Problems

Use molecular modeling software for the following problems:

13.1 Which of the following obey the 18-electron rule?

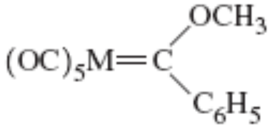
a. $Fe(CO)_5$
b. $[Rh(bipy)_2Cl]^+$
c. $(\eta^5\text{-}Cp^*)Re(\theta O)_3$, where $Cp^* = C_5(CH_3)_5$
d. $Re(PPh_3)_2Cl_2N$
e. $Os(CO)(\equiv CPh)(PPh_3)_2Cl$
f. The CE complexes in **Table 13.3**

13.2 Which of the following square-planar complexes have 16-electron valence configurations?

a. $Ir(CO)Cl(PPh_3)_2$
b. $RhCl(PPh_3)_3$
c. $[Ni(CN)_4]^{2-}$
d. *cis*-$PtCl_2(NH_3)_2$

13.3 On the basis of the 18-electron rule, identify the first-row transition metal for each of the following:

a. $[M(CO)_7]^+$
b. $H_3CM(CO)_5$
c. $M(CO)_2(CS)(PPh_3)Br$
d. $[(\eta^3\text{-}C_3H_3)(\kappa^5\text{-}C_5H_5)M(CO)]^-$



e.
f. $[(\eta^4\text{-}C_4H_4)(\eta^5\text{-}C_5H_5)M]^+$
g. $(\eta^3\text{-}C_3H_5)(\eta^5\text{-}C_5H_5)M(CH^3)(NO)$ (has linearly coordinated NO)
h. $[M(CO)_4I(diphos)]^-$ (diphos = 1,2-bis(diphenylphosphino)ethane)

13.4 Determine the metal–metal bond order consistent with the 18-electron rule for the following:

a. $[(\eta^5\text{-}C_5H_5)Fe(CO)_2]_2$
b. $[(\eta^5\text{-}C_5H_5)Mo(CO)_2]_2^{2-}$

13.5 Identify the most likely second-row transition metal for each of the following:

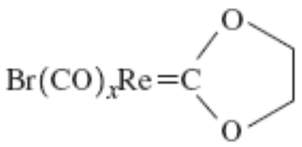
a. $[M(CO)_3(NO)]^-$
b. $[M(PF_3)_2(NO)_2]^+$ (contains linear M — N — O)
c. $[M(CO)_4(m_2\text{-}H)]_3$
d. $M(CO)(PMe_3)_2Cl$ (square-planar complex)

13.6 On the basis of the 18-electron rule, determine the expected charge on the following:

a. $[Co(CO)_3]^z$
b. $[Ni(CO)_3(NO)]^z$ (contains linear M — N — O)
c. $[Ru(CO)_4(GeMe_3)]^z$
d. $(\eta^3\text{-}C_3H_5)V(CNCH_3)_5]^z$
e. $[(\eta^5\text{-}C_5H_5)Fe(CO)_3]^z$
f. $[(\eta^5\text{-}C_5H_5)_3Ni_3(\mu_3\text{-}CO)_2]^z$

13.7 Determine the unknown quantity:

a. $[(\eta^5\text{-}C_5H_5)W(CO)_x]_2$ (has W—W single bond)



b.

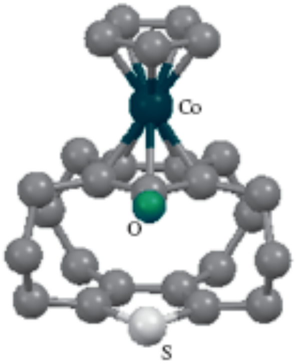
c. $[(CO)_3Ni{-}Co(CO)_3]^z$

d. $[Ni(NO)_3(SiMe_3)]^z$ (contains linear M — N — O)

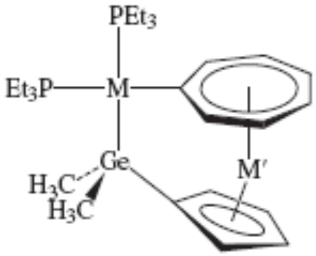
e. $[(\eta^5\text{-}C_5H_5)Mn(CO)_x]^2$ (has Mn═Mn bond)

