Name _____ Test 2 (10/23)
CHEM 0211 (Adv. Inorganic) Fall 2019

1. (12 pts.) Describe what each of the following symmetry operations are.

a. a σ_h operation

1. _____

2. _____

b. a C_2 operation

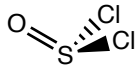
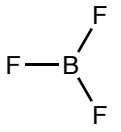
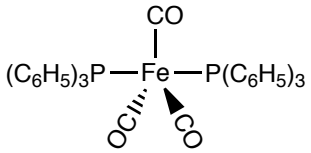
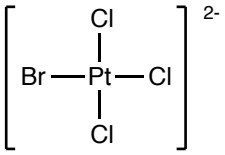
3. _____

c. an S_4 operation

4. _____

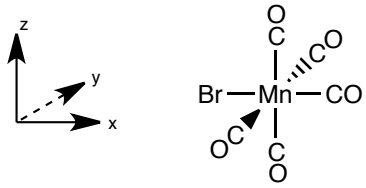
5. _____

2. (16 pts.) Determine the point group for each of the following molecules. Wedge and dashed 3D representations have been provided.

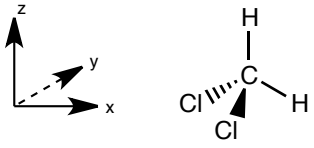
a. 	b. 
d. 	d. 

3. (12 pts.) Perform the indicated operations on the following molecules, and draw a 3D representation, using wedge and dash notation where appropriate, for the resulting view.

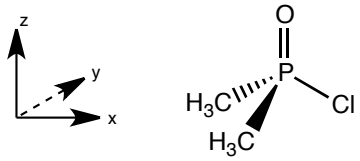
a. Perform a reflection through the yz plane that contains the Mn atom



b. Perform an inversion through the C atom



c. Perform a C_3 on the axis that contains the P to O bond.

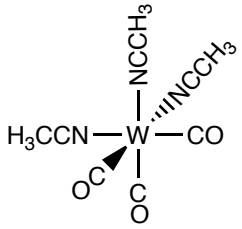


4. (10 pts.) Determine the irreducible representation for the reducible representation listed at the bottom of the following character table.

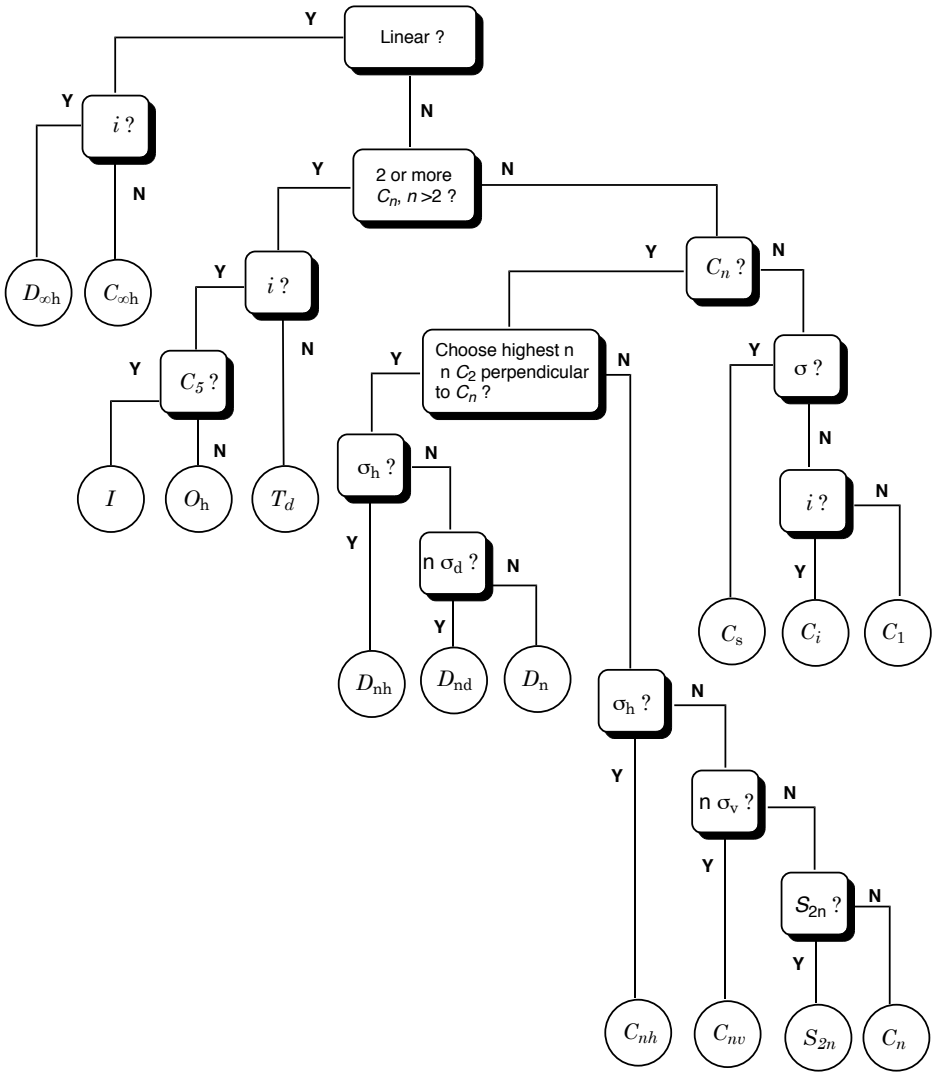
T_d	E	8 C_3	3 C_2	6 S_4	6 σ_d		
A_1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_2	1	1	1	-1	-1		
E	2	-1	2	0	0		$2z^2 - x^2 - y^2$, $x^2 - y^2$
T_1	3	0	-1	1	-1	(R_x, R_y, R_z)	
T_2	3	0	-1	-1	1	(x, y, z)	(xy, xz, yz)
Γ	**8**	**2**	**0**	**2**	**-2**		

