

# CHEM 5378-P01-Spring 2024

## Advanced Physical Chemistry

Department of Chemistry and Physics

Brailsford College of Arts & Sciences

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**Office Hours:** T, F: 8:30 am – 9:30 am; M, R: 8:30 am – 9:50 am or by appointments

**Course Location:** Room 203, E. E. O'Banion Science Building

**Class Meeting Days & Times:** M, 10:00 am – 12:40 pm

**Course Abbreviation and Number:** CHEM 5378

**Section Number and CRN:** P01 - 24853

**Catalog Description:** (3-0) Credit 3 semester hours. An independent study course dealing with advanced topics of special interest in modern physical chemistry in areas including experimental and theoretical thermodynamics, chemical kinetics, collision and transition state theories, atomic and molecular spectra, quantum mechanical systems, photochemistry, structure of crystals and liquids, surface chemistry, macro-molecules, and gas phase reactions.

**Prerequisites:** MATH 2043; CHEM 3413 CHEM3423.

**Co-requisites:** None

**Required Text:** "Physical Chemistry", K. J. Laidler, Meiser, and Sanctuary, Edition:4th

**Recommended Text:** "Physical Chemistry", P. W. Atkins, Oxford, Edition: 5<sup>th</sup>, 1994  
Physical Chemistry", R. A. Alberty and R. Sibley, Wiley 1998

### Access to Learning Resources:

PVAMU Library:  
Telephone: (936) 261-1500;  
web: <http://www.tamu.edu/pvamu/library/>

University Bookstore:  
Telephone: (936) 261-1990;  
web: <https://www.bkstr.com/Home/10001-10734-1?demoKey=d>

## Course Overview:

CHEM 5783 is a lecture course focusing on a deeper understanding of fundamental principles of Physical Chemistry. The course will emphasize the study of elementary thermodynamics, chemical kinetics and reaction transition theory, elements of quantum theory, and molecular spectroscopy. The course will present the underlying theory of chemical phenomena through theoretical and practical problems. A major emphasis will be placed upon solution of numerical problems as a way of demonstrating the underlying theory and practical applications of Physical Chemistry. Many activities will require use of computer skills as an adjunct to the development of problem-solving abilities and the skill to synthesize and apply knowledge in new contexts.

**Course Learning Objectives/Accrediting Body** *American Chemical Society (ACS)* **Standards Met:** A, C, E, F

At the end of this course, the student will

- Understand how to derive and apply rate equations for chemical reactions
- Understand the concept of the order of a reaction with respect to one reactant and to the overall order
- Demonstrate knowledge of the definition of rate constant and a rate coefficient
- Understand the role of temperature and use of the Arrhenius Equation for determining reaction rates and Activation Energies
- Demonstrate a basic knowledge of classical electromagnetic theory
- Understand the Bohr Model and its role in the development of Quantum Mechanics
- Understand the historical development of quantum mechanics and the way that its postulates led to the formulation of modern quantum mechanics.
- Understand the central role of the Schrodinger Equation to explain simple systems
- Understand how chemical spectroscopy is concerned with a coupling mechanism between classical electromagnetic waves and quantum mechanical atoms and molecules
- Understand how absorption, spontaneous emission, and stimulated emission are described by the Einstein coefficient and provide the basic theoretical framework for chemical spectrometers
- Understand the role of electric and magnetic moments in chemical systems and their importance to spectroscopy
- Understand the different spectroscopic studies in the various electromagnetic regions and how these relate to chemical structure
- Understand the difference between absorption spectroscopy and Raman spectroscopy
- Understand the concept of molecular term symbols

## **COURSE OUTLINE:**

### **Sections**

### **TOPIC**

#### **Section 1**

**Structure-Property Relationships: Mechanical Analysis  
Literature Study Project with Report**

#### **Section 2**

**A brief review of thermodynamics  
Quiz**

#### **Section 3**

**Chemical Kinetics I. The Basic Ideas**

- 9.1 Rates of Consumption and Formation
  - 9.2 Rate of Reaction
  - 9.3 Empirical Rate Equations
  - 9.4 Analysis of Kinetic Results
  - 9.5 Techniques for Very Fast Reactions
  - 9.6 Molecular Kinetics
  - 9.7 The Arrhenius Equation
  - 9.8 Potential-Energy Surfaces
  - 9.9 The Pre-exponential Factor
  - 9.10 Reactions in Solution
  - 9.11 Reaction Dynamics
  - 10.1 Evidence of a complex mechanism
  - 10.2 Rates of Composite Reactions
  - 10.3 Rate Equations for Composite Mechanisms
  - 10.4 Rate Constants, rate Coefficients, and Equilibrium Const
  - 10.5 Photochemical Reactions
- Exam 1**

