

General Course Information

CHEM 111–22S1 Chemical Principles and Processes

0.125 EFTS 15 Points
First 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 BRDG022, or
- 6) 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

Owen Curnow, owen.curnow@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)

- Prof Paul Kruger (topics 1 to 3): paul.kruger@canterbury.ac.nz
- A/Prof Laura Revell (topic 4): laura.revell@canterbury.ac.nz
- A/Prof Greg Russell (topic 5): greg.russell@canterbury.ac.nz
- A/Prof Deborah Crittenden (topics 6 & 7): deborah.crittenden@canterbury.ac.nz
- A/Prof Greg Russell (topic 8): greg.russell@canterbury.ac.nz
- A/Prof Owen Curnow (topics 9 & 10): owen.curnow@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.

On-line laboratory assignments/experiments: The on-line laboratory assignments are an essential part of CHEM111, which are run when we are unable to run the labs in-person. All on-line lab assignments are compulsory and assessable; you must satisfactorily complete all on-line labs to pass the course. For each on-line assignment you will be supplied with a word document for the lab experiment, a PowerPoint file and videos. You will be required to upload your assignment in pdf format to a portal on the CHEM111 LEARN laboratory webpage. Each assignment will have an advertised submission deadline. 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 also forms part of your overall lab grade), even though the labs will be on-line. The on-line laboratory-associated assessment is 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, Thursday 5 May (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 exam** 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: will be run online with assignments

Laboratory allocations: You must allocate yourself to a lab stream through [MyTimetable](#) 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 [laboratory coordinators](#) to be assigned to a lab stream.

These lab streams will be used for marking your on-line laboratory assignments so it's important you allocate yourself.

All CHEM111 on-line laboratory assignments are compulsory and assessed; 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 on-line assignment you will be supplied with a word document for the week's experiment, a PowerPoint file and videos. The assignment should be completed and submitted through an on-line portal by an advertised deadline (details will be provided through the CHEM111 LEARN laboratory page).

Laboratory manuals: will be available to download from the on-line laboratory page of the CHEM111 LEARN website <https://learn.canterbury.ac.nz/course/view.php?id=12534§ion=4>

Completion of on-line safety quiz and laboratory assignments

You are expected to complete every CHEM111 on-line assignment and to complete the CHEM111 on-line safety quiz.

If you cannot complete your assignment, you should contact the [laboratory coordinators](#) **in advance** to check that your reason is deemed valid. For an exemption, you will need to provide documented evidence **via e-mail**, 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 [laboratory coordinators](#).

Students who are unable to complete an assignment 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.

Important note: a medical certificate should be obtained **in the period around the missed lab assignment**. 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 [laboratory coordinators](#) 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 assignment, 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 [course coordinator](#) 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 on-line laboratories is judged unsatisfactory you will not be given a pass in the laboratory course and will FAIL CHEM111.

Laboratory Safety (information for completing safety quiz)

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. **(No purchase needed for chemistry on-line lab assignments)**

Laboratory coats must be worn at all times in the laboratory and should not be worn outside of the laboratory environment. **(No purchase needed for chemistry on-line lab assignments)**

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 air buds 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 5½ 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.

1. Atoms and the Periodic Table (2 lectures); *Chemistry*³ 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); *Chemistry*³ 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.

5. Introduction to Thermodynamics (5 lectures); *Chemistry*³ 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); *Chemistry*³ 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); *Chemistry*³ 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); *Chemistry*³ 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); *Chemistry*³ 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, *Chemistry*³ by Burrows *et al.*

1: ATOMS AND THE PERIODIC TABLE

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

(1.i) Atoms and the mole (*Chemistry*³ 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 ${}_{92}^{235}\text{U}$;
- 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 (*Chemistry*³ 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 ns , np and nd 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; *Chemistry*³ 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)

At the end of this section you should:

- 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 (*Chemistry*³ 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 (*Chemistry*³ 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 (*Chemistry*³ 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; *Chemistry*³ 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 (*Chemistry*³ 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 stratosphere**: its production, photochemistry and removal;

5: INTRODUCTION TO THERMODYNAMICS

(5 lectures; *Chemistry*³ 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)

At the end of this section you should:

- 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, C_p** , and **heat capacity at constant volume, C_v** , and understand how these are related to enthalpy and internal energy, respectively.

(5.iii) Calorimetry (*Chemistry*³ 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 (*Chemistry*³ 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; *Chemistry*³ 1st ed. Chap. 8, 2nd and 3rd eds. Chap. 9)

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

At the end of this section you should:

- 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)

At the end of this section you should:

- 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 (*Chemistry*³ 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; *Chemistry*³ 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

$$K = \frac{a_L^l a_M^m}{a_B^b a_C^c} \quad \text{for the equilibrium } bB + cC \rightleftharpoons lL + mM;$$

- 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)

At the end of this section you should:

- 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 (*Chemistry*³ 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; *Chemistry*³ 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 (*Chemistry*³ 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

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

- 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; *Chemistry*³ 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 $\Delta_{\text{vap}}H$ 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)

At the end of this section you should:

- 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** K_w ;
- 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 (*Chemistry*³ 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 (*Chemistry*³ 1st ed. 6.4, 2nd and 3rd eds. 7.4)

At the end of this section you should:

- 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 - 2021

Policy on 'Dishonest or Improper Practice'

The University has strict guidelines regarding 'dishonest or improper practice' in relation to the completion and submission of examinable material. Dishonest practice or breach of instructions is involved in tests or other work submitted for credit may lead to any or all the following penalties (p 57 of the 2019 UC Calendar under regulation 6 of the Academic Integrity and Breach of Instruction Regulations):

- i. expulsion from the University;
- ii. suspension from enrolment in the University or in particular courses for such period as deemed fit;
- iii. denial of credit or partial credit;
- iv. assignment of an X grade in any course or courses;
- v. a fine;
- vi. a reprimand;
- vii. unpaid community work.

Plagiarism, collusion, copying, and ghost writing are considered 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.
- **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 coordinator](#).

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: On rare occasions, you may not be able to sit a test due to other important commitments. In such cases, you must contact the [course coordinator](#) to arrange alternative procedures. **This must be done well in advance of the set date for the test.**

Past tests and exams:

Past tests can be found at: <http://learn.canterbury.ac.nz/course/view.php?id=4632>

Past exams can be found at: <http://library.canterbury.ac.nz/exams/>

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+	A	A-	B+	B	B-	C+	C	C-	D	E
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, [Assoc Prof Greg Russell](#) (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 [Equity and Disability Service](#), phone: 369 3334 (or ext. 93334), email: eds@canterbury.ac.nz.

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