

**Instructor:** [Dr. A.P. Hitchcock](#) ABB 422 aph@mcmaster.ca

**Objectives:** This course treats molecular spectroscopy at an intermediate level, with emphasis on basic principles and applications to the determination of geometric and electronic structure of molecules. Classical optical methods as well as electron, synchrotron, and laser spectroscopies will be treated.

**Background:** The course prerequisite is Chem 3BA3 or its equivalent. I will assume you have had previous exposure to basic principles of quantum mechanics, operator methods, group theory and simple spectroscopic models (hydrogen atom, rigid rotor, harmonic oscillator etc.). We will build on this background.

**Text:** J. Michael Hollas, [Modern Spectroscopy, 4th Edition](#), (Wiley, 2004) (**required**)

**Assignments:** There will be regular assignments during the term.

**Laboratory:** While there is no formal lab with this course, you will carry out one experiment in electron spectroscopy (core excitation or valence photoionization (photoelectron) spectroscopy) and analyze your results with the aid of a quantum molecular calculation.

**Testing:** There will be regular quizzes and a student presentation of independent study on a selected topic. There will not be a final exam.

**Grading:** The grade will be determined as:

- 20% exercise assignments
- 20% lab/computer assignment
- 30% periodic quizzes (3 or 4)
- 30% student presentation (independent study)

### Course Outline

Topic	Hollas
Interaction of Radiation and Matter	1, 2, 3
Symmetry	4
Rotational spectroscopy	5
Vibrational spectroscopy	6
Electronic Spectroscopy	7
Synchrotron and Electron Spectroscopies	8
Lasers and Laser Spectroscopies	9

**Supplementary References** (**R** = on reserve in Thode Library).

In many cases you will wish to review the subject matter in your 3BA3 text.

<http://www.umsl.edu/~chemist/cgi-test/mybooks.pl?category=46> is a rather complete list of texts on Molecular Spectroscopy

Classical quantum mechanics, group theory and spectroscopy

I.N. Levine, Quantum Chemistry 5<sup>th</sup> edition (Prentice Hall, 2000) **R**

J.I. Steinfeld, Molecules and Radiation: An Introduction to Modern Molecular Spectroscopy (MIT Press, US, 1985).(Dover reprint, 2006) QC454.M6S83 **R**

F.A. Cotton, Chemical Applications of Group Theory, 3<sup>rd</sup> edition (Wiley, 1990). **R**

### Electron Spectroscopy

Stefan Hufner, Photoelectron Spectroscopy: Principles and Applications, (Springer, 2003)

J.H.D. Eland, Photoelectron Spectroscopy, (Buttersworth, 1985) QC454.P48E38

Thompson, et al., Auger Electron Spectroscopy, (Wiley, 1985) QD96 .P54

### Synchrotron Spectroscopy

J. Stöhr, NEXAFS Spectroscopy, (Springer Tracts in Surface Science, Vol 25, 1992)

T.K. Sham (ed) Chemical Applications of Synchrotron Radiation, Advanced Series in Physical Chemistry Vol 12A, (World Scientific, 2002)

### Laser Spectroscopy

W. Demtroder, Laser Spectroscopy, (Springer, 2002)

LM.D. Levinson, Introduction to Non linear Laser Spectroscopy (Academic, 1982) QC454.L3L48.

S. Stenholm, Foundations of Laser Spectroscopy (Wiley, 1984) QC454.L3S75.

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