

QUANTUM CHEMISTRY AND SPECTROSCOPY
(CHEMISTRY 570)
Fall 2017

Instructor: Dr. Kostas Vogiatzis
Office: Bu 319
Office Hours: Mondays 12:30 – 1:30
Wednesdays 12:30 – 1:30
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Class Schedule: Every Monday, Wednesday, Friday, 11:15-12:05, Buehler 476

Textbook: "Quantum Chemistry" - Second Edition
Donald McQuarrie (University Science Books, Mill Valley, CA 2008).

Suggested Books For Mathematics

- A. "Guide to Essential Math" - Second Edition
S. M. Blinder (Elsevier, 2013)
- B. "Quantum Chemistry" - Second Edition (*Math Chapters*)
Donald McQuarrie (University Science Books, Mill Valley, CA 2008).
- C. "Mathematics for Physical Chemistry" – Fourth Edition
Robert G. Mortimer (Elsevier, 2013)

Grading:

First Midterm Exam:	25%
Second Midterm Exam:	25%
Paper:	25%
Problem Sets:	25%

Topics:

1. Introduction to Quantum Mechanics
2. Particle in a box
3. The harmonic oscillator and vibrational spectroscopy
4. The rigid rotor and rotational spectroscopy
5. The hydrogen atom and electron spin
6. Many-electron atoms and molecules: structure and bonding
7. The Hartree-Fock method

Paper: A list of topics relevant with quantum chemistry and spectroscopy will be given. Each student will choose one of these topics and give a 20-minute presentation in the class (plus 5 minutes for questions).

LECTURES

TOPICS

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| I. | Introduction to Quantum Mechanics (Chapters 1 and 2) |
| 2 | The Dawn of Quantum Theory |
| 2 | The Classical Wave Equation |

	II.	Particle in a Box (Chapters 3 and 4)
1		The Schrödinger Equation
3		Particle in a Box
3		The Postulates and General Principles of Quantum Mechanics
	III.	The Harmonic Oscillator and Vibrational Spectroscopy (Chapter 5)
2		The Harmonic Oscillator
3		Vibrational Spectroscopy

First Midterm Exam

	IV.	The Rigid Rotor and Rotational Spectroscopy (Chapter 6)
1		Structure and Rotation of Rigid Bodies
2		Introduction to Rotational Spectroscopy
	V.	The Hydrogen Atom and Electron Spin (Chapters 7-8)
4		The Hydrogen Atom
4		Approximate Methods
	VI.	Many Electron Atoms and Molecules (Chapters 9-11)
4		Many Electron Atoms
4		The Chemical Bond
3		Qualitative Theory of Chemical Bonding

Second Midterm Exam

	VII.	Hartree-Fock Theory (Book A, Chapter 12)
2		The Hartree-Fock-Roothaan Method
1		Introduction to post-Hartree-Fock Methods

TOTAL

Lectures: 41

Paper Presentation: 1 (extended)