

JOHN JAY COLLEGE OF CRIMINAL JUSTICE
The City University of New York
524 West 59th Street, New York, NY, 10019

Syllabus for CHE 302, Section 01, Lab/Rec 1-2
Physical Chemistry II
Quantum Mechanics, Theoretical Spectroscopy,
and Scientific Programming/Data Analysis

Professor's name: Nicholas Petraco

Lecture location: 3.79

Laboratory location: 4.69

Contact hours: Fridays 12:00 and Open Door Policy

E-mail address: npetraco@gmail.com

Course website: <https://npetraco.github.io/CHE302/>

Course description:

This is a one-semester seminar course in basic quantum chemistry, theoretical spectroscopy, optics, materials and scientific data analysis pertinent to forensic scientists. It is designed to give a forensic scientist a thorough understanding of the physical principles behind the spectroscopic/optical methods they use in the lab and how to analyze the data they obtain. The course is also intended to prepare students for graduate work in forensic science or chemistry. As such, the course material is intended to further develop critical thinking and problem solving skills.

Learning outcomes:

By the end of the course students will be able to:

- Solve chemical problems, especially those related to forensic science, using the methods of quantum mechanics, classical mechanics and optics. Analyze the physicochemical/materials data obtained from different sources using scientific computing software R (<http://www.r-project.org/>), Mathematica and other scientific software.
- Identify compounds and various materials commonly encountered in forensic science, by spectroscopy and microscopy. Utilize scientific data from literature searches of the scientific literature.
- Acquire deep understanding of physical phenomena that lead to the appearance of molecular spectra and the formation of images in optical and electron microscopy.

- Describe various perspectives how physicochemical and materials systems work. Recognize the importance of the knowledge at the interface of physics, chemistry, computing, engineering and forensic science.
- Collect and analyze molecular and atomic spectra. Extract information about chemical compounds from their spectral characteristics.
- Recognize the importance of accuracy and objectivity in collecting physicochemical data, especially with applications to the law.

Course pre-requisites or co-requisites

Students should have taken PHYS 203/204 (General Physics I and II with Calculus), CHE 320 (Instrumental Methods I), MAT 241/242 (Calculus I and II) and be enrolled in CHE 321 (Instrumental Methods II).

Requirements / course policies

Unethical/unprofessional conduct which includes cheating will result in a failing grade and referral for additional action. *Attendance in lecture laboratory and recitation is mandatory.* More than five unexcused absences from any of these components will result in an automatic failing grade. Unexcused lateness or early departure will count as ½ an absence, up to 30 minutes. After 30 minutes you will be marked absent.

Required Electronic Text and Resources:

Physical Chemistry: A Molecular Approach.

D. A. McQuarrie and J. D. Simon

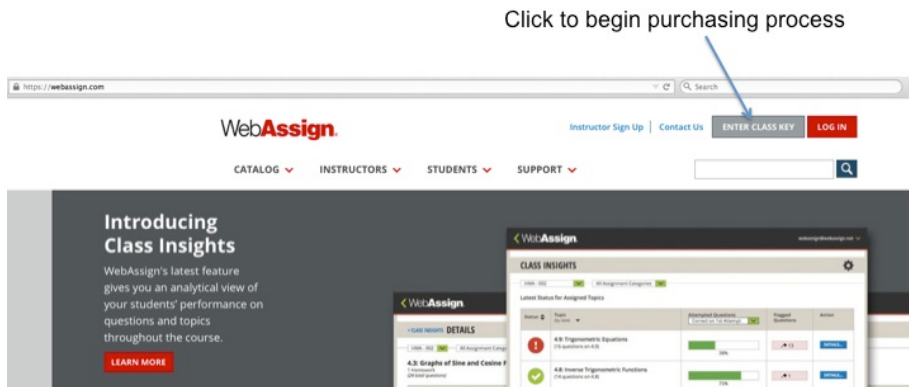
- The Assignments/Electronic Text can be purchased on **WebAssign**:

<https://webassign.com/>

- In order to purchase, got to:

<https://www.webassign.net/wa-auth/class-key/enroll>

and click on “Enter Class Key” **FOR YOUR SECTION:**



- You should see a place to enter the class key:



Support

Let's get you enrolled in your courses!

Start by entering the Course Key provided by your instructor. Don't have a Course Key?
Reach out to your instructor to request it.

If your course is integrated with your campus Learning Management System (i.e. Blackboard, Brightspace by D2L, Canvas or Moodle), head there to enroll in your course or follow this [quick walkthrough](#).

Enter your Course Key


Enter your Course Key, Class Key or Course Registration Link

[What is a Course Key?](#)

ENROLL

- Students Registered for **Tuesday Rec/Lab** 3:05pm-5:45pm
 - Class Key: **jjay.cuny 7943 1849**
- Students Registered for **Thursday Rec/Lab** 3:05pm-5:45pm
 - Class Key: **jjay.cuny 3272 8247**

- After logging in/creating-account, eventually the website will prompt you to purchase the materials for the class:



WebAssign Instant Access for University Science Books'
Physical Chemistry: A Molecular Approach, Single Term
Instructor: Nicholas Petracco

Start Temporary Access

ENTER ACCESS CODE

An Access Code is an alpha-numeric code that is either printed on the card that came with your textbook, purchased electronically, or provided by Cengage Learning.

