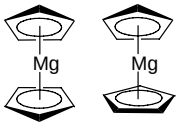
University of Windsor
Chemistry and Biochemistry
Chemistry 59-250, Fall Term 2005

Assignment 2

Question #1
Identification of Point Groups

Determine the point groups for the following molecules:

(a) ClF_4^{-1} D_{4h}
(b) PF_6^{-1} O_h
(c) carbon disulfide, CS_2 $D_{\infty h}$
(d) cyanogen, N≡C-C≡N $D_{\infty h}$
(e) nitrate, NO_3^{-1} D_{3h}
(f) carbon monoxide, CO $C_{\infty v}$
(g) ozone, O_3 C_{2v}
(h) phosphonium cation, PH_4^{+1} T_d
(i) sulphur dioxide, SO_2 C_{2v}
(j) acetone (with the highest symmetry possible), $H_3CC(O)CH_3$ C_{2v}
(k) thionyl fluoride, OSF_2 C_s
(l) $CHFCl_2$ C_s
(m) boric acid (planar), $B(OH)_3$ C_{3h}
(n) allene, $H_2C=C=CH_2$ D_{2d}
(o) AsF_4^{-1} C_{2v}
(p,q) the two common conformations of magnesocene:



D_{5h} D_{5d}
(r) H_3C-CFBrCl C_1
(s) XeF_4 D_{4h}
(t) buckminsterfullerene, C_{60} I_h

Question #2

More VBT

Use localized bonding models to describe the bonding in the molecules from (a) to (o) in Question #1. Use VSEPR and VBT for each of the non-terminal atoms. You must draw pictures to show the shapes of the hybridized orbitals and how they interact with other orbitals to form bonds! The electron configuration boxes do not show the shapes and are not advised.

Note that you have to draw pictures of the orbitals – I have not done so here only to save time and space!

(a) ClF_4^{-1} Cl: AX_4E_2 so square planar and $(sp^3d^2\text{-}2p)\sigma$ Cl-F bonds

(b) PF_6^{-1} P: AX_6 so octahedral and $(sp^3d^2\text{-}2p)\sigma$ P-F bonds

(c) carbon disulfide, CS_2 C: AX_2 so linear and $(sp\text{-}3p)\sigma$ C-S bonds and 2 perpendicular $(2p\text{-}3p)\pi$ C-S bonds

(d) cyanogen, N≡C-C≡N C: AX_2 so linear and $(sp\text{-}sp)\sigma$ C-C bonds; $(sp\text{-}2p)\sigma$ C-N bonds and 2 perpendicular $(2p\text{-}2p)\pi$ C-N bonds

(e) nitrate, NO_3^{-1} N: AX_3 so trigonal planar and $(sp^2\text{-}2p)\sigma$ N-O bonds and one $(2p\text{-}2p)\pi$ N-O bond

(f) carbon monoxide, CO Both atoms are terminal so just use atomic orbitals: $(2p\text{-}2p)\sigma$ C-O bonds and 2 perpendicular $(2p\text{-}2p)\pi$ C-O bonds

(g) ozone, O_3 O: AX_2E so bent and $(sp^2\text{-}2p)\sigma$ O-O bonds and one $(2p\text{-}2p)\pi$ O-O bonds

(h) phosphonium cation, PH_4^{+1} P: AX_4 so tetrahedral and $(sp^3\text{-}1s)\sigma$ P-H bonds

(i) sulphur dioxide, SO_2 S: AX_2E so bent and $(sp^2\text{-}2p)\sigma$ S-O bonds, one $(3p\text{-}2p)\pi$ S-O bond and one $(3d\text{-}2p)\pi$ S-O bond

(j) acetone (with the highest symmetry possible), $H_3CC(O)CH_3$

methyl C: AX_4 so tetrahedral and three $(sp^3\text{-}1s)\sigma$ C-H bonds, one $(sp^3\text{-}sp^2)\sigma$ C-C bond each

ketone C: AX_3 so trigonal planar and one $(sp^2\text{-}2p)\sigma$ C-O bond and one $(2p\text{-}2p)\pi$ C-O bond

(k) thionyl fluoride, OSF_2 S: AX_3E so pyramidal and two $(sp^3\text{-}2p)\sigma$ S-F bonds, one $(sp^3\text{-}2p)\sigma$ S-O bond, and one $(3d\text{-}2p)\pi$ S-O bond

(l) $CHFCl_2$ C: AX_4 so tetrahedral and one $(sp^3\text{-}1s)\sigma$ C-H bond, one $(sp^3\text{-}2p)\sigma$ C-F bond, and two $(sp^3\text{-}3p)\sigma$ C-Cl bonds

(m) boric acid (planar), $B(OH)_3$

B: AX_3 so trigonal planar and three $(sp^2\text{-}sp^3)\sigma$ B-O bonds

O: AX_2E_2 so bent and one $(sp^3\text{-}1s)\sigma$ O-H bond for each hydroxyl group

(n) allene, $H_2C{=}C{=}CH_2$

methylene C: AX_3 trigonal planar and two $(sp^2\text{-}1s)\sigma$ C-H bonds, one $(sp^2\text{-}sp)\sigma$ C-C bond each

central C: AX_2 so linear and one $(sp\text{-}sp^2)\sigma$ C-C bond (as above) and perpendicular $(2p\text{-}2p)\pi$ C-C bonds to each methylene carbon atom

(o) AsF_4^{-1} As: AX_4E so see-saw (disphenoidal) and $(sp^3d\text{-}2p)\sigma$ As-F bonds

Question #3
More Point Groups

Draw a picture and determine the point group for EACH of the possible structural arrangements of $AsF_nCl_{(5-n)}$ for n = 0 to 5. *I.e. start with $AsCl_5$ and end with AsF_5.* Assuming a static structure, indicate the number and relative intensities of the signals that you would expect to see in the ^{19}F NMR spectrum of each molecule.

$AsCl_5$ (and AsF_5): D_{3h} ; no ^{19}F signal for $AsCl_5$, 3:2 signal ratio for AsF_5

$AsF_{ax}Cl_4$ (and $AsCl_{ax}F_4$): C_{3v} ; one signal for $AsF_{ax}Cl_4$, 3:1 for $AsCl_{ax}F_4$

$AsF_{eq}Cl_4$ (and $AsCl_{eq}F_4$): C_{2v} ; one signal for $AsF_{eq}Cl_4$, 2:2 for $AsCl_{eq}F_4$

$AsF_{(ax)2}Cl_3$ (and $AsCl_{(ax)2}F_3$): D_{3h} ; one signal for $AsF_{(ax)2}Cl_3$, one signal for $AsCl_{(ax)2}F_3$

$AsF_{ax}F_{eq}Cl_3$ (and $AsCl_{ax}Cl_{eq}F_3$): C_s ; 1:1 for $AsF_{ax}F_{eq}Cl_3$, 2:1 for $AsCl_{ax}Cl_{eq}F_3$

$AsF_{(eq)2}Cl_3$ (and $AsCl_{(eq)2}F_3$): C_{2v} ; one signal for $AsF_{(eq)2}Cl_3$, 2:1 for $AsCl_{(eq)2}F_3$