#### **Section 4**

**Quantum Mechanics and Atomic Structure**

- 11.1 Electromagnetic Radiation and the Old Quantum Theory
  - 11.2 Bohr's Atomic Theory
  - 11.3 The Foundations of Quantum Mechanics
  - 11.4 Schrödinger's Wave Mechanics
  - 11.5 Quantum-Mechanical Postulates
  - 11.6 Quantum Mechanics of Some Simple Systems
  - 11.7 Quantum Mechanics of Hydrogenlike Atoms
  - 11.8 Physical Significance of the Orbital Quantum Numbers
  - 11.9 Angular Momentum and Magnetic Moment
  - 11.10 The Rigid Linear Rotor
  - 11.11 Spin Quantum Numbers
  - 11.12 Many-Electron Atoms
  - 11.13 Approximate Methods in Quantum Mechanics
- Exam 2**

#### **Section 5**

**The Chemical Bond and Foundations of Chemical Spectroscopy**

12.5 Symmetry in Chemistry  
13.1 Emission and Absorption Spectra  
13.2 Atomic Spectra  
13.3 Pure Rotational Spectra of Molecules  
13.4 Vibrational-Rotational Spectra of Molecules  
13.5 Raman Spectra  
13.6 Electronic Spectra of Molecules  
**Quiz**

## Section 6

## Course Review and Final Exam

### Course Evaluation Methods

This course will utilize the following instruments to determine student grades:

**Exams** – written tests designed to measure knowledge of presented course material

**Exercises** – written assignments designed to supplement and reinforce course material

### Grading Matrix

Instrument	Value (points or percentages)	Total
Hour Exams	3 Exams at 100 points each	300
Literature Study		100
Final		200
<b>Total:</b>		<b>600</b>

### Grade Determination:

A = >90%

B = >80%

C = >70%

D = >60%

F = Below 59%

### Course Procedures

#### Submission of Selected Assignments:

TrueOutcomes is a web-based tool that Prairie View A&M University uses for assessment purposes. At least one of your assignments or examinations will be considered an "artifact" (an item of coursework that serves as evidence that course objectives are met) and will be loaded into TrueOutcomes. The assignment/exams(s) to be used as TrueOutcomes artifacts will be identified by your instructor.

TrueOutcomes also allows students to electronically post documents that can be used to create an electronic portfolio (e-portfolio) for future employment and/or educational endeavors. More information will be provided during the semester, but for general information, you can visit the TrueOutcomes web site at: [www.trueoutcomes.pvamu.edu](http://www.trueoutcomes.pvamu.edu).

### **Formatting Documents:**

Microsoft Word is the standard word processing tool used at PVAMU. If you're using other word processors, be sure to use the "save as" tool and save the document in either the Microsoft Word, Rich-Text, or plain text format.

### **Exam Policy**

Exams should be taken as scheduled. No makeup examinations will be allowed except under documented emergencies (See Student Handbook). Students with excused absences may be allowed to take a make-up exam at a time designated by the instructor.

### **Professional Organizations and Journals**

Students enrolled in Physical Chemistry are expected to take advantage of professional development activities available through such organizations as the American Chemical Society (ACS), American Institute of Chemical Engineers (AIChE), and the National Organization of Black Chemists and Chemical Engineers (NOBCChE).

## **University Rules and Procedures**

### **Disability statement (See Student Handbook):**

Students with disabilities, including learning disabilities, who wish to request accommodations in class should register with the Services for Students with Disabilities (SSD) early in the semester so that appropriate arrangements may be made. In accordance with federal laws, a student requesting special accommodations must provide documentation of their disability to the SSD coordinator.

### **Academic misconduct (See Student Handbook):**

You are expected to practice academic honesty in every aspect of this course and all other courses. Make sure you are familiar with your Student Handbook, especially the section on academic misconduct. Students who engage in academic misconduct are subject to university disciplinary procedures.

### **Forms of academic dishonesty:**

1. Cheating: deception in which a student misrepresents that he/she has mastered information on an academic exercise that he/she has not mastered; giving or receiving aid unauthorized by the instructor on assignments or examinations.
2. Academic misconduct: tampering with grades or taking part in obtaining or distributing any part of a scheduled test.
3. Fabrication: use of invented information or falsified research.
4. Plagiarism: unacknowledged quotation and/or paraphrase of someone else's words,

ideas, or data as one's own in work submitted for credit. Failure to identify information or essays from the Internet and submitting them as one's own work also constitutes plagiarism.

