

COURSE CONTENT FOR CY1101

Academic Year	2021/22	Semester	1
Course Coordinator	ZHANG Zhengyang and QIAO Yuan		
Course Code	CY1101		
Course Title	Molecule		
Pre-requisites	By permission		
No of AUs	4		
Contact Hours	On-line activities		- 11 hours
	Lectures -		- 22 hours
	Mid-term assessments		- 4 hours
	Laboratory experiments		- 30 hours
Proposal Date	16 June 2021		

Course Aims

The course provides an introduction to modern chemistry with the focus on molecules that are used to build key fundamental understandings of inorganic, organic, biological and physical chemistry. You will understand the nature of chemical bonds in structures of compounds, reaction mechanisms, kinetics and thermodynamics, and basic spectroscopic methods used to monitor the progress of reactions. The course comprises basic laboratory skills, and virtual laboratory simulations, linked to the course syllabus to provide you with hands on application of the key concepts and principles learned during the duration of the course thus further enhancing their understanding. You will understand the role that chemistry plays in other sciences, such as physics, biology, or earth science, and apply chemistry knowledge to solve real life problem in science or engineering related problems.

Intended Learning Outcomes (ILO)

By the end of this course, you (as a student) would be able to:

1. Chemical Kinetics

- Determine the average reaction rate over a specified period of time and estimate instantaneous reaction rate from a graph of concentration versus time.
- Relate the rate of consumption of any reactant to the rate of formation of any product using reaction stoichiometry.
- Find the reaction order with respect to each reactant, the overall reaction order, and the units of the rate constant from a given rate law.
- Predict the change in reaction rate when the concentration of a reactant changes by a specified amount.
- Determine the rate law and rate constant using initial rate and concentration data.
- Use the integrated rate law to determine the half-life and the concentrations remaining at various times for a zeroth order, first order and second order reactions.
- Interpret potential energy diagrams and suggest geometries for successful collisions and transition states using collision theory.
- Calculate rate constants, temperatures, and activation energy using the Arrhenius equation.

- i) Given a reaction mechanism, write the overall reaction, identify intermediates, and determine the molecularity for each elementary step.
- j) Illustrate and interpret Gibbs energy profiles for reactions.
- k) Explain how a catalyst speeds up a reaction and the difference between heterogeneous and homogeneous catalysis.

2. Applications of Aqueous Equilibria

- a) Write a balanced equation for a neutralization reaction, calculate the equilibrium constant, and determine whether the pH after neutralization is greater than, equal to, or less than 7.
- b) Calculate the effect of a common-ion on concentrations, pH, and percent dissociation in a solution of a weak acid.
- c) Calculate the pH of a buffer solution and the change in pH on addition of a strong acid or a strong base.
- d) Use the Henderson–Hasselbalch equation to calculate the pH of a buffer solution and to prepare a buffer solution that has a given pH.
- e) Calculate the pH at various points in a strong acid–strong base, weak acid–strong base, weak base–strong acid, diprotic acid–strong base titration.
- f) Write the equilibrium-constant expression for dissolution of an ionic compound, and calculate the value of its K_{sp} .
- g) Calculate ion concentrations and the solubility of an ionic compound from its K_{sp} .
- h) Describe how the presence of molecular and ionic species will affect the solubility of an ionic compound.
- i) Calculate solubility in a solution that contains a common ion.
- j) Use the formation constant K_f to calculate ion concentrations in a solution that contains a complex ion.
- k) Calculate the ion product IP for an ionic compound, and determine whether a precipitate will form when various solutions are mixed.

3. Thermochemistry

- a) Explain the terms system and surroundings.
- b) Calculate the heat and work involved.
- c) Describe the difference between heat capacity, specific heat capacity, molar heat capacity, and perform calculations using these properties.
- d) Describe the characteristics of a state function.
- e) Describe enthalpy change and calculate changes of enthalpy during phase changes and chemical reactions.
- f) Apply Hess's law to calculate enthalpy changes (ΔH).
- g) Describe enthalpy changes of formation (ΔH_f) and use them to calculate enthalpy changes during reactions.
- h) Describe and use enthalpy changes of combustion (ΔH_c) and enthalpy changes of solution.

4. Thermodynamics

- i) Explain and calculate expansion work.
- j) Describe the First, Second and Third Laws of thermodynamics.
- k) Calculate internal energy change from enthalpy change and vice versa.
- l) Describe how to use a bomb calorimeter to measure energy changes of combustion.
- m) Describe spontaneous changes.