5. (10 pt.) Determine the number of CO stretching vibrations that would be visible in the IR spectrum of trisacetonitrilecarbonyltungsten.

a. Determine the point group for the molecule.
b. Determine the reducible representation for the CO stretching vibrations.
c. Determine the irreducible representations for the CO stretching vibrations.
d. Determine the number of CO stretching bands that you would expect to see in the IR spectrum of the molecule.



Point Group Assignment Tree



$$\left(\begin{array}{c}\text{number of irreducible}\\ \text{representations of a given}\\ \text{type needed}\end{array}\right) = \frac{1}{\text{order}} \Sigma_{\text{classes}} \left(\begin{array}{c}\text{\# operations}\\ \text{in class}\end{array}\right)\left(\begin{array}{c}\chi \text{ of the irreducible}\\ \text{representation}\end{array}\right)\left(\begin{array}{c}\chi \text{ of the reducible}\\ \text{representation}\end{array}\right)$$

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, yx)

C_{3h}	E	$2\ C_3$	σ_h	$2\ S_3$		
A'	1	1	1	1	R_z	$x^2 + y^2, z^2$
A''	1	1	-1	-1	z	
E'	2	-1	2	-1	(x,y)	$(x^2 – y^2, xy)$
E''	2	-1	-2	1	(R_x, R_y)	(xz, yz)

C_{3v}	E	$2\ C_3$	$3\ \sigma_v$		
A_1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	-1	R_z	
E	2	-1	0	(x, y), (R_x, R_y)	$(x^2 – y^2, xy)$, (xz, yz)

O_h	E	$8\ C_3$	$6\ C_2$	$6\ C_4$	$3\ C_2$ (C_4^2)	i	$6\ S_4$	$8\ S_6$	$3\ \sigma_h$	$6\ \sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_{2g}	1	1	-1	-1	1	1	-1	1	1	-1		
E_g	2	-1	0	0	2	2	0	-1	2	0		$(2z^2 – x^2 – y^2, x^2 – y^2)$
T_{1g}	3	0	-1	1	-1	3	1	0	-1	-1	(R_x, R_y, R_z)	
T_{2g}	3	0	1	-1	-1	3	-1	0	-1	1		(xy, yz, xz)
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1		
A_{2u}	1	1	-1	-1	1	-1	1	-1	-1	1		
E_u	2	-1	0	0	2	-2	0	1	-2	0		
T_{1u}	3	0	-1	1	-1	-3	-1	0	1	1	(x, y, z)	
T_{2u}	3	0	1	-1	-1	-3	1	0	1	-1		