Contents **Page**

Whilst every effort has been made to ensure the information contained in this booklet is accurate going to print, students should contact Course Director(s) for a module they have a query about.

Summary of Course Structure 2016-17

Modules	Credits	Examination/assessment
Semester I		
CH311 -– Organic Chemistry	5	2 h Exam paper
CH326 – Analytical Chemistry & Molecular Structure	5	2 h Exam paper
CH333 – Experimental Chem. 1	5	Continuous Assess
CH332 – Drug Design & Discovery	10	2 h Exam paper (50 %) & Continuous assessment (50%)

CH333 consists of the laboratory classes to accompany CH311 and CH326

Semester II		
CH307- Inorganic Chemistry	5	2 h Exam paper
CH313 - Physical Chemistry	5	2 h Exam paper
CH334 – Experimental Chem. 2	5	Continuous Assess
CH3103 – Validation in the Pharmaceutical & Medical Device	5	2 h Exam paper
CH3101 - Computers in Chemical Research	10	Continuous Assess

CH334 consists of the laboratory classes to accompany CH307 and CH313

Please note the credit weighting of these modules.

Schedule

Semester I

CH311 – First Lecture is in the Dillon @ 9.00 am, Monday, 5th September

& Lab. Registration @ First Lecture

CH326 – First Lecture is in the Dillon @ 10.00 am, Tuesday, 6th September

CH332 – First Lecture is in the Dillon @ 9.00 am, Tuesday 6th September

CH332 – First Lab in Software Engineering Suite @ 2.00 pm, Monday, 12th September

Semester II

CH313 – First Lecture is in the Dillon @ 9.00 am, Monday, 9th January

CH3103 – First Lecture is in the Dillon @ 9.00 am, Tuesday, 10th January

CH307 – First Lecture is in the Dillon @ 10.00 am, Tuesday, 10th January

CH3101 - First Lab in Arts/Science Computer Suite @ 2.00 pm, Monday, 10th January

CH311 - Organic Chemistry with Learning Outcomes

Staff: Dr. Fawaz Aldabbagh (Co-ordinator), Prof. Paul Murphy, Dr. Peter Crowley and Dr. Niall Geraghty

Heterocyclic Chemistry (8.5 h + 0.5 h, FA)

An understanding of what makes a molecule aromatic; an understanding of the effect of the N atom in pyridine and pyrrole on reactivity in comparison to benzene; an understanding of the basicity of pyridine and piperidine; draw resonance structures of pyridine and pyrrole to designate positions of nucleophilic and electrophilic substitution; designate the NMR chemical shifts of pyridine and pyrrole; an understanding of the use of pyridine and DMAP in ester formation; an understanding of the use of pyridine N-oxide in electrophilic aromatic substitution; an understanding of the mechanisms of nucleophilic and electrophilic aromatic substitution onto pyridine and pyrrole; draw mechanisms for the nitration, formylation, acetylation and chlorination of pyrrole; an understanding of the effect of a fused benzene ring on reactivity of indole; an understanding of the Mannich and Vilsmeier reaction onto indole; compare and contrast electronic structure, aromaticity and reactivity of pyrrole, furan and thiophene; write mechanisms for electrophilic aromatic substitutions onto thiophene and furan; an understanding of the Diels-Alder reaction in terms of orbital theory, mechanism, kinetic and thermodynamic control; an understanding of the reactivity of thiophene and oxidized forms to the Diels-Alder reaction; an understanding of the effect of the N atom of diazoles, triazoles and tetrazoles on electronic structure (aromaticity), basicity (acidity) and reactivity towards electrophiles; the drawing of tautomeric forms of all azoles is expected, as well as resonance forms of salts; an understanding of the biological significance of imidazole (enzymes), nitroimidazoles (antibiotics) and tetrazoles (isosteres of carboxylic acids); an understanding of the mechanism of 1,3-dipolar cycloaddition to give tetrazoles.

Physical Organic Chemistry (8.5 h + 0.5 h, PM)

Acid-base chemistry (3 h)
Write expressions for Ka and *p*Ka
Use Ka and *p*Ka to draw conclusions about acid and base strength
To know or predict a molecule or functional groups protonation state at a defined *p*H
To understand and be able to explain chemical factors that have an effect on acidity and basicity and to apply these concepts when comparing relative acidities of different substances
To be able to relate *p*Ka to other properties (e.g. leaving group ability, nucleophilicity).

