School of Physical and Chemical Sciences

Te Kura Matū



General Course Information

CHEM 111–22S2 Chemical Principles and Processes

0.125 EFTS 15 Points Second Semester 2022

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Description

This course deals with a series of topics in physical and inorganic chemistry and is a prerequisite for those students wishing to proceed to a BSc majoring in Chemistry or majoring in other subjects while including advanced chemistry courses. This course also meets the chemistry requirement for entry into the BE (Hons) degree.

Topics covered are: atoms and the periodic table; chemical bonding; reduction and oxidation reactions; properties of gases; introduction to thermodynamics; kinetics; chemical equilibrium; Gibbs energy and the second law of thermodynamics; aqueous chemistry; acid-base equilibrium.

Students should note that in the Science Faculty the average student should undertake approximately three hours of additional study for each hour of lectures at the 100-level.

Prerequisites

The prerequisites for CHEM111 are:

- 1) NCEA: at least 14 level-3 credits in Chemistry, or
- 2) CIE: at least a D grade in A Level Chemistry, or at least an A grade in ASL Chemistry, or
- 3) IB: at least Grade 4 in HL Chemistry or Grade 6 in SL Chemistry
- 4) CHEM114, or
- 5) at least B+ grade in TRNS006, or
- equivalent preparation approved by the Head of School.

Goals of the Course

To provide a solid understanding of basic principles of physical chemistry and related areas.

Course Coordinator

A/Prof Vladimir Golovko, vladimir.golovko@canterbury.ac.nz

Laboratory coordinators

Dr Anthea Lees, anthea.lees@canterbury.ac.nz. Contact Anthea for morning lab session queries

Dr Justine Cottam justine.cottam@canterbury.ac.nz. Contact Justine for afternoon lab session queries.

Lecturers (list of topics is on pages 8 & 9)

- A/Prof Vladimir Golovko (topics 1 to 3): vladimir.golovko@canterbury.ac.nz
- Prof Stephen Ashworth (topic 4): S.Ashworth@uea.ac.uk
- A/Prof Greg Russell (topic 5): greg.russell@canterbury.ac.nz
- A/Prof Laura Revell (topic 6): laura.revell@canterbury.ac.nz
- A/Prof Deborah Crittenden (topic 7); deborah.crittenden@canterbury.ac.nz
- A/Prof Greg Russell (topic 8): greg.russell@canterbury.ac.nz
- Prof Ian Shaw (topics 9 & 10): ian.shaw@canterbury.ac.nz

Timetable

36 Lectures and 12 tutorials: Check the web (http://www.canterbury.ac.nz/courses/) for confirmation of times and venues, which may be subject to change. Generally, three lectures and one tutorial will be held each week each week in the time slots labelled Lectures A-D. Some lecturers will instead incorporate their tutorials into their lectures.

Laboratory experiments: The laboratory sessions are an essential part of CHEM111. All experiments are compulsory and assessable; you must satisfactorily complete all experiments to pass the course. For each experiment you will be supplied with a lab manual, a PowerPoint information file and experiment videos. You will be required to complete your results sheets during the laboratory session and hand them in to be marked. Prior to each lab assignment you are required to read and understand the introduction, theory and experimental sections for that experiment in the lab manual. During the first week of term, you will be instructed about laboratory procedures and safety. You will also be required to complete an on-line safety quiz (this is marked and forms part of your overall lab grade). The laboratory experiments are worth 15% of your course mark. Additionally, this material will be assessed in the test and exam.

Assessment

Laboratory (including safety quiz and timelines): 15%
BestChoice on-line problems: 5%
Mid-semester test: 30%
Final exam: 50%

Failure to achieve a mark of at least 40% in the final exam will result in a grade no higher than a restricted pass (R grade). Grades are often scaled up to ensure consistency between semesters but may be scaled down if necessary.

Examination and Test

- Test: Mid semester, 1.5 hours duration, Friday 23 September (evening), time and venue to be advised.
- Exam: End of semester, 2.5 hours duration, time and venue to be advised.

BestChoice on-line problems

BestChoice is a computer-based service provided by the University of Auckland. It contains a comprehensive selection of exercises ("topics") that cover most aspects of CHEM111 course material. You should use these topics both to reinforce the lecture material and also as revision for tests and exams. You are required to achieve a total of at least 1300 marks in the assessable topics (marked with orange flags to the right on the BestChoice website) to obtain the maximum 5% grade allocated for BestChoice. There are also additional revision topics available that you may find useful but which do not count towards your final grade. These are indicated by the preface "More" and are not marked by an orange flag.

The total marks available from the assessable section is approximately 2,250. If you collect fewer than 1300, you will be given a proportionate assessment mark, e.g. 650 marks would translate to 2.5 out of 5, because 650 is half of 1,300. Note that many *BestChoice* questions are worth 5-10 marks, with one mark being assigned for each step of working. Also note that if you get a *BestChoice* question wrong, then you may try again to get it correct. As long as you eventually get the correct answer, this will be logged as a correct answer for your assessment mark.

There are no weekly deadlines for completing *BestChoice* questions. Rather, you should complete these questions at your own pace and according to your own needs. In other words, it is self-directed learning. However, it is clearly desirable to work consistently with *BestChoice*, striving to achieve at least 100 marks every week. The only *deadline* in terms of marks is *on midnight after the final* <u>exam</u> for the course.

Textbook: The course textbook is *Chemistry*³ by Burrows *et al.* (either the 2nd or 3rd edition may be used). It is recommended that students have a copy. Other resources will be available via the *Learn* website (see below).

Problems manual: The CHEM111 *Problems Manual* is available via the *Learn* website: http://learn.canterbury.ac.nz/. There are two folders. The "Problems" folder contains sets of problems related to various sections of the course. Some of these problems may be used by lecturers as exercises for tutorials, but even if they are not, you should attempt them as examples of the types of questions that might be asked in the class test or exam. The second "Solutions" folder contains worked solutions for each of the problems. You should refer to these only after you have made a genuine attempt to answer the problems yourself.

