Name_____

Chem 370 - Spring, 2018
Test I
February 26, 2018

1. (16 points) Fill in the symbols for the missing elements in the portion of the periodic table shown below.

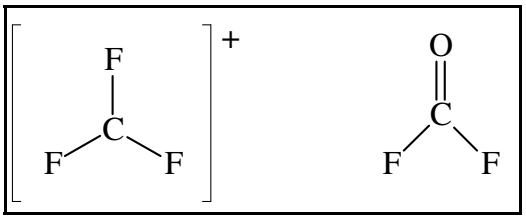
									C
V									

2. (32 points; 4 points each part). Fill in the blanks.

a. Name the shape of each of the following molecules, based on VSEPR considerations.

IF_7 _____ IF_5 _____

b. In terms of ligand close packing (LCP) theory, briefly explain why $F_2C{=}O$ has a longer C–F bond length (131.7 pm) and smaller F–C–F angle (107.6°), compared to CF_3^+ (123.5 pm, 120°).



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Name_____

c. As indicated by the equation $\sum_{R_c} g_c \chi_i(R_c)\chi_j(R_c) = h\delta_{ij}$, for a group of order h the sum of the squares of the characters for any irreducible representation is equal to _____, but the sum of the products of the characters for any two different irreducible representations is equal to _____.

d. The group D_{3h} has an order $h = 12$. List the four possible orders (g) for its subgroups (excluding $g = 1$ for the trivial subgroup C_1). (Do not attempt to name the subgroups.)

_____

e. Consider the A_u irreducible representation of the group C_{4h}. Judging from the Mulliken symbol, the representation is _____ (symmetric/antisymmetric) with respect to the C_4 axis, and _____ (symmetric/antisymmetric) with respect to inversion.

f. Circle the correct answer among each of the following choices.

The shortest bonds: NF_3 PF_3 AsF_3 NF_4^+

The smallest bond angle: NF_3 PF_3 AsF_3 NF_4^+

g. The valence configuration of $_{27}Co$ is _____, and the valence configuration of the Co^{2+} ion is _____.

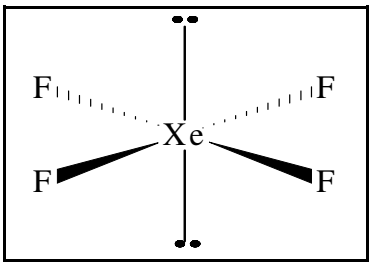
h. With the aid of the D_{3h} character table shown on the last page, give the irreducible representations that would result from the following direct products:

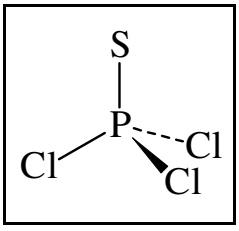
$A_2'' \times A_2'' =$ $A_1'' \times E' =$

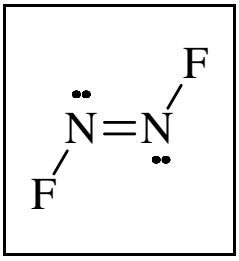
Name_____

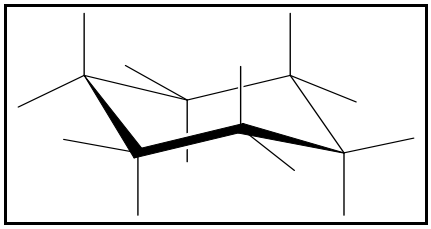
3. (20 points) Give the point group of each of the following.

O=C=C=C=O



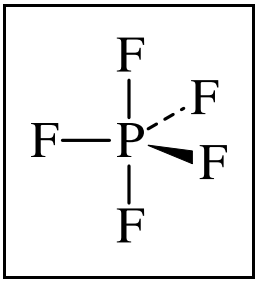






Name_____

4. (32 points) Consider PF_5:



Determine the number of frequencies, their symmetries, and the infrared and Raman activities of the normal modes of PF_5. Show your work on the worksheet on page 5. A D_{3h} character table is shown below the worksheet. From your work in the worksheet, write out the composition of Γ_{3n}, identify the species that comprise Γ_{trans} and Γ_{rot}, and then indicate the symmetries of the genuine normal modes that comprise Γ_{3n-6}. When you have written out the composition of Γ_{3n-6}, you should be able to identify which species are infrared active, which species are Raman active, and which species are polarized in the Raman spectrum. Note the species and number of frequencies that may be coincident in both spectra, as well as any silent modes that would not be active in either spectrum. Once you have completed your work, summarize your results in the table below. For each category (infrared, Raman, polarized, coincidences, silent modes), give the total number of frequencies and indicate the specific numbers of frequencies of each symmetry species. **Don't forget that there are six (6) atoms in the molecule.**

Type	Total Active Frequencies	Number of Each Symmetry Species
Infrared		
Raman		
Polarized		
Coincidences		
Silent modes		

Name_____

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
N_i								
χ_i								
Γ_{3n}							Σ	Σ/h
A_1'								
A_2'								
E'								
A_1''								
A_2''								
E''								

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A_1'	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2'	1	1	−1	1	1	−1	R_z	
E'	2	−1	0	2	−1	0	(x, y)	$(x^2 - y^2, xy)$
A_1''	1	1	1	−1	−1	−1		
A_2''	1	1	−1	−1	−1	1	z	
E''	2	−1	0	−2	1	0	(R_x, R_y)	(xz, yz)

$\Gamma_{3n} =$

$\Gamma_{trans} =$ $\Gamma_{rot} =$

$\Gamma_{3n-6} =$