Mechanism (5 h)
To understand and be able to use a variety of experiments for determining reaction mechanism. These include kinetics, kinetic isotope effects, substituent effects (Hammett plots & LFERs), product identification, trapping & competition experiments, cross-over experiments, isotope scrambling & labelling, stereochemical analysis. To be able to propose and write organic reaction mechanisms (e.g. acid and base promoted hydrolysis of esters; acid catalysed formation/hydrolysis of acetals/ketals)

Natural Product Chemistry (8.5 h + 0.5 h, PC)
This aspect of the course focuses on biological molecules in particular, proteins. "*Foundations of Chemical Biology*" (Oxford Primer) is an excellent text book 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 centre.

- Reactions of hydroxyl groups at non-anomeric carbon atoms.
- Glycosides. Glycoside synthesis. Disaccharides.

Lipids
- Biological lipids. Bilayers and Membranes
- Chemical structures of terpenes and steroids
- Isoprene building block. Cyt P450 oxidation reactions
- Squalene – intermediate in Cholesterol synthesis
- Biological activity (hormones signalling)

Synthesis and Stereochemistry (8.5 h + 0.5 h, NG)

- 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,

CH333 Experimental Chemistry 1

The laboratory course is included in CH333, and provides students with experience of a range of reactions which are important from the synthetic point of view, an introduction to techniques associated with biological chemistry, and hands-on experience of important analytical techniques, both spectroscopic and chromatographic. Computer based techniques such as molecular modelling and database searching are also introduced during the course.

Also see CH333 module description.

CH326 - Analytical Chemistry & Molecular Structure with Learning Outcomes

Staff: Dr. Niall Geraghty (Co-ordinator)

Topic	Lectures	Lecturer
Surface Analysis	4	A. Ryder
NMR	8	N. Geraghty
Crystal Diffraction	4	A. Erxleben
Gas Chromatography	2	N. Geraghty
HPLC	4	N. Geraghty
Mass Spectrometry	4	P. O'Leary
Thermal analysis	4	A. Ryder
XRF	2	A. Ryder

Surface Analysis:

- A basic understanding of the workings of a secondary ion mass spectrometer (SIMS), an x-ray photoelectron spectrometer (XPS), a scanning electron microscope (SEM) and an energy dispersive x-ray analysis system (EDS).
- An understanding of the kinds of chemical and structural information that these instruments can provide about the surface of materials.
- Their application to the analysis of the surface of biomaterials

Crystal Diffraction:

- 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

Nuclear Magnetic Resonance (NMR) Spectroscopy:

- 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
- An understanding of how the movement of nuclei between these energy state gives rise to the absorption and emission of energy and thus to the production of a spectrum
- 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 characterise signals in an NMR spectrum as being shielded/upfield/low frequency or deshielded/downfield/high frequency
- A recognition that nuclei in the same environment are termed chemically equivalent
- 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 determine the number of sets of chemically equivalent nuclei, for example protons, in a molecule from the number of signals in its NMR spectrum
- 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, TMS, added to the sample, and is referred to as the chemical shift (δ) of the signal and/or of the nucleus responsible for it
- A recognition that a nucleus close to a electronegative atom, and in most cases (but not always) close to a π bond (alkene, aromatic system) will appear downfield/has a large chemical shift (δ)
- 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 (vicinal 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 = n+1, where n is the number of protons on the adjacent carbon
- The ability to explain splitting (coupling) patterns in terms of the interaction between the coupled protons considered as bar magnets
- The ability to use a correlation table to link an IR absorption band with a particular functional group
- 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 (containing only C, H, and O atoms) based on spectroscopic 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
- An understanding of how proton-proton spin decoupling can be used to identify signals in a 1H-NMR due to coupled protons
- The ability to describe how ^{1}H-NMR spectroscopy is used in medicine in the form of magnetic resonance imaging (MRI)
- The ability to describe how an MRI scanner works
- An appreciation of what is meant by a 2-D NMR spectrum (COSY)

Chromatography

Gas Chromatography:

- Discussion of how, on a molecular level, separation occurs in chromatography, emphasising 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 analyse 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
- An knowledge of the various types of HPLC column 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

Mass Spectrometry:

- A basic understanding of the workings of the basic forms of mass spectrometer including
    - Sample introduction (Direct insertion probe, GC, LC systems)
    - Ionisation methods (electron impact, chemical, electronspray, laser desorption)
    - Mass analysers (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 ionisation 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 Mc Clafferty type rearrangement

- An understanding and ability to recognise or apply the isotope effect.
- An appreciation of the importance of resolution as applied to HRMS.