Web-based resources: Various learning resources (lecture and lab material, reference links, quizzes, discussion forums, etc.) for this course are available via the University of Canterbury's *Learn* web site (http://learn.canterbury.ac.nz/). This site will also be used regularly as a means of communication and information distribution for all of your Canterbury courses. You should familiarise yourself with *Learn* as soon as possible.

Learning Outcomes

Develop skills in the critical analysis of chemical information Develop problem-solving skills in chemistry Enhance applied mathematical skills relevant to chemistry Develop a working understanding of:

- Atomic structure and periodicity
- Chemical bonding and material properties
- Chemical reactions, especially redox reactions
- Quantities and dimensions (IUPAC conventions and SI units)
- Physical models and the properties of gases
- Thermochemistry, including the 1st law of thermodynamics
- Entropy and the 2nd and 3rd laws of thermodynamics
- Gibbs energy and its relationship to chemical equilibrium
- Chemical kinetics, reaction mechanisms and integrated rate laws
- Equilibria, equilibrium constants and Le Châtelier's principle
- The chemistry of water
- Acid-base equilibria

LABORATORY CLASSES

Laboratory allocations: You must allocate yourself to a lab stream through <u>MyTimetable</u> before the laboratory classes begin. If you do not do this before the start of term you will be allocated into a laboratory class. If you enrol late and your lab session does not appear on your timetable, you will also need to contact the <u>laboratory coordinators</u> to be assigned to a lab stream.

All CHEM111 laboratory experiments are compulsory and assessed and worth 15% of your total mark.

Laboratory organization: Each laboratory is overseen by a laboratory supervisor. They will be accompanied by demonstrators and together they will be responsible for grading your lab assignments and answering queries. If you encounter difficulties during the on-line lab assignments, please consult any demonstrator, the supervisor or lab coordinators Anthea/Justine. We will provide you with email details for these.

Laboratory assessment: For each experiment you will be supplied with a results sheet for the week's experiment and be expected to read a PowerPoint file and watch a video on LEARN prior to the laboratory class (details will be provided through the CHEM111 LEARN laboratory page).

Laboratory manuals: will be available to collect when you collect your lab coat and an electronic copy is available to download of the CHEM111 LEARN website https://learn.canterbury.ac.nz/course/view.php?id=13752§ion=4

Attendance at laboratory experiments

You are expected to complete every CHEM111 experiment and to complete the CHEM111 safety quiz.

If you cannot complete an experiment, you should contact the <u>laboratory coordinators</u> in advance to check that you reason is deemed valid. For an exemption, you will need to provide documented evidence via email, e.g. a copy of a letter from a team manager, or funeral notice, or letter from a doctor or counsellor. You should retain the original copy of the letter and send a scanned or photographed copy by e-mail to the <u>laboratory coordinators</u>.

Students who are unable to complete an experiment because of any circumstances described below should, in the first instance, contact the laboratory coordinators.

Absences due to illness, injury or other medical condition will be excused only if you provide a medical certificate from a registered medical practitioner, registered dental surgeon, registered midwife or a student counsellor.

<u>Important note</u>: a medical certificate should be obtained in the period around the missed lab experiment. A retrospectively obtained medical certificate must be accompanied by evidence (e.g. a letter from a relevant medical professional) confirming that an appointment was made on or near the day of the missed lab. In all cases where a medical appointment was not made (and evidenced) around the time of the missed lab, a reason must be provided by the health professional as to why the medical certificate could not have been obtained near the time of the missed lab.

Absences due to bereavement (the death of a family member or close friend) will be excused, provided a copy of the death notice is provided.

Absence to attend a national sporting or cultural event may be excused, but you must contact the laboratory coordinators in advance of the event and provide any supporting documentation that is requested.

Absence due to other emergencies or other unforeseen circumstance may be excused if you immediately provide appropriate evidence. You need to contact the <u>laboratory coordinators</u> as soon as practical.

Any unexcused absences may constitute an unsatisfactory record and result in you failing the laboratory requirement and hence CHEM111. At the very least, you will be assigned a mark of zero for the experiment which will reduce your final mark.

Exemptions: Students who are repeating CHEM111 may, on the basis of their results in a previous year, be exempted from attending laboratories. Students who wish to apply for exemption should contact the <u>course coordinator</u> by email by the end of the second week of the semester. You must obtain formal exemption to be excused from the laboratory section of the course.

If your overall completion of laboratories is judged unsatisfactory you will not be given a pass in the laboratory course and will FAIL CHEM111.

Laboratory Safety

Safety glasses and laboratory coats must always be worn when you are in the laboratory.

Purchasing safety glasses and laboratory coats

Approved safety glasses and laboratory coats may be purchased from the University. To purchase: go to https://www.canterbury.ac.nz/science/current-students/shop/

The collection point for purchases is inside the southern entry to the Ernest Rutherford Building. Thursday 14th July and Friday 15th July between the hours of 9.00 – 10.00am

Monday to Friday for the first two weeks of the semester at 9.00 - 10 am and 1.00 - 2.00 pm,

Safety glasses of an approved design must be worn at all times in the laboratory. If you normally wear prescription glasses you must either wear safety glasses over them or they must have plastic or toughened-glass lenses and be fitted with side protectors. Safety glasses are not supplied.

You must wear approved safety glasses in the laboratory and they must be put on before entering the lab and removed after leaving lab.

Laboratory coats must be worn at all times in the laboratory and should not be worn outside of the laboratory environment.

Suitable footwear must be worn at all times in the laboratory. This means footwear that is closed to spills and that covers all of your feet. No open-topped, open-toed, or backless footwear – and absolutely no gumboots, jandals or sandals. Students who come to a laboratory in bare feet or unsuitable footwear will not be allowed to enter the laboratory.

Bags may be stored in lockers outside the lab. They must not be taken into the lab although computers may be stored on the side benches and it is recommended valuables should remain with you.

