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**Third Year 2014-2015**

Summary of Course Structure – for Biopharmaceutical Chemistry Students

**Semester One Module Descriptions**

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## Summary of Course Structure 2012-13

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**Note** – BPC Summer industrial work placements (12 weeks approx) are coordinated by Dr. Aldabbagh, and will involve a competitive application and interview process. NUI Galway students have been placed at the following companies; Roche, GSK, UCB, MSD, and Coca Cola. The successful completion of a summer placement will lead to the award of the Certificate in Professional Practice, and is awarded credit as part of CH451 (Fourth Year module).
Schedule

Semester I

CH331 – First Lecture is in the Dillon @ 9.00 am, Monday, 8th September
& Lab. Registration @ First Lecture

CH326 – First Lecture is in the Dillon @ 10.00 am, Thursday, 11th September

CH332 – First Lecture is in the Dillon @ 9.00 am, Tuesday, 9th September

CH332 – First Lab starts on Monday October 20th in the Software Engineering Suite, which is located very close to Physical Chemistry at 2.00 pm

Semester II

CH307 – First Lecture is in the Dillon @ 9.00 am, Monday, 12th January

CH330 – First Lecture is in the Dillon @ 9.00 am, Tuesday, 13th January

CH338 – First Lecture is in the Dillon @ 10.00 am, Tuesday, 13th January

CH3102 - First Lab in Arts/Science Computer Suite @ 2.00 pm, Friday, 16th January

Full Semester One and Semester Two Timetables are posted on the School of Chemistry website
Organic Chemistry – CH311 with Learning Outcomes

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

Heterocyclic Chemistry (9 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 & Peptide Synthesis (9 h, PM)

Acid-base chemistry (3 h)
Write expressions for Ka and pKa
Use Ka and pKa 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 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 pKa to other properties (e.g. leaving group ability, nucleophilicity).

Mechanism (4 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 write organic reaction mechanisms (e.g. acid and base promoted hydrolysis of esters; acid catalysed formation/hydrolysis of acetals/ketals)

Peptide synthesis (2 h)
To be able to describe how to carry out peptide synthesis, including solid phase peptide synthesis

Natural Product Chemistry (9 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.

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 (9 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 carbocyclic 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 auxiliary) 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.

Also see CH333 module description below.
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.
- 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 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 regular 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).
# Analytical Chemistry & Molecular Structure – CH326 with Learning Outcomes

Staff: Dr. Niall Geraghty (Co-ordinator)

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<td>Crystal Diffraction</td>
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<td>Gas Chromatography</td>
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**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

**Gas Chromatography:**
- Explain at both phenomenological and theoretical levels the separation of molecules using chromatography
- Explain the function(s) of the instrumentation used in gas chromatograph, to include descriptions of the instrumentation

**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 affect 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 ($\delta$) 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 $\pi$ bond (alkene, aromatic system) will appear downfield/has a large chemical shift ($\delta$)
• The ability to use a $^1$H-NMR correlation table to relate the $\delta$ value of a signal to the type of proton responsible for it
• 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
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• A recognition that a nucleus close to a electronegative atom, and in most cases (but not always) close to a $\pi$ bond (alkene, aromatic system) will appear downfield/has a large chemical shift ($\delta$)
• The ability to use a $^1$H-NMR correlation table to relate the $\delta$ 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 $\delta$ 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)

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, electrospray, 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.
CH334 Experimental Chemistry 2

Staff: Dr. Andrea Erxleben (Co-ordinator), Dr. Tim Higgins, Dr. Luca Ronconi, Prof. Heny Curran, Prof. Donal Leech, Dr. Alan Ryder

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 stoichiometric 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).
LECTURES (32 lectures, 4 tutorials)

1. Complex Formation by the Transition Metals (8 lectures, TH)
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 endeavour 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 stabilisation 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.

2. Biological Functions of Metals (4 lectures, TH)
Here we explore how the chemical properties of metallic elements are exploited by biological systems. The student will be expected to:
- Describe the roles found for metal cations in biological systems and relate these roles to the chemical properties of the cations.
- Describe the structural features of metallo-proteins and relate these features to biological functions.
- Give examples that illustrate the variety of roles metallo-proteins perform in biological systems.

3. Comparative Chemistry of the Transition Metals (4 lectures, AE)
This lecture series 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.

