

Problem set 8

1. Interpret the following spectroscopic data:

(a) The IR spectrum of $[\text{Co}_3(\text{CO})_{10}]^-$ has peaks at 2071, 2006, 1999, 1975, 1865 and 1584 cm^{-1} .

(b) At 178 K, the ^1H NMR spectrum of $[(\mu\text{-H})_3\text{Ru}_4(\text{CO})_{12}]^-$ exhibits three signals due to two isomers:

A: $\delta -15.9$, d, $J = 2.5$ Hz, relative integral 2

$\delta -19.1$, t, $J = 2.5$ Hz, relative integral 1

B: $\delta -17.4$, s, relative integral 3.7

At room T, the cluster exhibits a singlet at $\delta -16.9$.

(c) The ^{13}C NMR spectrum of $\text{Rh}_6(\text{CO})_{16}$ shows two signals ($\delta 180$, d, $J = 70$ Hz and $\delta 232$, q, $J = 26$ Hz). However, the ^{13}C NMR spectrum of $[\text{Rh}_6(\text{CO})_{15}]^{2-}$ shows just one signal ($\delta 209$, septet, $J = 14$ Hz).

2. Do the following molecules conform to the Effective Atomic Number rule: $\text{Co}_2(\text{CO})_8$ (dimer), $\text{FeRu}_2(\text{CO})_{12}$ (triangle), $\text{H}_4\text{Ru}_4(\text{CO})_{12}$ (tetrahedron), $[\text{Os}_5(\text{CO})_{15}]^{2-}$ (trigonal bipyramid), $\text{Os}_6(\text{CO})_{21}$ (raft), $\text{Ru}_5\text{C}(\text{CO})_{15}$ (square-based pyramid), $[\text{Co}_6\text{C}(\text{CO})_{15}]^{2-}$ (trigonal prism), $[\text{Co}_6(\text{CO})_{15}]^{2-}$ (octahedron) and $[\text{Os}_8(\text{CO})_{22}]^{2-}$ (bicapped octahedron)?

3. Use PSEPT to predict the structure of the following clusters: $\text{Fe}_5\text{C}(\text{CO})_{15}$, $[\text{Re}_4(\text{CO})_{16}]^{2-}$, $\text{H}_2\text{Os}_6(\text{CO})_{18}$ and $\text{Os}_9(\text{CO})_{25}$. Discuss the possibility of isomers for $\text{Os}_9(\text{CO})_{25}$.

4. Use the condensation principle to decide which of the following M_8 cluster geometries corresponds to (i) $\text{Rh}_8\text{C}(\text{CO})_{19}$, (ii) $\text{Rh}_8\text{C}_2(\text{CO})_{18}$, (iii) $[\text{Re}_8\text{C}(\text{CO})_{24}]^{2-}$ and (iv) $[\text{Ir}_8(\text{CO})_{22}]^{2-}$.

