Ollscoil na Gaillimhe
University of Galway

Scoil na nEolaíochtaí
Bitheacha agus Ceimiceacha

School of Biological
and Chemical Sciences

Chemistry

3BS Information Booklet

Academic Year 2023 – 2024

Compiled by Dr. David Cheung
Revised: August 2023

Contents

Course Structure and Schedule

	Module (ECTS Credits)	Examination/Assessment	
		Two-Hour Exam Paper	Continuous Assessment
Semester I	CH311 - Organic Chemistry (5)	80%	20%
	CH326 - Analytical Chemistry & Molecular Structure (5)	80%	20%
	CH333 - Experimental Chemistry I (5)	-	100%
	CH332 - Drug Design & Drug Discovery (10, elective)	50%	50%
Semester II	CH307 - Inorganic Chemistry (5)	80%	20%
	CH313 - Physical Chemistry (5)	80%	20%
	CH334 - Experimental Chemistry II (5)	-	100%
	CH3101 - Computers in Chemical Research (10)	-	100%
	CH3103 - Validation in the Pharmaceutical and Medical Devices Industry (5, elective)	65%	35%

Semester I Schedule

CH311 First lecture in Dillon Theater on Monday, September 4th 2023, at 9am
CH326 First lecture in Dillon Theater on Tuesday, September 5th 2023, at 10am
CH332 First lecture in Dillon Theater on Tuesday, September 5th 2023, at 9am
First practical class on Monday, September 11th 2023, at 2pm (details on registration and final timetable to be provided in due course)
CH333 First practical class in Organic Chemistry Teaching Laboratory on Tuesday, September 12th 2023, at 2pm (details on registration and final timetable to be provided in due course)

Semester II Schedule

CH307 First lecture in Dillon Theater on Tuesday, January 9th 2024, at 10am
CH313 First lecture in Dillon Theater on Monday, January 8th 2024, at 9am
CH334 First practical class in Inorganic Chemistry Teaching Laboratory on Tuesday, January 9th 2024, at 2pm (details on registration and final timetable to be provided in due course)
CH3101 First practical class in Software Engineering Suite (ISS228A) on Friday, January 12th 2024, at 2pm
CH3103 First lecture in Dillon Theater on Wednesday, January 10th 2024, at 9am

While every effort has been made to ensure that this booklet is accurate, students should contact Module Coordinator(s) with queries. Any updates will be communicated through Canvas

CH311 - Organic Chemistry

Instructors: Prof. Paul Murphy (Coordinator), Prof. Peter Crowley, Dr. Eddie Myers

MODULE DELIVERY

1. **Physical Organic Chemistry, Reaction Mechanism (9 h + 2 h tutorial, PM)**
   At the end of this lecture series students should be able to:
   - Write expressions for K_a and pK_a.
   - Use K_a and pK_a to draw conclusions about acid and base strength.
   - To know or predict a molecule or functional groups protonation state at a defined pH.
   - To understand and explain chemical factors that have an effect on acidity and basicity.
   - To be able to relate pK_a to other properties (*e.g.* leaving group ability, nucleophilicity).
   - To understand how various types of experiments are used to study reaction mechanism, including kinetics, kinetic isotope effects, substituent effects (Hammett plots & LFERs), product identification, trapping & competition experiments, cross-over experiments, isotope scrambling & labelling, stereochemical analysis, computational methods.
   - To be able to write reasonable mechanisms for well-known reactions such as acid- and base-promoted hydrolysis of esters; acid-catalyzed formation/hydrolysis of acetals/ketals.
   - To solve problems based on the material covered.

2. **Biomolecular Chemistry (10 h + 2h tutorial, PC)**
   This aspect of the course focuses on biological molecules in particular, proteins. "*Foundations of Chemical Biology*" (Oxford Primer) is an excellent textbook that will also be useful for fourth year.

   Amino acids, peptides and proteins
   - Structures and properties of the amino acids.
   - Primary, secondary, tertiary and quaternary structures of proteins.
   - Isoelectric point.
   - The hydrophobic effect.
   - Interactions between proteins and small molecules (*e.g.* carbohydrates, lipids).

   Carbohydrates
   - Monosaccharides: classification and configuration.
   - Reactions at the anomeric center.

   Lipids
   - Biological lipids, bilayers and membranes.
   - Chemical structures of terpenes and steroids.

3. **Synthesis and Stereochemistry (10 h + 2 h tutorial, EM)**

   Synthesis
   - A general understanding of what organic synthesis involves, and of the difficulties associated with the synthesis of a polyfunctional molecule which can exist in different stereoisomeric forms.
   - An understanding of the reason why the synthesis of a complex organic molecule is undertaken.
   - A recognition of the different classes into which syntheses can be divided.
   - The ability to calculate the yield of a multistep synthesis.
   - The ability to distinguish between linear and convergent syntheses, and an appreciation of the advantages of the former.
   - An understanding of the basic concept underpinning retrosynthetic analysis.
   - The ability to describe what the following terms involve and to provide simple examples of each one: disconnection, functional group interconversion, synthon, synthetic equivalents.
   - The ability to carry out multistep retrosynthetic analyses based on the use of Grignard reactions, redox reactions involving carbonyl groups, catalytic hydrogenation, alkyl halide/alcohol interconversions, Friedel-Craft reactions, aldol reactions and Michael reactions.
   - The ability to carry out the retrosynthetic analyses of six-membered carbocylic rings based on Diels-Alder reactions and Robinson annulations.
   - A general understanding of the protecting group approach, of why it may be necessary, of what is involved, and of the disadvantages associated with it.
   - An understanding of the circumstances under which the carbonyl groups in ketones and aldehydes need to be protected, and of how this is done.

- An understanding of the circumstances under which alcohol groups need to be protected, and of how this is done.