- n) Apply changes in entropy and Gibbs energy to assess the spontaneity of processes or reactions.
- o) Predict the sign of the entropy change (ΔS) given the chemical equation or a molecular diagram.
- p) Using the relationship between the Gibbs free energy (ΔG) and spontaneity, predict the sign of ΔG , ΔH , ΔS .
- q) Use ΔH and ΔS to determine the temperature at which a reversible system is at equilibrium.

5. ^1H NMR Spectroscopy

- a) Describe typical requirements for reference compounds for ^1H .
- b) Explain what leads to signal multiplicity in ^1H NMR.
- c) Describe typical requirements for reference compounds for ^1H NMR.
- d) Correlate the number of peaks to the number of nuclei environments in ^1H NMR.
- e) List and explain the different regions of ^1H NMR spectrum.
- f) State the factors that local magnetic field depends on.
- g) Explain shielding and deshielding in ^1H NMR
- h) Illustrate the formation of doublet, triplet, quartet, quintets, etc. in ^1H NMR
- i) Explain and depict coupling pattern in ^1H NMR.
- j) Predict the intensity ratios using Pascal's triangle and tree diagrams in ^1H NMR

6. Molecular orbital theory

- a) Interpret the different energies of bonding and antibonding orbitals
- b) Sketch graphical addition of AOs to form MOs
- c) Define Molecular orbital
- d) Sketch qualitative MO diagrams for H_2^+ ion
- e) Fill in the electrons in MO diagrams
- f) Construct simple MO diagrams for diatomic molecules (involving s orbitals)
- g) Calculate bond order for simple diatomic molecules
- h) Relate bond orders to bond strengths and stability in diatomic molecules
- i) Compose MO diagrams for heteronuclear diatomic molecules
- j) Estimate validity of MO diagrams for heteronuclear diatomic molecules

7. Molecule structures: bonding and stereochemistry

- a) Explain electronegativity, polarity and inductive effects.
- b) Recognize the differences among types of bonds: nonpolar covalent bond, polar covalent bond, ionic bond, H-bond.
- c) Be able to convert the resonance structures of molecules by applying the 5 rules of resonance forms.
- d) Explain the difference between structural isomers and stereoisomers.
- e) Recognize both types of configurational isomers – E/Z isomers and isomers with chiral centres.
- f) Recognize enantiomers and assign the configuration of chiral centres as R or S using the Cahn-Ingold-Prelog sequence rules.
- g) Convert a hashed-wedged line structure into a Fischer projection (and vice versa).
- h) Recognize diastereomers and the difference between diastereomers and enantiomers.

8. Molecule reactions: survey of reactions with alkyl halide

- a) Recognize the difference in curved arrows in drawing mechanisms.
- b) Recognize the basic types of organic reactions: Addition, elimination, substitution, rearrangement.
- c) Explain why different carbon-halogen bonds in alkyl halide react differently from one another.
- d) Explain how alkyl halide react in S_N2 and S_N1 reactions
- e) Explain how alkyl halide react in E2 and E1 reactions.
- f) Describe the factors that affect S_N2 versus S_N1 reactions.
- g) Describe the factors that affect E2 versus E1 reactions.
- h) Describe the factors that influence substitution versus elimination reactions.

9. Sweet molecules: carbonyl chemistry in biological systems

- a) Recognize structures of hemiacetal, hemiketal, acetal, ketal.
- b) Recognize the α - and β - anomers of carbohydrate.
- c) Recognize the nucleophilic addition to carbonyl compounds to obtain hemiacetal or hemiketal.
- d) Recognize enolization of carbonyl under acidic and basic conditions.
- e) Explain the interconversion between cyclic α and β -anomers and open-chain carbonyl.
- f) Recognize the difference in retaining glycosidase and inverting glycosidases.

10. Nature's chemical reagents: ATP

- a) Explain why monosaccharides exist in phosphate esters in biological systems.
- b) Explain why ATP is kinetically stable, but thermodynamically activated molecule.
- c) Recognize reactions that involve ATP in nature: kinases, and nucleotidyl transfer.
- d) Recognize the Nature's logic for building polysaccharide

11. Nature's catalysts: Enzymes

- a) Explain basic enzyme kinetic terms: V_{max} , K_m , K_d , K_i .
- b) Explain the difference between competitive inhibitor and non-competitive inhibitor
- c) Perform Lineweaver-Burk Plot.
- d) Recognize the four types of proteases: aspartyl protease, zinc(metallo) protease, serine and cysteine proteases.
- e) Recognize the inhibitors for particular type of proteases.