Food or drink may not be consumed in the laboratory. Water bottles are not allowed in the laboratory. **Smoking and vaping** is prohibited everywhere on the university campus.

No headphones or wireless headphones to be worn in labs

Only those students who are enrolled in CHEM111 are permitted to enter the laboratories. You must not bring anyone else into the laboratories.

Anyone waiting for you must do so outside the laboratory rooms.

SUMMARY OF COURSE CONTENT

This outline is provided as a study guide and indicates the topics covered in the tests and examinations. Appropriate chapter references are given for the course textbook, *Chemistry*³ by Burrows *et al.* The detail and depth of treatment will be defined by the lecture material rather than by the textbook references, which may sometimes contain additional material that may be helpful to understanding, but which will not be examinable.

ASSUMED MATERIAL

Some knowledge of the following material will be assumed. It will be briefly revised rather than covered at length. This includes:

- The mole concept, relative atomic mass, molar mass, chemical stoichiometry (*Chemistry*³ Chap.1).
- Basic principles of atomic structure; electron configurations; quantum numbers; the periodic table; atomic and ionic radii (*Chemistry*³ 1st ed. Chap. 2, 2nd and 3rd eds. Chap. 3). You should also be familiar with the formation of and typical properties of ionic and covalent compounds, and have a basic understanding of the ionic lattice and closest-packed structures (*Chemistry*³ 1st ed. Chaps. 2 & 5, 2nd and 3rd eds. Chaps. 3 and 6).
- The basic principle of the conservation of energy; bond energy (*Chemistry*³ 1st ed. Chap. 14, 2nd and 3rd eds. Chap. 13).
- Oxidation and reduction (*Chemistry*³ Chap. 1).

MATHEMATICAL PREPARATION

You are expected to:

- be capable of performing simple numerical manipulations including cross multiplication;
- have a knowledge of logarithms and exponentials;
- have some acquaintance with basic calculus (gradient and differentiation, area and integration);
- be familiar with the use of SI units.

There is a helpful section entitled "Maths toolkit" near the end of *Chemistry*³. Chapter 10 of the Problems Manual might also be useful.

Lecture Course Outline

The following is a brief outline of the content of the CHEM 111 lecture course. (The numbers of lectures indicated are approximate.) A more detailed description of the topics, which you may use as a study guide, can be found below under the heading "Learning Objectives for CHEM 111".

In the week after the mid-semester break there will be a test based on the material covered in topics 1 to 5; that is, to the end of the topic "Introduction to Thermodynamics" (or approximately the first $5\frac{1}{2}$ weeks of lectures). At the conclusion of the course there will be a final examination. In this, material from the whole course may be examined, but the topics covered after the cut-off point for the test (i.e. Sections 6 to 10) will be given greater weight.

- Atoms and the Periodic Table (2 lectures); Chemistry³ 1st ed. Chaps. 1 & 2, 2nd and 3rd eds. Chaps. 1 & 3
- Revision of atomic structure, atomic mass, quantum numbers and atomic orbitals. Electronic configurations, the aufbau principle and Hund's rule.
- The periodic table periodicity, electronegativity, ionization energy, electron affinity, etc.
- 2. Chemical Bonding (2 lectures); *Chemistry*³ 1st ed. Chaps. 1, 3, 4 & 5, 2nd and 3rd eds. Chaps. 1, 4, 5 & 6
- Chemical bonding: ionic, covalent and metallic bonding.
- Lewis structures and the octet rule.
- Molecular geometry, VSEPR theory.
- 3. Reduction and Oxidation Reactions (2 lectures); Chemistry³ Chap. 1
- Redox and related reactions, oxidation numbers, balancing redox equations.
- 4. Properties of Gases (5 lectures); *Chemistry*³ 1st ed. Chaps. 1, 3 & 7, 2nd and 3rd eds. Chaps. 1, 4 & 8
- Intermolecular forces, kinetic vs potential energies and states of matter.
- Gas laws (units of pressure, Boyle's, Charles's and Avogadro's laws).
- The ideal gas equation (density calculations, molar mass of gaseous substances, gas stoichiometry).
- Quantities and dimensions (IUPAC conventions and SI units).
- The kinetic theory of gases.
- Dalton's law of partial pressures.
- Grahams law of effusion.
- Global warming and physical principles of carbon capture technologies.
- Atmospheric ozone depletion and reactivity of gas molecules.
- Introduction to Thermodynamics (5 lectures); Chemistry³ 1st ed. Chap. 14, 2nd and 3rd eds. Chap. 13
- Systems, states and state functions; heat and work; pressure-volume work.
- First law of thermodynamics; conservation of energy; internal energy and enthalpy.
- Calorimetry; heat capacities C_p and C_V.
- Thermodynamic cycles as a generalisation of Hess's law and Kirchhoff's law; standard states; use of tables of state functions.
- 6. Kinetics (5 lectures); Chemistry³ 1st ed. Chap. 8, 2nd and 3rd eds. Chap. 9
- Reaction rates and rate laws.
- Experimental kinetics measurements.
- Concentration-time plots and the integrated rate equations for zero-order and first-order processes.
- Activation energies; the Arrhenius law and temperature dependence of reaction rates.
- Mechanisms of complex reactions, molecularity and catalysis.

7. Chemical Equilibrium (3 lectures); *Chemistry*³ 1st ed. Chaps. 15 & 16, 2nd and 3rd eds. Chaps. 14 & 15

- Equilibrium constants.
- Calculations of equilibrium concentrations of reactants and products.
- Le Chatelier's principle. Reaction quotients and the direction of spontaneous change of a reaction.

8. Thermodynamics II (5 lectures); Chemistry³ 1st ed. Chaps. 15 & 16, 2nd and 3rd eds. 14 & 15

- The concept of entropy change as driving force.
- Second law of thermodynamics; calculations using entropy as a state function.
- Gibbs energy; relationship of Gibbs-energy change to entropy change.
- Relationship of the standard Gibbs-energy change to the equilibrium constant. Temperature dependence of the equilibrium constant.

