



**UNIVERSITY OF CALGARY
FACULTY OF SCIENCE
DEPARTMENT OF CHEMISTRY
COURSE SYLLABUS
WINTER 2022**

1. **Course:** Chemistry 471, Physical Chemistry: Kinetics and Spectroscopy – Winter 2022

LEC	DAYS	TIME	ROOM	INSTRUCTOR	OFFICE	EMAIL	OFFICE HOURS
L01	MWF	11:00-11:50	SA104 or Online	Dr. Yujun Shi	SB 301	shiy@ucalgary.ca	TBA

Course website: d2l.ucalgary.ca [CHEM 471 L01-(Winter 2022)- Physical Chemistry: Kinetics and Spectroscopy]
 Departmental Office: Room SB 605 | Tel: 403-220-5385 | e-mail: chem.info@ucalgary.ca

2. **Course Description:** Reaction kinetics and transport kinetics in the gas phase and in solution. Rotational, vibrational, electronic and nuclear magnetic resonance spectra.
3. **Recommended Textbook(s):**
1. *Thermodynamic, Statistical Thermodynamics, and Kinetics, 4th edition* by Thomas Engel and Philip Reid and published by Pearson.
 2. *Quantum Chemistry and Spectroscopy, 4th edition* by Thomas Engel and published by Pearson.

Other REQUIRED course materials (available from the bookstore):

- Lab coat & safety glasses
- A non-programmable scientific calculator (Casio FX 260 or equivalent)

4. **Course contents and associated textbook references:**

Note: Not all sub-sections of each textbook chapter will be covered.

Part I. Kinetics (Chapters 16 – 19 in Textbook 1)

Chapter 1. Kinetic Theory of Gases

- 1.1 Introduction to Kinetics (Section 18.1)
- 1.2 Kinetic Theory of Gas – An Overview (Section 16.1)
- 1.3 Velocity Distribution and Molecular Speed Distribution (Sections 16.2 – 16.4)
- 1.4. Molecular Collision Frequency (Sections 16.6 – 16.7)

Chapter 2. Elementary Chemical Kinetics

- 2.1 Reaction Rates (Section 18.2)
- 2.2 Rate Laws (Section 18.3)
- 2.3 Integrated Rate Laws (Section 18.5)
- 2.4 Reaction Mechanisms (Section 18.4)
- 2.5 Sequential First-Order Reactions (Section 18.7)
- 2.6 Parallel Reaction (Section 18.8)
- 2.7 Temperature Dependence of Rate Constants (Section 18.9)
- 2.8 Reversible Reactions and Equilibrium (Section 18.10)

Chapter 3. The Kinetics of Complex Reactions

- 3.1 Complex Reactions vs Simple Reactions (Section 19.1)
- 3.2 The Pre-equilibrium Approximation (Section 19.2)
- 3.3 The Lindemann Mechanism (Section 19.3)
- 3.4 Michaelis-Menton Enzyme Kinetics (Sections 19.4)
- 3.5 Kinetics of Photochemical Processes (Section 19.9)

Chapter 4. Diffusion Kinetics

- 4.1 Mass Transport – Diffusion (Section 17.1 and 17.2)
- 4.2 Fick's First Law of Diffusion (Section 17.2)
- 4.3 Fick's Second Law of Diffusion (Section 17.3)
- 4.4 Diffusion and Viscosity of Liquids – the Stokes-Einstein Equation (Section 17.8)

Chapter 5. Collision Theory and Activated Complex Theory

- 5.1 Collision Theory
- 5.2 Activated Complex Theory (Transition State Theory) (Section 18.14)
- 5.3 Potential Energy Surface (Section 18.13)

Part II. Spectroscopy (Chapters 8, 14, and 17 in Textbook 2)**Chapter 6. Rotational and Vibrational Spectroscopy of Diatomic Molecules**

- 6.1 Introduction to Spectroscopy (Section 8.1)
- 6.2 Pure Rotational Spectroscopy of Diatomic Molecules (Section 8.6)
- 6.3 Vibrational Spectroscopy of Diatomic Molecules (Sections 8.3 – 8.4)

Chapter 7. Electronic Spectroscopy

- 7.1 The Energy of Electronic Transitions vs Rotational and Vibrational Transitions (Section 14.1)
- 7.2 The Electronic Spectroscopy of Diatomic Molecules (Sections 14.2 – 14.4)
- 7.3 UV-Visible Absorption Spectroscopy of Organic Molecules (Section 14.5)
- 7.4 Fluorescence and Phosphorescence (Sections 14.6 – 14.8)
- 7.5 Absorption, Spontaneous Emission, and Stimulated Emission (8.2)

Chapter 8. Nuclear Magnetic Resonance Spectroscopy

- 8.1 Nuclear Angular Momentum and Magnetic Moment (Section 17.1)
- 8.2 The Nuclear Zeeman Effect – The Larmor Frequency (Section 17.2)
- 8.3 The Mechanism of Magnetic Resonance
- 8.4 The Chemical Shift (Section 17.3)
- 8.5 Spin-spin Coupling – The Fine Structure (Section 17.4)

5. Laboratory Experiments: (3 experiments and 1 independent project, *see schedule*)

- Experiment 1. Determination of the bond dissociation energies in gaseous phase using UV-Vis spectroscopy (part A) and solvent effects on fluorescence spectra (part B)
- Experiment 2. The kinetic isotope effect in the hydrolysis of acetone (part A) and determination of the reaction order using the method of initial rates (part B)
- Experiment 3. Theory of electron transfer reactions and their effect on fluorescence
- Experiment 4. Independent Research Project