

Name _____ Key _____

Chem 370 - Spring, 20019**Test I****March 8, 2019**

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

						B	C	N
						Al	Si	P
Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As
Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb
Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi

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.

SeF₄ irregular tetrahedron SeF₄²⁻ square planar

b. In terms of ligand close packing (LCP) theory, briefly explain why the C-F bond length in CF₄ (131.6 pm) is longer than that in CF₃⁺ (124.7 pm).

The fluorine atoms are close packed and the F...F distance is virtually the same in both (215.5 pm). As a result of geometry, the tetrahedral geometry does not allow the F atoms to come as close to the central C as in a trigonal plane.

c. From your knowledge of the meanings of Mulliken symbols and principles derived from the Great Orthogonality Theorem, fill in the missing characters in the C_{4v} character table shown below.

C _{4v}	E	2C ₄	C ₂	2σ _v	2σ _d
A ₁	1	1	1	1	1
A ₂	1	1	1	-1	-1
B ₁	1	-1	1	1	-1
B ₂	1	-1	1	-1	1
E	2	0	-2	0	0

Name _____ Key _____

- d. The group D_3 consists of six operations (including E). Grouped by class, these are E , $2C_3$, $3C_2$. Other than C_1 , it has two subgroups; viz., the cyclic groups C_2 and C_3 . List all the operations of each subgroup and give its order (g). (Don't forget, every group has E .)

$$C_2: \underline{E, C_2} \quad g = \underline{2}$$

$$C_3: \underline{E, C_3, C_3^2} \quad g = \underline{3}$$

- e. Among the following, circle the *two* whose infrared and Raman spectra would show completely different frequencies (i.e., mutual exclusion):



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



- g. Give the valence configuration of each of the following:



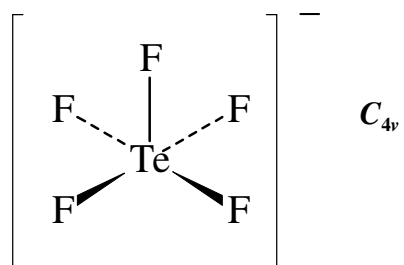
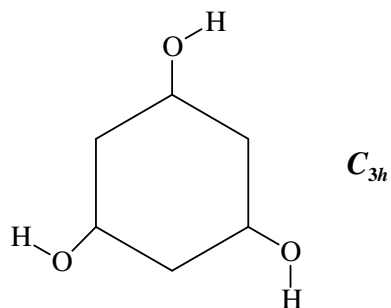
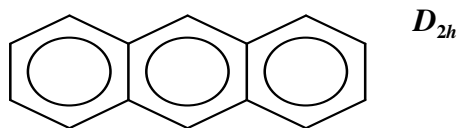
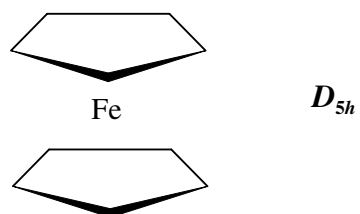
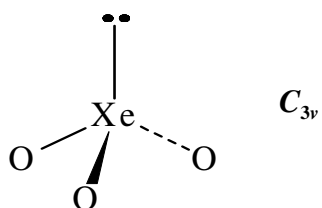
- h. With the aid of the D_{2h} character table shown on the last page, give the irreducible representations that would result from the following direct products:

$$A_g \times A_u = A_u$$

$$B_{2u} \times B_{3u} = B_{1g}$$

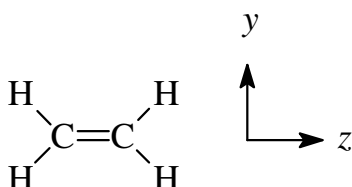
Name _____

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



Name _____ Key _____

4. (32 points) Consider ethylene, C_2H_4 , with the axis orientations shown below. (Feel free to make a model with your kit.)



Using the worksheet on the next page, determine the number of frequencies, their symmetries, and the infrared and Raman activities of the normal modes of ethylene. Identify any polarized Raman bands and the number of frequencies that should be coincident between the two spectra. A separate D_{2h} character table is shown on the final page of this test packet; feel free to remove it for your working convenience. Do not write anything on the character table that you want graded, and take it with you or dispose of it at the end of the test. Once you have completed all your work, summarize your results in the table below, giving the number of frequencies and their symmetry species.

Type	Frequencies	Symmetry Species
Infrared	5	$2B_{1u} + 2B_{2u} + B_{3u}$
Raman	6	$3A_{1g} + B_{2g} + 2B_{3g}$
Polarized	3	$3A_{1g}$
Coincidences	0	—
Silent modes	1	A_{1u}

Name _____ Key _____

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$	$h = 8$	
N_i	6	2	0	0	0	0	2	6		
χ_i	3	-1	-1	-1	-3	1	1	1		
Γ_{3n}	18	-2	0	0	0	0	2	6	Σ	Σ/h
A_{1g}	18	-2					2	6	24	3
B_{1g}	18	-2					-2	-6	8	1
B_{2g}	18	2					2	-6	16	2
B_{3g}	18	2					-2	6	24	3
A_{1u}	18	-2					-2	-6	8	1
B_{1u}	18	-2					2	6	24	3
B_{2u}	18	2					-2	6	24	3
B_{3u}	18	2					2	-6	16	2

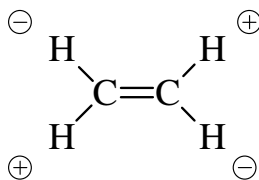
$$\Gamma_{3n} = 3A_{1g} + B_{1g} + 2B_{2g} + 3B_{3g} + A_{1u} + 3B_{1u} + 3B_{2u} + 2B_{3u}$$

$$\Gamma_{\text{trans}} = B_{1u} + B_{2u} + B_{3u} \quad \Gamma_{\text{rot}} = B_{1g} + B_{2g} + B_{3g}$$

$$\Gamma_{3n-6} = 3A_{1g} + B_{2g} + 2B_{3g} + A_{1u} + 2B_{1u} + 2B_{2u} + B_{3u}$$

R (pol) R R — ir ir ir

Bonus (4 points) One of the normal modes of ethylene is depicted below, where \oplus and \ominus indicate motion above and below the plane of the molecule, respectively. Give the Mulliken symbol for this mode, and indicate its infrared and Raman activity.

Mulliken symbol A_{1u} i.r./Raman activity **none (silent mode)**