13.8 Determine the unknown quantity:

a. The hapticity of the lower ring in the mixed superphane (See S. Gath, R. Gleiter, F. Rominger, C. Bleiholder, *Organometallics*, **2007**, *26*, 644. Structure generated with CIF data, with hydrogen atoms omitted for clarity.)



b. The *third* row 16-electron transition metal **M** on the left and the *first* row 16-electron transition metal on the right (See M. Tamm, A. Kunst, T. Bannenberg, S. Randoll, P. G. Jones, *Organometallics* **2007**, *26*, 417.)



13.9 **Figure 13.35** shows examples of complexes containing both C_5H_5 and CO ligands for group 4–8 transition metals. What complexes containing both ligands would be consistent with the 18-electron rule for first row transition metals in groups 9–11? Consider complexes containing one or two metal atoms.

13.10 Nickel tetracarbonyl, $Ni(CO)_4$, is an 18-electron species. Using a qualitative molecular orbital diagram, explain the stability of this 18-electron molecule. (See A. W. Ehlers, S. Dapprich, S. V. Vyboishchikov, G. Frenking, *Organometallics*, **1996**, *15*, 105.)

13.11 The Re — O stretching vibration in $Re(^{16}O)I(HC \equiv CH)_2$ is at 975 cm^{-1}. Predict the position of the Re — O stretching band in $Re(^{18}O)I(HC \equiv CH)_2$ (See J. M. Mayer, D. L. Thorn, T. H. Tulip, *J. Am. Chem. Soc.*, **1985**, *107*, 7454.)

13.12 The compound $W(O)Cl_2(CO)(PMePh_2)_2$ has v (CO) at 2006 cm^{-1}. Would you predict v (CO) for $W(S)Cl_2(CO)(PMePh_2)_2$ to be at higher or lower energy? Explain briefly. (See J. C. Bryan, S. J. Geib, A. L. Rheingold, J. M. Mayer, *J. Am. Chem. Soc.*, **1987**, *109*, 2826.)

13.13 The vanadium–carbon distance in $V(CO)_6$ is 200 pm but only 193 pm in $[V(CO)_6]^-$. Explain.

13.14 Describe, using sketches, how the following ligands can act as both σ donors and π acceptors:

a. CN^-
b. $P(CH_3)_3$
c. SCN^-

13.15

a. Account for the following trend in IR frequencies:
   $[Cr(CN)_5(NO)]^{4-}$ v (NO) = 1515 cm^{-1}
   $[Mn(CN)_5(NO)]^{3-}$ v (NO) = 1725 cm^{-1}
   $[Fe(CN)_5(NO)]^{2-}$ v (NO) = 1939 cm^{-1}

b. The ion $[RuCl(NO)_2(PPh_3)_2]^+$ has N — O stretching bands at 1687 and 1845 cm^{-1}. The C — O stretching bands of dicarbonyl complexes typically are much closer in energy. Explain.

13.16 Sketch the π molecular orbitals for the following:

a. CO_2
b. 1,3,5-Hexatriene
c. Cyclobutadiene, C_4H_4
d. Cyclo-C_7H_7

13.17 For the hypothetical molecule $(\eta^4\text{-}C_4H_4)Mo(CO)_4$:

a. Assuming C_{4v} geometry, predict the number of IR-active C—O bands.

b. Sketch the π molecular orbitals of cyclobutadiene. For each, indicate which *s*, *p*, and *d* orbitals of Mo are of suitable symmetry for interaction. (Hint: Assign the *z* axis to be collinear with the C_4 axis.)

13.18 Using the D_{5h} character table in **Appendix c** :

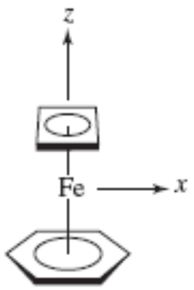
a. Assign symmetry labels (labels of irreducible representations) for the group orbitals shown in **Figure 13.27** .
b. Assign symmetry labels for the atomic orbitals of Fe in a D_{5h} environment.
c. Verify that the orbital interactions for ferrocene shown in **Figure 13.28** are between atomic orbitals of Fe and group orbitals of matching symmetry.

