

CHEM 363– Physical Chemistry

General Information - 2007

SUMMARY OF COURSE CONTENT

The topics treated in this course are:

- physical chemistry applied to technical chemistry;
- molecular electronic spectroscopy;
- introduction to quantum mechanics and the approximate methods used in quantum chemistry;
- molecular symmetry and group theory;
- polymer physical chemistry;
- use of electrochemistry for the study of redox properties of species in solution.

THIS COURSE IN CONTEXT

This course runs over both semesters. It counts 28 points towards a Bachelor of Science degree. Normally it is taken in conjunction with other 300-level chemistry lecture courses as well as an appropriate chemistry laboratory course (see below). CHEM 363 is part of the Honours programme in chemistry. It is highly recommended for students intending to proceed to 400-level courses in Chemistry, especially CHEM 463, CHEM 466 and CHEM 467.

Prerequisites:

- 1) CHEM 263 or CHEM 223*
- 2) CHEM 233 and either CHEM 273 or CHEM 243*
- 3) CHEM 282
- 4) 36 points from courses in Mathematics and Statistics or ENGR 102.

* Entry with these prerequisites only with the permission of the Head of Department

For students who are in the Honours Programme in chemistry, CHEM 382 is a **co-requisite** course for CHEM 363 (see below).

Course Coordinator: Dr Robert Maclagan (Room 636)

General enquiries about 300-level courses should be directed either to the 300-level course coordinator (Prof Murray Munro, Room 758), or to the Head of Department (Prof Bryce Williamson, Room 530).

LECTURES AND LECTURERS

Lectures will be held on Mondays and Wednesdays at 9 am in Room 431 of the Chemistry Department.

The lectures for this course will be given by:

Professor Michael Buback	Phone 364 2987 ext 4973,	Room 730
	email: michael.buback@canterbury.ac.nz	
Assoc Prof Alison Downard	Phone 364 2501,	Room 660
	email: alison.downard@canterbury.ac.nz	
Professor Leon Phillips	Phone 364 2425,	Room 632
	email: leon.phillips@canterbury.ac.nz	
Assoc Professor Robert Maclagan	Phone 364 2456,	Room 636
	email: robert.maclagan@canterbury.ac.nz	
Assoc Prof Greg Russell	Phone 364 2458,	Room 634
	email: greg.russell@canterbury.ac.nz	
Prof Bryce Williamson	Phone 364 2439,	Room 530
	email: bryce.williamson@canterbury.ac.nz	

The order of lectures will be: Buback (8), Phillips (8), Maclagan (7), Williamson (8), Russell (8), Downard (8).

TUTORIALS

Tutorials for this course will be held at least every second week, as arranged by lecturers at the time. They will be held on Wednesdays at 12 pm in Room 431 of the Chemistry Department.

Tutorials will involve revision and expansion of lecture material; active student participation is expected.

ASSESSMENT

Final overall course marks will be determined as follows:

- 10% from assignment-based assessment, details to be advised
- 15% from a test held mid-way through the year
- 15% from a test held three-quarters of the way through the year
- 60% from the final examination

MARKS AND GRADES

The following numbers should be considered to be a guide to the expected grades under normal circumstances. The Department reserves the right to adjust mark/grade conversions, if necessary. This will occur only where statistical analysis of marks indicates that the numerical distribution, and subsequently arising grades, is anomalous. Any such adjustments will **not** be made to the detriment of students' grades.

Grade:	A+	A	A-	B+	B	B-	C+	C	D	E
Minimum mark %:	85	80	75	70	65	60	55	50	40	0

TERM TESTS

Two tests will be held during the year.

Test details:

First test: 50 mins duration, worth 15% of the overall course mark, to be held on Wednesday 23 May in Room 431 of the Chemistry Department (time to be announced). It will cover material from the first 16 lectures (given by Buback and Phillips).

Second test: 50 mins duration, worth 15% of the overall course mark, to be held on Wednesday 22 August in Room 431 of the Chemistry Department (time to be announced). It will cover material from lectures 17 through 31 (given by Maclagan and Williamson).

Note that performance in these tests will be the main criterion for assessing aegrotat applications in the event of illness or incapacity during the final examinations.

