UNIVERSITY OF CALGARY
FACULTY OF SCIENCE
DEPARTMENT OF CHEMISTRY
COURSE SYLLABUS
WINTER 2021

1. **Course:** Chemistry 471, Physical Chemistry: Kinetics and Spectroscopy – Winter 2021

LEC	DAYS	TIME	ROOM	INSTRUCTOR	OFFICE	EMAIL	OFFICE HOURS
L01	MWF	12:00-12:50	Online	Dr. Yujun Shi	SB 301	shiy@ucalgary.ca	TBA

Course website: d2l.ucalgary.ca [CHEM 471 - (Winter 2021) - Physical Chemistry: Kinetics and Spectroscopy]
Departmental Office: Room SA 229 | Tel: 403-220-5341 | 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 Transport Phenomena (Section 17.1)
4.2 Diffusion – Mass Transport (Section 17.2)

4.3 Fick's First Law of Diffusion (Section 17.2)
4.4 Fick's Second Law of Diffusion (Section 17.3)

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 NMR Spectrometer
8.5 The Chemical Shift (Section 17.3)
8.6 Spin-spin Coupling – The Fine Structure (Section 17.4)
8.7 Pulsed NMR Spectroscopy – Fourier Transform NMR (Section 17.6)

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