

Things You Should Know

Chapter 4: Vibrational Spectroscopy

Be able to define the following terms (using words, equation, or figures):

Fundamental Band	Hot band	Overtone
Band origin	Null gap	P- Branch
R-branch	Band head	Combination differences
Normal modes/coordinates	Combination level	Combination band
Raman effect		

Concepts and Exercises:

1. Be able to use raising and lowering operators to derive vibrational selection rules for diatomic molecules.
2. Know what causes the breakdown of vibrational selection rules. Be able to demonstrate this semi-quantitatively.
3. Be able to analyze a vibration-rotation spectrum of a diatomic molecule using the technique of combination differences. From this analysis, find molecular constants such as B_e , R_e , and α .
4. You should have a qualitative understanding of normal modes of vibration. What are they, how do they arise?
5. Be able to use group theory to determine the symmetry of the normal modes of vibration.
6. Use group theory to determine which vibrational transitions will be allowed by symmetry.
7. Be able to explain the overall shape of a rovibrational spectrum of a symmetric top molecule.
8. Be able to describe the physical principle behind Raman Scattering and understand its advantages over normal infrared spectroscopy.
9. Be able to do all the exercises.