Stereochemistry

- The ability to distinguish between constitutional isomers and stereoisomers.
- An understanding of the difference between conformational and configurational stereoisomers.
- An understanding of the stereochemical possibilities, chirality/enantiomerism, in systems containing one asymmetric carbon.
- An appreciation of the concepts of absolute configuration, specific rotation and enantiomeric excess.
- The ability to interpret the significance of the stereochemical descriptors, (+), (-), R and S, both on their own and in combination.
- An understanding of the structural possibilities in systems containing more than one asymmetric carbon: identical, enantiomers and diastereomers.
- A recognition of the importance of a plane of symmetry in a molecule: meso stereoisomers.
- The ability to define and recognize racemization, epimers, epimerization and anomers.
- The recognition that chirality can arise in molecules containing tetrahedral atoms other than carbon: sulfoxides, etc.
- The recognition that chirality can arise in non-tetrahedral systems: allenes, atropisomers (biphenyls), helicenes.
- An understanding of the concept of resolution, the separation of enantiomers.
- The ability to describe, and to discuss the advantages and disadvantages of the three methods by which resolution can be achieved: mechanical separation, decomposition and the use of a resolving agent.
- The ability to recognize and distinguish between enantioselective and diastereoselective reactions.
- The ability to describe a number of diastereoselective reactions and to explain why they are stereoselective.
- An appreciation of why the synthesis of chiral molecules (asymmetric synthesis) is important.
- An understanding of the difficulties involved in carrying out reactions with chiral molecules in terms of retaining chirality.
- An appreciation that there are three different methods of making a chiral molecule: starting with a chiral pool molecule, carrying out a resolution, or using an enantioselective reaction.
- The ability to describe, and to discuss the advantages and disadvantages of, asymmetric synthesis involving chiral pool molecules.
- The ability to describe, and to discuss the advantages and disadvantages of, asymmetric synthesis involving resolution.
- The recognition that enantioselective reactions occur under the influence of a chiral group (chiral auxillary) which can be in the reagent, the substrate or the catalyst.
- The ability to provide examples of all the above methods of carrying out asymmetric synthesis.

Related practicals are included in the laboratory-based Module CH333 - Experimental Chemistry I. Experience will be gained in a range of synthetically important reactions, techniques associated with biological chemistry, as well as analytical techniques, both spectroscopic and chromatographic. Molecular modelling and database searching are also introduced (see description of the CH333 Module for details).

CH326 - Analytical Chemistry & Molecular Structure

Instructors: Dr. Andrea Erxleben, Dr. Mihai Lomora, Prof. Olivier Thomas (Coordinator)

MODULE DELIVERY

1. **Crystal Diffraction (8 lectures+1 tutorial, AE)**
   - An understanding of the following terms: unit cell, crystal system, Bravais lattice, space group, Miller indices.
   - An understanding of the information that can be obtained from X-ray powder diffraction data.
   - The ability to index simple X-ray powder diffraction patterns and to calculate the unit cell parameters from X-ray powder data of cubic structures.
   - An understanding of the relevance of polymorphism.
2. **Chromatography (8 lectures+1 tutorial, ML)**
   - Gas Chromatography (GC)
     - Discussion of how, on a molecular level, separation occurs in chromatography, emphasizing how this chromatographic principle underpins all forms of chromatography.
     - GC instrumentation: injections systems, columns and detectors.
     - Quantifying column performance: column efficiency.
     - Applications.
   - High Performance Liquid Chromatography (HPLC)
     - The ability to describe the chromatographic separation process in terms of a stationary phase (SP) and a mobile phase (MP).
     - An understanding that the number of peaks in a chromatogram indicates the number of components in the sample and of the reasons why this is not always true.
     - An understanding that the area of a peak is proportional to the amount of a substance in a sample.
     - An understanding of how the retention time of a component in a sample can be used to identify it, and of the limitations of this approach to identifying a substance.
     - An understanding of what preparative chromatography involves.
     - An understanding of the advantages and disadvantages of classical liquid chromatography (LC).
     - An understanding of the advantages and disadvantages of gas chromatography (GC).
     - A particular understanding of why the analysis of involatile/water soluble substances, a group which includes most biological substances/pharmaceuticals, is difficult/impossible by GC.
     - An appreciation that the importance of HPLC in the pharmaceutical industry is due to its ability to efficiently analyze such of involatile/water soluble substances.
     - An appreciation that the separating ability of a chromatography system is directly related to SP surface area, and thus to the size of the particles in packed columns.
     - An appreciation that HPLC is more efficient than classical LC because of the smaller particles used, but that this requires a powerful pump to establish an adequate mobile phase flow.
     - The ability to describe a simple isocratic HPLC system in terms of solvent reservoir/pump, injection valve, column, detector, and PC/data system.
     - An understanding of what a gradient HPLC system involves and what advantages it provides.
     - An understanding of why an injection valve is required and how it operates.
     - A knowledge of the various types of HPLC columns available in terms of their physical size and that of the packing material used.
     - An appreciation of how a fixed wavelength UV/visible detector operates.
     - An appreciation of how a variable wavelength UV/visible detector operates.
     - An appreciation of how a diode array detector operates.
     - An appreciation of how a fluorescence detector operates.
     - An understanding of the relative merits of UV/visible, diode array and fluorescence detectors.
     - An appreciation of the relative merits of GC and HPLC as analytical tools.
     - The ability to identify the key experimental features in a published HPLC method with a view to using it.
     - An understanding of what an adsorption HPLC column is, and of the retention mechanism through which it operates.
     - An understanding of what is implied by the term “chemically bound stationary phase”.
     - An understanding of what a normal phase HPLC column is, and of the retention mechanism through which it operates.
     - An understanding of what a reverse phase (RP) HPLC column is, and of the retention mechanism through which it operates.
     - A precise understanding of why RP columns are the most commonly used HPLC column.

- An understanding of how chiral HPLC operates and of how it can be used to determine the enantiomeric excess of a compound.

