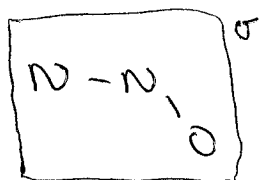


CHEM 721 – INORGANIC STRUCTURE AND BONDING
EXAM 1 – OCTOBER 2, 2000

NAME Key

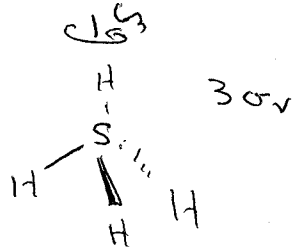
1. For the following molecules and ions, determine the correct symmetry point group.
[20 pts]

a. N_2O (N-N-O, bent)



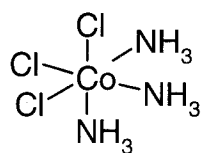
C_s

b. SiH_3I

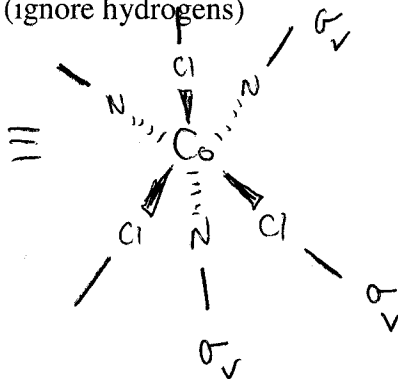


C_{3v}

c. *fac*- $Co(NH_3)_3Cl_3$

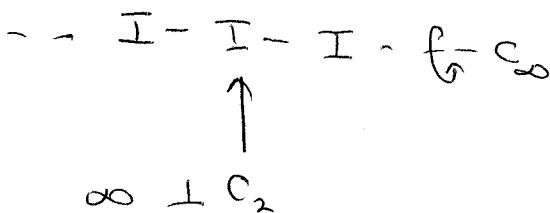


(ignore hydrogens)



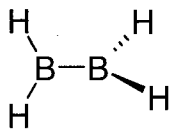
C_{3v}

d. I_3^- (linear)



$D_{\infty h}$

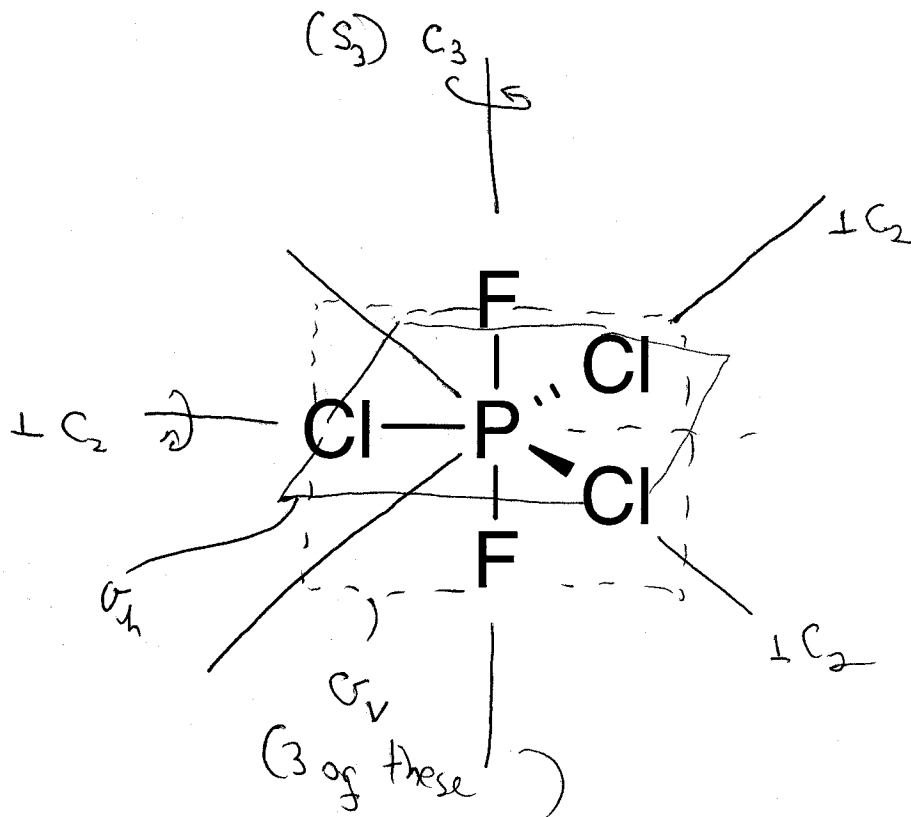
e. H_2B-BH_2 (BH_2 planes twisted 90°)



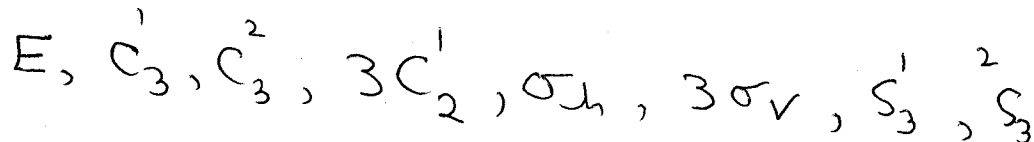
D_{2d}

same as allene ($H_2C=C=CH_2$)

2. The following questions refer to the trigonal bipyramidal molecule, PCl_3F_2 , shown below.



- a. Using the figure above, diagrammatically show all symmetry elements and list all associated symmetry operations. [15 pts]



- b. Determine the point group symmetry of the molecule. [5 pts]



3. What symmetry operation must be present in order for a molecule to have a superimposable mirror image? [10 pts]

improper rotation axis

4. The character table for the point group D_{3h} is shown below.

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)

- a. What is the order of the group? [5 pts]
12
- b. How many symmetry classes are present in the group? [5 pts]
6
- c. Which irreducible representation is the totally symmetric representation? [5 pts]
 A_1'
- d. To what irreducible representations do the following atomic orbitals belong : [8 pts]

i.) p_z A_2''

ii.) s A_1'

iii.) d_{xz} E''

iv.) d_{z^2} A_1'

- e. Determine the direct products of the following representations in D_{3h} . [10 pts]

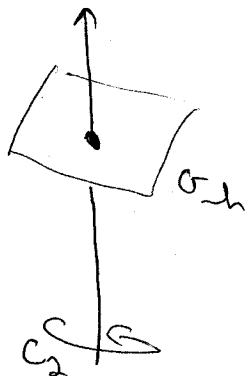
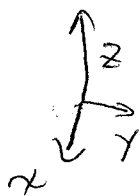
i.) $A_2' \times A_2'' = A_1''$

ii.) $E' \times A_1'' = E''$

5. Below is an incomplete character table for the point group C_{2h} . There is one irreducible representation that is missing.

C_{2h}	E	C_2	i	σ_h
A_g	1	1	1	1
B_g	1	-1	1	-1
	1	1	-1	-1
B_u	1	-1	-1	1

- a. Deduce the characters of this representation and complete the table. [8 pts]
- b. Which Mulliken symbol is appropriate for this representation? [3 pts]
- A_u
- c. To which representations would the vectors x , y , and z belong. (The z axis is along the principal rotation axis and the x and y axes are in the horizontal mirror plane.) [6 pts]



	E	C_2	i	σ_h	
z	1	1	-1	-1	$\equiv A_u$
y	1	-1	-1	1	$\equiv B_u$
x	1	-1	-1	1	$\equiv B_u$