9. Aqueous Chemistry (3 lectures); Chemistry³ 1st ed. Chaps. 1, 6 & 25, 2nd and 3rd eds. 1, 7 & 25

- Structure and bonding of water. Intermolecular forces, hydrogen-bonding.
- Physical properties of water. Polarisability, dielectric constant.
- Ice and other hydrogen-bonded systems.
- Ion hydration, mobility and hydrolysis. The dissolution process.
- Water as a solvent for: non-polar covalent, polar covalent, hydrogen-bonding covalent and extended lattice covalent compounds, metals, gases, and ionic solids.
- Qualitative solubility predictions.

10. Acid-Base Equilibrium (4 lectures); Chemistry³ 1st ed. Chap. 6, 2nd and 3rd eds. Chap. 7

- Acids and bases. Self-ionisation of water. Amphoterism.
- Calculations of pH in solutions of acids, bases, salts, titrations and applications of the buffer equation.

Learning Objectives for CHEM 111

Appropriate chapter and section references are given for the course textbook, Chemistry³ by Burrows et al.

1: ATOMS AND THE PERIODIC TABLE

(2 lectures; Chemistry³ 1st ed. Chaps. 1 & 2, 2nd and 3rd eds. Chaps. 1 & 3)

(1.i) Atoms and the mole (Chemistry³ 1st ed. 1.3 & 2.8, 2nd and 3rd eds. 1.3 & 3.8)

At the end of this section you should:

- be able to define the terms atomic number, mass number and isotope in formulating the composition
 of an atom in terms of its constituent neutrons, protons and electrons;
- understand the meaning of symbolism such as $^{235}_{92}$ U;
- know the definitions of Avogadro's number and the mole (mol), the SI unit for amount,
- understand the concept of relative molar mass and know how it is related to the actual mass of a given
 amount of a substance.

(1.ii) Atomic orbital and electronic structure (Chemistry³ 1st ed. 2.3–2.6, 2nd and 3rd eds. 3.3–3.6)

At the end of this section you should:

- know the allowed *quantum numbers* n, l, and m_l for the *electron orbitals* of an atom and be able to distinguish valid and invalid combinations of these quantum numbers;
- be able to describe the **shapes** and **relative energies** of the of *n*s, *n*p and *n*d orbitals of an atom for n = 1 3;
- be able to state the number of orbitals within each orbital level and shell, and what is meant by the term degenerate;
- be able to use the **aufbau principle** and **Hund's rule** to assign **electron configurations** for atoms with atomic number up to Z < 30 (Zn);
- be aware of special cases for the electron configurations of chromium and copper.

2: CHEMICAL BONDING

(2 lectures; Chemistry³ 1st ed. Chaps. 1, 3, 4 & 5, 2nd and 3rd eds. Chaps. 1, 4, 5 & 6)

(2.i) Chemical bonding (*Chemistry*³ 1st ed. 5.7, 2.7, 3.3, 4.1 & 4.3, 2nd and 3rd eds. 6.7, 3.7, 4.3, 5.1 & 6.3)

- have a general understanding about the differences between *ionic*, *covalent* and *metallic bonding*, along with the parameters that determine the type of bonding that occurs in a given compound;
- be able to describe what is meant by the valence electrons of an atom in terms of the atom's electronic configuration;

- be able to describe the concepts of *ionisation energy*, *electron affinity* and *electronegativity*, and understand qualitatively how they relate to an atom's electronic configuration and position in the periodic table;
- be able to use the above ideas to describe the formation of *ionic compounds*, identify combinations of atoms likely to form *ionic salts* and describe, in general terms, the arrangement of atoms in an *ionic* solid:
- be able to use the above ideas to describe the formation of metallic compounds and identify combinations of atoms likely to form metals and alloys;
- understand the concept of covalent bonding in terms of shared electron pairs and be able to give examples of covalently bonded molecules;
- be able to use the Lewis dot model and the octet rule to construct representations for the electronic structures of simple covalent molecules;
- expand the ideas of the Lewis model to include double bonds, triple bonds and lone pairs.
- (2.ii) Molecular geometry (Chemistry³ 1st ed. 4.1 & 4.2, 2nd and 3rd eds. 5.1 & 5.2)

At the end of this section you should:

- understand the concept of formal charge in the context of the Lewis model, and be able to use the
 concept to determine the most likely Lewis structure from amongst two or more possibilities;
- understand the concept and consequences of resonance in the context of Lewis structures;
- know some of the exceptions to the octet rule and how they can be accommodated in the Lewis model:
- understand the principles of the **VSEPR** (**valence shell electron pair repulsion**) **model** and be able to use it to predict the shapes and geometries of molecules;
- understand how variations of the **bond angles** of similar covalent compounds can be qualitatively understood in terms of the VSEPR model.

3: REDUCTION AND OXIDATION REACTIONS (2 lectures; *Chemistry*³ Chap. 1)

(3.i) Reduction and oxidation reactions (Chemistry³ 1st ed. 1.4, 2nd and 3rd eds. 1.4)

At the end of this section you should:

- know the definitions of reduction and oxidation processes and reducing and oxidising agents;
- be able to assign oxidation numbers to atoms in compounds;
- be able to state the criteria for a *redox reaction* and be able to distinguish redox reactions from other reaction types;
- for any redox reaction, decide which element is oxidised and which is reduced.
- (3.ii) Ion-electron half reactions and redox titrations (Chemistry³ 1st ed. 1.4–1.5, 2nd and 3rd eds. 1.4–1.5)

At the end of this section you should:

know what is meant by the terms ion-electron reduction and oxidation half reactions;

- be able to derive balanced redox equations using ion-electron half equations for oxidation and reduction processes in acidic and basic solutions;
- be able to calculate the amount and concentration of a reactant from volumetric redox analysis.