3. Mass Spectrometry (8 lectures+1 tutorial, OT)

- A basic understanding of the workings of the basic forms of mass spectrometer including:
  - Sample introduction (direct insertion probe, GC, LC systems).
  - Ionization methods (electron impact, chemical, electrospray, laser desorption).
  - Mass analyzers (magnetic sector, double focusing including kinetic filter, time of flight including reflectron, quadrupolar).
  - Ion detection.
- An understanding of the basics of fragmentation, when and how it occurs and its prevalence with different molecule types and ionization techniques.
- An ability, given a molecule and its mass spectrum (EI or CI) to deduce the fragmentations, and their mechanisms, leading to the main peaks; fragmentations covered will center on alpha radical initiated cleavage, adjacent bond cleavage, and McLafferty type rearrangement.
- An understanding and ability to recognize or apply the isotope effect.
- An appreciation of the importance of resolution as applied to HRMS.

4. Nuclear Magnetic Resonance (NMR) Spectroscopy (8 lectures+ 1 tutorial, OT)

- An understanding of how some nuclei, behaving like tiny bar magnets, can line up with and against an external magnetic field and so exist in two energy states.
- An understanding of how the size of the external field affects the energy gap between these two states.
- The ability to describe how an NMR spectrum of a molecule is obtained in terms of the basic structure of the spectrometer and of sample preparation.
- An understanding of how the environment of a nucleus in a molecule affects the signal it produces and that thus the environment of a nucleus in a molecule can be determined from the signal it produces.
- An understanding that the electron cloud surrounding the nucleus lowers the effective magnetic field in the vicinity of the nucleus, thus shielding it.
- The ability to characterize signals in an NMR spectrum as being shielded/upfield/low frequency or deshielded/downfield/high frequency.
- The ability to recognize the effect of symmetry on the number of sets of chemically equivalent protons and thus on the number of signals produced by a molecule.
- The ability to predict the number of signals that would be observed in the ^{1}H NMR spectrum of a molecule on the basis of its structure.
- An understanding that the position, or frequency, of a signal in the spectrum is determined relative to that of a standard and is referred to as the chemical shift (δ) of the signal and/or of the nucleus responsible for it.
- The ability to use a ^{1}H NMR correlation table to relate the δ value of a signal to the type of proton responsible for it.
- The ability to use the integration (area) of the signals in a ^{1}H NMR spectrum to determine the relative number of protons responsible for each signal.
- An understanding that the splitting of a signal for a proton is due to an interaction (scalar coupling) of that proton with the protons attached to the atom (usually a carbon atom) next to the atom (again usually a carbon atom) carrying the proton producing the signal.
- The ability to deduce the number of protons on an adjacent carbon based on the multiplicity of the splitting shown by a particular proton (none, doublet, triplet, quartet), given that the multiplicity is equal to (2n +1), where n is the number of protons on the adjacent carbon.
- An understanding that the standard form of ^{13}C NMR spectrum does not show C-H coupling and, thus, consists of a series of lines in which each set of chemically equivalent carbons appears as a single line.
- An appreciation that the chemical shift of a carbon signal is affected by the same factors that determine the shift of a proton signal.
- The ability to use a ^{13}C NMR correlation table to relate the δ value of a signal to the type of carbon responsible for it.
- The ability to determine the number of hydrogens attached to a particular carbon using a ^{13}C NMR DEPT spectrum.
- The ability to deduce the structure of simple molecules based on NMR data, usually in the form of actual spectra, the above concepts and simple spectroscopic correlation tables.
- An appreciation of the existence of long-range and geminal coupling, and of the concept of diastereotopic protons.
- An appreciation of the issues relating to the ^{1}H NMR spectra of molecules containing N-H and O-H bonds.

The practicals related to the topics dealt with within the course are included in the laboratory-based Module CH333 - Experimental Chemistry I (see description of the CH333 Module for details).

CH332 - Drug Design & Drug Discovery

Instructors: Dr. David Cheung (Coordinator), Prof. Olivier Thomas, TBC

MODULE DELIVERY

The Module is delivered in 24 lectures (2 one-hour lectures per week).

1. **Computational Approaches to Drug Design (12 lectures, DC)**
   - Role of modelling in drug design.
   - Describing molecular structure.
   - Molecular Models and Force Fields.
   - Molecular Docking.
   - Challenges of modelling proteins and prediction of protein structure.
   - Molecular Dynamics.
   - Thermodynamics of protein-ligand binding.

   Learning outcomes
   At the end of this course students will be able to:
   - Describe the applications of molecular modelling in drug design.
   - Discuss the origin of the potential energy surfaces and relate features of this to the conformation of molecules.
   - Explain the different terms in a typical molecular mechanics force field
   - Describe Molecular Docking and its use in drug discovery
   - Discuss the different levels of protein structure and methods for prediction of this.
   - Describe the application of molecular dynamics simulation to investigate biomolecular structure and function
   - Critically analyze literature on the use of molecular modelling in drug design.

   Continuous Assessment
   Continuous assessment for the Computational Approaches to Drug Design component will take place across the course. The principal objectives of the course are:
   - To develop a practical capability to visualize and modify molecular structures on a computer.
   - To be able to compute binding energies.
   - To be able to analyze data from MD simulations.
   - To illustrate the principles dealt with in the lecture course.

   Recommended readings
   Students may consult the following textbooks (available in the library):
   - A.R. Leach, *Molecular Modelling: Principles and Applications*
   - A: Hinchliffe, *Molecular Modelling for Beginners*

2. **Natural Products in Drug Discovery (6 lectures, OT)**
   This lecture series covers relevant topics relating to modern natural products chemistry and its role in drug discovery and development. Main outcomes are:
   - Historical and current importance of natural products as drugs and drug leads, anti-infective, anticancer but also others.
   - The most important natural sources for bioprospection and drug discovery: plants, microbes.
   - Natural product chemistry: principles for the extraction, isolation and structure elucidation steps.
   - Basic concepts of bioactivity guided isolation process.
   - Main metabolic pathways leading to specialized metabolites or natural products.
   - New perspectives for natural products in drug discovery: sources like the marine biodiversity, extreme environments; dereplication processes, collaborative databases.