### **Nonacademic misconduct (See Student Handbook)**

The university respects the rights of instructors to teach and students to learn. Maintenance of these rights requires campus conditions that do not impede their exercise. Campus behavior that interferes with either (1) the instructor's ability to conduct the class, (2) the inability of other students to profit from the instructional program, or (3) campus behavior that interferes with the rights of others will not be tolerated. An individual engaging in such disruptive behavior may be subject to disciplinary action. Such incidents will be adjudicated by the Dean of Students under nonacademic procedures.

### **Sexual misconduct (See Student Handbook):**

Sexual harassment of students and employees at Prairie View A&M University is unacceptable and will not be tolerated. Any member of the university community violating this policy will be subject to disciplinary action.

### **Attendance Policy:**

Prairie View A&M University requires regular class attendance. Excessive absences will result in lowered grades. Excessive absenteeism, whether excused or unexcused, may result in a student's course grade being reduced or in assignment of a grade of "F". Absences are accumulated beginning with the first day of class.

### **Student Academic Appeals Process**

Authority and responsibility for assigning grades to students rests with the faculty. However, in those instances where students believe that miscommunication, errors, or unfairness of any kind may have adversely affected the instructor's assessment of their academic performance, the student has a right to appeal by the procedure listed in the Undergraduate Catalog and by doing so within thirty days of receiving the grade or experiencing any other problematic academic event that prompted the complaint.

# Technical Considerations for Online and Web-Assist Courses

## Minimum Hardware and Software Requirements:

- Pentium with Windows XP or PowerMac with OS 9
- 56K modem or network access
- Internet provider with SLIP or PPP
- 8X or greater CD-ROM
- 64MB RAM
- Hard drive with 40MB available space
- 15" monitor, 800x600, color or 16 bit
- Sound card w/speakers
- Microphone and recording software
- Keyboard & mouse
- Netscape Communicator ver. 4.61 or Microsoft Internet Explorer ver. 5.0 /plug-ins
- Participants should have a basic proficiency of the following computer skills:
  - Sending and receiving email
  - A working knowledge of the Internet
  - Proficiency in Microsoft Word
  - Proficiency in the Acrobat PDF Reader
  - Basic knowledge of Windows or Mac O.S.

**Netiquette (online etiquette):** students are expected to participate in all discussions and virtual classroom chats when directed to do so. Students are to be respectful and courteous to others in the discussions. Foul or abusive language will not be tolerated. When referring to information from books, websites or articles, please use ADA standards to reference sources.

**Technical Support:** Students should call the Prairie View A&M University Helpdesk at 936-261-2525 for technical issues with accessing your online course. The helpdesk is available 24 hours a day/7 days a week. For other technical questions regarding your online course, call the Office of Distance Learning at 936-261-3290 or 936-261-3282

## Communication Expectations and Standards:

All emails or discussion postings will receive a response from the instructor within 48 hours.

You can send email anytime that is convenient to you, but I check my email messages continuously during the day throughout the work-week (Monday through Friday). I will respond to email messages during the work-week by the close of business (5:00 pm) on the day following **my receipt** of them. Emails that I receive on Friday will be responded to by the close of business on the following Monday.

## Submission of Assignments:

Assignments, Papers, Exercises, and Projects will distributed and submitted through your online course. Directions for accessing your online course will be provided. Additional assistance can be obtained from the Office of Distance Learning.

## Discussion Requirement:

Because this is an online course, there will be no required face to face meetings on campus. However, we will participate in conversations about the readings, lectures, materials, and other aspects of the course in a true seminar fashion. We will accomplish this by use of the discussion board.

Students are required to log-on to the course website often to participate in discussion. It is strongly advised that you check the discussion area daily to keep abreast of discussions. When a topic is posted, everyone is required to participate. The exact use of discussion will be determined by the instructor.

**It is strongly suggested** that students type their discussion postings in a word processing application and save it to their PC or a removable drive before posting to the discussion board. This is important for two reasons: 1) If for some reason your discussion responses are lost in your online course, you will have another copy; 2) Grammatical errors can be greatly minimized by the use of the spell-and-grammar check functions in word processing applications. Once the post(s) have been typed and corrected in the word processing application, it should be copied and pasted to the discussion board.