

## General Course Information

### CHEM 211 Molecules

0.125 EFTS      15 Points  
First Semester    2024

#### Description

The topics covered in this course are: atomic structure and bonding in covalent molecules; p-block chemistry, solids and the modern periodic table; and principles of chemical characterisation.

This course is required to major in chemistry and is preferably taken in conjunction with other 200-level chemistry courses.

#### Timetable

**Lectures and tutorials:** three hours per week. The course comprises 27 lectures and 7 tutorials. Each lecturer will advise the schedule of lectures and tutorials.

Students should note that in the Science Faculty, the average student should plan to spend approximately 4.5 hours of additional study for each hour of lecture at the 200-level.

#### Course Coordinator

Assoc. Prof. Vladimir Golovko

Room: Julius von Haast 632, ext 95942, email: [vladimir.golovko@canterbury.ac.nz](mailto:vladimir.golovko@canterbury.ac.nz)

*Email me if you have any queries about the course.*

#### Assessment

In order, with course component indicated:

Tutorials/assignment assessment (Crittenden)	12%
Test (Crittenden)	21%
Tutorials/assignment assessment (Golovko)	6%
Tutorials/assignment assessment (Curnow)	6%
Final examination (Golovko, Curnow)	55%

Lecturers will notify the class about their requirements for the tutorial/assignment assessments, including due dates.

#### Examination and Formal Tests

**Test:** 2 hours in person, details will be available on the CIS and 'My Timetable'.

**Exam:** 2 hours in person, details to be advised.

#### Textbooks

The general textbook for the course is:

A. Burrows, J. Holman, A. Parsons, G. Pilling and G. Price, *Chemistry*<sup>3</sup>, OUP, any edition. This textbook is available in the library, where copies are in the high demand section.

For Professor Crittenden's part of the course, the following is an easy-to-read supplement to the general textbook: M. J. Winter, '*Chemical Bonding*', M.J. Winter, Oxford Chemistry Primers, Oxford University Press, 1994

The following Primer is a relatively inexpensive text that will be useful in Dr Golovko's lectures: N. C. Norman, *Periodicity and the s- and p-Block Elements*. OUP, Primer No. 51.

## Prerequisites

CHEM 111

## Goal of the Course

To build on principles from first year chemistry in developing an understanding of the fundamental principles of chemical bonding, and chemical periodicity and materials, and chemical (elemental and molecular) characterisation. This course will provide a solid foundation for further study in all aspects of chemistry.

## Summary of the Course Content

### **Block 1: ATOMS AND COVALENT MOLECULES** (9 lectures, 2 tutorials)

Textbook coverage: *Chemistry*<sup>3</sup> 2.1-2.6; 3.1-3.2; 3.4-3.12, 4.6 and 4.1-4.5 (1st edition); 3.1 -3.6; 4.1-4.2; 4.5-4.12, 5.6 and 5.1-5.5 (2<sup>nd</sup> to 4<sup>th</sup> editions).

Further reading: M. J. Winter, 'Chemical Bonding', M.J. Winter, Oxford Chemistry Primers, Oxford University Press, 1994: Chapters 1-6

We 'fill in' and extend the concepts introduced in CHEM111. We start by studying the shapes, energies and electron densities of atomic orbitals in H-like atoms. This is then extended to many electron atoms. The bonding in diatomic and polyatomic molecules and molecular ions will be examined using two theoretical frameworks: molecular orbital theory and valence bond theory.

**Assoc. Prof. Deborah Crittenden, Room Julius von Haast 520, ext 95087,**  
[deborah.crittenden@canterbury.ac.nz](mailto:deborah.crittenden@canterbury.ac.nz)

### **Block 2: PRINCIPLES OF CHEMICAL CHARACTERISATION** (9 lectures, 2 tutorials)

Textbook coverage: *Chemistry*<sup>3</sup> chapters 11-13 (1<sup>st</sup> edition); chapters 10-12 (2<sup>nd</sup> to 4<sup>th</sup> editions).

**Spectroscopic principles:** electromagnetic radiation; spectroscopic equipment; energy levels and quantisation; single-electron transitions; emission; absorption; transition intensities and selection rules.

**Atomic spectroscopy:** Atomic emission spectroscopy; inductively coupled plasma-optical emission spectroscopy.

**Molecular spectroscopy:** molecular dynamics, rotational microwave spectroscopy, vibrational infrared and Raman spectroscopy; vibrations of anharmonic oscillators; vibrations of polyatomic molecules; molecular electronic transitions;  $\pi \rightarrow \pi^*$  transitions of organic molecules; vibrational progressions.

**Nuclear magnetic resonance (NMR) spectroscopy:** nuclear spin; Zeeman effect; NMR transitions of a proton; NMR spectrometers; key information from NMR -- chemical shifts, spin-spin multiplets, CH, OH and NH signals.

