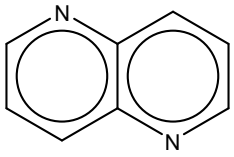
Group Theory Mini-Exam – March 3, 2020 (50 pts)

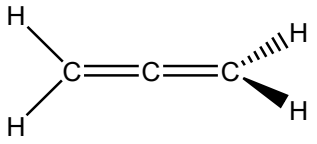
1. (10 pts) Please determine the **point group** for each molecule below.

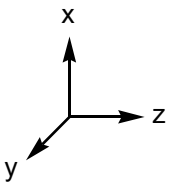
   a. PF_5

   b.



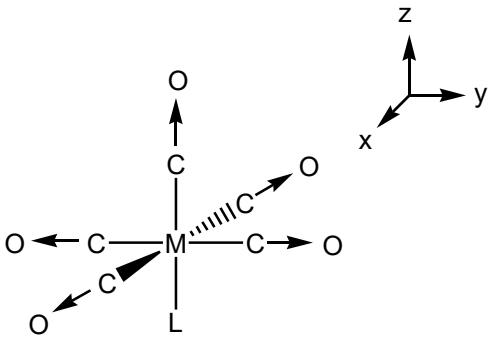
2. (8 pts) Please generate the **transformation matrix** for the ***$C_2(z)$* operation** of the ***D_{2d}*** point group by operating on a point, (x, y, z). What is the **character** of the matrix? (It may help to consider allene, a molecule with D_{2d} symmetry, shown below.)





3. (10 pts) Consider the carbonyl stretches in $ML(CO)_5$, depicted with vectors below. Please **<u>generate a reducible representation</u> (Γ_R)** showing how these vectors transform under the operations of the C_{4v} point group. (This would be the first step toward predicting the number of C-O peaks in the IR spectrum.)

   <u>Hint:</u> Recall that σ_v planes tend to contain the most bonds; σ_d planes tend to lie between bonds.



C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$	
Γ_R						C-O stretches

4. (8 pts) Please **reduce the reducible representation (Γ_R)** below. Show your work and clearly indicate your final answer.

C_{3v}	E	$2C_3$	$3\sigma_v$
Γ_R	12	0	2

5. (14 pts) The reducible representation in Question 4 represents all 3N molecular motions in ammonia, NH_3. Please use the C_{3v} character table and the irreducible representations from your answer above to complete the following questions.

   a. Which irreducible representation(s) describe(s) **translational** motions?

   b. Which irreducible representation(s) describe(s) **rotational** motions?

   c. Which irreducible representation(s) describe(s) **vibrational** motions?

   d. How many **vibrations** are expected for NH_3? Are all of these represented in your answer to (c)? Explain briefly.

   e. How many **peaks** should be visible in the IR spectrum of ammonia? Briefly explain how you arrived at your answer.

   f. How many **peaks** should be visible in the Raman spectrum of ammonia? Briefly explain how you arrived at your answer.