13.19 Dibenzenechromium, $(\eta^4\text{-}C_6H_6)_2Cr$, is a sandwich compound having two parallel benzene rings in an eclipsed conformation. For this molecule,

a. Sketch the π orbitals of benzene.
b. Sketch the group orbitals, using π orbitals of the two benzene rings.
c. For each of the 12 group orbitals, identify the Cr orbital(s) of suitable symmetry for interaction.
d. Sketch an energy-level diagram of the molecular orbitals.

13.20 Although the bonding in the proposed ferrocene isomer $(\eta^4\text{-}C_4H_4)(\eta^6\text{-}C_6H_6)$ has been studied theoretically, synthesis of this molecule has not been reported (C. M. Brett, B. E. Bursten, *Polyhedron*, **2004**, *23*, 2993). For this molecule:

a. What is its point group?
b. Generate a (reducible) representation using as a basis the *p* orbitals of the C_4H_4 and C_6H_6 rings that can participate in interactions.
c. Reduce this representation to its irreducible components, and match these with the appropriate orbitals on Fe.



13.21 Predict the number of IR-active C — O stretching vibrations for $W(CO)_3(\eta^6\text{-}C_6H_6)$ assuming C_{3v} geometry.

13.22 In this chapter, the assertion was made that highly symmetric binary carbonyls of T_d and O_h symmetry should show only a single C — O stretching band in the infrared. Check this assertion by analyzing the C — O vibrations of $Ni(CO)_4$ and $Cr(CO)_6$ by the symmetry method described in **Chapter 4**.

13.23 $Mn_2(CO)_{10}$ and $Re_2(CO)_{10}$ have D_{4d} symmetry. How many IR-active carbonyl stretching bands would you predict for these compounds?

13.24 When tungsten hexacarbonyl is refluxed in butyronitrile, C_3H_7CN, product **X** is formed first. Continued reflux converts **X** to **Y**, and very long reflux (several days) converts **Y** to **Z**. However, even refluxing for several weeks does not convert compound **Z** into another product. In addition, in each reaction step, a colorless gas is liberated.

The following infrared bands are observed (cm^{-1}):

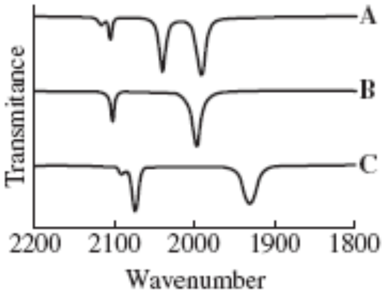
X:	2077	**Y:**	2017	**Z:**	1910
	1975		1898		1792
	1938		1842		

a. Propose structures of **X**, **Y**, and **Z**. Where more than one isomer is possible, determine the isomer that is the best match for the infrared data. (Note: a weak band in **Y** may be obscured by other bands.)

b. Account for the trend in the position of the infrared bands in the sequence X → Y → Z.

c. Suggest why **Z** does not react further when refluxed in butyronitrile. (See G. J. Kubas, *Inorg. Chem.* **1983**, *22*, 692.)

13.25 The infrared spectra of *trans*- and *cis*-$[Fe(CO)_2(CN)_4]^{2-}$ and of $[Fe(CO)(CN)_5]^{3-}$ are shown below.



a. Which stretching bands occur at lower energy, those for the CO ligand or those for the CN^- ligand? Explain.
b. How many $C-O$ and $C-N$ stretching bands would you predict for each of these complexes on the basis of their symmetry? Match the complexes with their spectra. (Reproduced with permission Inorg. Chem., 41, 1670. Copyright 2002. American Chemical Society.)

13.26 Samples of $Fe(CO)(PF_3)_4$ show two carbonyl stretching bands, at 2038 and 2009 cm^{-1}.

a. How is it possible for this compound to exhibit two carbonyl bands?
b. $Fe(CO)_5$ has carbonyl bands at 2025 and 2000 cm^{-1}. Would you place PF_3 above or below CO in the spectrochemical series? Explain briefly. (See H. Mahnke, R. J. Clark, R. Rosanske, R. K. Sheline, *J. Chem. Phys.*, **1974**, *60*, 2997.)