4: PROPERTIES OF GASES

(5 lectures; Chemistry³ 1st ed. Chaps. 1, 3 & 7, 2nd and 3rd eds. Chaps. 1, 4 & 8)

(4.i) Molecular interactions and the gas laws (*Chemistry*³ 1st ed. 1.7 & 1.8, 7.1 & 7.2, 2nd and 3rd eds. 1.7 & 1.8, 8.1 & 8.2)

At the end of this section you should be able to:

- predict whether a collection of atoms or molecules will exist as a gas, liquid or solid at room temperature and pressure, given information about their interactions;
- state the gas laws of Boyle, Charles, and Avogadro;
- know how the gas laws are combined in the ideal gas equation.

(4.ii) Kinetic molecular theory and the ideal gas equation (*Chemistry*³ 1st ed. 7.4 & 7.5, 2nd ed. 8.4 & 8.5)

At the end of this section you should be able to:

- estimate the average velocity of a collection of identical gas molecules given temperature and mass information;
- provide a molecular level explanation for temperature and pressure;
- rationalize the ideal gas equation in terms of both empirical and theoretical arguments;
- use the ideal gas equation to calculate the pressure, volume, temperature and amount of a gas.
- (4.iii) Mixtures of gases (Chemistry³ 1st ed. 7.3–7.5, 2nd and 3rd eds. 8.3–8.5)

At the end of this section you should be able to:

- define Dalton's law both mathematically and in words;
- use Dalton's law to calculate the partial pressure of a gas in a mixture of gases;
- define Graham's law both mathematically and in words;
- explain the role of Graham's law in the **separation of gases** from mixtures;
- list and explain the principles behind different carbon capture and storage technologies.
- (4.iv) Physical versus chemical properties of gases (*Chemistry*³ 1st ed. 1.8 & 3.2–3.3, 2nd and 3rd eds. 1.8 & 4.2–4.3)

At the end of this section you should be able to:

- explain the relative reactivities of different gases, based upon bond order arguments;
- predict trends in **boiling points** based upon molecular properties and intermolecular interactions;

- explain why O₂ and CO have different chemical and biological properties despite having very similar physical properties.
- (4.v) Atmospheric chemistry and physics (*Chemistry*³ 1st ed. 1.1 & boxes 27.2 & 27.6, 2nd ed. 1.1 & boxes 27.2 & 27.6)

At the end of this section you should be able to:

- describe the greenhouse effect in terms of the physical properties of CO₂ and H₂O and other greenhouse gases;
- state the role and *chemistry of ozone in the stratospher*e: its production, photochemistry and removal;

5: INTRODUCTION TO THERMODYNAMICS

(5 lectures; Chemistry³ 1st ed. Chap. 14, 2nd and 3rd eds. Chap. 13)

(5.i) Systems, states and state functions (*Chemistry*³ 1st ed. 14.1, 14.2 & 14.5, 2nd and 3rd eds. 13.1, 13.2 & 13.5)

At the end of this section you should:

- know what is meant by the term thermodynamics and appreciate that thermodynamics can provide an
 understanding of the roles of heat and work in chemical and physical processes;
- understand what is meant by the terms system and surroundings;
- know the differences between open, closed and isolated systems;
- understand the definition and importance of state functions in thermodynamics;
- know the definitions of, and conventions relating to, the processes of heat and work in thermodynamics;
- be able to state the *first law of thermodynamics* in a practically useful form and understand its equivalence with the principle of *conservation of energy*;
- know how to calculate the work done on a system expanding or contracting against an external pressure.

(5.ii) Changes of state (*Chemistry*³ 1st ed. 14.1 & 14.5, 2nd and 3rd eds. 13.1 & 13.5)

- know how to use the first law to calculate the energy exchanged between the surroundings and system
 by heat (for processes at constant volume);
- know the definition and importance of *enthalpy* and how to calculate enthalpy changes using the first law (for processes at *constant volume*);
- understand the concept of *internal energy* and its importance, and know how it and enthalpy are interrelated;
- know that heat is related to temperature by the heat capacity of the system;
- know that heat is related to temperature by the specific heat or specific heat capacity of a substance.

know the interrelationship between heat capacity at constant pressure, Cp, and heat capacity at constant volume, Cv, and understand how these are related to enthalpy and internal energy, respectively.

(5.iii) Calorimetry (Chemistry³ 1st ed. 14.6, 2nd and 3rd eds. 13.6)

At the end of this section you should:

- understand the operating principles of calorimeters;
- understand the significance of the heat capacities C_p and C_V as they apply to calorimetry;
- understand how calorimeters are used for experimental measurements of enthalpy and internal energy changes;

(5.iv) Thermodynamic cycles (Chemistry³ 1st ed. 14.3, 2nd and 3rd eds. 13.3)

At the end of this section you should:

- know what is meant by the standard state of a substance;
- know what is meant by a standard molar thermodynamic property of a substance;
- know what is meant by a thermodynamic cycle;
- understand *Hess's law* and be able to calculate the unknown enthalpy change of a process from known enthalpy changes for other related processes.
- (5.v) Tabulations and temperature dependence (*Chemistry*³ 1st ed. 14.3 & 14.4, 2nd and 3rd eds. 13.3 & 13.4)

At the end of this section you should:

- be able define the **standard molar enthalpy of formation** of a substance;
- be able to calculate the standard molar enthalpy change of a chemical reaction from tabulated thermodynamic data;
- understand that the enthalpy change of a process is temperature dependent;
- understand the basis of *Kirchoff's law* and know how to use it to interrelate the enthalpy changes of a process at different temperatures.

6: KINETICS

(5 lectures; Chemistry³ 1st ed. Chap. 8, 2nd and 3rd eds. Chap. 9)

(6.i) Rates of reactions (Chemistry³ 1st ed. 8.1–8.5, 2nd and 3rd eds. 9.1–9.5)

- be able to define what is meant by the rate of a reaction;
- know the factors that influence the rate of a reaction;

- be able to describe methods by which changing concentrations are monitored experimentally;
- be able to define the terms rate law, rate coefficient (or rate constant) and reaction order.

