

Modern Techniques in Structural Elucidation of Organic Compounds

Spectroscopic Techniques in Structural Elucidation



Water (H_2O)
or
Ethanol ($\text{C}_2\text{H}_5\text{OH}$)
or
Hexane (C_6H_{14})

a. UV-Vis- Spectroscopy

b. IR-Spectroscopy

c. NMR- Spectroscopy

Books: Any book on organic spectroscopy

Lectures mainly follow:

Introduction to Spectroscopy by D. L. Pavia, G. M. Lampman, G. S. Kriz
and J. R. Vyvyan

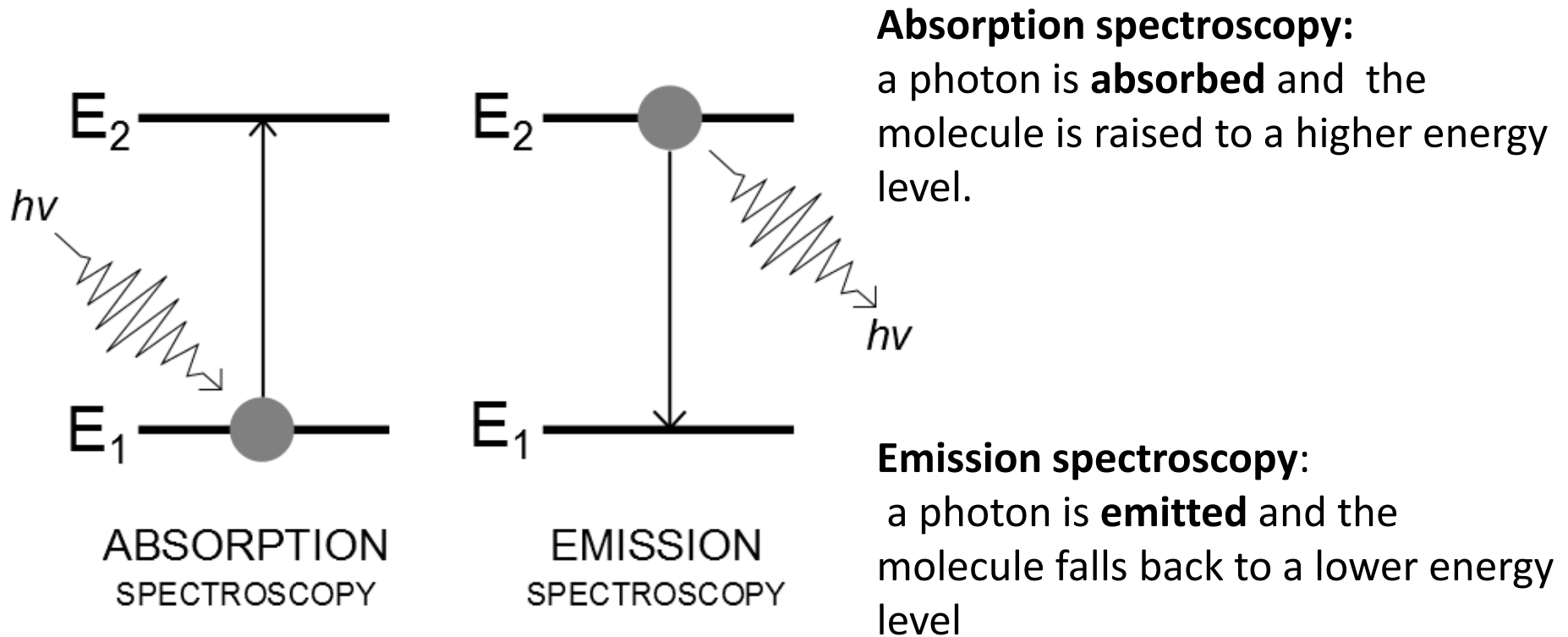
Organic Chemistry by P. Y. Bruice

Organic Chemistry by J. Clayden, N. Greeves and S. Warren

Spectroscopy

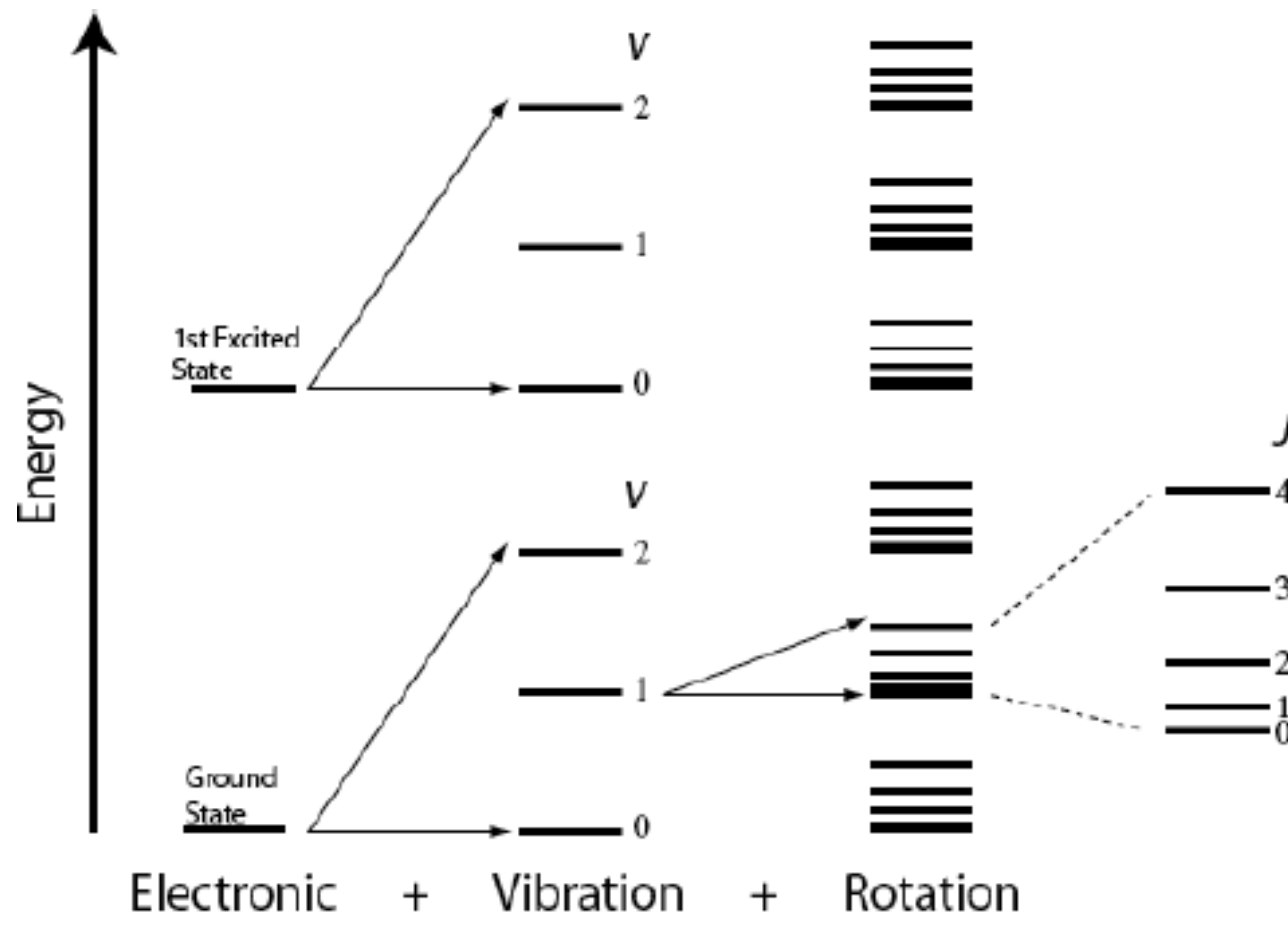
molecular spectroscopy is the study of the interaction of electromagnetic (EM) radiation with Molecule

based on the analysis of EM radiation that is emitted, absorbed, or scattered by molecules