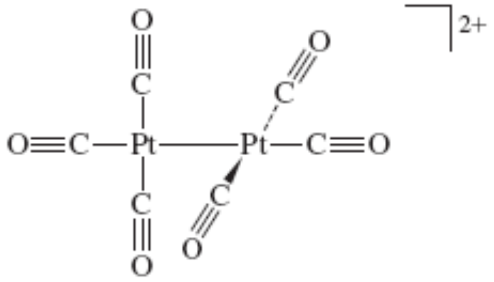
13.27 Evidence has been reported for two isomers of $Ru(CO)_2(PEt_2)_3$, one with the carbonyls occupying axial positions in a trigonal-bipyramidal structure and the other with the carbonyls occupying equatorial positions. Could infrared spectroscopy distinguish between these isomers? How many carbon–oxygen stretching vibrations would be expected for each? (See M. Ogasawara, F. Maseras, N. Gallego-Planas, W. E. Streib, O. Eisenstein, K. G. Caulton, *Inorg. Chem.*, **1996**, *35*, 7468.)

13.28 Account for the observation that $[Co(CO)_3(PPh_3)_2]^+$ has only a single carbonyl stretching frequency.

13.29 In addition to the hexacarbonyl complexes shown in **Section 13.4.1**, the ion $[Ir(CO)_6]^{3+}$ has been reported. Predict the position of the carbonyl stretching vibration in this complex. (See C. Bach, H. Willner, C. Wang, S. J. Rettig, J. Trotter, F. Aubke, *Angew. Chem.*, *Int. Ed.*, **1996**, *35*, 1974.)

13.30 Pathways to a variety of homoleptic transition-metal carbonyl cations have now been developed.

a. Three such cations are $[Hg(CO)_2]^{2+}$, $[Pt(CO)_4]^{2+}$ and $[Os(CO)_6]^{2+}$. Predict which of these has the lowest energy carbon–oxygen stretching vibration in the infrared. (See H. Willner, F. Aubke, *Angew. Chem.*, *Int. Ed.*, **1997**, *36*, 2402.)
b. The cation $[\{Pt(CO)_3\}_2]^{2+}$ is believed to have the structure shown, with D_{2d} symmetry. Predict the number of carbon–oxygen stretching bands observable in the infrared for this ion, and predict the approximate region in the spectrum where these bands might be observed.



13.31 The Raman spectrum of $Mo(CO)_6$ in pyridine has bands at 2119 and 2015 cm^{-1}. Microwave irradiation of this solution yielded three products with the following Raman bands:

Compound **J**: 2071, 1981 cm^{-1}

Compound **K**: 1892 cm^{-1}

Compound **L**: 1600 cm^{-1}

a. Determine the irreducible representations matching the Raman-active bands of $Mo(CO)_6$.
b. On the basis of the Raman data, propose structures of **J**, **K**, and **L.**
   (See T. M. Barnard, N. E. Leadbeater, *Chem. Commun.*, **2006**, 3615.)

- **13.32** One of the first thionitrosyl complexes to be reported was $(\eta^5\text{-}C_5H_5)Cr(CO)_2(NS)$. This compound has carbonyl bands at 1962 and 2033 cm^{-1}. The corresponding bands for $(\eta^5\text{-}C_5H_5)Cr(CO)_2(NO)$ are at 1955 and 2028 cm^{-1}. On the basis of the IR evidence, is NS behaving as a stronger or weaker acceptor in these compounds? Explain briefly. (See T. J. Greenough, B. W. S. Kolthammer, P. Legzdins, J. Trotter, *Chem. Commun.*, **1978**, 1036.)

- **13.33** The ^{14}N and ^{15}N derivatives of $TpOs(NS)Cl_2$ [Tp = hydrotris(1-pyrazolyl)borate, a tridentate ligand] have been prepared. The ^{14}N derivative has a nitrogen–sulfur stretch at 1284 cm^{-1}. Predict the N—S stretch for the ^{15}N derivative. (See T. J. Crevier, S. Lovell, J. M. Mayer, A. L. Rheingold, I. A. Guzei, *J. Am. Chem. Soc.*, **1998**, *120*, 6607.)