(6.ii) Rate laws (*Chemistry*³ 1st ed. 8.4 & 8.5, 2nd and 3rd eds. 9.4 & 9.5)

At the end of this section you should:

- know how to demonstrate that a reaction is zeroth order and be able determine the rate coefficient;
- know how to use the integrated rate law to demonstrate that a reaction is first order and be able to determine the rate coefficient;
- be able to determine the rate law and the rate coefficient from a set of initial rates and initial concentrations.

(6.iii) First-order reactions (*Chemistry*³ 1st ed. 8.4 & 8.5, 2nd and 3rd eds. 9.4 & 9.5)

At the end of this section you should:

- be able to use the *initial conditions* of a first-order reaction to determine the concentrations of the reaction components after some elapsed time;
- be able to define what is meant by the terms lifetime and half-life of a first-order reaction;
- be able to determine the half-life of a first-order reaction from the rate coefficient or vice-versa.

(6.iv) Collision and transition state theories (*Chemistry*³ 1st ed. 8.4 & 8.5, 2nd and 3rd eds. 9.4 & 9.5)

- understand the distinction between *elementary* and *complex reactions*;
- know the definition of the molecularity of an elementary reaction;
- know that a complex reaction can be represented by a reaction mechanism involving a series of elementary steps;
- know that the rate coefficients of most reactions increase dramatically with temperature in a manner empirically described by the *Arrhenius equation*;
- know that the Arrhenius equation can be understood in terms of transition state theory;
- be able to define the terms reaction coordinate, transition state, activation energy and activation barrier;
- be able to use rate coefficients at different temperatures to determine the activation energy of a reaction;
- know how to use the Arrhenius equation and the rate coefficient at one temperature to determine a rate coefficient at any other temperature.

(6.v) Mechanisms of complex reactions (Chemistry³ 1st ed. 8.4 & 8.5, 2nd and 3rd eds. 9.4 & 9.5)

At the end of this section you should:

- understand what is meant by the mechanism of a reaction;
- know that kinetics measurements can provide information about the mechanism of a reaction;
- be able to define the terms *intermediate* and *catalyst* as they apply to chemical kinetics;
- know that reaction rates are increased by catalysis;
- understand that catalysis can be explained by reaction mechanisms involving lower effective activation barriers due to the presence of reaction intermediates;
- know the distinctions between, and examples of, *homogenous*, *heterogeneous*, and *enzyme* catalysis.

7: CHEMICAL EQUILIBRIUM

(3 lectures; Chemistry³ 1st ed. Chaps. 15 & 16, 2nd and 3rd eds. Chaps. 14 & 15)

(7.i) Equilibrium constants (*Chemistry*³ 1st ed. 1.9, 16.1 & 15.6, 2nd and 3rd eds. 1.9, 15.1 & 14.6)

At the end of this section you should:

- understand that chemical equilibria are dynamic processes;
- know that a state of dynamic equilibrium exists when the rates of forward and reverse processes are equal;
- know how the equilibrium constant of a chemical process relates to the (kinetics) rate coefficients of the forward and reverse processes;
- know that the equilibrium constant of a chemical process of specified direction and stoichiometry is dependent on temperature but otherwise is independent of the reaction conditions;
- know how to find the equilibrium constant for a reaction that can be expressed as the sum of several reactions whose equilibrium constants are known;
- know that the thermodynamic equilibrium constant relates to the equilibrium thermodynamic activities
 of reactants and products as described by the equation

$$K = \frac{a_{\rm L}^{\ l} \, a_{\rm M}^{\ m}}{a_{\rm B}^{\ b} \, a_{\rm C}^{\ c}}$$
 for the equilibrium $b{\rm B} + c{\rm C} \ \rightleftharpoons l{\rm L} + m{\rm M};$

 know the working rules for estimating activities in terms of the concentrations and partial pressures of the reaction components.

(7.ii) Equilibrium calculations (*Chemistry*³ 1st ed. 16.4, 2nd and 3rd eds. 15.4)

- know how to calculate the equilibrium constant from the final (equilibrium) concentrations (or partial pressures) of one component and the initial conditions of the reaction system;
- know how to calculate the concentrations (or partial pressures) of components in a system at equilibrium, given the initial state of the system and the value of the equilibrium constant;

(7.iii) Direction of spontaneous change (Chemistry³ 1st ed. 16.2 & 16.5, 2nd and 3rd eds. 15.2 & 15.5)

At the end of this section you should:

- know the definition of a reaction quotient and understand its distinction from an equilibrium constant;
- know that the direction of spontaneous change of a process can be predicted by comparing the values
 of the reaction quotient and the equilibrium constant;
- understand **Le Chatelier's principle** and be able to use it to predict the direction of spontaneous change of a system that is not at equilibrium.

8: THERMODYNAMICS II

(5 lectures; Chemistry³ 1st ed. Chaps. 15 & 16, 2nd and 3rd eds. Chaps. 14 & 15)

(8.i) Entropy and the second and third laws of thermodynamics (*Chemistry*³ 1st ed. 15.1–15.4, 2nd and 3rd eds. 14.1–14.4)

At the end of this section you should:

- understand qualitatively the concepts of spontaneous change and entropy, including that entropy is a state function;
- be able to qualitatively predict whether entropy increases or decreases for a chemical process, including phase transitions;
- be able to state the **second law of thermodynamics**, and understand qualitatively the manner in which all processes are driven by a net increase of the entropy of the universe;
- be able to state a form of the third law of thermodynamics and understand its meaning;
- know what is meant by an absolute standard molar entropy;
- know how to calculate the entropy change of a process from tabulated absolute standard molar entropies
 of the reaction components.

