School of Physical and Chemical Sciences

UNIVERSITY OF CANTERBURY
Te Whare Wānanga o Waitaha
CHRISTCHURCH NEW ZEALAND

General Course Information

CHEM 211
Molecules

0.125 EFTS 15 Points
First Semester 2022

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 9 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: Beatrice Tinsley 427, ext 95942, email: 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: 1 hour, details will be available on the CIS and 'My Timetable'.
Exam: 2 hours, details to be advised.

Textbooks
The general textbook for the course is:
A. Burrows, J. Holman, A. Parsons, G. Pilling and G. Price, *Chemistry*^{3}, 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, 3 tutorials)**

Textbook coverage: *Chemistry*^{3} 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 (2nd and 3rd 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 Beatrice Tinsley 326, ext 95087,
deborah.crittenden@canterbury.ac.nz

Block 2: PERIODICITY AND TRENDS **(9 lectures, 3 tutorials)**

Textbook coverage: *Chemistry*^{3} 2.6, 2.7, 3.3, 5 and selected parts of chapters 26 & 27 (1st Edition); 3.6, 3.7, 4.3, 6 and selected parts of 26 & 27 (2nd and 3rd 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, Room Beatrice Tinsley 427, ext 95942,
vladimir.golovko@canterbury.ac.nz

Block 3: PRINCIPLES OF CHEMICAL CHARACTERISATION **(9 lectures, 3 tutorials)**

Textbook coverage: *Chemistry*^{3} chapters 11-13 (1st edition); chapters 10-12 (2nd and 3rd 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 form 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 patters; high-resolution MS.

Assoc. Prof. Owen Curnow, Room Beatrice Tinsley 420, ext 94239
owen.curnow@canterbury.ac.nz

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 (*1st 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_2 and how they can be applied in medical therapeutics

b) 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 (*2nd 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

c) a broad understanding of some of the methods employed in the characterisation of chemical substances. (*3rd 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.

GENERAL INFORMATION 2022

Chemistry Department 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 Department of Chemistry 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. 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

***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 will be at the discretion of the course coordinator. Please contact the coordinator if your assessment is likely to be late.

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