

Chem 315, Fall 2000
Answers to Problem Set #4

P4.7) MA_3B_3 two isomers (fac vs mer), $MA_2B_2C_2$ five isomers

P4.8) BF_3 is D_{3h} , NF_3 is C_{3v} , and ClF_3 is C_{2v} . Looking at the irreducible representation one can tell the difference between the molecule based on their point group and what symmetries are IR and Ramon active.

Ex.4.10) 5 in the plane [(4x2)-8], 1 perpendicular to the plane (total vibrational modes $3(4)-6=6$, $6-5=1$)

Ex.4.11) SF_6 if Oh, and have no vibrations which are both IR and Ramon active, BF_3 is D_{3h} and E' is both IR and Ramon active.

a) D_{2h} . Key symmetry elements are: C_2 , 2 C_{∞} , ? σ_h .

b) oh. C_4 , multiple C_3 , ? σ_h , multiple ? σ_v .

c) D_{5d} . C_5 , 5 C_{∞} , no ? σ_h , 5 ? σ_v .

d) D_{3d} . C_3 , 3 C_{∞} , no ? σ_h , 3 ? σ_v .

e) **Two options:** 1) if you ignore the angle between two silicon and oxygen atoms - D_{3h} . C_3 , 3 C_{∞} , ? σ_h , 3 ? σ_v . 2) If you do consider the angle between these atoms (150°), then C_{2v} . C_2 , no C_{∞} , no ? σ_h , 2 ? σ_v .

f) D_{2h} C_2 , 2 C_{∞} , ? σ_h .

g) D_{3h} C_3 , 3 C_{∞} , ? σ_h , ? σ_v 's.

h) T_d multiple C_3 , multiple ? σ_v .

i) D_{3h} (trig. bipyramide) C_3 , 3 C_{∞} , ? σ_h , ? σ_v 's, or C_{4v} (sq. pyramide) C_4 , no C_{∞} , no ? σ_h , 4 ? σ_v .

j) T_d multiple C_3 , multiple ? σ_v .

k) D_{3h} (eclipsed) C_3 , 3 C_{∞} , ? σ_h , ? σ_v 's; D_{3d} (staggered) C_3 , 3 C_{∞} , ? σ_h , ? σ_v 's; D_3 (intermediate) C_3 , 3 C_{∞} , no mirror planes.