(8.ii) Gibbs energy (Chemistry³ 1st ed. 15.5 & 15.6, 2nd and 3rd eds. 14.5 & 14.6)

At the end of this section you should:

- be able to calculate the entropy change of the surrounding associated with an process occurring in the system and understand that an exothermic process increases the entropy of the surroundings;
- be able to calculate the entropy change of a phase transition from the associated enthalpy change and critical temperature;
- be able to define Gibbs energy;
- understand that a spontaneous process (*i.e.* one for which $\Delta S_{\text{universe}}$ is positive) corresponds to a negative Gibbs energy change for a system;
- know that the Gibbs energy change for a system at constant temperature and pressure is given by

$$\Delta G = \Delta H - T \Delta S$$
:

 understand how this equation dictates changes in the spontaneity of physical and chemical processes with temperature;

- know what is meant by a standard Gibbs energy change and know how to use tabulated data to determine
 the standard Gibbs energy change for a process;
- be able to calculate the Gibbs energy change for a system under non-standard conditions.

(8.iii) Gibbs energy and equilibrium (*Chemistry*³ 1st ed. 16.1, 16.2 & 16.5, 2nd and 3rd eds. 15.1, 15.2 & 15.5)

At the end of this section you should:

 know that the thermodynamic equilibrium constant K of a reaction is related to the standard Gibbs energy change by

$$\Delta G^{\circ} = -RT \ln K$$
 or $K = \exp(-\Delta G^{\circ}/RT)$

- understand that the thermodynamic definition of equilibrium implies a temperature dependent equilibrium constant consistent with *Le Châtelier's principle*;
- be able to determine the enthalpy and entropy changes of a process from the equilibrium constants at two or more temperatures according to the *Van't Hoff equation*.

9: AQUEOUS CHEMISTRY

(3 lectures; Chemistry³ 1st ed. Chaps. 1, 6 & 25, 2nd and 3rd eds. Chaps. 1, 7 & 25)

(9.i) Physical properties of water (*Chemistry*³ 1st ed. 1.8, 4.2, 4.3, 18.3 & 25.3, 2nd and 3rd eds. 1.8, 5.2, 5.3, 17.3 & 25.3)

At the end of this section you should:

- understand the *molecular structure* of water in terms of its *Lewis structure* and *VSEPR* principles;
- be able to rationalise the trends of bond-length, bond-strength and bond-angle for the hydrides (CH₄, NH₃, H₂O and HF) of the second-row elements in terms of valency and electronegativity;
- know and understand trends of *polarity* of the hydrides (CH₄, NH₃, H₂O and HF) of the second-row elements in terms of geometric structure and electronegativities;
- understand how intermolecular forces arise from interactions between charged, polar and polarisable molecules;
- be able to describe the phenomenon of van der Waals interactions in terms of dipole-dipole, dipole-induced-dipole and dispersion forces;
- be able to describe the phenomenon of hydrogen bonding and its significance in determining the high boiling point and Δ_{vap}H of water, as well as the open structure and low density of ice.

(9.ii) Water as a solvent (*Chemistry*³ 1st ed. 1.8 & 18.4, 2nd and 3rd eds. 1.8 & 17.4)

- understand the way in which enthalpy changes associated with the breaking and making of intermolecular bonds constitute the driving force for dissolution processes;
- be able to provide a thermodynamic rationale for the effectiveness of water as a solvent for polar and ionic compounds;

• know the definition of the **enthalpy of hydration** of an ion and understand how and why it is affected by the size and charge of the ion.

(9.iii) Aqueous ionic solutions (*Chemistry*³ 1st ed. 17.2 & 26.3, 2nd and 3rd eds. 16.2 & 26.3)

At the end of this section you should:

- know the definition of *ionic mobility* in aqueous solutions and understand its dependence on the charge density of a solute ion;
- understand that H⁺ and OH⁻ ions have anomalously large mobilities that can be explained by hydrogen-bonding interactions;
- be able to rationalise the **solubility** of ionic compounds as a balance between the **enthalpy of hydration** and the **lattice energy** of the undissolved solute;
- know and be able to use simple rules for predicting the effect of cation and anion size on the solubility of ionic compounds in water;
- know the definition of the term electrolyte and be able to give examples of hydrolysis reactions;
- know what is meant by percentage hydrolysis and how it can be used to classify strong and weak electrolytes.

10: ACID-BASE EQUILIBRIUM (4 lectures; *Chemistry*³ 1st ed. Chap. 6, 2nd and 3rd eds. Chap. 7)

(10.i) Acids and bases in the Brønsted-Lowry scheme (*Chemistry*³ 1st ed. 6.1 & 6.2, 2nd and 3rd eds. 7.1 & 7.2) *At the end of this section you should:*

- know the definition of acid and base in the Brønsted-Lowry scheme;
- know the definitions of the terms conjugate acid and conjugate base;
- understand the definitions of the *ionisation* (or *dissociation*) *constants* K_a (for an acid) and K_b (for a base);
- be able to classify acids and bases as strong or weak according to the values of their ionisation constants
 (and know the descriptors strong or weak are not the same as concentrated or dilute);
- know that water is amphiprotic and amphoteric with an auto-ionisation (self-dissociation) constant Kw;
- be able to define the *logarithmic parameters* pH, pOH, pK_a, pK_b and pK_w; understand the meanings of these parameters and the relationships between them;
- be able to calculate the pH (and pOH) of strong-acid and strong-base solutions of **stated concentration**;
- know how to derive and use the Henderson-Hasselbalch equation;
- be able to calculate the pH (and pOH) of weak-acid and weak-base solutions from K_a and K_b values, along with the stated concentration of the solution;
- understand the concept of polyprotic acids.

(10.ii) Salts and buffer solutions (Chemistry³ 1st ed. 6.3, 2nd and 3rd eds. 7.3)

At the end of this section you should:

- know the definition of a salt and its classification in terms of the strength or weakness of its precursor acid and base;
- be able to calculate the pH and percentage hydrolysis of a salt solution;
- know what is meant by the terms buffer, common-ion effect and buffer action;
- be able to calculate the pH of a buffer solution with a given composition;
- understand the principles behind preparation of a buffer solution that will be effective at a given pH.