Thermal analysis:

- A basic understanding of the workings of thermogravimetric analysis (TGA, DTA) and scanning calorimetry (DSC) instruments
- An understanding of the chemical information that these instruments can provide
- Their application to the understanding of thermal transitions occurring inorganic, organic, polymeric, and biological materials

XRF Analysis:

- A basic understanding of the fundamental theory underpinning workings of X-Ray Fluorescence (XRF).
- A basic understanding of the workings and operation of a Energy Dispersive XRF (ED-XRF) and Wavelength Dispersive XRD (wd-XRF).
- An understanding of the major matrix effects (absorption and intensity enhancement) that occur in XRF measurements.

CH333 Experimental Chemistry 1

Staff: Dr. Fawaz Aldabbagh (Co-ordinator), Dr. Peter Crowley, Dr. Andrea Erxleben, Dr. Niall Geraghty and Dr. Alan Ryder

Learning Outcomes

- 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.
- Demostrate competence in organic compound characterization techniques, and analysis of spectroscopic data such as HPLC, GC, IR, UV, MS and NMR spectroscopy.
- Demostrate competence in report writing, interpretation of laboratory results, and relate experimental data with theoretical and mechanistic aspects covered in associated lecture modules (CH331 and CH336).
- Carry out procedures in solving crystal structures, and other solid state techniques such as SEM, EDX.
- Demonstrate competence in the thermal analysis of polymers.
- Demonstrate an understanding in protein handling and purification

The module is graded through continuous assessment by submission of written reports to laboratory class supervisors with each experiment graded out of 100%. At the end of the course each student will undergo a 10 minute interview assessment, which is also graded out of 100% (equivalent to the grade for one laboratory experiment).

CH332 - Drug Design and Drug Discovery with Learning Outcomes

Staff: Dr David Cheung (Co-ordinator), Dr. Fawaz Aldabbagh, Prof. Olivier Thomas

Schedule: **Lectures (24)** Tuesday / Thursday 9-10 am
Computer labs (10) Monday 2-5 pm

Assessment:
Continuous assessment – reports based on computer labs
Final written paper – Answer four questions

Computational approaches to Drug Design (DC)

This is a 12 lecture course covering the following:

- Role of modelling in drug design
- Describing molecular structure
- Molecular Models and Force Fields
- Molecular Docking
- Molecular Dynamics
- Challenges in modelling biomolecules: Solvation, prediction of protein structure, and thermodynamics of protein-ligand binding

Learning outcomes

Students will gain an appreciation of
- Applications of molecular modelling in drug design
- The importance of three-dimensional molecular structure
- Potential energy surfaces and how these relate to the structure of molecule
- Molecular mechanics force fields
- Molecular docking and molecular dynamics calculations
- Challenges in modelling biomolecular structure and function

Practicals
The Molecular Modelling Practical Course will take place over a 10 week period (3 hrs per week). Attendance records are taken at practical classes and performance at each laboratory class will be assessed on a weekly basis. Part of the marks will be awarded for this continuous assessment.

The principal objectives of the laboratory 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 perform and analyse data from MD simulations.
- To be able to critically compare theoretical and experimental molecular data.
- To illustrate the principles dealt with in the lecture course.

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

Some Heterocyclic Drugs (FA)

This is a 6 lecture taught course. The learning outcomes are as follows:

- The student should be able to identify and write the structure of all nucleotides and nucleosides derived from DNA and RNA. Also know the structure of ATP and NAD^+.
- Student should know the numbering and stereochemistry about a ribose or deoxyribose ring.

- The student should be familiar with primary and secondary structure of DNA, biosynthesis and replication.
- The student should be familiar with the Watson-Crick Model of DNA (B-DNA)
- The student should have an understanding of the mode of action of AZT used on HIV patients.
- The student should be able to propose a synthesis of AZT from thymidine
- The student should be able to propose a biosynthesis for *S*-adenosyl methionine, and describe its methylation to form caffeine in terms of a reaction mechanism.
- The student should describe the biosynthesis of cAMP from ATP with a reaction mechanism.
- The student should be able to derive the structure of NADPH from NADH, and write mechanisms for asymmetric reductions.
- The student should be able to write the "ping-pong" mechanism for NQO1 reduction of quinones if provided with the isoalloxazine ring of $FADH_2$.
- The student should be able to write the mechanism for mitomycin C bioreductive activation (one and two-electron), and explain the formation of cross-linked adducts with DNA.

