Things You Should Know

Chapter 2: Overview of Molecular Spectroscopy

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

Born-Oppenheimer Approximation	Potential Energy Surface
Spherical Harmonics	Absorption
Stimulated Emission	Spontaneous Emission
Einstein A and B coefficients	Homogeneous Broadening
Natural Line Broadening	Pressure Broadening
Inhomogeneous Broadening	Doppler Effect

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Concepts and Exercises:

1. Know the basic principle of the Born-Oppenheimer approximation.

2. Be able to interpret simple figures in which we draw an electronic potential curve for a diatomic molecule with the vibrational and rotational levels superimposed on it. Understand how this picture results from the approximate separation of the electronic, vibrational and rotational motion in the Hamiltonian.

3. Know the general approach used to go beyond the Harmonic oscillator and Rigid Rotor approximations for diatomic molecules.

4. Be able to describe the physical significance of each term in the expression for the energy levels of a diatomic molecule.

5. Know in which wavelength regions different types of spectra occur.

6. Be able to discuss all the factors that determine the intensity of a spectroscopic transition.

7. Know where the various types of selection rules come from.

8. Know the various sources of spectral broadening and be able to calculate the contributions of each type under a particular set of conditions.

9. Be able to do all the assigned exercises.

Things You Should Know

Chapter 3: Rotational Spectroscopy

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

Moment of inertia	Rotational Constant
Centrifugal Distortion	Principal axis

Concepts and Exercises:

1. Be able to calculate the moments of inertia for linear or planer molecules.
2. Be able to classify molecules into rotational types.
3. Know the rotational selection rules for linear and symmetric top molecules.
4. Know the other requirements for rotational spectra (permanent dipole moment).
5. Understand the pattern of energy levels for both linear and symmetric top molecules in the rigid rotor approximation. Know the basic appearance of the spectrum and be able to calculate r_e for a linear molecule.
6. Be able to do all the exercises.

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.

Things You Should Know

Chapter 5: Electronic Spectroscopy

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

Fundamental Band	Hot band	Progression
Sequence band	Band origin	Null gap
P- Branch	R-branch	Band head
Combination differences	Franck-Condon Principle	

Concepts and Exercises:

1. Know the physical basis Franck-Condon principle for electronic transitions and be able to use it to predict the overall structure of an electronic band.

2. Be able to analyze a simple electronic spectrum of a diatomic molecule using combination differences.

3. Know the various processes described by a Jablonski diagram.

4. Be able to do all the exercises related to this chapter.