| | | | |
|---|---|---|---|
| **Academic Year** | 2020/21 | **Semester** | 1 |
| **Course Coordinator** | ZHANG Zhengyang and Felipe GARCÍA | | |
| **Course Code** | CM9001 | | |
| **Course Title** | Conceptual Chemistry with Laboratory | | |
| **Pre-requisites** | By permission | | |
| **No of AUs** | 4 | | |
| **Contact Hours** | On-line activities - 11 hours<br>Lectures - - 22 hours<br>Mid-term assessments - 4 hours<br>Laboratory experiments - 30 hours | | |

**Course Aims**

The course provides an introduction to modern chemistry that are used to build key fundamental understandings of bonding theories, inorganic, organic and physical chemistry. Students 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.

**Intended Learning Outcomes (ILO)**

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

**1. <u>Molecular orbital theory</u>**

a) Interpret atomic quantum numbers
b) Recognise wavefunctions and their angular and radial parts
c) Define radial distribution function (RDF)
d) Construct an RDF from a wavefunction graphically
e) Represent s, p and d orbital graphically
f) Interpret the different energies of bonding and antibonding orbitals
g) Sketch graphical addition of AOs to form MOs
h) Define Molecular orbital
i) Sketch qualitative MO diagrams for $H_2^+$ ion
j) Fill in the electrons in MO diagrams
k) Construct simple MO diagrams for diatomic molecules (involving s orbitals)
l) Calculate bond order for simple diatomic molecules
m) Relate bond orders to bond strengths and stability in diatomic molecules
n) Describe the differences between s-p mixing and not-mixed MO diagrams
o) Reproduce the MO diagrams for groups 13 to 16
p) Discuss the nature of the interactions underlying s-p mixing
q) Compose MO diagrams for heteronuclear diatomic molecules
r) Estimate validity of MO diagrams for heteronuclear diatomic molecules
s) Reproduce the MO diagram of simple triatomic molecules.

**2. <u>Transition Metals and Coordination Chemistry</u>**

a) Define coordination compounds and metal complexes

b) Identify different types of ligands and their structures
c) Name simple coordination complexes
d) Define and identify isomers in coordination chemistry
e) Draw different isomers for square planar and octahedral complexes
f) Identify optical isomerism
g) Explain the bonding in coordination compounds
h) Cite and formulate the basics of crystal field theory
i) Draw molecular orbital splitting for different coordination geometry
j) Compare and contrast Tetrahedral & Square Planar Ligand Field
k) Depict the splitting diagram of the d orbitals for $\sigma$- donor ligands
l) Depict the splitting diagram of the d orbitals for $\sigma$-donor and $\pi$-acceptor ligands
m) Depict the splitting diagram of the d orbitals for $\sigma$-donor and $\pi$-donor ligands

**3. <u>$^{13}$C NMR Spectroscopy</u>**

a) Define and identify high spin and low spin complexes
b) Calculate magnetic moments
c) Discuss the color of simple metal complexes
d) State the formula for chemical shift and describe it.
e) Describe typical requirements for reference compounds for $^{1}$H and $^{13}$C NMR.
f) Correlate the number of peaks to the number of nuclei environments in $^{13}$C NMR.
g) List and explain the different regions of $^{13}$C NMR spectrum.
h) State the factors that local magnetic field depends on.
i) Explain shielding and deshielding effects on NMR chemical shift.
j) Illustrate the formation of doublet, triplet and quartet.
k) Explain coupling in $^{13}$C NMR.
l) Predict the intensity ratios using Pascal’s triangle.

**4. <u>$^{1}$H NMR Spectroscopy</u>**

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

**5. <u>Infrared Spectroscopy</u>**

a) List the benefits of infrared spectroscopy.
b) Explain how the vibrations of a diatomic can be classified.
c) List the vibrational frequencies for different functional groups.
d) Identify functional groups by their typical vibration frequencies.
e) List the factors affecting strength of IR absorption.
f) Identify doubly and triply bonded species by the position of their typical vibrational frequencies.
g) Identify a range of species containing X–H bonds within the region: 2500 – 4000 $cm^{-1}$

6. **Chemical Kinetics**

a) Determine the average reaction rate over a specified period of time and estimate instantaneous reaction rate from a graph of concentration versus time.
b) Relate the rate of consumption of any reactant to the rate of formation of any product using reaction stoichiometry.
c) 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.
d) Predict the change in reaction rate when the concentration of a reactant changes by a specified amount.
e) Determine the rate law and rate constant using initial rate and concentration data.
f) 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.
g) Interpret potential energy diagrams and suggest geometries for successful collisions and transition states using collision theory.
h) 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.