Natural Products in Drug Discovery (OT)

This part of the course will cover relevant topics relating to the modern natural products chemistry and its role in drug discovery and development. The students will learn:

- Historical and current importance of natural products as drugs and drug leads
- The most important natural sources for drug discovery
- Advantages and challenges in natural product chemistry
- Basic concepts of bioactivity guided isolation process
- Methods used in natural product chemistry / drug discovery
- Most important natural product classes relevant in drug research

CH334 Experimental Chemistry 2

Staff: Dr. Andrea Erxleben (Co-ordinator), Dr. Luca Ronconi, Prof. Heny Curran, Dr. Alan Ryder, Dr. Pau Farras, Dr. Constantina Papatriantafyllopoulou

This laboratory based module complements third year inorganic chemistry and physical lecture courses.

Learning Outcomes

- demonstrate competence in recording, interpreting and reporting experimental data and laboratory results
- set-up and perform tests to verify fundamental physical chemistry theories in the laboratory; e.g. chemical kinetics, viscosity, temperature dependence of equilibrium, miscible liquids, rotational-vibrational spectra, and electrochemistry in anodising aluminium
- set-up and carry out inorganic syntheses (coordination compounds, polyoxometallates)
- relate laboratory results to the properties (oxidation states, structures) and reaction mechanisms of compounds of the transition metals (coordination compounds, polyoxometallates) covered in the associated inorganic lecture module
- demonstrate competence in inorganic spectroscopy (IR, UV, NMR spectroscopy of coordination compounds)
- demonstrate competence in stoichimetric calculations

The module is graded through continuous assessment by weekly submission of written reports to laboratory class supervisors with each experiment graded out of 100%. At the end of the course each student will undergo a 10 minute interview assessment, which is also graded out of 100% (equivalent to the grade for one laboratory experiment).

CH307 – Inorganic Chemistry Course Outline with Learning Outcomes

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

LECTURES (30 lectures, 4 tutorials)

1. **Introduction to 3rd Year Inorganic Chemistry Laboratory (2 lectures, LR1)**
   The laboratory component of the inorganic chemistry course is included in the CH334 Module "Experimental Chemistry II" (see relevant module description elsewhere).
   This lecture series will provide a general introduction into the experimental work to be carried out, mainly dealing with the properties of coordination compounds of transition metals.
   The practical experiments include:
   - an investigation of the oxidation states of vanadium;
   - the kinetics of oxidation of alcohols by chromium(VI);
   - synthesis and spectroscopic characterization of acetylacetonate derivatives of copper(II) and vanadium(IV);
   - synthesis, spectroscopic characterization and redox properties of polyoxometallates (POMs) of molybdenum(VI);
   - synthesis, spectroscopic characterization and reactivity of acetylacetonate derivatives of cobalt(III).

2. **Comparative Chemistry and Kinetics of Transition Metals (6 lectures + 1 tutorial, AE)**
   This lecture series is comprised of two parts.
   The first will give an introduction into the chemistry of chromium and vanadium. The following topics will be covered: general properties of Cr and V, oxidation states, species in aqueous solution, halides, oxides and oxohalides, coordination compounds, biological relevance of V. The learning outcomes that will be assessed will include the student being able to:
   - describe the general properties of V and Cr in different oxidation states;
   - describe the pH-dependent equilibria of V species in water;
   - write down balanced equations for the formation and reactions of V and Cr halides, oxides and oxohalides;
   - describe the coordination chemistry of V and Cr;
   - describe the biological relevance of V;
   - describe Cr-Cr multiple bonds;
   - interpret Frost-Ebsworth diagrams.

   The second part will discuss in detail the reaction mechanisms of ligand substitution reactions and of electron transfer reactions in transition metal complexes. The learning outcomes that will be assessed will include the student being able to:
   - describe the dissociative, associative and interchange mechanism for substitution reactions of coordination compounds;
   - plot reaction profiles for the dissociative, associative and interchange mechanisms;
   - interpret kinetic data in terms of the type of mechanism;
   - derive and apply the rate law for substitution reactions of Pt(II) complexes;
   - apply the concept of the *trans* effect to predict substitution products in Pt(II) complexes;
   - describe the Eigen-Wilkins mechanism;
   - describe the conjugate-base mechanism;
   - describe the inner-sphere and outer-sphere mechanism for electron-transfer reactions;
   - apply the Marcus-Hush equation.

