

CHM 201- Spectroscopic and other physical methods

Total: 38 classes (time: 15 -15.55 pm;
MON, WED and FRI)

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Office hours dedicated for **CHM 201**: 16:00-18:00 hrs (or by appointment)

CHM 201- Spectroscopic and other physical methods

[Cr:3, Lc:2, Tt:1, Lb:0]

Part -I: Introduction to spectroscopy (approx. 5 classes)

- 1) Introduction
- 2) Properties of light
- 3) Electromagnetic field
- 4) Reflection, refraction, diffraction, interference etc
- 5) Simple instruments that can be used for spectral measurements
- 6) How a spectra can be represented
- 7) Resolution/sensitivity, resolving power etc
- 8) Width, intensity, line shape, Maxwell-Boltzmann distributions
- 9) Fourier Transform spectroscopy

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Part -II: Microwave spectroscopy (approx. 5 classes)

- 1) Rotation of a molecule
- 2) Rotational spectra
- 3) Diatomic molecules
- 4) Rigid rotor
- 5) Intensity and spectral line shape
- 6) Isotope substitution
- 7) Non-rigid rotor
- 8) Spectra of non-rigid rotor
- 9) Polyatomic molecules
- 10) Symmetric top
- 11) Asymmetric top
- 12) Applications

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Part -III: Infrared spectroscopy (approx. 6 classes)

- 1) The vibrating diatomic molecule
- 2) Simple harmonic oscillator model
- 3) Energy –zero-point energy
- 4) The anharmonic oscillator
- 5) Morse potential curve
- 6) Examples ...HCl
- 7) Ro-vibrational spectroscopy
- 8) Example ...CO
- 9) Born-Oppenheimer breakdown in ro-vibrational spectra
- 10) The vibration on polyatomic molecules
- 11) Example ...H₂O, CO₂
- 12) Overtones and combination bands
- 13) Ro-vibration of linear / symmetric top molecules
- 14) IR analysis and applications

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Part -IV: Raman spectroscopy (approx. 5 classes)

- 1) Quantum and classical theory of Raman spectra
- 2) Rotational Raman spectra
- 3) Symmetric /spherical and asymmetric top
- 4) Vibrational Raman
- 5) Examples... H₂O, CO₂
- 6) Mutual exclusion principle
- 7) Vibrational/rotational fine structure
- 8) Instrumentation
- 9) Applications

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Part -V: Electronic spectroscopy (approx. 6 classes)

- 1) Electronic wavefunction
- 2) The shape of atomic orbitals
- 3) Atomic quantum numbers
- 4) The energies of Atomic Orbitals
- 5) The Hydrogen atom spectrum
- 6) Electronic angular momentum
- 7) The fine structure of H-atom
- 8) Many electron system
- 9) Term symbols
- 10) The spectrum of Helium atom
- 11) Atomic absorption spectroscopy (basics)
- 12) Photoelectron spectroscopy
- 13) The Zeeman effect

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Part -VI: EPR and NMR spectroscopy (approx. 5 classes)

- 1) General introduction to EPR
- 2) Basic working principles
- 3) General introduction to NMR
- 4) Basic working principles
- 5) Applications

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Part -VII: Tutorials (approx. 5 classes)

- 1) Problem solving and understanding of molecular structure:
- 2) From rotational spectroscopy
- 3) From infrared spectroscopy
- 4) From Raman spectroscopy
- 5) From EPR and NMR spectroscopy
- 6) Structural analysis of molecules using all spectroscopic tools – CHM 211

Recommended reading

1. C. N. Banwell, E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th Ed, Tata McGraw-Hill, New Delhi (1995).
2. D. L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Spectroscopy, 3rd Ed, Cengage, India Edition (2001).
3. W. Kemp, Organic Spectroscopy, 3rd Ed, Palgrave, New York (1991).
4. I. N. Levine, Physical Chemistry, 5th Ed, Tata McGraw-Hill, New Delhi (2007).

Suggested further reading

1. Gordon M. Barrow. Introduction to Molecular Spectroscopy, McGraw-Hill, New York, (1962). Paperback (2021)
2. P. F. Bernath, Spectra of Atoms and Molecules, 2nd Ed, Oxford University Press, USA (1995). J. M. Hollas, Modern Spectroscopy, 4th Ed, John Wiley & Sons Inc, England (2004).
3. Robert M. Silverstein - Spectrometric Identification of Organic Compounds 7th ed John Wiley & Sons Inc, England (2005).

Fundamentals of Molecular Spectroscopy

Fourth edition

C. N. BANWELL

*Lecturer in Chemistry
University of Sussex*

Grading Policy

Quiz/Surprise quizzes = 10 marks

Midsem 1 = 20 marks

Midsem 2 = 20 marks

Endsem exam = 50 marks

Total = 100 marks

Quizzes = Open book, anytime

James Webb Space Telescope



Cosmic Cliffs, Carina Nebula (NIR and MIR cameras and spectrometers)



THANK YOU