

## 4.3: Application to Vibrational Spectroscopy

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Learning objectives for this unit are to:

- Know the number of expected vibrational modes in a molecule containing "N" atoms
  - Generate reducible representations using a degrees of freedom basis set or a simple bond stretching basis set
  - Decompose reducible representations within a point group into their irreducible components using the great orthogonality theorem
  - Assign the irreducible representations to translations, rotations and vibrations
  - Determine which vibrational modes are IR active and Raman active
  - Use Mulliken symbols to predict the molecular deformations that correspond to a particular vibrational mode
  - Apply the selection rules for IR and Raman active modes to experimental scenarios
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