3. **Complex Formation by the Transition Metals (8 lectures + 1 tutorial, PF)**
   Here we explore how crystal field theory (CFT) and molecular orbitals (MOs) theory are used to explain properties of transition metal coordination compounds. The student will endeavor to:
   - use point group character tables and orbital repulsions 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;
   - calculate 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;

- use laboratory measured properties in conjunction with crystal field theory to predict the geometries adopted by coordination compounds of transition metals in a variety of oxidation states, using a number of common ligands;
- draw MOs energy level diagrams and pictorial representations for the bonding in coordination compounds with σ-donor, π-donor and π-acceptor ligands;
- compare CFT and MOs approaches to describing the bonding in coordination compounds;
- correlate MOs diagrams with spectroscopic properties of coordination compounds and account for the order of ligands in the spectrochemical series.

4. Organometallic Compounds of the d-Block Elements (8 lectures + 1 tutorial, CP)

This lecture series details the structure, bonding and reactivity of organometallic complexes comprising d-block metal ions. On completion of this course students will:

- have a thorough understanding of most types of organometallic complexes along with a detailed knowledge of the various organic ligands (*e.g.* CO, NO, PR_3) used in their construction;
- be able to use MOs theory to describe the bonding in organometallic complexes;
- understand the 18-electron rule (and its limitations) and apply it to any type of organometallic species;
- understand various reaction mechanisms (*e.g.* β-H elimination, alkyl migration, oxidative addition) observed for organometallic complexes;
- have an excellent understanding of the catalytic capabilities of certain organometallic complexes (*e.g.* Grubbs and Schrock types).

5. Nuclear and Isotopic Chemistry (6 lectures + 1 tutorial, LR)

This lecture series will cover the basic concepts of nuclear chemistry and radioactivity. The learning outcomes that will be assessed are:

- 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).

Suggested references:

- C. E. Housecroft, A. G. Sharpe, *Inorganic Chemistry*, 4th Ed., Pearson Education Ltd., **2012**.
- Lecture notes, slides and literature papers provided on Blackboard in due course

PRACTICALS

The laboratory component is included in the CH334 Module "Experimental Chemistry 2" (see module description above). The main objectives are:

- To provide an appreciation of the scientific method in the observation, recording and interpretation of experimental data.
- To illustrate the chemical principles dealt with in the lecture course.
- To familiarise the student with important techniques fundamental to all chemical work.

The practicals are to be written up as a **separate report** and handed up in the lab each week.
To derive full benefit from the course the student should read details of the experiment to be performed **before doing each practical**.
The experiments include the following:

1. An investigation of the oxidation states of vanadium.
2. Kinetics of oxidation of alcohols by chromium(VI).
3. Preparation and investigation by infrared spectroscopy of bis(pentane-2,4-dionato)oxovanadium(IV) and some of its adducts with N-donor ligands.
4. Polyoxometallates: synthesis, characterisation and reduction of a heteropolytungstate.
5. Tris(pentane-2,4-dionato)cobalt(III), $[Co(pd)_3]$: synthesis, reactions and spectra

CH313 - Physical Chemistry with Learning Outcomes

Staff: Dr. Paul Kavanagh (Co-ordinator), Prof. Henry Curran, Dr. David Cheung and Dr. Alan Ryder

Text Book: *"Elements of Physical Chemistry", 5th Edition, by Atkins and De Paula, available in the library and in the university book shop, price €36.00.*

Molecular Interactions (4 h, HC): Chapter 15 of textbook

Students will understand that:

- A 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.

Chemical Kinetics (4 h, HC): Chapters 10 and 11 of textbook

Students will be able to:

- Derive the rate law for a first and second order reaction and from that determine the half-life for a reaction and the rate of reaction.
- Determine the kinetics for an elementary reaction.
- Explain the kinetics associated with flow reactors and jet-stirred reactors.
- Understand how the rate constant of a reaction varies with temperature, and derive the frequency A-factor and activation energy of a reaction given the rate constant and different temperatures.
- Appreciate and understand the dependence of kinetics on thermodynamics of reactants and products.

Phase diagrams of mixtures (4 h, PK): Chapter 6 of textbook

Students will understand that:

- The equilibria between phases (at constant pressure) are represented by lines on a temperature-composition phase diagram, and the relative abundance of phases is obtained by using the lever rule.
- A regular solution is one in which the entropy of mixing, but not the enthalpy of mixing, is the same as an ideal solution.
- An azeotrope is a mixture that vaporizes and condenses without a change in composition; a eutectic is a mixture that freezes and melts without change of composition.