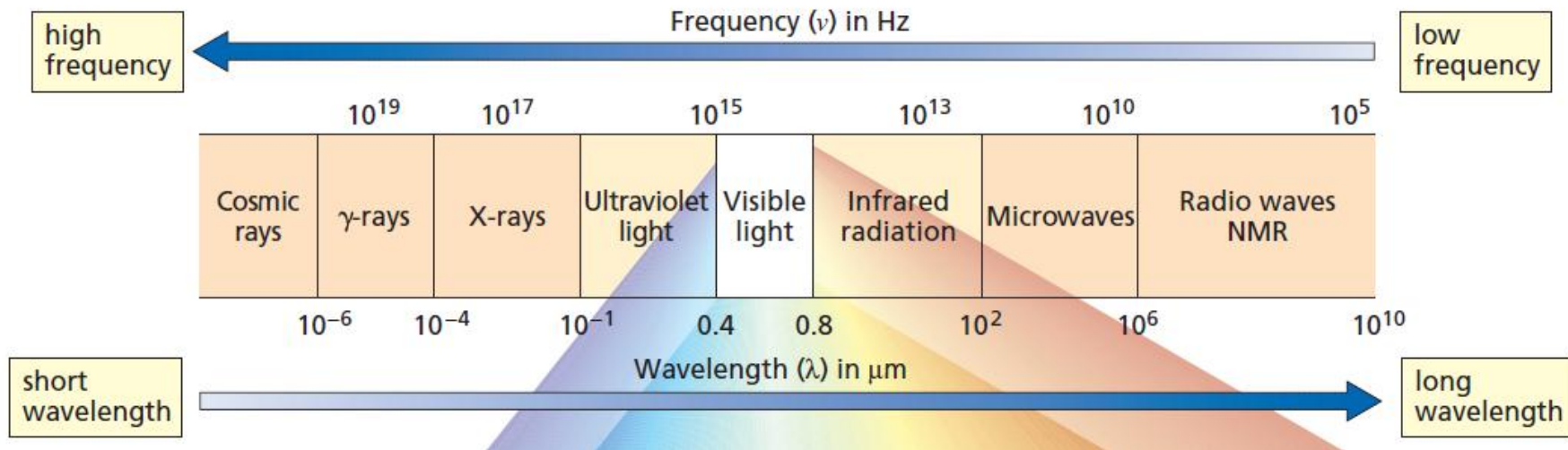


give information on: molecular structure (bond lengths, strengths, energy levels, etc...)

Spectroscopy: Molecular Energy Levels



Spectroscopy: Electromagnetic (EM) Radiation



EM region	Wavelength (nm)	Energy (K cal/mole)	Molecular Energy level
UV	200-300	143-95	Electronic
visible	400-700	71-41	
infrared	1000-10000	29-2.9	Vibrational
microwave	10^7 - 10^9	3×10^{-3} - 3×10^{-4}	Rotational
radiowave	10^{11}	3×10^{-6}	Nuclear spin precession

Ultraviolet \rightarrow electronic (UV-Visible spectroscopy)

Infrared \rightarrow vibration (Infra red spectroscopy)

Microwave \rightarrow rotation (rotational spectroscopy)

Radio \rightarrow nuclear spin in magnetic field (NMR-spectroscopy)

Looking forward

UV spectroscopy:

Basic principle, Beer–Lambert law, Chromophore, etc.