Name _____ Test 2 (10/29)
CHEM 0211 (Adv. Inorganic) Fall 2021

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

a. an C_3 operation

1. _____

2. _____

b. a σ_v operation

3. _____

4. _____

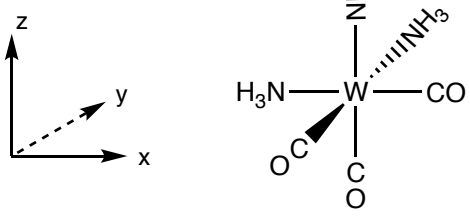
c. an *i* operation

5. _____

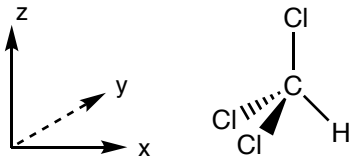
6. _____

2. (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.

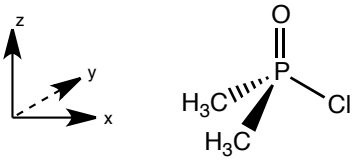
a. Perform and inversion through the W atom.



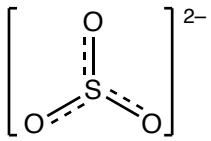
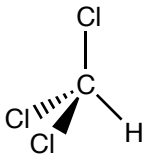
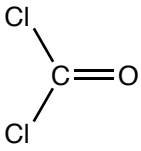
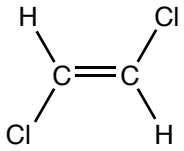
b. Perform a reflection through the yz plane that contains the C atom



c. Perform a S_3 on the axis that contains the P to O bond.



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

a. 	b. 
d. 	d. 

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

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)
Γ	**5**	**2**	**-1**	**3**	**0**	**-3**		

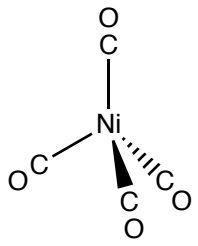
5. (10 pt.) Determine the number of CO stretching vibrations that would be visible in the IR spectrum of nickel tetracarbonyl. Nickel tetracarbonyl is in the T_d point group

a. Determine the reducible representation for the CO stretching vibrations.

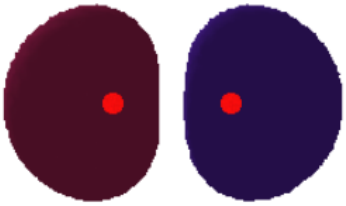
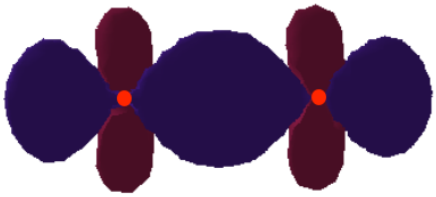
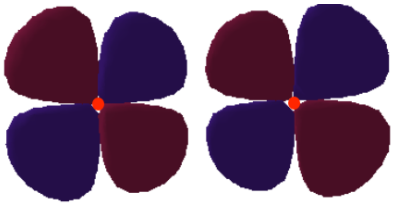
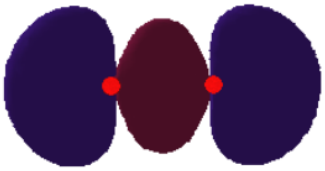
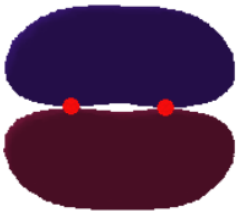
b. Determine the irreducible representations for the CO stretching vibrations.

c. Determine the number of CO stretching bands that you would expect to see in the IR spectrum of the molecule.

