Problem Set 1

(1) Determine the point groups of the following molecules:

(a) CH_4
(b) $CHCl_3$
(c) CH_2Cl_2
(d) $Fe(CO)_5$
(e) $Cr(CO)_6$
(f) $Mn(CO)_5Cl$
(g) *cis*-$Fe(CO)_4Cl_2$
(h) *trans*-$Fe(CO)_4Cl_2$
(i) *fac*-$Cr(CO)_3(^{13}CO)_3$
(j) *mer*-$Cr(CO)_3(^{13}CO)_3$
(k) tris(ethylenediamine)Cr(III)
(l) *cis*-1,2-dichloroethane
(m) *trans*-1,2-dichloroethane
(n) allene
(o) $(\eta^6\text{-}C_6H_6)Cr(CO)_3$
(p) $(\eta^5\text{-}C_5H_5)Mn(CO)_3$
(q) staggered ferrocene
(r) $(\eta^8\text{-}C_8H_8)_2U$
(s) $(\eta_3\text{-}C_3H_5)_2Ni$
(t) borazine
(u) $Ru_3(CO)_{12}$
(v) $Fe_3(CO)_{12}$
(w) $[Mo_2Cl_9]^{3-}$
(x) S_8
(y) $[Re_2Cl_8]^{2-}$
(z) carbon suboxide (OC_3O)

Note: This problem is intended to refresh your ability to name molecular point groups. If you are unfamiliar with the structures of some of the above, you should look them up in an appropriate textbook. If you desire additional practice assigning point groups, I would suggest you do the problems in Cotton pp. 61-67.

(2) Find the transformation of a general Cartesian point (a,b,c) under each of the following products of symmetry operations. For each product, determine whether the operations commute. If possible, determine a single symmetry operation that performs the same transformation.

(a) $C_2^x \bullet C_2^y$
(b) $C_2^x \bullet C_4^z$
(c) $i \bullet \sigma_z$
(d) $C_4^x \bullet i$
(e) $C_4^x \bullet \sigma_{x=y}$
(f) $\sigma_x \bullet \sigma_y$

(3) Draw a cube and label the corners 1 through 8. For one operation of each of the following classes of operations of the O_h point group, construct a matrix that describes the permutation of the corners under the operation.

(a) E
(b) C_3
(c) C_4
(d) i
(d) S_4
(e) S_6
(f) σ_h
(h) σ_d

Abbreviated Point Group Flow Chart