Macromolecules (4 h, DC): Chapter 16 of textbook

Students will understand that:

- Many proteins are monodisperse, while a synthetic polymer is polydisperse.
- The definitions of number-average molar mass and weighted-average molar mass and the difference between the two.
- Techniques for the determination of the mean molar masses of molecules and in particular viscosity measurements and gel permeation chromatography.
- An understanding of the different categories of polymers.
- The classification of polymers and the main properties of thermoplastics, elastomers and thermosets.
- The properties of amorphous and crystalline polymers.
- 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.
- The mechanical properties of polymers and how they are influenced by the glass transition temperature, molar mass and molar mass distribution.
-

Surface Chemistry (4 h, DC): Chapter 18 of textbook

Students will understand that:

- Adsorption is the attachment of molecules to a surface; the substance that adsorbs is the adsorbate and the underlying material is the adsorbent or substrate. The reverse of adsorption is desorption.
- The fractional coverage, θ, is the ratio of the number of occupied sites to the number of available sites.
- Techniques for studying the rates of surface processes include flash desorption, surface Plasmon resonance (SPR), and gravimetry by using a quartz crystal microbalance (QCM).
- Physisorption is adsorption by a van der Waals interaction; chemisorption is adsorption by formation of a chemical bond.
- The Langmuir isotherm is a relation between the fractional coverage and the partial pressure of the adsorbate, $\theta = K\pi/(1+K\pi)$
- The isosteric enthalpy of adsorption is determined from a plot of ln K versus $1/T$.
- The BET isotherm is an isotherm applicable when multilayer adsorption is possible.
- The sticking probability, *s*, is the proportion of collisions with the surface that successfully lead to adsorption.

Electrochemistry(4 h, PK): Chapter 16 of textbook

Students will understand that:

- 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.

Quantum Chemistry (4 h, AR): Chapter 12 of 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 hν. Einstein proposed that *atoms* oscillating in a solid with frequency ν could acquire or discard energy in quanta of magnitude hν.
- 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 wavefunction, Ψ, contains all the dynamical information about a system and is found by solving the appropriate Schrödinger equation, $-(\bar{h}^2/2m)\mathrm{d}^2\psi/\mathrm{d}x^2 + \mathrm{V}\psi = \mathrm{E}\psi$, 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 wavefunction 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 wavefunctions 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 wavefunctions are $\Psi_n(x) = (2/L)^{1/2}\sin(n\pi x/L)$.
- Because wavefunctions do not decay abruptly to zero, particles may tunnel into classically forbidden regions. Two aspects of tunnelling include radioactivity and scanning tunnelling microscopy.
- The energy levels of a particle of mass m on a circular ring of radius r are $E_{m_I} = m_I^2\hbar^2/2I$ where I is the moment of inertia, $I = mr^2$ and $m_I = 0, \pm1, \pm2$, etc.
- The angular momentum of a particle on a ring is quantized and confined to the values $J_z = m_I\hbar$, $m_I = 0, \pm1, \pm2$, 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 $E_v = (v + ½)h\upsilon$, where $\upsilon = (1/2\pi)(k/m)^{1/2}$ and v = 0, 1, 2, …

Spectroscopy (4 h, AR): Chapter 19 of textbook

Students will understand that:

- 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. D 3 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 $\Delta J = \pm1$, $\Delta K = 0$; 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 are $E_v = (v + 1/2)hcv$ with $v = 0, 1, 2, \ldots$, 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 centre of inversion, then no modes can be both infrared and Raman active.

CH3103-Validation Enterprise with Learning Outcomes

Staff: Dr. Constantina Papatriantafyllopoulou (Co-ordinator), Dr Ray McCarthy and Prof. Michael J. Hynes

Schedule: **Lectures (18)** Wednesday 9-10 am / Thursday 9-10 am / Thursday 11-12 am (Semester 2)

Assessment:
Continuous assessment –Project to be undertook along with a presentation.
Final written paper

Attendance:
Attendance at all lectures is compulsory.

Validation Course Outline (18 lectures): This module covers pertinent topic concerning validatory requirements within the bio-, pharmaceutical and chemical industries. Detailed insights into the inner workings of industry are also given.

Validation: Learning Outcomes:

• The student 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.

• The student will be introduced to the concept of Good Manufacturing Practice (GMP) and Good Laboratory (GLP) in relation to the pharmaceutical and chemical industries.

• Students will then learn of the numerous and pertinent aspects of Cleaning Validation with respect to the manufacturing industry.

• A broad knowledge of the subject of Equipment qualification (which includes Design, Installation, Process and Performance Qualification) is given.