END-OF-YEAR EXAMINATION

The final 3-hour examination will cover the whole year's work. .

Exam details: Not available at the time of preparation. To be published in term 1.

LABORATORIES

This course has no component of laboratory work. However, for students who are undertaking an Honours degree in chemistry, the laboratory course CHEM 382 (“Instrumental Methods”) is a **co-requisite** course for CHEM 363.

Because laboratory work is extremely important in chemistry, it is **highly recommended** that other students (i.e. non-Honours CHEM 363 students) also take an appropriate laboratory course in conjunction with this course. The appropriate courses to take are CHEM 282 (“Measurement and Analysis”) or, if that (or equivalent work) has already been completed, CHEM 382 (“Instrumental Methods”).

TEXTBOOKS

The general textbook for the course is:

- P.W. Atkins, *Physical Chemistry*, 6th or 7th ed.

A recommended textbook is:

- P.W. Atkins and R.S. Friedman, *Molecular Quantum Mechanics*, 3rd ed.

The above textbooks are available in the library, where copies will be on reserve. Students are advised to consult their lecturers before purchasing the recommended textbook.

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 (2007 Calendar, p 81 and pp 351-2 of 2007 Enrolment Handbook under the headings ‘Cheating’ and ‘Discipline’).

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.
- **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

Aegrotat applications: If you feel that illness, injury, bereavement or other critical circumstances has prevented you from completing an item of assessment or affected your performance, you should complete an aegrotat application form, available from the Registry or the Student Health and Counselling Service. This should be done **within seven days** of the due date for the required work or the date of the 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 further details on aegrotat applications, please refer to pages 351 and 353 of the University's 2007 Enrolment Handbook.

Missing of tests: In rare cases a student will not be able to sit a test because of involvement in representative sport or cultural groups. In such cases the student should consult the Course Coordinator and the Head of Department, and a course of action (usually the sitting of an equivalent test at a different time) will be arranged. **This should be done well in advance of the set date for the test.**

Submission of reports and assignments: 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.

Academic liaison: Prof Murray Munro (Room 758, phone 364 2434) is the coordinator of 200-level and 300-level chemistry courses. His interest is in the academic performance and well-being of all such students. Anyone experiencing problems with their 300-level chemistry courses or requiring guidance about their B.Sc. in Chemistry should get in contact with Prof Munro.

Liaison committee: There is a small staff-student liaison committee that includes a representative from each of the second, third and fourth year classes. Student representatives will be selected from each class early in the first term.

Computer equipment: The University provides several student computer facilities. There is also a suite of PCs in Room 540 on the 5th floor of the Chemistry Department which 300-level chemistry students are welcome to use for chemistry assignments and laboratory exercises OUTSIDE THE TIMES WHEN THESE COMPUTERS ARE NEEDED FOR THE CHEM 282 and 382 LABORATORY COURSES. Commonly-used programs such as Word and Excel have been loaded onto these PCs.

Please note that these computers are provided for your use in Chemistry courses only and are not to be used for work for other departments. Abuse of this privilege will result in access to the computers being denied.

Common room: A common room for 300-level chemistry students has been incorporated into the 4th floor of the Chemistry Department, in the entrance to room 431. This is your “space” and you are encouraged to make full use of it and its amenities. Comments and suggestions about this room should be directed to Professor Munro (Room 758).

Bryce E Williamson
Head of Department
February 2007

CHEM 363

Physical Chemistry

Course Content - 2007

Professor Michael Buback (Room 730)

(8 lectures)

Applied Physical Chemistry

The objective of these lectures is to familiarize students with basic concepts of technical chemistry and to outline the close links between physical chemistry and technical chemistry.

Topics to be covered include:

- General aspects of technical chemistry
- Basic vocabulary of technical chemistry
- Estimates of chemical equilibria for technical reactions up to high pressure
- Estimates of phase equilibria for chemical reactions in wide ranges of T and p
- Kinetics of chemical processes in wide ranges of T and p
- Heat transfer kinetics and apparatus for heat exchange
- Basic types of continuously operated chemical reactors
- Mass and heat balances for the basic types of chemical reactors

Reference book:

Levenspiel, O., *Chemical Reaction Engineering*, Wiley, New York 1998 (available in Engineering Library)

Professor Leon Phillips (Room 632)

(8 lectures)

Electronic Spectroscopy

This section builds on the spectroscopy and quantum mechanics introduced in CHEM 263. Topics will be chosen from the following.