**Mass spectrometry (MS):** mass spectrometry processes – electron impact, chemical ionisation, fast-atom bombardment, electrospray ionisation, time-of-flight and magnetic sector mass analysers; mass spectra; isotopic patterns; high-resolution MS.

**Assoc. Prof. Owen Curnow, Julius von Haast 634, ext 94239**  
[owen.curnow@canterbury.ac.nz](mailto:owen.curnow@canterbury.ac.nz)

### **Block 3: PERIODICITY AND TRENDS** (9 lectures, 3 tutorials)

Textbook coverage: *Chemistry*<sup>3</sup> 2.6, 2.7, 3.3, 5 and selected parts of chapters 26 & 27 (1<sup>st</sup> Edition); 3.6, 3.7, 4.3, 6 and selected parts of 26 & 27 (2<sup>nd</sup> to 4<sup>th</sup> Editions).

Further reading: N.C. Norman, "Periodicity and the s- and p-Block Elements", Oxford Chemistry Primers, Oxford University Press, 2007: Chapters 5, 26 & 27

**The modern periodic table:** isotopes; many electron atoms; electron spin, the aufbau and Pauli principles; anomalous electronic configurations; structure of the periodic table; shielding and penetration; effective nuclear charge and Slater's rules

**Atomic properties, periodicity and trends:** ionization energy; electron affinity; electronegativity

**Oxidation state and valence:** p-block elements; inert pair effect; bonding; orbital energies; element size & coordination number

**Bond energies:** homo- vs. hetero- nuclear s- and p- block elements

**Bonding:** structure in the p-block elements: groups 14-17; bond types, van Arkel triangle, predicting bond types.

**Solid state and introduction to materials chemistry** (bonding in solids): covalent network structures; structures based on the packing of spheres; the ionic model; calculating lattice energy; metallic bonding, band theory; insulators; semiconductors; LEDs.

**Assoc. Prof. Vladimir Golovko, Julius von Haast 632, ext 95942,**  
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## Learning Outcomes

By the end of this course, students should have:

- a) a broad understanding of atomic theory and bonding theories that can be applied to diatomic and larger molecules (*1<sup>st</sup> tutorial assessment and test*).  
Specifically, they should be able to:
- Outline our modern understanding of atomic structure
  - Describe atomic structure for one-electron and many-electron atoms in terms of orbitals, quantum numbers and energy levels
  - Derive electron configurations for atoms
  - Qualitatively account for atomic orbital energy ordering
  - Develop, with explanation, bonding schemes for homonuclear and heteronuclear diatomic molecules using Molecular Orbital Theory, and understand how the theory is applied to polyatomic molecules
  - Develop, with explanation, bonding schemes for homonuclear and heteronuclear diatomic molecules and polyatomic molecules using a localised bonding approach
  - Describe excited states of O<sub>2</sub> and how they can be applied in medical therapeutics
- b) a broad understanding of some of the methods employed in the characterisation of chemical substances. (*2<sup>nd</sup> tutorial assessment and final exam*)  
Specifically, they should be able to:
- Understand the physical principles that underpin spectroscopic techniques.
  - Have a general understanding of the spectroscopic techniques of electronic absorption and emission, microwave infrared and Raman; and nuclear magnetic resonance spectroscopy, and how they are used in the characterisation of chemical substances.
  - Have a general understanding of the techniques of mass spectrometry.
- c) an in-depth understanding of the basis of the Periodic Table, the periodic properties of the elements, p-block chemistry and the structures and properties of solids (*3<sup>rd</sup> tutorial assessment and final exam*).  
Specifically, they should be able to:
- Develop appreciation of the evolution of the Periodic Table and understanding of its structure in the light of atomic structure of the elements
  - Rationalize concepts of effective nuclear charge, as well as shielding and penetration of electrons occupying different orbitals using foundations of atomic structure (radial distribution functions *etc.*)
  - Apply numerical skills to calculate effective nuclear charge according to Slater's rules and screening percentage
  - Give definitions of the key atomic properties (ionization energy, electron affinity and electronegativity) and be able to explain periodicity and specific trends for each property
  - Discuss in detail trends in the oxidation states, homonuclear and heteronuclear bond energies
  - Explain in detail differences between the key types of chemical bonding (covalent, ionic and metallic) and predict type of bonding using van Arkel triangles
  - Rationalize properties of technologically important solid state materials (insulators, conductors and semiconductors) in the light of band theory

## GENERAL INFORMATION | TE KIMI MŌHIOHIO 2024

### ***Policy on 'Dishonest Practice' / Ngā Takahitanga me ngā Tinihanga***

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 – see the online guidelines in relation to ['Academic Integrity'](#).