4. Inorganic Kinetics (4 lectures, AE)
This lecture series 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.

5. Organometallic Compounds of the d-Block Elements (8 lectures, DM)
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, PR₃) 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).

6. Nuclear and Isotopic Chemistry (4 lectures, 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:
➢ Lecture notes and slides.

PRACTICALS
The laboratory component is included in the CH334 Module “Experimental Chemistry 2” (see module description below). 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.
5. Tris(pentane-2,4-dionato)cobalt(III), [Co(pd)_3]: synthesis, reactions and spectra.
Physical Chemistry – CH330 with Learning Outcomes

Staff: Prof. Henry Curran (Co-ordinator), Dr. Another and Dr. Alan Ryder


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, Another): 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, Another): 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, Another): 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, \( \theta \), 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, Another): 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, \( j = j_0 e^{\left( (1-\alpha)\eta - \alpha \eta \right)} \), where \( \eta \) is the overpotential, \( \eta = E' - E_i \), \( \alpha \) is the transfer coefficient, and \( j_0 \) 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 \( \alpha \) 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 \( T\lambda_{\text{max}} = \text{constant} \); the Stefan-Boltzmann law states that the emission of a black body is proportional to \( T^4 \). Planck proposed that electromagnetic oscillators of frequency \( v \) could acquire or discard energy in quanta of magnitude \( h v \).
• Einstein proposed that atoms oscillating in a solid with frequency \( v \) could acquire or discard energy in quanta of magnitude \( h v \).
• 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 \( E_k = h v - \phi \), where \( \phi \) is the work function of the metal. The de Broglie relation for the wavelength, \( \lambda \), of a particle of linear momentum \( p \) is \( \lambda = \hbar / p \).
A wavefunction, $\Psi$, contains all the dynamical information about a system and is found by solving the appropriate Schrödinger equation, $-(\hbar^2 / 2m)\frac{d^2\psi}{dx^2} + V\psi = E\psi$, 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 $\delta V$ is proportional to $\psi^2\delta V$, where $\psi$ 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 $E_n = n^2\hbar^2 / 8mL^2$, with $n = 1, 2, \ldots$ 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 $E_n = (n_1^2/L_1^2 + n_2^2/L_2^2 + n_3^2/L_3^2)(\hbar^2/8m)$, with $n = 1, 2, \ldots$ 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 tunneling include radioactivity and scanning tunneling microscopy.

The energy levels of a particle of mass $m$ on a circular ring of radius $r$ are $E_{\phi_n} = \frac{m^2\hbar^2}{2I}$ where $I$ is the moment of inertia, $I = mr^2$ and $m_1 = 0, \pm 1, \pm 2, \ldots$.

The angular momentum of a particle on a ring is quantized and confined to the values $J_z = m_1 \hbar$, $m_1 = 0, \pm 1, \pm 2, \ldots$.

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 $E_v = (v + \frac{1}{2})\hbar\nu$, where $\nu = (1/2\pi)(k/m)^{1/2}$ and $v = 0, 1, 2, \ldots$.

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. Another contribution to linewidth is lifetime broadening: $\delta E = \hbar/\tau$, where $\tau$ 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 $E_J = \hbar BJ(J+1)$ with $J = 0, 1, 2, \ldots$, where $B = h/(4\pi\hbar$) is the rotational constant of a molecule with moment of inertia $I$.
- The Pauli principle states for fermions $\Psi(B,A) = -\Psi(A,B)$ and for bosons $\Psi(B,A) = \Psi(A,B)$. 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 are $E_v = (v + 1/2)\hbar c v$ with $v = 0, 1, 2, \ldots$, where $v = (1/2\pi)(k/\mu)^{1/2}$ 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.
Drug Design and Drug Discovery – CH332 with Learning Outcomes

Staff: Prof. Robert Woods (Co-ordinator), Dr. Fawaz Aldabbagh, Dr. Another

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

Assessment:
Continuous assessment – reports based on computer labs
Final written paper – Answer four questions (one question per main topic).

Attendance:
Attendance at all lectures and labs is compulsory. Students will not be eligible to sit the final written exam if they have missed more than 3 lectures and 3 labs without a medical cert.