   Continuous Assessment
   The Natural Products Chemistry practical component will take place over a six-week period (2 groups, 3 laboratory sessions each, 3 h per week). Attendance records are taken at practical classes and performance will be assessed at the end of the practical. Part of the marks will be awarded for this Continuous Assessment.
   - Extraction of the metabolites from a common marine macroalga *Halidrys siliquosa*.
   - Fractionation of the extract into families of metabolites of different polarities. Use of solid phase extraction and applications of basic principles of chromatography: normal and reversed phase. Polarity of solvents.
   - Analysis of some fractions by mass spectrometry and nuclear magnetic resonance. Drawing of the isolated molecules and structure elucidation.
   - Propose metabolic pathways of the isolated metabolites based on basic rules.

Recommended readings

Students may consult the following textbooks (available in the library):

- P.M. Dewick, *Medicinal Chemistry, a Biosynthetic Approach*
- G.M.L. Cragg; D. Kingston, D.J. Newman, *Anticancer Agents from Natural Products*

3. TBC

CH333 - Experimental Chemistry I

Instructors: Gerard Fahy, Roisin Doohan, Prof. Peter Crowley, Dr. Eddie Myers, Prof. Paul Murphy, Dr. Mihai Lomora, Dr. Andrea Erxleben, Prof. Olivier Thomas (Coordinator)

COURSE OUTLINE WITH LEARNING OUTCOMES

This laboratory-based Module complements the 3rd Year Organic Chemistry (CH311) and Analytical Chemistry & Molecular Structure (CH326) lecture-based Modules (which students **must** also take).

Attendance to laboratory sessions is **mandatory**.

On successful completion of this Module, the learner will be able to:

- Demonstrate an understanding in protein handling and purification.
- Demonstrate competence in setting up organic and organometallic reactions, work up and standard purification techniques, such as distillation, chromatography and recrystallization.
- Demonstrate competence in mole and yield calculations.
- Demonstrate competence in reaction rate monitoring and reporting.
- Demonstrate competence in organic compound characterization techniques, and analysis of spectroscopic data such as HPLC, GC, IR, UV, MS and NMR spectroscopy.
- Demonstrate competence in report writing, interpretation of laboratory results, and relate experimental data with theoretical and mechanistic aspects covered in the associated lectures (*i.e.* Modules CH311 and CH326).
- Carry out procedures in solving crystal structures.
- Demonstrate competence in the thermal analysis of polymers.

The Module is graded through Continuous Assessment by submission of written reports to laboratory class supervisors with each experiment graded out of 100%.

CH307 - Inorganic Chemistry

Instructors: Dr. Pau Farras, Dr. Constantina Papatriantafyllopoulou, Dr. Luca Ronconi (Coordinator)

COURSE OUTLINE WITH LEARNING OUTCOMES (LO)

This Module will provide insights into the specific roles of metals and ligands in the broad field of coordination chemistry. Specific areas to be discussed include the coordination and organometallic chemistry of transition metals and f-block elements, inorganic kinetics and principles of nuclear chemistry.

The associated practical component of the course is carried out as part of the laboratory-based Module CH334 - Experimental Chemistry II (see description of the CH334 Module for details).

On successful completion of this Module, the learner will be able to:

- LO1 explain the bonding and structural features of transition metal coordination compounds based on the Crystal Field Theory (CFT) and the Molecular Orbitals (MOs) models;
- LO2 explain the structure, bonding and reactivity of transition metals in the various oxidation states;
- LO3 predict the spectroscopic properties of transition metal coordination compounds using theoretical models;
- LO4 discuss the mechanisms of dissociative, associative and interchange reactions of selected transition metals, including the interpretation of kinetic data;
- LO5 describe the structure, bonding and reactivity of organometallic complexes;
- LO6 classify the types of organometallic complexes on the basis of the coordinated ligands;
- LO7 illustrate the catalytic activity of selected organometallic complexes and draw the associated mechanisms of reaction;
- LO8 correlate the general features of lanthanides and actinides to their reactivity, coordination and organometallic chemistry;
- LO9 recognize the basic principles of radioactivity and nuclear chemistry, to include radioactive decays, the interaction of radiations with matter, nuclear reactions and common applications of radioisotopes.

MODULE DELIVERY

The Module will be delivered in 30 lectures (normally 3 one-hour lectures per week) and 3 one-hour tutorials (normally grouped at the very end of the course). 3 one-hour duration in-class tests (making up for the Continuous Assessment component of the Module, worth 20% the overall final mark) will be held during the teaching semester according to the timetable provided.

Specifically, the following topics will be dealt with.

1. **Introduction to 3rd Year Inorganic Chemistry Laboratory (2 lectures, LR1)**
   This lecture series will provide a general introduction to the experimental work to be carried out, with a focus on the following practical experiments:
   - investigation of the oxidation states of vanadium;
   - oxidation of ethanol by Cr(VI);
   - synthesis and characterization of acetylacetonate derivatives of V(IV) and Cu(II);
   - investigation of the aqueous chemistry of Fe(III), Fe(II), Cu(II) and Ag(I);
   - the cycle of copper.

   See description of the CH334 Module for details.