- **13.34** The compound $[Ru(CO)_6][Sb_2F_{11}]_2$ has a strong infrared band at 2199 cm^{-1}. The spectrum of $[Ru(^{13}CO)_6][Sb_2F_{11}]_2$ has also been reported. Would you expect the band observed at 2199 cm^{-1} for the ^{12}C compound to be shifted to higher or lower energy for the analogous ^{13}C compound? (See C. Wang, B. Bley, G. Balzer-Jöllenbeck, A. R. Lewis, S. C. Siu, H. Willner, F. Aubke, *Chem. Commun.*, **1995**, 2071.)

- **13.35** Predict the products of the following reactions:

a. $\mathrm{Mo(Co)_6 + Ph_2P—CH_2—PPh_2} \overset{\Delta}{\rightarrow}$
b. $(\eta^5\text{-}\mathrm{C_5H_5})(\eta^1\text{-}\mathrm{C_3H_5})\mathrm{Fe(Co)_2} \overset{h\nu}{\rightarrow}$
c. $(\eta^5\text{-}\mathrm{C_5Me_5})\mathrm{Rh(Co_2)} \overset{\Delta}{\rightarrow}$ (dimeric product, contains one CO per metal)
d. $V(CO)_6 + NO \rightarrow$
e. $W(CO)_5[C(C_6H_5)(OC_2H_5)] + BF_3 \rightarrow$
f. $[(\eta^5\text{-}C_5H_5)Fe(CO)_2]_2 + Al(C_2H_5)_3 \rightarrow$

- **13.36** Complexes of formula $Rh(CO)(phosphine)_2Cl$ have the C — O stretching bands shown below. Match the infrared bands with the appropriate phosphine.

Phosphines: $P(p\text{-}C_6H_4F)_3$, $P(p\text{-}C_6H_4Me)_3$, $P(t\text{-}C_4H_9)_3$, $P(C_6F_5)_3$; ν(CO), cm^{-1}: 1923, 1965, 1984, 2004

- **13.37** For each of the following sets, which complex would be expected to have the highest C — O stretching frequency?

a.	$Fe(CO)_5$	$Fe(CO)_4(PF_3)$	$Fe(CO)_4(PCl_3)$	$Fe(CO)_4(PMe_3)$
b.	$[Re(CO)_6]^+$	$W(CO)_6$	$[Ta(CO)_6]^-$	
c.	$Mo(CO)_3(PCl_3Ph)_3$	$Mo(CO)_3(PCl_2Ph)_3$	$Mo(CO)_3(PPh_3)_3$	$Mo(CO)_3py_3$ (py = pyridine)

- **13.38** When $Cr(CO)_5(PH_3)$ and $Cr(CO)_5(NH_3)$ are oxidized by one electron:

a. What is the change in LFSE?
b. Does the C—O distance increase or decrease? Explain briefly.
c. When $Cr(CO)_5(PH_3)$ is oxidized, what is the effect on the Cr—P distance? Explain briefly.
d. When $Cr(CO)_5(NH_3)$ is oxidized, what is the effect on the Cr—N distance? Explain briefly. (T. Leyssens, D. Peeters, A. G. Orpen, J. N. Harvey, *New J. Chem.*, **2005**, *29*, 1424.)

- **13.39** Arrange the following complexes in order of the expected frequency of their *ν*(CO) bands. (See M. F. Ernst, D. M. Roddick, *Inorg. Chem.*, **1989**, *28*, 1624.)