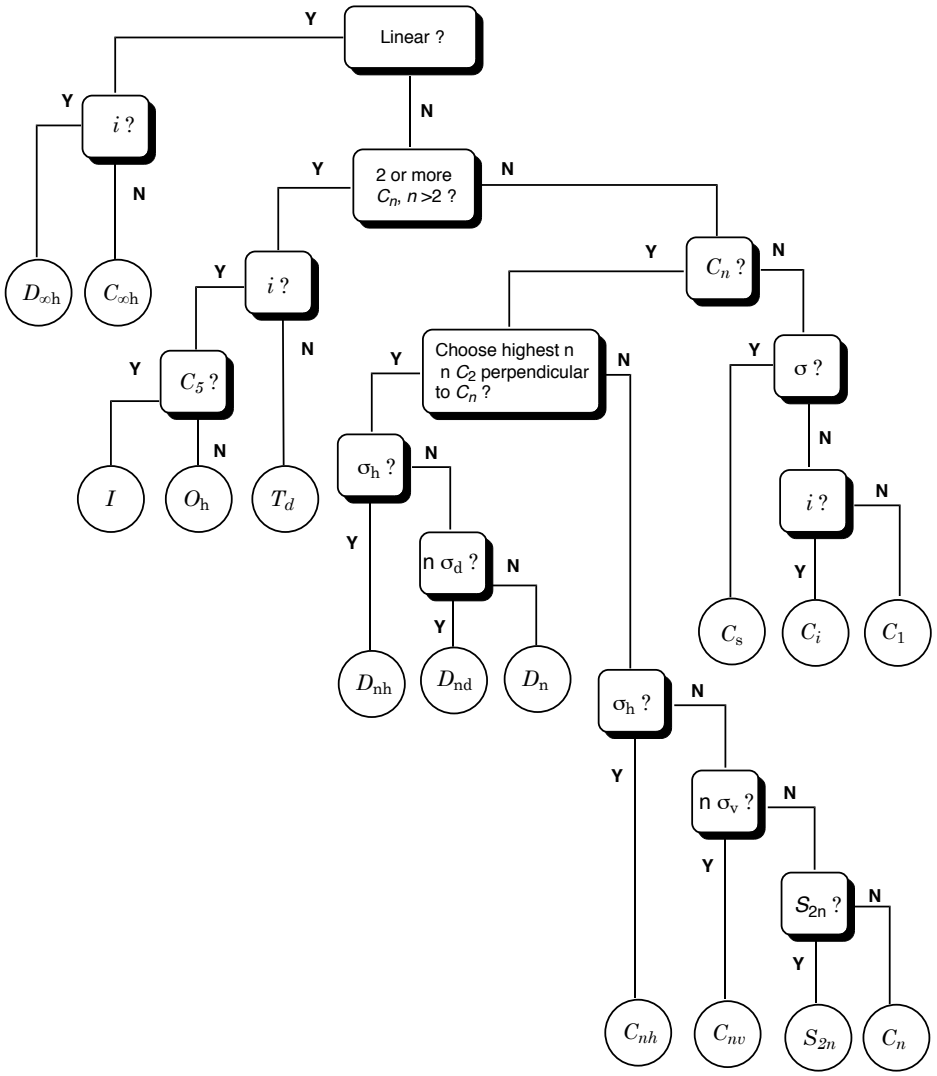
T_d	E	8 C_3	3 C_2	6 S_4	6 σ_d		
A_1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_2	1	1	1	-1	-1		
E	2	-1	2	0	0		$2z^2 - x^2 - y^2$, $x^2 - y^2$
T_1	3	0	-1	1	-1	(R_x, R_y, R_z)	
T_2	3	0	-1	-1	1	(x, y, z)	(xy, xz, yz)



6. Graphical representations of molecular orbitals from diatomic molecules are pictured below.
   a. (3 pts. each) Determine whether the following orbitals would be bonding or antibonding.
   b. (2 pts. each) Determine the symmetry of the orbital, σ, π, or δ/
   c. (2 pts. each) Determine whether the orbitals are gerade or ungerade

i. MO made from two s orbitals 	ii. MO made from two d_{z^2} orbitals 
iii. MO made from two p_z orbitals 	iv. MO made from two d_{xz} orbitals 
v. MO made from two p_z orbitals 	vi. MO made from two p_x orbitals 

Point Group Assignment Tree



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