Approaches to Drug Design (RW)

Basic concepts of Molecular Modelling:
• Relative energy versus absolute energy versus thermodynamics.
• Potential energy functions, energy minimization and validating theory with experiment

Databases as sources of information:
• The Cambridge Chemical Structure Database (CCSD),
• The Protein Data Bank (PDB)

Modelling Solvent Effects in Molecular Interactions
• The role of solvent: Hydrogen bonding and explicit models
• Implicit models and the dielectric
• Computing intermolecular interaction energies

Challenges in Modelling Biomolecules:
• Protein folding and conformational sampling
• Levinthal’s Paradox and the theory of protein folding
• The fundamentals of protein structure
• Homology modelling: Theory, application and model validation
• The structure and thermodynamics of protein ligand complexes

Computational Approaches to Characterize Biomolecular Interactions
• The strengths and weaknesses of Computational Docking
• Blind versus focused docking and virtual library screening
• Molecular Dynamics simulation techniques
• The importance of convergence in molecular simulations
• Computing binding free energies


Students will gain an understanding of:

Potential Energy Functions
Energy Minimization: Steepest Descent/Conjugate Gradient/Grid Searching
Automated ligand docking
Molecular dynamics (MD) simulations
Computing ligand binding energies from MD data
The importance of water in modelling
Approaches to predicting the 3D structure of proteins
The structure and thermodynamic properties of protein secondary elements
The structure and thermodynamics of protein-ligand interactions
How to compare theoretical and experimental data

Practicals
The Molecular Modelling Practical Course will take place over a 12 week period (6 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.

The practicals are to be written up as a separate Report and handed up in the lab each week. The experiments are to be done in sequence. To derive full benefit from the course the student should, before coming to the laboratory, read details of the experiment to be performed.

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 isalloxazine ring of FADH₂.
- 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.
CH339-Validation Enterprise with Learning Outcomes

Staff: Dr. Another (Co-ordinator) and Dr Ray McCarthy

Schedule: Lectures (18) Tuesday/ Wednesday / Thursday 9-10 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.
**CH335- Industrial Chemistry: Learning Outcomes**

Staff: Dr. Judith Wurmel

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

**Assessment:** Final written paper and optional continuous assessment worth 10%

**Attendance:**
Attendance at all lectures is compulsory.

Detailed insights into the inner workings of the chemical and pharmaceutical industry are given, including specific examples of chemistry carried out in industry.

**Industrial Chemistry (18 lectures): Learning Outcomes. Students will be expected to have knowledge about the following topics.**

- The structure of the Medical device and Chemical and Pharmaceutical industries.
- The top US and European chemical companies.
- A knowledge of the top inorganic and organic chemical production tables.
- The factors which push chemicals to the top of these production lists.
- The European chemical industry and the numbers employed in it.
- Base chemicals and their source and their conversion to other bulk chemicals.
- Relationship between the oil industry and chemical production.
- What the major chemicals produced are used for.
- Economic factors and the chemical industry.
- The importance of research and development in the industry.
- Industrial chemical processes versus laboratory chemical processes.
- Batch processes versus flow or continuous processes.
- Homogeneous versus heterogeneous catalysis.
- The chlor-alkali industry and why it is so large.
- How environmental factors have led to continued improvements in this industry and in the cell types used.
- The aluminium smelting industry.
- Raw material sources in the chemical industry.
- The Frasch process for sulphur production.
- The importance of the catalytic processes for the synthesis of ammonia.
- Raw materials for carbon based compounds.
- Refinery processes.
- Fischer-Tropsch synthesis.
- Syn-gas
- Getting oxygen into organics.
- Transition metal catalysed reactions.
- The Oxo-Process and the Wacker process.
- Monsanto acetic acid process.
- Zeigler-Natta processes and polymer stereochemistry.
- Metallocene catalysts.
- Olefin or alkene metathesis.
CH3102- Introduction to Research and Communication
Please note this module is worth 5 credits.

**Semester 2**

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Contact Person for Elective modules in Biochemistry

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Electives in semester 1 are one of the following:

Cell Biology BI309 or Molecular Biology BI319

Electives in semester 2 are two of the following:

Validation (CH339)
Industrial Chemistry (CH335)
Protein Biochemistry (BI321)
Or Cell Signalling (BI313)

Industrial Chemistry and Validation will be taught Tues/Wed/Thurs 9-10am in Semester 2.