2. **Coordination Compounds and their Properties (10 lectures + 1 tutorial, PF)**
   This lecture series will deal with the exploitation of the Crystal Field Theory (CFT) and the Molecular Orbitals (MOs) models to explain the properties of transition metal coordination compounds.
   Specifically, the following topics will be covered:
   - calculation of the crystal field stabilization energies for coordination compounds of the transition metals in a variety of oxidation states, using a number of common ligands and for common geometries;
   - exploitation of laboratory measured properties in conjunction with CFT to predict the geometry adopted by coordination compounds of transition metals in a variety of oxidation states, using a number of common ligands;
   - use of the point group character tables and orbital repulsion considerations to explain the d orbital splitting patterns and the symbolism used in labelling for common geometries found in coordination compounds of the transition metals;
   - drawing of MOs energy level diagrams and pictorial representations for the bonding in coordination compounds with σ-donor, π-donor and π-acceptor ligands;
   - correlation of MOs diagrams with spectroscopic properties of coordination compounds and accounting for the order of ligands in the spectrochemical series;
   - description of the dissociative, associative and interchange mechanisms for substitution reactions in coordination compounds;

- interpretation of kinetic data in terms of the type of mechanism.

3. **Organometallic Chemistry and f-Block Elements (10 lectures + 1 tutorial, CP)**
   This lecture series will deal with the structure, bonding and reactivity of organometallic complexes, and the chemistry, properties and applications of the f-block elements.
   Specifically, the following topics will be covered:
   - description and classification of the most common types of organometallic complexes based on the various organic ligands (*e.g.* CO, NO, PR_3) used in their construction;
   - the 18-electron rule, its limitations, and its application to organometallic species;
   - description of the common reaction mechanisms observed for organometallic complexes (*e.g.* β-H elimination, alkyl migration, oxidative addition);
   - the catalytic activity of selected organometallic complexes (*e.g.* Grubbs and Schrock types) and the associated mechanisms of reaction.
   - general features of lanthanides and actinides (electron configuration, properties of the f orbitals, lanthanoid and actinoid contraction and their consequences, oxidation states and their stability in water, simple binary derivatives);
   - lanthanides and actinides complexes (aqua complex ions, common coordination and organometallic compounds, coordination numbers and geometries);
   - applications of lanthanides (redox reagents and catalysts in organic reactions, MRI contrast agents, shift reagents, luminescent sensors).

4. **Nuclear and Isotopic Chemistry (8 lectures + 1 tutorial, LR2)**
   This lecture series will deal with the basic concepts of nuclear chemistry and radioactivity.
   Specifically, the following topics will be covered:
   - the nuclear structure and its involvement in the origin of radioactivity and nuclear reactions;
   - the nuclide symbolism and definitions (isotopes, nuclear binding energy, nuclei stability band, half-life);
   - the radioactive decays and the interaction of radiations with matter;
   - radiation measurement and detection;
   - natural radioactivity and the radioactive series;
   - nuclear reactions (fission and fusion) and nuclear waste handling and cleanup;
   - isotopic labelling;
   - applications of radioisotopes (radiotracers, radiometric dating, nuclear medicine).

RECOMMENDED TEXTBOOKS AND REFERENCE MATERIAL

- C.E. Housecroft, A.G. Sharpe, *Inorganic Chemistry*, 5^{th} Ed., Pearson Education Ltd.: 2018
- S. Cotton, *Lanthanide and Actinide Chemistry*, John Wiley & Sons Ltd.: Chichester, 2006
- Lecture notes, slides and literature papers provided in due course on Blackboard

CH313 - Physical Chemistry

Instructors: Dr. David Cheung, Prof. Henry Curran (Coordinator), Prof. Donal Leech, Dr. Chongwen Zhou

TEXTBOOK

P.W. Atkins, J. De Paula, *Elements of Physical Chemistry*, 5th Ed. (available in the library)

MODULE DELIVERY

1. Molecular Interactions (5 h, HC, Chapter 15 of the textbook)

Students will understand that:

- Van der Waals force is an attractive interaction between closed-shell molecules with a potential energy that is inversely proportional to the sixth power of the separation.
- A polar molecule is a molecule with a permanent electric dipole moment; the magnitude of the dipole moment is the product of the partial charge and the separation.
- Dipole moments are approximately additive.
- The equations for potential energies of interaction for (i) charge/charge, (ii) charge/dipole, (iii) dipole/dipole, (iv) London (dispersion) interaction.
- A hydrogen bond is an interaction of the form X–H···Y, where X and Y are N, O, or F.
- The Lennard-Jones (6,12)-potential is a model of the total intermolecular potential energy.

2. Spectroscopy (10 h, CZ, Chapter 19 of the textbook)

Students will understand that:

Students will understand that:

- Energy is quantised, with transitions allowed between energy states
- The Beer-Lambert law relates intensity of absorption of radiation to concentration of the absorbing species
- The Franck-Condon principle states that because nuclei are much more massive than electrons an electronic transition takes place faster than the nuclei can respond.
- A selection rule is a statement about when the transition dipole is non-zero.
- A gross selection rule specifies the general features a molecule must have if it is to have a spectrum of a given kind. The gross selection rule for MIR absorption is that there must be a change in dipole moment during the motion for the vibration to be IR active. For Raman spectroscopy there must be a change in polarizability for the molecule/vibration to be Raman active
- A specific selection rule is a statement about which changes in quantum number may occur in a transition. The specific selection rule for vibrational spectroscopy is $\Delta\nu=\pm1$.
- The vibrational energy levels of a molecule are given by:

$$E_\upsilon = (\upsilon + \tfrac{1}{2})hc\tilde{\nu}, \text{ where } \tilde{\nu} = \frac{1}{2\pi c}\sqrt{\frac{k}{\mu}}$$

