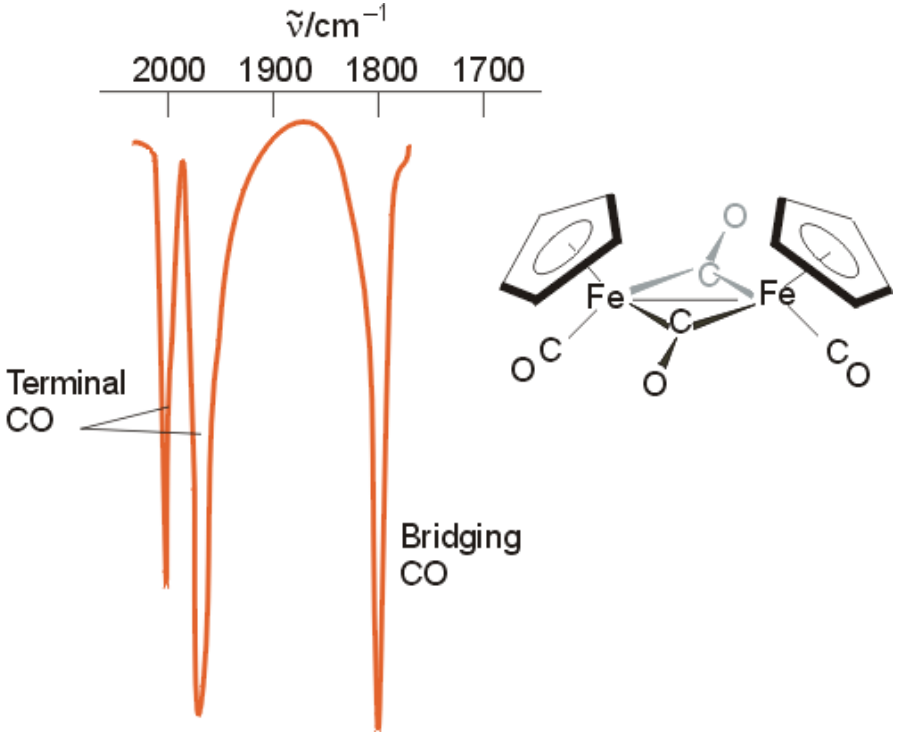


Figure 5. Cyclic voltammetry of (a) $[PhBP^{iPr}_3]FeCl$ (**2**) and (b) $[PhBP_3]$-FeCl in 0.4 M [TBA][PF_6]/THF, scan rate = 50 mV/s, V vs $Ag/AgNO_3$.



IR Spectroscopy of CO Ligands

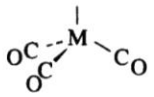
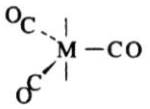
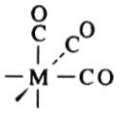
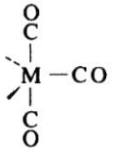
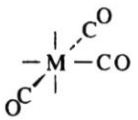
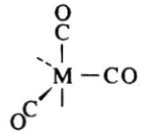
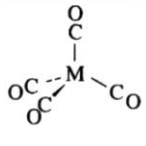
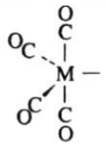
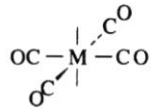
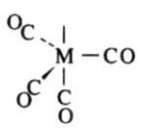
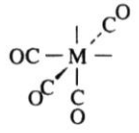
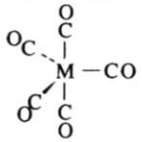
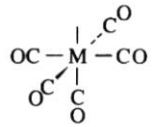
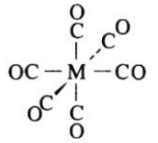




IR Spectroscopy of CO Ligands

How many peaks to expect in IR spectroscopy?

Table 4-2 Carbonyl Stretching Bands[a]

Number of Carbonyls	Coordination Number 4	5	6
3			
IR bands:	2	1	2
			
IR bands:		3	3
			
IR bands:		3	
4			
IR bands:	1	4	1
			
IR bands:		3	4
5			
IR bands:		2	3
6			
IR bands:			1

[a]Adapted with permission from G. L. Miessler and D. A. Tarr, Inorganic Chemistry, Prentice-Hall, Englewood Cliffs, NJ, 1991, 457.