1. The following questions relate to benzene:
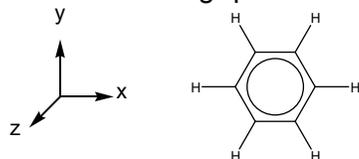
   a. Determine a reducible representation for all 3N motions of this molecule and reduce it to find the symmetries of the translations, rotations and vibrations.

      NOTE: The C_2 axis is colinear with C_6 ($=C_6^3$); the C_2' and C_2'' are perpendicular C_2 axes: C_2' axes lie along C-H bonds and C_2'' axes lie between C-H bonds. Similarly, the σ_v planes contain C-H bonds while the σ_d planes lie between them.

   b. How many vibrations should benzene contain? Does your list of vibrational symmetries in (a) correctly represent this number of vibrational motions? Briefly explain how this can be the case.

   c. How many peaks do you expect to observe in the IR spectrum of benzene? In the Raman spectrum?

   d. Next, let's focus on only the **6 C-H stretches** of benzene, represented by 6 vectors ($v_1 - v_6$) along the C-H bonds. Generate a new reducible representation that shows how these stretches transform under the operations of the group.

   e. What are the symmetries of the individual C-H stretching vibrations? How many C-H stretching peaks do you expect to observe in the IR spectrum of benzene?

   f. You should have found in (e) that one of the C-H stretches has b_{1u} symmetry. Use a projection operator to project one of the six stretching vectors (I chose v_1); then, use your projection to determine the appearance of the b_{1u} C-H stretching vibration and draw a diagram.

      NOTE regarding the operations in each class: $2C_6 = C_6^1$ and C_6^5; $2C_3 = C_3^1$ and C_3^2; $2S_3 = S_3^1$ and S_3^5 (where, in this case, S_3^5 looks like S_3^2); $2S_6 = S_6^1$ and S_6^5

2. Consider the silane derivative below (in the staggered conformation, as shown):
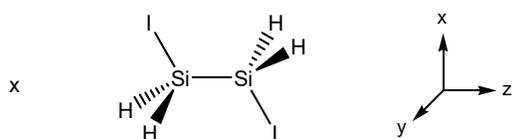
   a. Obtain a representation (Γ_R) based on all 3N molecular motions.

   b. Reduce Γ_R and specify the symmetries of translations, rotations and vibrations of the molecule.

   c. Which vibrations are IR-active? Raman-active? Specify how many peaks you would expect to find in each spectrum.

   d. Will the IR and Raman spectra be distinguishable from each other? (That is, will their peaks occur at the same frequencies?) Briefly, why or why not?

3. Returning to the silane derivative in Problem 2 above, suppose that we were specifically interested in the **Si-I vibrations**, rather than all vibrations of the molecule. Determine a reducible representation for these vibrations alone, reduce it to find their symmetries, and determine the number of Si-I peaks expected in the IR and Raman spectra.

4. One of the vibrations of square-planar XeF$_4$ is diagrammed below:
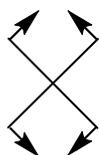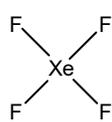
D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$
Γ										

e. Use the arrows shown to determine a representation (Γ) for the vibration; compare to the character table to determine its symmetry.

> **Note:** In the D_{4h} group, the C$_2$ class refers to the C$_2$ axis that is colinear with the C$_4$ axis (= C$_4{}^2$). The C$_2'$ and C$_2''$ classes refer to perpendicular C$_2$ axes: C$_2'$ axes are along the bonds of the molecule, while C$_2''$ axes are between the bonds. Similarly, the σ$_v$ planes contain the bonds while the σ$_d$ planes lie between them.

f. Is the vibration IR-active? Raman-active? Justify your answers in a few words.