Molecular Spectroscopy

Plan of the lecture curse
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Summer Semester 2009 r. A color labels a three-hours lecture

I. Introdution: Optical Transitions in Atoms and Molecules

A. Spectrum of Electromagnetic Waves

B. Light polarization. How to produce polarized light

II. Optical Transitions and the spectral line shape

A. Types of optical transitions. Einstein coefficients

B. Lambert-Beer Law. Low optical density approximation.

C. Spectral line shapes. Homogeneous (Lorentz) and Inhomogeneous (Doppler) broadening.

B. Line broadening mechanisms in gases and in solid state.

III. Atomic structure and spectroscopy

A. Interference of matter waves, Schrödinger equation

B. Wave functions and energy levels of hydrogen atom, quantum numbers

C. Spin-orbital interaction in hydrogen atom

D. Structure of multi-electron atoms. Self-consisting field, electron configurations, quantum numbers

E. The nomenclature of atomic terms in the LS approximation, parity of the atomic terms.

F. Transition dipole moments, selection rule for the dipole radiation transitions.

G. The physical meaning of the selection rules for the quantum number ***M***.

H. Fine and hyperfine structure of spectral lines

I. Time-independent Perturbation Theory

J. Interaction with external fields: Stark Effect and Zeeman Effect

K. Radiation transitions, electric dipole and multipole radiation. Selection rules for the magnetic dipole radiation.

IV. Molecular Spectroscopy

A. Rotational Structure in Molecular Spectra

1) Born-Oppenheimer Approximation

2) Rigid Spherical Top, Symmertic/Linear Top,

3) Asymmertic Top, Non-rigid Top

4) Selection rules in rotational spectra of diatomic molecules

5) Intensities of rotational spectra

B. Vibrational wave functions and vibrational energy levels of a diatomic molecule

1) Vabrational transitions in diatomic molecules

2) Ro-vibrational transitions in molecules

C. Electronic wave functions and energy levels in the molecular ion H_2^+. Bonding and antibonding orbitals.

D. The symmetry of one-electron orbitals, method LCAO. Self-consistent field, Hartree-Fock equation. Electronic configurations and terms of a multi-electron diatomic molecule.

E. Chemical bonds, electronic configurations and terms of homo-atomic diatomic molecules of the 1^{st} and the 2^{nd} periods of the Periodic Table.

F. Chemical bonds, electronic configurations and terms of hetero-atomic diatomic molecules

G. Electronic transitions in molecules. Yablonski diagram.

1) Selection rules for electronic transitions in diatomic molecules

2) Frank-Condon principle

V. Molecular dissociation and molecular predissociation

VI. Nonlinear processes in molecules

А. Thompson scattering of light on molecules

Б. Rahman scattering of light on molecules

Б. Harmonic generation

VIII. Experimental technique

A. Non-coherent light sources

1) Sources of broad-band radiation

2) Sources of narrow-band radiation

3) Synchrotron radiation

B. Coherent light sources

1) Princips of laser radiation

2) Properties of laser radiation

3) Properties, design and applications of different types of lasers

4) Free-electron lasers

C. Radiation detectors: photodiodes, photomultipliers, microchannel plates

D. Spectral devices: gratings, monochromators, spectrometers

IX. Experimental methods of molecular spectroscopy

A. Photoelectron spectroscopy

B. Absorption spectroscopy

C. Cavity ring-down spectroscopy

D. Photo-acoustic spectroscopy

E. Laser induced fluorescence spectroscopy (LIF)

F. Ionization spectroscopy

G. Rahman spectroscopy

H. Quantum beat spectroscopy

E. Femtosecond laser spectroscopy