$Mo(CO)_4(F_2PCH_2CH_2PF_2)$

$Mo(CO)_4[(C_6F_5)_2PCH_2CH_2P(C_6F_5)_2]$

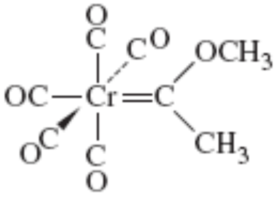
$Mo(CO)_4(Et_2PCH_2CH_2PEt_2)$ (Et = C_2H_5)

$Mo(CO)_4(Ph_2PCH_2CH_2PPh_2)$ (Ph = C_6H_5)

$Mo(CO)_4[(C_2F_5)PCH_2CH_2P(C_2H_5)]$

- **13.40** Free N_2 has a stretching vibration (not observable by IR; why?) at 2331 cm^{-1}. Would you expect the stretching vibration for coordinated N_2 to be at higher or lower energy? Explain briefly.

- **13.41** The ^1H NMR spectrum of the carbene complex shown below shows two peaks of equal intensity at 40 °C. At –40 °C, the NMR shows four peaks, two of a lower intensity and two of a higher intensity. The solution may be warmed and cooled repeatedly without changing the NMR properties at these temperatures. Account for this NMR behavior.



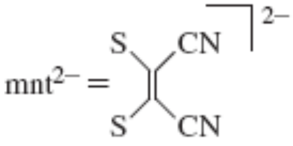
- **13.42** The ^1H NMR spectrum of $(C_5H_5)_2Fe(CO)_2$ shows two peaks of equal area at room temperature but has four resonances of relative intensity 5:2:2:1 at low temperatures. Explain. (See C. H. Campbell, M. L. H. Green, *J. Chem. Soc., A*, **1970**, 1318.)

- **13.43** Of the compounds $Cr(CO)_5(PF_3)$ and $Cr(CO)_5(PCl_3)$, which would you expect to have

  a. The shorter $C—O$ bonds?
  b. The higher energy $Cr—C$ stretching bands in the infrared spectrum?

- **13.44** Select the best choice for each of the following:

a. Higher N—O stretching frequency:
$[Fe(NO)(mnt)_2]^-$ $[Fe(NO)(mnt)_2]^{2-}$



b. Longest N — N bond:
N_2
$(CO)_5Cr{:}N \equiv N$
$(CO)_5Cr{:}N \equiv N{:}Cr(CO)_5$

c. Shorter Ta — C distance in
$(\eta^5\text{-}C_5H_5)_2Ta(CH_2)(CH_3)$:
Ta — CH2 Ta — CH3

d. Shortest Cr — C distance:
$Cr(CO)_6$

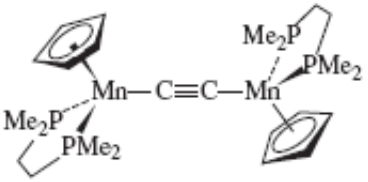
Cr — CO in *trans*-$Cr(CO)_4I(CCH_3)$
Cr — CCH3 in *trans*-$Cr(CO)_4I(CCH_3)$

e. Lowest C — O stretching frequency:
$Ni(CO)_4$
$[Co(CO)_4]^-$
$[Fe(CO)_4]^{2-}$

- **13.45** The dimanganese complex shown can be oxidized reversibly by 1–3 electrons. X-ray crystal structures for the neutral complex and the ions having charges of 1^+1 and 2^+ have provided the following bond distances for the atoms in the MnCCMn chain:

Complex	Mn—C(Å)	C—C(Å)
MCCM	1.872	1.271
[MCCM] $^{+}$	1.800	1.291
[MCCM] $^{2+}$	1.733	1.325

Account for the trends in Mn—C and C—C distances. Be sure to take into account the relevant orbitals. (See S. Kheradmandan, K. Venkatesan, O. Blacque, H. W. Schmalle, H. Berke, *Chem–Eur. J.*, **2004**, *10*, 4872.)