- Experimental methods: jet cooling, matrix isolation, the use of lasers in spectroscopy.
- Electronic spectroscopy: interactions of electrons with radiation; quantum-mechanical description of electronic transitions; selection rules.
- Many-electron atoms: the electronic Hamiltonian; configurations; terms and states; coupling of electronic angular momenta.
- Diatomic molecules: description of states and transitions in terms of angular momenta and symmetry; spin-orbit coupling; vibronic spectra.
- Polyatomic molecules: rotational states; group theoretical description of states and selection rules; vibronic spectra and vibronic coupling.

Quantum Chemistry

The objective of these lectures is to introduce students to some of the fundamental principles of quantum mechanics and the approximate methods used in quantum chemistry.

Topics to be covered:

- classical mechanics
- postulates of quantum mechanics;
- immediate consequences of the postulates;
- approximate methods: variation principle, linear variation method, perturbation theory;
- angular momentum theory for a single particle;

Molecular Symmetry and Group Theory

Modern physical theories provide powerful means by which to describe molecular properties. However, as the number of particles (electrons and nuclei) is increased, 'brute force' application of these techniques can be unwieldy and difficult to conceptualise. Group theory is a mathematical technique with many applications, one of which allows the symmetry of a molecule to be utilised to reduce complexity and to aid the interpretation of experimental data and theoretical results.

In the first part of this course some of the elementary concepts of group theory will be introduced with reference to molecular symmetry. In the second part, applications of group-theoretical techniques will be presented: to molecular vibrations, molecular-orbital theory and molecular (vibrational) spectroscopy.

Course summary:

- *Group theory*: multiplication tables; groups; basis functions; representations and character, irreducible representations; character tables.
- *Molecular vibrations*: internal coordinates; symmetrised coordinates.
- *Molecular orbitals*: symmetry adapted linear combinations of atomic orbitals.
- *Products of functions*: Cartesian products; overlap integrals.
- *Spectroscopic selection rules*: Laporte selection rule; vibrational (infrared and Raman) selection rules.

Reference books (available in the library):

- R.L. Carter, *Molecular Symmetry and Group Theory*
- G. Davidson, *Group Theory for Chemists*
- F.A. Cotton, *Chemical Applications of Group Theory*

Dr Greg Russell (Room 634)

(8 lectures)

Polymer Physical Chemistry

The objective of these lectures is to familiarize students with some aspects of the physical chemistry of polymers.

Topics to be covered include:

- step-growth polymerization and the Carothers equation for number-average molecular weights;
- chain-growth polymerization;
- the kinetics of free-radical polymerization;
- copolymers, copolymerization and the copolymer composition equation;
- number-average molecular weights in free-radical polymerization: the Mayo equation;
- molecular weight distributions, as illustrated by free-radical polymerization;

Reference books (all available in the library):

- P.C. Painter and M.M. Coleman, *Fundamentals of Polymer Science: An Introductory Text*, 1994
- A. Rudin, *The Elements of Polymer Science and Engineering*, 1982
- R.J. Young and P.W. Lovell, *Introduction to Polymers*, 1991
- S.F. Sun, *Physical Chemistry of Macromolecules*, 1994

Dr Alison Downard (Room 660)

(8 lectures)

Electrochemistry

Electrochemistry is a discipline which finds applications in all branches of chemistry as well as in biology, biochemistry and engineering. The objective of these lectures is to introduce the concepts and techniques of electrochemistry which may be applied to the study of redox properties of species in solution.

Course outline:

- Introduction: overview of an electrochemical experiment; information from electrochemical experiments; nature of electrode processes.
- *Mass transport limited rates*: modes of mass transport; diffusion.
- *Electron transfer limited rates*: standard heterogeneous rate constants; Butler-Volmer equation.
- *Interaction of electron transfer and mass transport*: potential step experiment; steady-state voltammetry.
- *Cyclic voltammetry*: reversible, quasi-reversible and irreversible systems.