

Spectroscopy

Exercises Chapter 4C

1. For a molecule belonging to the D_{2h} point group, deduce whether the following vibrational transitions from the ground vibrational state are allowed in the infrared and/or Raman spectrum. State the direction of the transition moment and/or the component of the polarizability involved.
 - a. to the $v=2$ level of a b_{1g} vibration
 - b. to the $v=1$ level of an a_u or b_{2u} vibration
 - c. to the combination level involving $v=1$ of a b_{1u} and $v=1$ of a b_{3g} vibration
 - d. to the combination level involving $v=2$ of an a_u vibration and $v=1$ of a b_{2g} vibration.
2. The infrared spectrum of N_2O has three fundamental bands. Assuming that the structure of N_2O is linear, explain how this spectrum allows you to distinguish between NNO and NON. Sketch the normal modes.
3. Fill in the table with a YES or a NO to indicate allowed spectroscopic transitions. For vibrational and vibrational Raman transitions, indicate the symmetry species of the vibrational modes to which transitions are allowed.

| Molecule | Pure Rotational | Vibrational | Vibrational Raman |
|----------|-----------------|-------------|-------------------|
| H_2O | | | |
| SF_6 | | | |
| CS_2 | | | |
| N_2O | | | |
| allene | | | |
| Cl_2 | | | |

4. For the molecules BF_3 (D_{3h} symmetry) and cis-diimide $HN=NH$ (C_{2v} symmetry):
 - a. Determine the number and symmetries of the normal modes of vibration.
 - b. Determine which of these modes will appear in an infrared spectrum and which will appear in a Raman spectrum.