• The student will then be introduced to the cutting-edge field of Process Analytical Technology (PAT) and will begin to understand its immense relevance to the future of pharmaceutical manufacturing.

• Students will 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.

CH3101 Computers in Chemical Research 2016 - 2017, Semester 2

Staff: .Dr. Niall Geraghty (Course Co-ordinator), Dr. David Cheung, Dr. Peter Crowley, Prof. Henry Curran, Dr. Andrea Erxleben, Dr. Pau Farras, Dr. Paul Kavanagh and Dr. Pat O'Leary.

Course Outline: 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.

Schedule: Semester 2, Monday and Friday, 2.00-5.00, computer workshops in the Arts-Science Computer Suite

Assessment: Continuous assessment based on two workshop reports each week. An extended essay, poster and presentation, on an individual topic that will be given to each student at the beginning of the semester, are also part of the assessment process.

Learning Outcomes

On completion of the course the student will be able to:

- produce scientific written reports and that includes communication of chemical information such as structures, tables of data, other figures such as molecular graphics to present chemical information
- produce spreadsheets and graphs using Excel for inclusion in reports and for analysing data
- source information from the primary scientific literature using various resources such as online library, 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 a group
- 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 or biopharmaceutical chemistry
- to use protein and other structural databases
- to produce a poster suitable for a scientific conference
- to give a Powerpoint presentation

Week	Week beginning	Monday			Friday		
		Task	**Software**	**Lecturer**	**Task**	**Software**	**Lecturer**
1	9th January				Introduction and project assignment		
2	16th January	Report writing	MS Word	Dr. Andrea Erxleben	Molecular graphics	ChemDraw	Dr. Pat O'Leary
3	23rd January	Spreadsheets in the lab	MS Excel	Prof. Henry Curran	Technical writing	MS Word	Dr. Niall Geraghty
4	30th January	Data fitting and plotting	MS Excel	Prof. Henry Curran	Plagiarism	Turnitin	Dr. Pau Farras
5	6th February	Molecular modelling 1: structure building and optimization	Spartan '10	Dr. Niall Geraghty	Referencing	EndNote	Dr. Pau Farras
6	13th February	Molecular modelling 2: conformational analysis and conformational searching	Spartan '10	Dr. Niall Geraghty	Presentations	MS PowerPoint	Dr. Peter Crowley
7	20th February	e-Searching chemical literature	Reaxys, SciFinder and Web of Knowledge	Dr. Pat O'Leary	Presentations	MS PowerPoint	Dr. Peter Crowley
8	27th February	Working with proteins	PDB	Dr. Peter Crowley	Posters and how to produce them	MS PowerPoint	Dr. Paul Kavanagh
9	6th March	Working with databases	Cambridge Structural Database (CSD)	Dr. David Cheung	Project report and presentation preparation		
10	13th March	Project report and presentation preparation					
11	20th March	Project report and presentation preparation					
12	27th March	Project Presentations					

Week beginning		05-Sep	12-Sep	19-Sep	26-Sep	03-Oct	10-Oct	17-Oct	24-Oct	31-Oct	07-Nov	14-Nov	21-Nov
Third Year Chemistry: First Semester: 2016-2017													
Week no.	**Time**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
		CH311 - Organic Chemistry; first lecture											
Mon	**9**	**Natural Products**			**Heterocyclic**			**Phys Org**			**Stereochem**		
Dillon		**PC**			**FA**			**PVM**			**NG**		
CH332 - Approaches to Drug Design & Discovery													
Tue	**9**	**Drug Design**											
Dillon		**DC**											
		CH326 - Analytical Chemistry and Molecular Structure; first lecture											
Tue	**10**	**NMR**			**Mass Spec**	**XRF/TA**		**GC**	**Crystal Dif**	**SurfA**	**HPLC**	**TUT**	**SurfA**
Dillon		**NWG**			**POL**	**AR**		**NWG**	**AE**	**AR**	**NWG**		**AR**
		CH326 - Analytical Chemistry and Molecular Structure; second lecture											
Wed	**11**	**NMR**			**Mass Spec**	**XRF/TA**	**GC**		**Crystal Dif**	**SurfA**	**HPLC**	**TUT**	**SurfA**
Dillon		**NWG**			**POL**	**AR**	**NWG**		**AE**	**AR**	**NWG**		**AR**
CH332 - Approaches to Drug Design & Discovery													
Thu	**9**	**Drug Design**											
Dillon		**OT**						**FA**					
		CH311 - Organic Chemistry; second lecture											
Fri	**10**	**Natural Products**			**Heterocyclic**			**Phys Org**			**Stereochem**		
Dillon		**PC**			**FA**			**PVM**			**NG**		
		CH311 - Organic Chemistry; third lecture											
Fri	**11**	**Natural Products**			**Heterocyclic**			**Phys Org**			**Stereochem**		
Dillon		**PC**			**FA**			**PVM**			**NG**		
		CH326 - Analytical Chemistry and Molecular Structure; third lecture											
Fri	**12**	**NMR**		**Mass Spec**		**XFR/TA**	**GC**	**Crystal Diff**		**HPLC**		**TUT**	**TUT**
Dillon		**NWG**		**POL**		**AR**	**NWG**	**AE**		**NWG**			**AR**
Mon	2		**CH332 labs**										
T or W	**2**	**Registration**	**CH333 Labs**					**CH333 Labs**					
or T		**in lectures**	**Organic Practicals**					**Analytical Chemistry/Molecular Structure**					**Orals**
											Bank Holiday		