-
- μ = effective or reduced mass, for a diatomic AB, μ = mAXmB/(mA+mB)
- The number of vibrational modes for a non-linear molecule is 3N-6, for a linear molecule it is 3N-5 where N is the number of atoms in the molecule.
- Fluorescence is the spontaneous emission of light from molecules where the transitions occurs from states of the same multiplicity.
- Phosphorescence is the spontaneous emission of light from molecules where the transitions occurs from states of the different spin multiplicity.
- A spectrometer consists of a source of radiation, a dispersing element, and a detector.
- One contribution to the linewidth is the Doppler effect, which can be minimized by working at low temperatures. Another contribution to linewidth is lifetime broadening: $\delta E \approx \hbar/T$, where T is the lifetime of the state.
- The intensity of a transition is proportional to the square of the transition dipole moment.
- A selection rule is a statement about when the transition dipole is non-zero.
- A gross selection rule specifies the general features that a molecule must have if it is to have a spectrum of a given kind.
- A specific selection rule is a statement about which changes in quantum number may occur in a transition.
- The rotational energy levels of a linear rotor and a spherical rotor are given by E_J = hBJ(J+ 1) with J = 0, 1, 2, ..., where B = fl/4nl is the rotational constant of a molecule with moment of inertia I.
- The Pauli principle states for fermions Ψ(B,A)= - Ψ(A,B) and for bosons Ψ(B,A) = Ψ(AB). The consequences of the Pauli principle for rotational states are called nuclear statistics.
- The populations of rotational energy levels are given by the Boltzmann distribution in connection with noting the degeneracy of each level.

- The gross selection rule for rotational transitions is that the molecule must be polar.
- The specific selection rules for rotational transitions are $\Delta J = \pm 1$, $\Delta K = 0$; a rotational spectrum of a polar linear molecule and of a polar symmetric rotor consists of a series of lines at frequencies separated by 2B.
- In a Raman spectrum lines shifted to lower frequency than the incident radiation are called Stokes lines and lines shifted to higher frequency are called anti-Stokes lines.
- A Raman spectrometer consists of a monochromatic light source (usually a laser), sampling optics, a dispersive element (spectrometer), and a detector (usually a multi-channel CCD).
- The gross selection rule for rotational Raman spectra is that the polarizability of the molecule must be anisotropic.
- The specific selection rules for the rotational Raman transitions of linear molecules are $\Delta J = +2$ (Stokes lines), $\Delta J = -2$ (anti-Stokes lines).
- The vibrational energy levels of a molecule $E_v = (v + 1/2)hcv$ with v = 0, 1, 2,..., where $v= (1/2\pi c\}(k/\mu)^{1/2}$ and $\mu = m_A m_B/(m_A + m_B)$.
- The gross selection rule for vibrational absorption spectra is that the electric dipole moment of the molecule must change during the vibration.
- The specific selection rule for vibrational transitions is $\Delta v = \pm 1$.
- The number of vibrational modes of non-linear molecules is 3N-6; for linear molecules the number is 3N-5.
- Rotational transitions accompany vibrational transitions and split the spectrum into a P branch ($\Delta J = -1$), a Q branch ($\Delta J = 0$), and an R branch ($\Delta J = +1$). A Q branch is observed only when the molecule possesses angular momentum around its axis.
- The gross selection rule for the vibrational Raman spectrum of a polyatomic molecule is that the normal mode of vibration is accompanied by a changing polarizability.
- The exclusion rule states that if the molecule has a center of inversion, then no modes can be both infrared and Raman active.

3. **Electrochemistry (10 h, DL, Chapter 16 of the textbook)**
   Students will understand that:

- The molar conductivity of a strong electrolyte follows the Kohlrausch law
- Protons migrate by the Grotthus mechanism in aqueous solutions
- Conductivity measurements can be used to predict values of equilibrium constants for processes that produce or consume ions, such as acid dissociation
- A galvanic cell is an electrochemical cell in which spontaneous chemical reactions produces a potential difference
- An electrolytic cell is an electrochemical cell in which an external source of current is used to drive a non-spontaneous chemical reaction
- Cell potentials are related to the reaction Gibbs energy, and standard cell potentials can be used to predict thermodynamic functions (Gibbs energy, entropy, enthalpy and equilibrium constant) of processes
- The cell potential is related to concentration of species by the Nernst equation
- To induce electrolysis, the applied potential difference must exceed the cell potential at least by the cell overpotential
- Cell overpotential is the sum of the overpotentials at the anode and the cathode, and of the ohmic (iR) drop.
- An electric double layer consists of a sheet of positive charge at the surface of the electrode and a sheet of negative charge next to it in the solution (and vice versa).
- The Galvani potential difference is the potential difference between the bulk of the metal electrode and the bulk of the solution.
- The current density, j, at an electrode is expressed by the Butler-Volmer equation, $j = j_0 \left\{e^{(1-\alpha)f\eta} - e^{-\alpha f\eta}\right\}$, where η is the overpotential $\eta = E' - E_i$, α is the transfer coefficient, and i_0 is the exchange current density.
- A Tafel plot is a plot of the logarithm of the current density against the overpotential; the slope gives the value of α and the intercept at $\eta = 0$ gives the exchange-current density.
- Voltammetry is the study of the current through an electrode as a function of the applied potential difference.
- To induce current to flow through an electrolytic cell and bring about a non-spontaneous cell reaction, the applied potential difference must exceed the cell emf by at least the cell overpotential.

4. **Macromolecules (5 h, DC, Chapter 16 of the textbook)**
   Students will be able to:

- Quantify the distribution of molecular weights in a synthetic polymer
- Describe techniques for the determination of the mean molar masses of molecules and in particular viscosity measurements and gel permeation chromatography.
- Relate the conformation and viscosity of polymers in solution and the melt to their molecular weight
- Discuss the properties of amorphous and crystalline polymers.
- Describe how crystallinity in a polymer influences the physical properties.

- An understanding of the meaning of the glass transition temperature (T_g) and the main factors such as chain flexibility, steric effects, molar mass and branching and cross-linking which influence its magnitude.

7. Self-Assembly (5 h, DC, Chapter 16 of the textbook)

Students will be able to:

- Discuss the formation of surfactant micelles as an example of self-assembly.
- Predict the morphology of surfactant aggregates based on the relative geometries of the head and tail groups.
- Discuss the nature of liquid crystals, nematic and smectic types, and how they self-assemble as a result of packing and intermolecular forces.
- Describe how external control of molecular behavior can make a simple twisted nematic liquid crystal display cell.