Course Content

- 1. Chemical Kinetics
- 2. Thermochemistry
- 3. Thermodynamics
- 4. Acid-Base Equilibria
- 5. Applications of Aqueous Equilibria
- 6. 1H NMR Spectroscopy
- 7. Molecular orbital theory
- 8. Molecule structures: bonding and stereochemistry
- 9. Molecule reactions: survey of reactions with alkyl halide
- 10. Sweet molecules: carbonyl chemistry in biological systems
- 11. Nature's chemical reagent: ATP

12. Nature's catalysts: Enzymes

Assessment (includes both continuous and summative assessment)

Component	Course LO Tested	Related Programme LO or Graduate Attributes (Appendix 3)	Weighting	Team/Individual	Assessment Rubrics
Mid-term Test 1	1-4	Competence	15	Individual	See
Mid-term Test 2	7-9	Competence	15	Individual	Appendix 1
Laboratory	4-11	Competence	10	Individual	Appendix 2
Virtual Laboratory	1-4, 6, 7	Competence	10	individual	Appendix 3
Final examination	All	Competence	50	Individual	Appendix 1
Total			100%		

Formative feedback

You will be given feedback in four ways:

1. By response to postings on the course discussion board.
2. Through the marking of the mid-terms.
3. Through tutorial sessions and/or 1-on-1 discussions with the course instructor (pre-scheduling required)
4. General feedback will be provided to the students following the final exam.

Learning and Teaching approach

Approach	How does this approach support students in achieving the learning outcomes?
Online material and online lectures + laboratory online and hands-on	The bulk of the content will be delivered through online lectures and online material. This allows (a) extensive use of animations and laboratory videos and (b) use of interactive questions so that students may immediately test their learning.

Reading and References

A. Burrows, J. Holman, A. Parsons, G. Pilling, and G. Price "Chemistry³ (3rd Edition)", Oxford University Press, 2017. ISBN: 978-0-19-969185-2.

J.E. McMurry, R.C. Fay, J.K. Robinson "Chemistry (7th Edition)", Pearson Education, 2015. ISBN: 978-1-292-09275-1.

Course Policies and Student Responsibilities

(1) General

You are expected to complete all online activities in good time.

(2) Absenteeism

If you miss a session, you are expected to make up for the lost learning activities. If you miss one of the mid-term tests with a valid reason and approval (such as a medical certificate), then the total CA will come from the other mid-term test. If you miss both mid-term tests with a valid reason, then an additional make-up test will be set to obtain the total CA mark.

Academic Integrity

Good academic work depends on honesty and ethical behaviour. The quality of your work as a student relies on adhering to the principles of academic integrity and to the NTU Honour Code, a set of values shared by the whole university community. Truth, Trust and Justice are at the core of NTU's shared values.

As a student, it is important that you recognize your responsibilities in understanding and applying the principles of academic integrity in all the work you do at NTU. Not knowing what is involved in maintaining academic integrity does not excuse academic dishonesty. You need to actively equip yourself with strategies to avoid all forms of academic dishonesty, including plagiarism, academic fraud, collusion and cheating. If you are uncertain of the definitions of any of these terms, you should go to the [academic integrity website](#) for more information. Consult your instructor(s) if you need any clarification about the requirements of academic integrity in the course.

Course Instructors

Instructor	Office Location	Phone	E-mail
ZHANG Zhengyang	SPMS-CBC-03-02	6513 6059	zhang.zy@ntu.edu.sg
QIAO Yuan	SPMS-CBC-04-22	6904 4477	yuan.qiao@ntu.edu.sg

Planned Weekly Schedule

Week	Topic	Course LO	Readings/ Activities
1	Chemical Kinetics	1	Online lectures and materials
2	Applications of Aqueous Equilibria	2	Online lectures and materials
3	Thermochemistry	3	Online lectures and materials
4	Thermodynamics	4	Online lectures and materials
5	¹ H NMR Spectroscopy	5	Online lectures and materials
6	Mid-term Test 1	1-4	Online lectures and materials
7	Molecular orbital theory	6	Online lectures and materials
8	Molecule structures: bonding and stereochemistry	7	Online lectures and materials
9	Molecule reactions: survey of reactions with alkyl halide	8	Online lectures and materials
10	Sweet molecules: carbonyl chemistry in biological systems	9	Online lectures and materials
11	Nature's chemical reagent: ATP	10	Online lectures and materials
12	Mid-term Test 2	7-9	Online lectures and materials
13	Nature's catalysts: Enzymes	11	Online lectures and materials

The above schedule is for illustrative purposes and is subject to the exigencies of the calendar

Appendix 1: Assessment Criteria for midterm tests and exam

Mid-term Test 1 and 2 – MCQ questions (two tests worth 15 marks each).

