

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

a. an S_3 operation

1. _____

b. a σ_h operation

2. _____

c. a C_2 operation

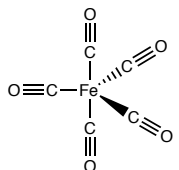
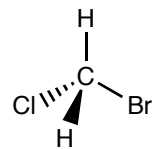
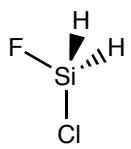
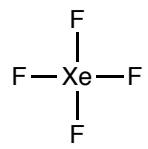
3. _____

4. _____

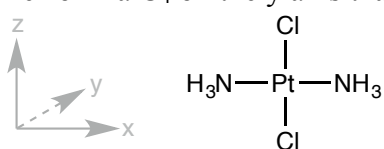
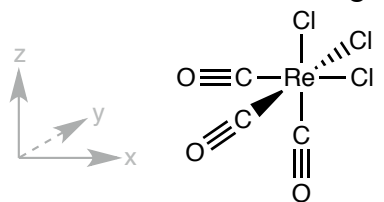
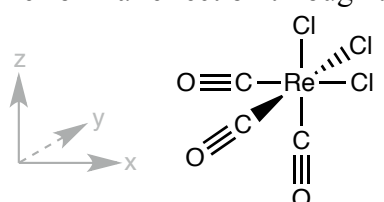
5. _____

2. (16 pts.) Determine the point group for each of the following molecules. Wedge and dashed

6. _____

<p>a.</p> 	<p>b.</p> 
<p>d.</p> 	<p>d.</p> 

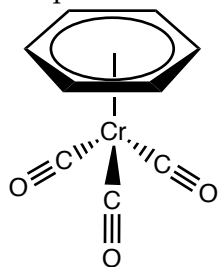
3D representations have been provided.

<p>a. Perform a C_4 on the y axis that goes through the Pt atom</p> 
<p>b. Perform an inversion through Re atom</p> 
<p>c. Perform a reflection through the yz plane that contains the rhenium atom</p> 

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.
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	7	1	3	1	3		

5. (10 pt.) Determine the number of CO stretching bands that you would expect to see in the IR spectrum of benzene tricarbonyl chromium. The molecule is in the C_{3v} point group.



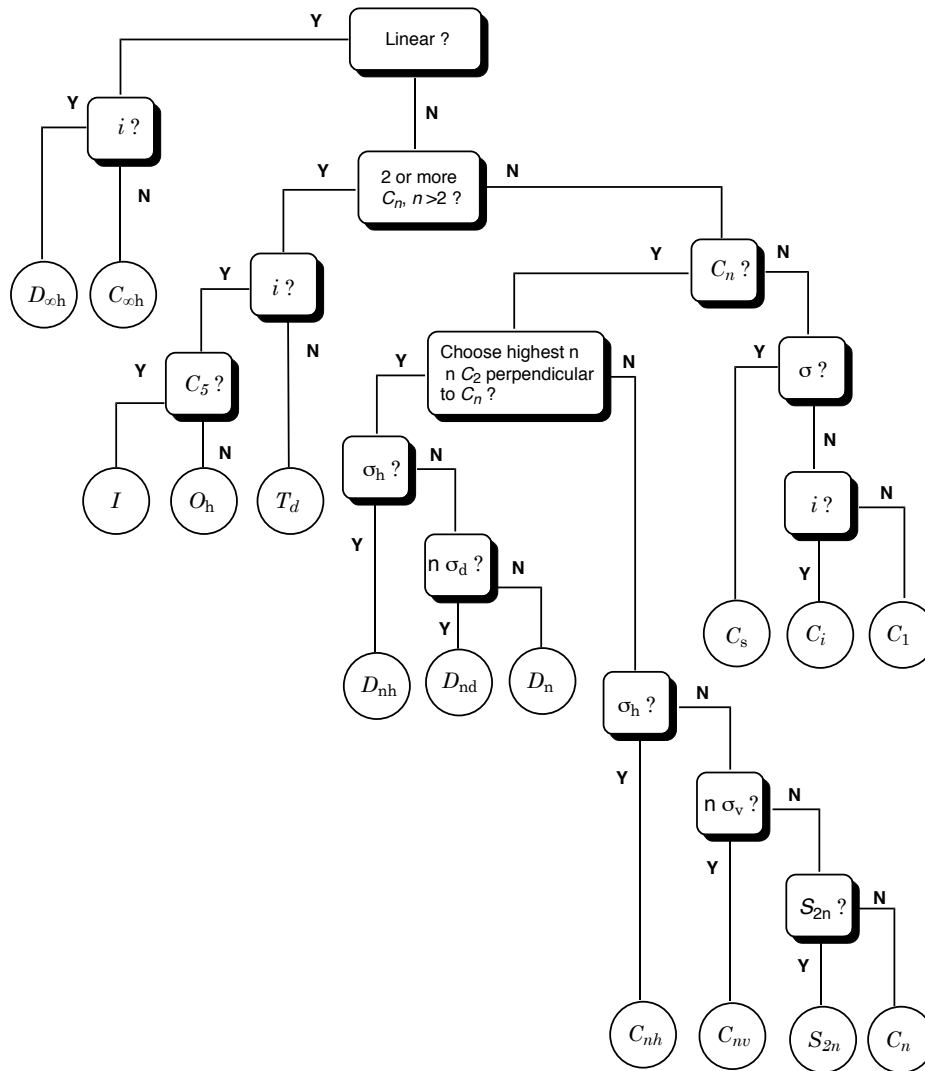
6. In class, we determined that the total number of IR-active vibrational modes for water was three. (a. 8 pts.) Determine the number of O–H stretching modes that are IR active for water, and (b. 2 pts.) compare this result to the conclusion that we reached in class; that is, are the results the same or different, explain.

C_{2h}	E	C_2	i	σ_h		
A_g	1	1	1	1	R_z	x^2, y^2, z^2, xy
B_g	1	-1	1	-1	R_x, R_y	xz, yz
A_u	1	1	-1	-1	z	
B_u	1	-1	-1	1	x, y	

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz

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

Point Group Assignment Tree



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