MCCM

- **13.46** Use the Covalent Bond Classification Method to classify these complexes with a $[ML_lX_xZ_z]^{Q\pm}$ formula. With charged species, reduce the formula to its equivalent neutral class.

  a. $W(CH_3)_6$
  b. $[W(\eta^5\text{-}C_5H_5)_2H_3]^+$
  c. $[Fe(CO)_4]^{2-}$
  d. $Mo(\eta^5\text{-}C_5H_5)(CO)_3H$
  e. $Fe(CO)_4I_2$
  f. $[Co(\eta^5\text{-}C_5H_5)_2]^+$

- **13.47** Use the Covalent Bond Classification Method to classify these hypothesized complexes with a $[ML_lX_xZ_z]^{Q\pm}$ formula. With charged species, reduce the formula to its equivalent neutral class. On the basis on the MLX plot for iron in **Section 13.7** , speculate on the likelihood that the following iron complexes have been prepared.

  a. $[FeCl_3(PPh_3)_3]^{3+}$
  b. $[FeCl_3(PPh_3)_2]^+$
  c. $[FeCl_2(PPh_3)_2]^+$

d. $FeCl_2(PPh_3)_2$

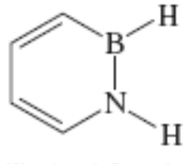
- **13.48** A solution of blue $Mo(CO)_2(PEt_3)_2Br_2$ was treated with a tenfold excess of 2-butyne to give **X**, a dark green product. **X** had bands in the ^1H NMR at δ 0.90 1.63 (2), and 3.16 (1). The peak at 3.16 was a singlet at room temperature but split into two peaks at temperatures below –20 °C. ^{31}P NMR showed only a single resonance. IR showed a single strong band at 1950 cm^{-1}. Molecular weight determinations suggest that **X** has a molecular weight of 580 ± 15. Suggest a structure for **X**, and account for as much of the data as possible. (See P. B. Winston, S. J. Nieter Burgmayer, J. L. Templeton, *Organometallics*, **1983**, *2*, 168.)

- **13.49** Photolysis at –78 °C of $[(\eta^5\text{-}C_5H_5)Fe(CO)_2]_2$ results in the loss of a colorless gas and the formation of an iron-containing product having a single carbonyl band at 1785 cm^{-1} and containing 14.7 percent oxygen by mass. Suggest a structure for the product.

- **13.50** Nickel carbonyl reacts with cyclopentadiene to produce a red diamagnetic compound of formula $NiC_{10}H_{12}$. The ^1H NMR spectrum of this compound shows four different types of hydrogen; integration gives relative areas of 5:4:2:1, with the most intense peak in the aromatic region. Suggest a structure of $NiC_{10}H_{12}$ that is consistent with this NMR spectrum

- **13.51** The carbonyl carbon–molybdenum–carbon angle in $Cp(CO)_2Mo[\mu\text{-}S_2C_2(CF_3)_2]_2MoCp$ ($Cp = \eta^5\text{-}C_5H_5$) is 76.05°. Calculate the ratio of intensities $I_{symmetric}/I_{antisymmetric}$ expected for the C—O stretching bands of this compound. (See K. Roesselet, K. E. Doan, S. D. Johnson, P. Nicholls, G. L. Miessler, R. Kroeker, S. H. Wheeler, *Organometallics*, **1987**, *6*, 480.)

- **13.52** The complex $(\pi\text{-}C_4BNH_6)Cr(CO)_3$ has recently been reported, the first example of the 1,2-dihydro-1,2-azaborine ligand. It has strong absorptions at 1898 and 1975 cm^{-1}, in comparison with 1892 and 1972 cm^{-1} for $(\pi\text{-}C_6H_6)Cr(CO)_3$. The C_4BNH_6 complex has carbon–carbon distances of 1.393, 1.421, and 1.374 Å, in order, in the ring.



1,2-dihydro-1,2-azaborine

a. Is the C_4BNH_6 ligand a (slightly) stronger or weaker acceptor than C_6H_6? Explain.

b. Account for the differences in the C—C distances in the ring. (See A. J. V. Marwitz, M. H. Matus, L. N. Zakharov, D. A. Dixon, S.-Y. Liu, *Angew. Chem., Int. Ed.*, **2009**, *48*, 973.)

- **13.53** Reaction of Ir complex **A** with C_{60} gave a black solid residue **B** with the following spectral characteristics: mass spectrum: $M^+ = 1056$; ^1H NMR: δ 7.65 ppm (multiplet, 2H), 7.48 (multiplet, 2H), 6.89 (triplet, 1H), and 5.97 (doublet, 2H); IR: $\nu(CO) = 1998\ cm^{-1}$.