7. **Thermochemistry: Chemical Energy**

a) Explain the terms system and surroundings.
b) Calculate the heat and work involved.
c) Describe the difference between hear 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 ($\Delta H$).
g) Describe enthalpy changes of formation ($\Delta H_f$) and use them to calculate enthalpy changes during reactions.
h) Describe and use enthalpy changes of combustion ($\Delta H_c$) and enthalpy changes of solution.
i) Explain and calculate expansion work.
j) Describe the First Law 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 ($\Delta S$) given the chemical equation or a molecular diagram.
p) Using the relationship between the Gibbs free energy ($\Delta G$) and spontaneity, predict the sign of $\Delta G$, $\Delta H$, $\Delta S$.
q) Use $\Delta H$ and $\Delta S$ to determine the temperature at which a reversible system is at equilibrium.

## 8. Acid-Base Equilibria

a) Identify Arrhenius acids and bases and Brønsted–Lowry acids and bases and conjugate acid–base pairs.
b) Predict the direction of a reaction based upon relative strengths of the conjugate acid–base pairs.
c) Predict the relative strengths of binary acids (HA) and oxoacids ($H_nYO_m$) based on their chemical structure.
d) Calculate the concentration of [$H_3O^+$] or [$OH^-$] using the value of $K$w.
e) Calculate the pH of a solution given [$H_3O^+$] or [$OH^-$].
f) Calculate the pH of a strong acid or base solution.
g) Calculate the value for $K_a$ given the initial concentration of a weak acid and its equilibrium pH.
h) Given the $K_a$ value for a weak acid and its initial concentration, calculate the pH, percent dissociation, and the concentration of all species present in solution.
i) Calculate the pH and the concentration of all species present in a solution of a diprotic acid.
j) Calculate the pH and equilibrium concentrations in a solution of a weak base.
k) Relate $K_a$, $K_b$, p$K_a$, and p$K_b$ for a conjugate acid–base pair.
l) Predict whether a salt is acidic, basic, or neutral and calculate the pH of the salt solution.
m) Identify the Lewis acid and Lewis base and use curved arrow notation to indicate donation of a lone pair of elections in Lewis acid–base reaction.

## 9. 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.

## 10. Isomerism and Stereochemistry

a) Recognize chain isomers, position isomers, and functional group isomers.

b) Explain the difference between structural isomers and stereoisomers.
c) Recognize conformational isomers and understand the factors (torsional strain, steric strain, and angle strain) that influence the conformation of organic molecules.
d) Recognize both types of configurational isomers – E/Z isomers and isomers with chiral centres.
e) Recognize enantiomers and assign the configuration of chiral centres as R or S using the Cahn-Ingold-Prelog sequence rules.
f) Convert a hashed-wedged line structure into a Fischer projection (and vice versa).
g) Recognize diastereomers and the difference between diastereomers and enantiomers.

**11. <u>Halogenalkanes: substitution and elimination</u>**

a) Explain why different carbon-halogen bonds in halogenalkanes react differently from one another.
b) Describe how halogenalkanes can be prepared from alkanes, alcohols, and alkenes.
c) Explain how halogenalkanes react in $S_N2$ and $S_N1$ reactions
d) Recognize the importance of tight ion pairs in some $S_N1$ reactons.
e) Explain how halogenalkanes 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.

**Course Content**

1. Molecular orbital theory
2. Transition Metals and Coordination Chemistry
3. $^{13}C$ NMR Spectroscopy
4. $^{1}H$ NMR Spectroscopy
5. Infrared Spectroscopy
6. Thermochemistry: Chemical Energy
7. Chemical Kinetics
8. Acid-Base Equilibria
9. Applications of Aqueous Equilibria
10. Isomerism and Stereochemistry
11. Halogenalkanes: substitution and elimination

**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 | 1-5 | Competence | 15 | Individual | See Appendix 1 |
| Mid-term Test 2 | 6-9 | Competence | 15 | Individual | |

| | | | | | |
|---|---|---|---|---|---|
| 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 "Chemistry$^3$ (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 |
| Felipe GARCÍA | SPMS-CBC-05-19 | 6592 1550 | FGarcia@ntu.edu.sg |

**Planned Weekly Schedule**

| Week | Topic | Course LO | Readings/ Activities |
|---|---|---|---|
| 1 | Molecular orbital theory | 1 | Online lectures and materials |
| 2 | Molecules and Transition Metals complexes | 2 | Online lectures and materials |
| 3 | Coordination Chemistry: | 2 | Online lectures and materials |
| 4 | $^{13}$C NMR Spectroscopy | 3 | Online lectures and materials |
| 5 | $^{1}$H NMR Spectroscopy | 4 | Online lectures and materials |
| 6 | Infrared Spectroscopy | 5 | Online lectures and materials |
| 7 | Mid-term Test 1 | 1-5 | |
| 8 | Thermochemistry: Chemical Energy | 6 | |
| 9 | Chemical Kinetics | 7 | Online lectures and materials |
| 10 | Acid-Base Equilibria | 8 | Online lectures and materials |
| 11 | Applications of Aqueous Equilibria | 9 | Online lectures and materials |
| 12 | Isomerism and Stereochemistry | 10 | Online lectures and materials |
| 12 | Mid-term Test 2 | 6-9 | |
| 13 | Halogenalkanes: substitution and elimination | 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.<br>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.<br>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.<br>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.<br>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.<br>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.<br>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.