5. Quantum Chemistry (5 h, CZ, Chapter 12 of the textbook)

Students will understand that:

- Wien's Law states that $T\lambda_{max}$ = constant; the Stefan-Boltzmann law states that the emission of a black body is proportional to T^4. Planck proposed that *electromagnetic oscillators* of frequency ν could acquire or discard energy in quanta of magnitude $h\nu$. Einstein proposed that *atoms* oscillating in a solid with frequency ν could acquire or discard energy in quanta of magnitude $h\nu$.
- The photoelectric effect is the ejection of electrons when radiation of greater than the threshold frequency is incident on a metal; the kinetic energy of the ejected electrons and frequency of the incident radiation are related by $E_k = h\nu\phi$ where ϕ is the work function of the metal. The de Broglie relation for the wavelength, λ, of a particle of linear momentum p is $\lambda = \eta/p$.
- A wave function, Ψ, contains all the dynamical information about a system and is found by solving the appropriate Schrödinger equation, $-(\bar{h}^2/2m)\mathrm{d}^2\psi/\mathrm{d}x^2 + V\psi = E\psi$, subject to constraints on the solutions known as boundary conditions.
- According to the Born interpretation, the probability of finding a particle in a small region of space of volume δV is proportional to $\psi^2\delta V$, where ψ is the value of the wave function in the region.
- According to the Heisenberg uncertainty principle, it is impossible to specify simultaneously, with arbitrary precision, both the momentum and position of a particle.
- The energy levels of a particle of mass m in a 1-D box of length L are $E_n = n^2h^2/8mL^2$, with n = 1, 2,… and the wave functions are $\Psi_n(x) = (2/L)^{1/2}\sin(n\pi x/L)$.
- The energy levels of a particle of mass m in a 3-D box of length L are $E_n = (n_1^2/L_1^2 + n_2^2/L_2^2 + n_3^2/L_3^2)(h^2/8m)$, with n = 1, 2,… and the wave functions are $\Psi_n(x) = (2/L)^{1/2}\sin(n\pi x/L)$.
- Because wave functions do not decay abruptly to zero, particles may tunnel into classically forbidden regions. Two aspects of tunneling include radioactivity and scanning tunneling microscopy.
- The energy levels of a particle of mass m on a circular ring of radius r are $E_{m_l} = m_l^2\hbar^2/2I$ where *I* is the moment of inertia, $I = mr^2$ and $m_l = 0, \pm1, \pm2$, etc.
- The angular momentum of a particle on a ring is quantized and confined to the values $J_z = m_l\hbar$, $m_l = 0, \pm1, \pm2$, etc.
- A particle undergoes harmonic motion if it is subjected to a Hooke's-law restoring force and has a parabolic potential energy, $V(x) = 1/2kx^2$.
- The energy levels of a harmonic oscillator are $E_v = (v + ½)h\nu$, where $\nu = (1/2\pi)(k/m)^{1/2}$ and v = 0, 1, 2,…

Related practicals are included in the laboratory-based Module CH334 - Experimental Chemistry II (see description of the CH334 Module for details).

CH334 - Experimental Chemistry II

Instructors: Prof. Henry Curran (Co-Coordinator/Physical Chemistry Practicals), Dr. David Cheung, Dr. Pau Farras, Prof. Donal Leech, Dr. Constantina Papatriantafyllopoulou, Dr. Luca Ronconi (Co-Coordinator/Inorganic Chemistry Practicals), Dr. Chong-Wen Zhou

COURSE OUTLINE WITH LEARNING OUTCOMES (LO)

This laboratory-based Module complements the 3rd Year Inorganic Chemistry (CH307) and Physical Chemistry (CH313) lecture-based Modules (which students **must** also take).

This course will involve the carrying out of experiments in areas such as inorganic syntheses, analysis and spectroscopic characterization of coordination compounds, correlation of the reactivity and aqueous chemistry of selected transition metal ions with their oxidation states, chemical kinetics, viscosity, temperature dependence of equilibrium, miscible liquids, rotational-vibrational spectra and electrochemistry.

Attendance to **all** laboratory sessions is **mandatory**.

On successful completion of this Module, the learner will be able to:

LO1 set up and carry out selected syntheses aimed at the generation coordination compounds;
LO2 relate laboratory results to the properties (*e.g.* oxidation states, structures, reactivity) of selected transition metals and their coordination compounds, covered in the associated inorganic chemistry lectures;
LO3 demonstrate competence in the spectroscopic characterization (*e.g.* IR, UV-Vis spectroscopy) of coordination compounds;
LO4 demonstrate competence in stoichiometric calculations;
LO5 set up and perform tests to verify fundamental physical chemistry theories in the laboratory;
LO6 relate experimental results to the physico-chemical principles dealt with in the associated physical chemistry lectures;
LO7 recognize the scientific method of planning, developing, conducting and reporting experiments to a scientifically acceptable standard;
LO8 apply important synthetic and analytical techniques relevant to the professional practice of chemistry;
LO9 implement safe work practices in a chemistry laboratory, to include awareness of common hazards and appropriate safety precautions.

MODULE DELIVERY

The Module is delivered in 10 practical sessions of 4 hours each (1 practical per week) split into two blocks (inorganic chemistry: practicals 1-5; physical chemistry: practicals 6-11).

The week following each block of practicals students will undergo an individual ten-minute oral examination related to the laboratory work carried out.

Specifically, the following practical experiments will be carried out.

1. **Inorganic Chemistry**
   - Investigation of the Oxidation States of Vanadium
   - Oxidation of Ethanol by Chromium(VI)
   - Synthesis and Characterization of Acetylacetonate Derivatives of Vanadium(IV) and Copper(II)
   - Investigation of the Aqueous Chemistry of Fe(III), Fe(II), Cu(II) and Ag(I)
   - The Cycle of Copper
2. **Physical Chemistry**
   - Rotational-Vibrational Spectrum of HCl
   - Beer-Lambert Law
   - Polymer Viscosity
   - Molar Conductivity
   - Nernst Equation
   - Cyclic Voltammetry of the Ferrocyanide/Ferricyanide Redox Couple

To derive full benefit from the course students should read details of the experiments to be performed **prior to attending the laboratory** and refer to the **literature resources** indicated in the laboratory manual.

