Chemistry 4000
Introduction to Inorganic Chemistry: The Different Perspectives of Bonding

Problem Set #2 Part A

Chapter 3-

1) a. Using VSEPR, explain why XeF_4 is a square planar molecule.

b. What is the point group of this molecule?

c. Is this molecule centrosymmetric?

d. Is this molecule linear?

e. How many degrees of freedom does this molecule have?

f. Draw a representation of the degrees of freedom that correspond to the 3 translations and the 3 rotations.

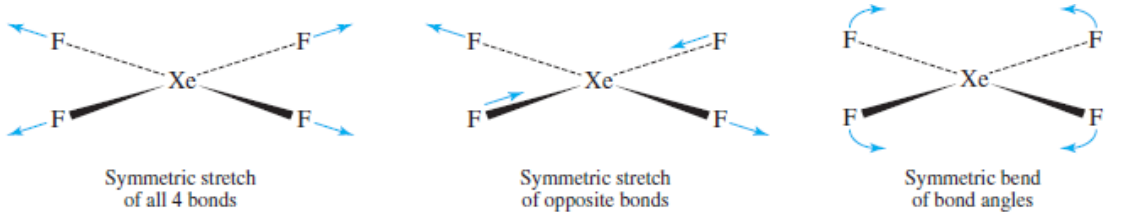
g. How many normal modes of vibration does this molecule have?

h. What are the symmetries (or irreducible representations) of the normal modes of vibration of this molecule?

i. Which modes are IR and/or Raman active?

j. Mathematically show that the sum of the irreducible representations equal the characters of the reducible representation.

k. Identify the symmetry (or irreducible representation) of these three specific vibrations.

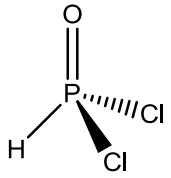


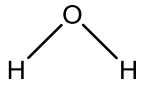
Symmetric stretch of all 4 bonds | Symmetric stretch of opposite bonds | Symmetric bend of bond angles

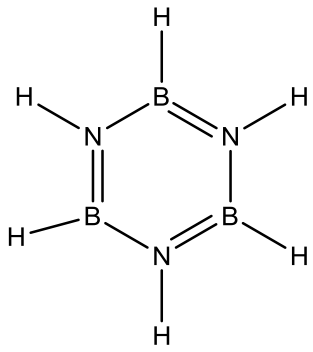
l.What would happen to the frequency of a Xe-F vibration if the F (in the form of ^{19}F) is substituted with ^{18}F?

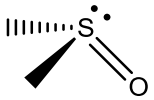
m. Determine the possible orbital hybridization of the central atom needed to engage in sigma bonds with the F substituents.

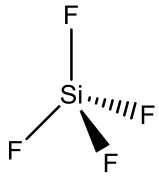
2. **Assign** the following molecules to their appropriate point groups and **identify** if they are **chiral** and if they have a **dipole moment**.

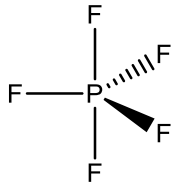


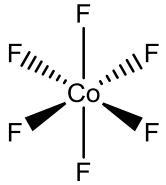


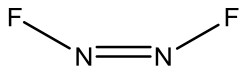


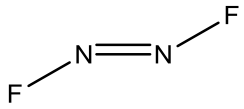












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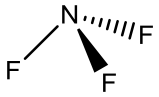
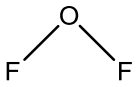
3. What are the symmetries of the normal modes of vibration of these molecules?





4. Unlike the water molecule, carbon dioxide has no dipole moment. How is it possible for it to have any of its vibrational modes to be infrared active?

5. Why is it that the O-H band in the IR broadens with H-bonding?

6. In an sp^3d hybridized phosphorus atom in a trigonal bipyramidal molecule, will the atom have a greater electronegativity when bonding through equatorial or axial orbitals? Explain.