Examples Include: Example-RXL XXXX 9999 X9X9 XX99 or PPJWJN2PP6SL5W

Please enter your code exactly as printed, including spaces.

If your Course Package requires an Access Code you should only have to enter it the first time you launch your course resources.

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Continue

- Purchase the **Single-term E-textbook AND the Homework**, which should be \$71.95:

A physical copy of the text is not required, but recommended. It is commonly available at very low cost (~\$30 - \$50), ISBN-10: 0935702997. John Jay Library does not own a copy unfortunately.

Grading:

The grades for this course are based on home works (10%), two exams (50%), a final (25%) and laboratory exercises (15%).

Course lecture/laboratory calendar:

Week/Days	Lecture Topics	Lab/Rec Topics	Notes	HW, Labs and Exam Dates
Aug 25	Course Overview Software Overview			
Aug 30, Sep 1	Classical Waves Math Review	Workshop: Intro to Mathematica Workshop: Intro to R		
Sep 6, Sep 8	Quantum Theory I	Workshop: A Little R Programming Lab 1		Sep 6: HW Set 1 Due
Sep 13, Sep 15	Quantum Theory II	HW/Lab QA		Sep 13: HW Set 2 Due Sep 14: Lab 1 Due
Sep 20, Sep 22	Postulates of Quantum Mechanics	Exam 1		Sep 20 HW Set 3 Due Exam 1, Tues Lab: Sep 20 Exam 1, Thurs Lab: Sep 22
Sep 27, Sep 29			No class	
Oct 4, Oct 6	Particle in a Box	HW QA	No class Oct 4 All welcome HW QA, Oct 6	Oct 6*: HW Set 4 Due
Oct 11, Oct 13	Quantum Oscillators	Workshop: Numerov Lab 2		
Oct 18, Oct 20	Angular Momentum	Lab 3 HW/Lab QA		Oct 18: HW Set 5 Due Oct 20: Lab 2 Due
Oct 25, Oct 27	The Atomic Model	Workshop: Generating Atomic Orbitals Lab 4		Oct 25: HW Set 6 Due Oct 27: Lab 3 Due
Nov 1, Nov 3	Molecular Orbital Theory	Workshop: Huckel MOs Lab 5		Nov 1: HW Set 7 Due Nov 3: Lab 4 Due
Nov 8, Nov 10	Vibrational Spectroscopy	Exam 2		Nov 10: Lab 5 Due Exam 2, Tues Lab: Nov 8 Exam 2, Thurs Lab: Nov 10
Nov 15, Nov 17	Electronic Spectroscopy	Workshop: Interferograms and Fourier Transforms Lab 6		Nov 15: HW Set 8 Due
Nov 22, Nov 24	Catch Up		No class Nov 24	Nov 22: HW Set 9 Due
Nov 29, Dec 1	Color Theory and Pigments	Workshop: Colorimetry Lab 7		Dec 1: Lab 6 Due
Dec 6, Dec 8	Intro to Statistical Mechanics			Dec 6: HW Set 10 Due Dec 8: Lab 7 Due
Dec 13	Review		Last Day of Class	
		Exam 3		Exam 3 Everyone: Dec 15 10:30am-12:30am

*Thursday **December 15: Exam III (Final Exam)**, 10:30am-12:30pm.

College wide policies for undergraduate courses (see the *Undergraduate Bulletin*, Chapter IV Academic Standards)

A. Incomplete Grade Policy

B. Extra Work During the Semester

C. Americans with Disabilities Act (ADA) Policies

“Qualified students with disabilities will be provided reasonable academic accommodations if determined eligible by the Office of Accessibility Services (OAS). Prior to granting disability accommodations in this course, the instructor must receive written verification of a student’s eligibility from the OAS which is located at L66 in the new building (212-237-8031). It is the student’s responsibility to initiate contact with the office and to follow the established procedures for having the accommodation notice sent

to the instructor.”

Source: *Reasonable Accommodations: A Faculty Guide to Teaching College Students with Disabilities*, 4th ed., City University of New York, p.3.
(http://www.jjay.cuny.edu/studentlife/Reasonable_Accommodations.pdf)

Statement of the College Policy on Plagiarism

Plagiarism is the presentation of someone else’s ideas, words, or artistic, scientific, or technical work as one’s own creation. Using the ideas or work of another is permissible only when the original author is identified. Paraphrasing and summarizing, as well as direct quotations require citations to the original source.

Plagiarism may be intentional or unintentional. Lack of dishonest intent does not necessarily absolve a student of responsibility for plagiarism.

It is the student’s responsibility to recognize the difference between statements that are common knowledge (which do not require documentation) and restatements of the ideas of others. Paraphrase, summary, and direct quotation are acceptable forms of restatement, as long as the source is cited.

Students who are unsure how and when to provide documentation are advised to consult with their instructors. The Library has free guides designed to help students with problems of documentation. (*John Jay College of Criminal Justice Undergraduate Bulletin*, <http://www.jjay.cuny.edu/academics/654.php> , see Chapter IV Academic Standards)