Question #1
Identification of Point Groups

Determine the point groups for the following molecules:

(a) ClF₄⁻¹  \( \text{D}_{4h} \)
(b) PF₆⁻¹  \( \text{O}_h \)
(c) carbon disulfide, CS₂  \( \text{D}_{\infty h} \)
(d) cyanogen, N≡C-C≡N  \( \text{D}_{\infty h} \)
(e) nitrate, NO₃⁻¹  \( \text{D}_{3h} \)
(f) carbon monoxide, CO  \( \text{C}_{\infty v} \)
(g) ozone, O₃  \( \text{C}_{2v} \)
(h) phosphonium cation, PH₄⁺  \( \text{T}_d \)
(i) sulphur dioxide, SO₂  \( \text{C}_{2v} \)
(j) acetone (with the highest symmetry possible), H₃C(C=O)CH₃  \( \text{C}_{2v} \)
(k) thionyl fluoride, OSF₂  \( \text{C}_s \)
(l) CHFCl₂  \( \text{C}_s \)
(m) boric acid (planar), B(OH)₃  \( \text{C}_{3h} \)
(n) allene, H₂C=CH₂  \( \text{D}_{2d} \)
(o) AsF₄⁻¹  \( \text{C}_{2v} \)
(p,q) the two common conformations of magnesocene:

\[ \text{D}_{5h} \quad \text{D}_{5d} \]
(r) H₃C-CFBrCl  \( \text{C}_1 \)
(s) XeF₄  \( \text{D}_{4h} \)
(t) buckminsterfullerene, C₆₀  \( \text{I}_h \)
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$_4^-$ Cl: AX$_4$E$_2$ so square planar and (sp$^3$d$^2$-2p)$\sigma$ Cl-F bonds
(b) PF$_6^-$ P: AX$_6$ so octahedral and (sp$^3$d$^2$-2p)$\sigma$ P-F bonds
(c) carbon disulfide, CS$_2$ C: AX$_2$ so linear and (sp-3p)$\sigma$ C-S bonds and 2 perpendicular (2p-3p)$\pi$ C-S bonds
(d) cyanogen, N≡C-C≡N C: AX$_2$ so linear and (sp-sp)$\sigma$ C-C bonds; (sp-2p)$\sigma$ C-N bonds and 2 perpendicular (2p-2p)$\pi$ C-N bonds
(e) nitrate, NO$_3^-$ N: AX$_3$ so trigonal planar and (sp$^2$-2p)$\sigma$ N-O bonds and one (2p-2p)$\pi$ N-O bond
(f) carbon monoxide, CO Both atoms are terminal so just use atomic orbitals: (2p-2p)$\sigma$ C-O bonds and 2 perpendicular (2p-2p)$\pi$ C-O bonds
(g) ozone, O$_3$ O: AX$_2$E so bent and (sp$^2$-2p)$\sigma$ O-O bonds and one (2p-2p)$\pi$ O-O bonds
(h) phosphonium cation, PH$_4^+$ P: AX$_4$ so tetrahedral and (sp$^3$-1s)$\sigma$ P-H bonds
(i) sulphur dioxide, SO$_2$ S: AX$_2$E so bent and (sp$^2$-2p)$\sigma$ S-O bonds, one (3p-2p)$\pi$ S-O bond and one (3d-2p)$\pi$ S-O bond
(j) acetone (with the highest symmetry possible), H$_3$C(O)CH$_3$
  methyl C: AX$_4$ so tetrahedral and three (sp$^3$-1s)$\sigma$ C-H bonds, one (sp$^3$-sp$^3$)$\sigma$ C-C bond each
  ketone C: AX$_3$ so trigonal planar and one (sp$^2$-2p)$\sigma$ C-O bond and one (2p-2p)$\pi$ C-O bond
(k) thionyl fluoride, OSF$_2$ S: AX$_3$E so pyramidal and two (sp$^3$-2p)$\sigma$ S-F bonds, one (sp$^3$-2p)$\sigma$ S-O bond, and one (3d-2p)$\pi$ S-O bond
(l) CHFCl$_2$ C: AX$_4$ so tetrahedral and one (sp$^3$-1s)$\sigma$ C-H bond, one (sp$^3$-2p)$\sigma$ C-F bond, and two (sp$^3$-3p)$\pi$ C-Cl bonds
(m) boric acid (planar), B(OH)$_3$
  B: AX$_3$ so trigonal planar and three (sp$^2$-sp$^3$)$\sigma$ B-O bonds
  O: AX$_2$E$_2$ so bent and one (sp$^3$-1s)$\sigma$ O-H bond for each hydroxyl group
(n) allene, H$_2$C=CH$_2$
  methylene C: AX$_3$ trigonal planar and two (sp$^2$-1s)$\sigma$ C-H bonds, one (sp$^2$-sp)$\sigma$ C-C bond each
  central C: AX$_2$ so linear and one (sp-sp$^2$)$\pi$ C-C bond (as above) and perpendicular (2p-2p)$\pi$ C-C bonds to each methylene carbon atom
(o) AsF$_4^-$ As: AX$_4$E so see-saw (disphenoidal) and (sp$^3$d-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