TEXTBOOK AND REFERENCE MATERIAL

- Experimental Chemistry II Laboratory Manual 2023 - 2024
- Lecture notes, slides and literature papers provided in due course on Canvas

CH3101 - Computers in Chemical Research

Instructors: Dr. David Cheung, Prof. Peter Crowley, Prof. Henry Curran, Prof. Pau Farras (Coordinator), Dr. Eddie Myers, Dr. Constantina Papatriantafyllopoulou

COURSE OUTLINE WITH LEARNING OUTCOMES

The course provides an opportunity for the student to become familiar with a wide range of software relevant to the working life of a professional Chemist or Biopharmaceutical Chemist. It involves a workshop approach which gives the student practical, hands-on experience of the software involved. The course will also allow the student to develop her/his communication skills in terms of both writing and oral presentations.

On successful completion of the course, the learner will be able to:

- produce scientific written reports for the communication and presentation of chemical information in terms of structures, tables of data and other figures, such as molecular graphics;
- produce spreadsheets and graphs using Excel for inclusion in reports and for analyzing data;
- source information from the primary scientific literature using various resources, such as online libraries, search engines, databases (*e.g.* SciFinder, Reaxys), and other related technology;
- prepare a chemistry or biopharmaceutical chemistry presentation, and use it to communicate knowledge to an audience;
- use various sources of chemical knowledge to independently research a topic and write a critical essay or report;
- carry out basic molecular modelling;
- demonstrate increased knowledge and understanding within chemistry and/or biopharmaceutical chemistry;
- use protein and other structural databases;
- produce a poster suitable for a scientific conference;
- give a PowerPoint presentation.

MODULE DELIVERY

The Module is delivered in 15 lectures (normally 2 three-hour lectures per week), finishing with an oral presentation.

Schedule (Semester II): Monday and Friday at 2.00-5.00pm. Computer workshops in the Software Engineering PC Suite, 1st floor, room 228A.

ASSESSMENT

Continuous assessment based on two workshop reports each week. An extended essay, poster and presentation on an individual topic (assigned to each student at the beginning of the semester) are also part of the assessment process. The final mark will consist of the average of all assignments, the presentation and final project report (all assignments with the same weight, while presentation and final project report will weight 2x and 3x, respectively).

Week	Week beginning	Monday			Friday		
		Task	Software	Lecturer	Task	Software	Lecturer
1	08/01/2024				Introduction and project assignment		
2	15/01/2024	Technical writing	MS Word	Dr. E. Myers	Report writing	MS Word	Dr. E. Myers
3	22/01/2024	Spreadsheets in the lab	MS Excel	Prof. H. Curran	Data fitting and plotting	MS Excel	Prof. H. Curran
4	29/01/2024	Molecular graphics	ChemDraw	Dr. P Farras	Plagiarism	Turnitin	Dr. P Farras
5	05/02/2024	BANK HOLIDAY			Referencing	EndNote	Dr. P. Farras
6	12/02/2024	e-Searching chemical literature	Reaxys, SciFinder and Web of Knowledge	Dr. P Farras	Visualisation of Molecular Structure	Visual Molecular Dynamics (VMD)	Dr. D. Cheung
7	19/02/2024	Working with proteins	PDB	Prof. P. Crowley	Molecular modelling 1: structure building and optimization	Spartan '10	Dr. D. Cheung
8	26/02/2024	Presentations	MS PowerPoint	Prof. P. Crowley	Molecular modelling 2: conformational analysis and conformational	Spartan '10	Dr. D. Cheung
9	04/03/2024	Posters and how to produce them	MS PowerPoint	Dr. C. Papatriantafyllopoulou			
10	11/03/2024	Project report and presentation preparation					
11	18/03/2024	Project Presentations					
12	25/03/2024						
	VENUE: Monday/Friday Software Eng - Arts & Sci - 1st F- 228A						

CH3103 - Validation in the Pharmaceutical and Medical Devices Industry

Instructors: Dr. Constantina Papatriantafyllopoulou (Coordinator), TBA

MODULE DELIVERY AND ASSESSMENT

The Module is delivered in 15 lectures (normally 3 one-hour lectures per week) and 1 two-hour practical.

The Module is assessed through a formal written examination at the end of Semester II (worth 65%) and Continuous Assessment (Project to be undertaken along with a presentation, worth 35%).

Attendance to lectures and the practical session is **mandatory**.

COURSE OUTLINE WITH LEARNING OUTCOMES

This module will cover relevant topics concerning validatory requirements within the (bio)pharmaceutical and chemical industries. Detailed insights into the inner workings of industry are also given.

On successful completion of this Module, the learner will:

- Be introduced to the concept of Validation and its role in the pharmaceutical industry; the Validation Masterplan (VMP) will then be discussed and its benefits outlined.
- Be introduced to the concept of Good Manufacturing Practice (GMP) and Good Laboratory Practice (GLP) in relation to the pharmaceutical and chemical industries.
- Learn of the numerous and pertinent aspects of Cleaning Validation with respect to the manufacturing industry.
- Apply the basic concepts of the course in a laboratory exercise.
- Be provided with a broad knowledge of the subject of Equipment qualification including Design, Installation, Process and Performance Qualification).
- Be introduced to the cutting-edge field of Process Analytical Technology (PAT) and understand its fundamental relevance to the future of pharmaceutical manufacturing.
- Be introduced to Medical Devices and will glean knowledge in the practical aspects of Quality Control, Good Manufacturing Practices and Drug Development in relation to the Medical Device Industry.