(10.iii) Strong-acid/strong-base titrations (*Chemistry*³ 1st ed. 6.4, 2nd and 3rd eds. 7.4)

At the end of this section you should:

- know the experimental set-up for performing an acid-base pH titration while monitoring the pH with a glass electrode;
- know the definitions of equivalence point and equivalence volume of an acid-base titration;
- be able to recognise the curves for pH titrations involving a strong acid and a strong base;
- be able to determine the unknown concentration of an acid or base from the equivalence point of a titration with a strong base or acid of known concentration;
- be able to calculate the pH at various points of a titration involving a strong acid and a strong base.

(10.iv) Titrations involving weak acids or bases (Chemistry³ 1st ed. 6.4, 2nd and 3rd eds. 7.4)

- be able to recognise the curves for pH titrations involving a strong acid and a weak base or vice versa;
- know what is meant by the buffer region of a titration curve;
- know how to estimate the pK_a of a weak acid (or pK_b of a weak base) from the **half-equivalence point** of its titration with a strong base (or strong acid);
- understand the principles of selection of an acid-base indicator suitable for a colorimetric titration;
- know the definition of the *endpoint* of a colorimetric titration and its distinction from the equivalence point.

GENERAL INFORMATION 2022

Policy on 'Dishonest Practice'

The University has strict guidelines regarding 'dishonest practice' and 'breach of instructions' in relation to the completion and submission of examinable material. In cases where dishonest practice is involved in tests or other work submitted for credit a department may choose to not mark such work ('Academic Integrity and Breach of Instruction Regulations').

The School of Physical and Chemical Sciences upholds this policy. It considers plagiarism, collusion, copying, and ghost writing to be unacceptable and dishonest practices:

- **Plagiarism** is the presentation of any material (text, data or figures, on any medium including computer files) from any other source without clear and adequate acknowledgement of the source.
- **Collusion** is the presentation of work performed in whole, or in part, in conjunction with another person or persons, but submitted as if it has been completed by the named author alone. This interpretation is not intended to discourage students from having discussions about how to approach an assigned task and incorporating general ideas that come from those discussions into their own individual submissions, but acknowledgement is necessary.
- Copying is the use of material (in any medium, including computer files) produced by another person or persons with or without their knowledge and approval. This includes copying of the lab reports (raw data may be shared within the group if permitted or required by the experiment) data analysis and interpretation of obtained results MUST be performed individually.
- **Ghost writing** is the use of other person(s) (with, or without payment) to prepare all or part of an item of work submitted for assessment.

Additional Information

Special consideration of assessment: If you feel that illness, injury, bereavement or any other critical extenuating circumstance beyond your control has prevented you from completing an item of assessment or affected your performance in that assessment, you may apply for special consideration. Special consideration is not available for items worth less than 10% of the course, including the following:

- Individual laboratory assessment items (see Attendance at Laboratory Classes)
- BestChoice problems

Applications for special consideration should be made **within five days** of the due date for the work or examination. In the case of illness or injury, medical consultation should normally have taken place shortly before, or within 24 hours after, the due date for the required work or the date of the test or examination. For details on special consideration, or to make an application, refer to the Examinations Office website http://www.canterbury.ac.nz/exams/. **You have the right to appeal any decision.**

Extensions of deadlines: Where an extension may be granted for an assessment item, this will be decided by application to the course co-ordinator.

Late withdrawal from the course: If you are prevented by extenuating circumstances from completing the course after the final date for withdrawing from the course, you may apply for special consideration for late discontinuation. For details on special consideration, or to make an application, refer to the Examinations Office website http://www.canterbury.ac.nz/exams/. Applications must be submitted within five days of the end of the main examination period for the semester.

Missing of tests: In rare cases a student will not be able to sit a test. In such cases, the student should consult with the course co-ordinator to arrange alternative procedures. This must be done well in advance of the set date for the test.

Past tests and exams: these can be found on our website using the link below: www.chem.canterbury.ac.nz/for/undergraduate.shtml

Marks and Grades: The following numbers should be considered as a guide to the expected grades under normal circumstances. The School reserves the right to adjust mark/grade conversions, if necessary.

Please note that for all invigilated assessments (tests and exams) worth 33% and above, failure to obtain a mark of at least 40% will result in a final grade no higher than an R at 100 and 200 level, and a C- at 300 level.

Grade: A+ Α B+ В B-C+ C C-D Ε Minimum mark %: 90 85 80 **75** 70 65 60 55 50 40 0

Reconsideration of Grades: Students should, in the first instance, speak to the course co-ordinator about their marks. If they cannot reach an agreeable solution, or have questions about their grade in a course, students should then speak to the Director of Undergraduate Studies, <u>Assoc Prof Greg Russell</u> (phone 3694228). Students can appeal any decision made on their final grade. You can apply at the Registry for reconsideration of the final grade within four weeks of the date of publication of final results. Be aware that there are time limits for each step of the appeals process.

Students with Disabilities: Students with disabilities should speak with someone at <u>Equity and Disability Service</u>, phone: 369 3334 (or ext. 93334), email: <u>eds@canterbury.ac.nz</u>).

Academic Advice: Assoc Prof Greg Russell is the coordinator of undergraduate chemistry courses. His interest is in the academic performance and well-being of all such students. Anyone experiencing problems with their chemistry courses or requiring guidance about their B.Sc. in Chemistry should get in contact with Greg.

Staff-Class Rep Liaison: Assoc Prof Greg Russell is in charge of liaison with students in chemistry courses. Your class will appoint a student representative to the liaison committee at the start of the semester. Please feel free to talk to the Academic Liaison or the student rep about any problems or concerns that you might have.

Greg Russell (greg.russell@canterbury.ac.nz, tel. 369 5129) Director of Undergraduate Studies School of Physical and Chemical Sciences 2022