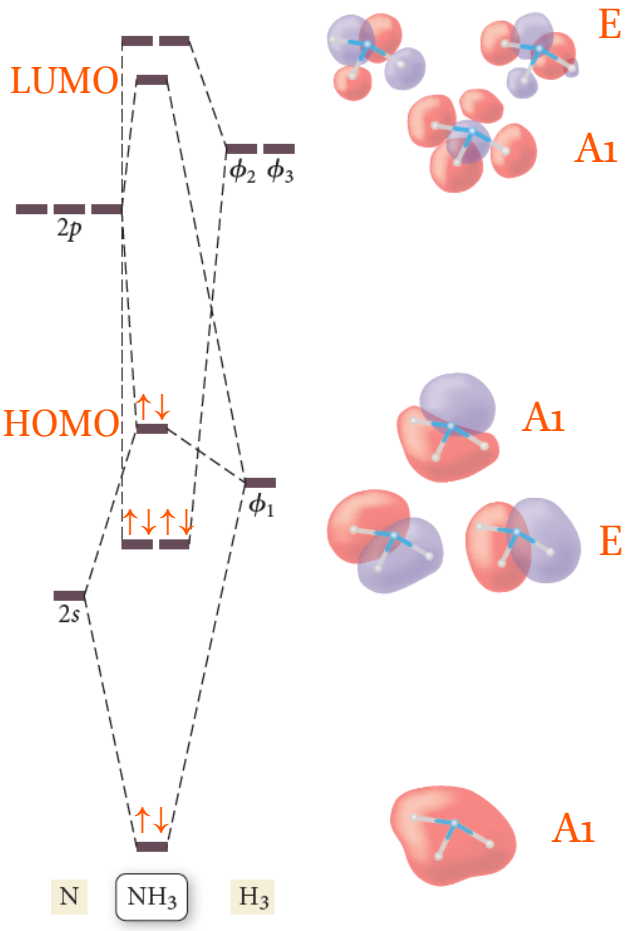
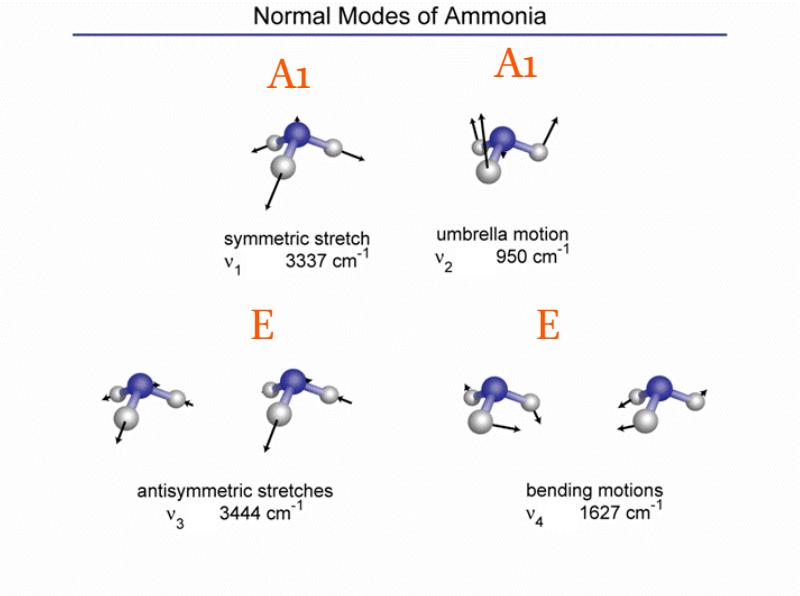
Quiz 10.2 – Applications of Symmetry and Group Theory

Name: Key

Irreducible Representations

Consider the ammonia molecule, which belongs to the C_{3v} symmetry point group. Below are figures showing the molecular orbitals and normal modes of ammonia. Assign each feature to the correct irreducible representation of the C_{3v} point group.





Which (if any) of the vibrational modes are "silent" in IR or Raman spectra

A2 would be silent in both IR and Raman, but there are no vibrational modes with this symmetry representation. All vibrations are active with both IR and Raman spectroscopy

Is the HOMO-LUMO transition allowed by symmetry? If so, what direction of light polarization can induce the transition?

There are 8 valence electrons (5 from N and 1 from each of the 3 Hs). Both the HOMO and LUMO have the A1 irreducible symmetry representation, so the transition should be allowed for z-polarized light.