Week beginning		09-Jan	16-Jan	23-Jan	30-Jan	06-Feb	13-Feb	20-Feb	27-Feb	06-Mar	13-Mar	20-Mar	27-Mar
Third Year Chemistry: Second Semester: 2016-2017													
Week no.	**Time**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
		CH313 - Physical Chemistry; first lecture											
Mon	9	Phases		Mol. Int.	Spect	Kinetics	Macro		Surface	Echem		Quantum	Tutorial
Dillon		PK		HC	AR	HC	DC		DC	PK	AN Other	AR	
		CH307 Inorganic Chemistry; first lecture											
Tue	10	Lab Intro	Organomet. Chem.			Comp. Chem./Kinetics		Test 1	Coord. Chem.		Nucl. Chem		Tutorial
Dillon		LR	CP			AE			PF		LR		AE
CH313 - Physical Chemistry; second lecture													
Tue	11	Phases	Mol. Int.		Spect	Kinetics	Macro	Surface		Echem	Quantum	Isotopes	Tutorial
Dillon		PK	HC		AR	HC	DC	DC		PK	AR	LR	
CH313 - Physical Chemistry; third lecture													
Wed	10	Phases	Mol. Int.	Spect		Kinetics	Macro	Surface	Echem		Quantum	Isotopes	Tutorial
Dillon		PK	HC	AR		HC	DC	DC	PK		AR	LR	
		CH307 Inorganic Chemistry; second lecture											
Wed	11	Lab Intro	Organomet. Chem.	Comp. Chem./Kinetic		Coord. Chem.			Nucl. Chem.		Test 2		Tutorial
Dillon		LR	CP	AE		PF			LR				PF
CH313 - Physical Chemistry; fourth lecture													
Fri	10	Phases	Mol. Int.	Spect	Kinetics		Macro	Surface	Echem	Quantum		Tutorial	Tutorial
Dillon		PK	HC	AR	HC		DC	DC	PK	AR			
		CH307 Inorganic Chemistry; third lecture											
Fri	11	Organomet. Chem		Comp. Chem./Kinetic		Coord. Chem.				Nucl. Chem.		Tutorial	Tutorial
Dillon		CP		AE		PF				LR		CP	LR
CH334 - Experimental Chemistry 2													
T or W or T	2	Practicals						Practicals					
		Inorganic Practicals					Inorg. Orals	Physical Practicals					Phy. Orals
CH3103 - Validation in the Pharmacetucal & Medical Device Industry													
Wed	9	Validation		Validation		Med Dev	Reach						
Dillon		CP		CP		RMC	MH						
CH3103 - Validation in the Pharmacetucal & Medical Device Industry													
Thu	9	Validation		Validation		Med Dev	Reach						
Dillon		CP		CP		RMC	MH						
CH3103 - Validation in the Pharmacetucal & Medical Device Industry													
Thu	11	Validation		Validation		Med Dev	Validation						
AC216		CP		CP		RMC	CP						
CH3101 Computers in Chemical Research													
Monday	2 to 5	Introductio	e-searching	lol. Graphic		MS Excel	Spartan '10		PCD	Powerpoint		Project Presentations	
Arts/Sci Computer Suite			POL	POL		HC	NG		PC	TBA			
Friday	2 to 5	TW	Report Writ	Plagiarism	Referencin	Audience	Presentations	Style	Summarie	Graphics	Project	Project Presentations	
Arts/Sci Computer Suite		TBA	AE	TBA	TBA	TBA	TBA	TBA	TBA	TBA			