Standards		
Fail standard (0-5 marks)	Pass standard (6-10 marks)	High standard (11-15 marks)
Answers to the questions are mostly incorrect.	Answers to the questions are mostly correct.	Answers to the questions are almost always correct.

Final exam – short answer questions and calculations (exam worth 50 marks).

Standards		
Fail standard (0-19 marks)	Pass standard (20-40 marks)	High standard (41 -50 marks)
Answers demonstrate the ability to repeat factual knowledge but not to apply it outside of the lecture context. Answers do not have a strong logical underpinning or maybe attempts to answer both ways at the same time.	Answers to the standard level question are correct and show the ability to apply concepts from the course, but a high level of critical thinking is absent. Answers are reasonably logical, but with gaps.	Answers to all questions show a high and consistent level of critical analysis of the information presented and creative solutions to the problems. Answers are highly logical and demonstrate strong reasoning. Answers are concise and to the point.

Appendix 2 – Assessment criterion for lab proforma

	Poor (1-3)	Acceptable (4-5)	Admirable (6-7)	Exceptional (8-10)
Overall presentation	Poorly organized report with frequent awkward phrases, poor word choices and wrong inferences/calculations. Lacks cohesion, style and fluidity.	Many passages are phrased poorly, contained awkward word choices, or many long sentences. Narrative is disorganized in many places. Multiple grammatical and/or spelling errors.	Minimal awkward phrasing or word choices. Minimal mistakes in calculations and explanations	Appropriate as a piece of scientific writing. Words were chosen carefully and appropriately. Sentence structure was clear and easy to follow. The report is free of spelling, punctuation, calculation and grammatical errors.
Answers to Proforma questions	Figures, graphs, and tables are poorly constructed; have missing titles, captions or numbers. Certain data reported are not mentioned in the text. Important data missing. Does not demonstrate an understanding of the important experimental concepts, forms inaccurate conclusions, suggests inappropriate improvements in the experiment and lacks overall justification of error. Address none of the specific points or questions posed in the proforma.	Most figures, graphs, and tables are included, but some important or required features are missing. Certain data reported are not mentioned in the text or are missing. Captions are not descriptive or incomplete. While some of the results have been correctly interpreted and discussed, partial but incomplete understanding of results is still evident. Student fails to make one or two connections to underlying theory. Address some of the specific points or questions posed in the proforma.	All data and associated figures, calculations etc. are presented. Demonstrates an understanding of most important experimental concepts, forms conclusions based on results and/or analysis but either lacks proper interpretation, suggests inappropriate improvements in the experiment or lacks overall justification of error. Address most of the specific points for questions posed in the proforma.	Relevant experimental data/calculation steps are presented which are used for answering proforma questions. Demonstrates a logical, coherent working knowledge and understanding of important experimental concepts, forms appropriate conclusions based on interpretations of results, includes applications of and improvements in the experiment, collected data and analysis and demonstrates accountability by providing justification for any errors. Address all specific questions posed in the proforma.

Appendix 3: Virtual laboratory experiments

Standards		
Simulations	Completed	Evaluation
1.- Ionic and Covalent Bonds -	Requisite	All four simulations must be completed by the end of the course
2.- Equilibrium -	Requisite	
3.- Nuclear Magnetic Resonance	Requisite	
4.- Basic Chemistry Thermodynamics	Requisite	
- The above schedule might change slightly and is subject to the availability of more appropriate simulations from Labster.		

Appendix 4: CBC Programme Learning Outcome

The Division of Chemistry and Biological Chemistry (CBC) offers an undergraduate degree major in Chemistry that satisfies the American Chemical Society (ACS) curricular guidelines and equips students with knowledge relevant to the industry. Graduates of the Division of Chemistry and Biological Chemistry should have the following key attributes:

1. Competence

Graduates should be well-versed in the foundational and advanced concepts of chemical science, be able to evaluate chemistry-related information critically and independently, and be able to use complex reasoning to solve emergent chemical problems.

2. Creativity

Graduates should be able to synthesize and integrate multiple ideas across the curriculum, and propose innovative solutions to emergent chemistry-related problems based on their training in chemistry.

3. Communication

Graduates should be able to demonstrate clarity of thought, independent thinking, and sound scientific analysis and reasoning through written and oral reports to audiences with varying technical backgrounds. They should also be able to effectively engage other professional chemists in collaborative endeavours.

4. Character

Graduates should be able to act in responsible ways and uphold the high ethical standards that the society expects of professional chemists.

5. Civic-mindedness

Graduates should be aware of the impact of chemistry on society, and how chemistry can be applied to benefit mankind. They should also be aware of and uphold the best chemical safety practices.