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

- **Plagiarism | Tārua Whānako** 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. Note that the use of **AI generative tools such as ChatGPT** for assessment work is *strictly forbidden*, except where the lecturer concerned has specifically granted approval.

- **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) (whether with or without payment) to prepare all or part of an item of work submitted for assessment.

### **Special consideration of assessment | Ngā Pairuri Motuhake**

'[Special Consideration](#)' for an item of assessment is for students who have covered the work involved but have been prevented from demonstrating their knowledge or skills at the time of the assessment due to unforeseen circumstances, whether illness, injury, bereavement, car crash or any other extenuating circumstance *beyond one's control*. Special Consideration for a test/exam may be because a student has not sat it or has done so with impaired performance. Applications can be submitted via the above link and must be made **no later than five working days after the assessment due date**. Note that special consideration is **not available for items worth less than 10% of the overall course mark**. In the case of illness or injury, medical consultation should normally have taken place either shortly before or within 24 hours after the due date for the required work or test/examination.

Note that you may be required to sit a special exam or your grade may not be changed if there is insufficient evidence of your performance from other invigilated assessment items in the course. **You have the right to appeal any decision.**

It is important to understand that Special Consideration is only available *where course work has been covered*, and the inability to demonstrate this fully is both *no longer possible* AND is due to *unexpected circumstances beyond one's control*. Thus Special Consideration is **NOT available for**:

- essays, assignments or quizzes where an extension of time is available to complete the assessment item (see below for the process to involved);
- missed lectures during the semester;
- experiencing examination anxiety;
- having several examinations or assessments close together;
- known impairment, such as chronic illness (medical or psychological), injury or disability unless medical evidence confirms that the circumstances were exacerbated, despite appropriate management, at the time of assessment;
- mistaking the date or time of an examination (this is a circumstance one can control!);
- failing to turn up to an examination or test because of sleeping in (a circumstance as above!);
- where applications are repeatedly made for the same or similar reason, then the application may be declined on the grounds that the reason is not unexpected;
- where the application is made at the time of the assessment but the supporting documentation is received significantly after this date or after the date results are released; or
- the application is made following the release of results (unless under exceptional circumstances).

### **Extensions of deadlines | Tononga Wā Āpiti**

Where an extension may be granted for an assessment item, this will be decided by application to the course co-ordinator and/or the lecturer concerned.

### **Late withdrawal from a 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 | Te Matangaro i ngā Whakamātautau**

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**

Past tests can be found on our [Chemistry Undergraduate](#) website. Past exams can be found on the [Library website](#).

### **Submission of reports and assignments**

**Reports (including lab reports) and assignments should be handed in on time.** Extensions will be granted only in exceptional circumstances (such as illness or bereavement). If an extension is required, as early as possible you should request it from the lecturer concerned.

*Note:* If you do not submit an assignment for assessment, you will be allotted zero marks, which will affect your final result. You should ensure that you pick up marked assignments and keep them until the end of the course as evidence that the work was completed and marked in the case that either is disputed. To guard against accidental loss, it would be prudent to keep photocopies or electronic copies of anything submitted.

### **Late Work**

Acceptance of late work for assessment will be at the discretion of the course coordinator and/or the lecturer concerned. If your assessment is likely to be late, please contact the relevant of these people **before the assessment is due**. Never assume that an extension will be automatically granted – some courses have the policy of no late work being accepted. A commonly exercised policy is to deduct 10% of the total marks for each day that the work is late, where weekends and public holidays also count as such days.

### **Marks and Grades | Taumata Ako**

The following numbers should be considered as a guide to the expected grades under normal circumstances.

**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; in general this requirement will not be applied at 300 level, but if it is then the course coordinator will inform the class and it will result in a final grade no higher than a C–.**

<b>Grade:</b>	<b>A+</b>	<b>A</b>	<b>A–</b>	<b>B+</b>	<b>B</b>	<b>B–</b>	<b>C+</b>	<b>C</b>	<b>C–</b>	<b>D</b>	<b>E</b>
<b>Minimum mark %:</b>	<b>90</b>	<b>85</b>	<b>80</b>	<b>75</b>	<b>70</b>	<b>65</b>	<b>60</b>	<b>55</b>	<b>50</b>	<b>40</b>	<b>0</b>

The School reserves the right to adjust this mark/grade conversion, up or down, to achieve consistency of assessments standards.

### **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](#). 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.

### **Student Accessibility Services | Te Whaikaha**

Students can speak with someone at [Student Accessibility Service](#), phone: 369 3334 (or ext. 93334), email: [sas@canterbury.ac.nz](mailto:sas@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](mailto:greg.russell@canterbury.ac.nz), tel. 369 5129)

Director of Undergraduate Studies  
School of Physical and Chemical Sciences  
2024