



NUI Galway  
OÉ Gaillimh



## 2<sup>nd</sup> Year Chemistry Information Booklet 2021–22

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*“If you put a spoonful of wine in a barrel full of sewage, you get sewage. If you put a spoonful of sewage in a barrel full of wine, you get sewage”*  
Schopenhauer’s law of entropy (from Murphy’s Law Complete, A. Bloch, 1990)

**Summary of Course Structure 2021/22  
Core Chemistry (CH201)**

<i>Code</i>	<i>CH204</i>	<i>CH203</i>	<i>CH202</i>	<i>CH205</i>
<i>Title</i>	<i>Inorganic Chemistry</i>	<i>Physical Chemistry</i>	<i>Organic Chemistry</i>	<i>Analytical &amp; Environmental Chemistry</i>
<i>ECTS</i>	5	5	5	5
<i>Semester</i>	<i>I</i>	<i>I</i>	<i>II</i>	<i>II</i>
<i>Lectures</i>	<i>4 hr/week</i>	<i>4 hr/week</i>	<i>4 hr/week</i>	<i>4 hr/week</i>
<i>Practical duration</i>	<i>4hr/week</i>	<i>4hr/week</i>	<i>4hr/week</i>	<i>4hr/week</i>
<i>Delivery</i>	<i>1<sup>st</sup> half Sem I</i>	<i>2<sup>nd</sup> half Sem I</i>	<i>1<sup>st</sup> half Sem II</i>	<i>2<sup>nd</sup> half Sem II</i>
<i>Assessment</i>				
<i>Examination:</i>	<i>2 hr Sem I</i>	<i>2 hr Sem I</i>	<i>2 hr Sem II</i>	<i>2 hr Sem II</i>
<i>MOSTLY 70% of final</i>			<i>65% of final mark</i>	
<i>Practical Marks 30% of final</i>	<i>Continuous Assessment+ MCQ</i>	<i>Continuous Assessment+ MCQ</i>	<i>Continuous Assessment</i>	<i>Continuous Assessment</i>
<i>Online Homework</i>			<i>5% of final mark</i>	

**Expected workload for each module**

<b>5 Credit Module</b>	<b>100–125 h</b>
Contact with staff:	~48 h
Examinations (written and practical)	~2hr
Autonomous learning:	~50–75 h (about 4 h/week)

Autonomous learning includes time spent working independently reporting on practicals, learning, revising, additional reading, studying.

**NOTE:** You pass **Chemistry (CH201)** by obtaining **40% or over** for each module, CH202, 203, 204, 205 AND a satisfactory performance in each evaluated component of the module

No candidate shall pass in an examination whose Laboratory Work, Computer Work, Project or Year's Work fails to satisfy the Science Examiners. Candidates at the Summer Examinations in Science who are deficient in their attendance at the academic exercises or in the submission of their Year's Work may, on the recommendation of the Board of Examiners, be excluded from admission into the relevant Autumn Examination.

**Persistent absence by a student from weekly laboratory sessions will mean that the student's laboratory work will fail to satisfy the examiners and the student will be prohibited from passing (i.e. they are incomplete) and will be excluded from admission into the relevant Autumn Examination and have to repeat the whole year.**

## Inorganic Chemistry I – CH204

Staff: Dr. Andrea Erxleben (Module co-ordinator), Dr. Pau Farras, Dr. Luca Ronconi

**Text Book:** "Inorganic Chemistry" C. E. Housecroft and A. G. Sharpe; 4<sup>th</sup> Ed.; Pearson Education Ltd.: Harlow, 2012.

### Lecture Course Outline:

1. Structure in the Solid State (4 lectures, A. Erxleben)
2. Titrations, Calculations and Redox Reactions (2 lectures, L. Ronconi)
3. Molecular Structure & Bonding (6 lectures, L. Ronconi)
4. Comparative Chemistry of the Elements (6 lectures, A. Erxleben)
5. Co-ordination Compounds (6 lectures, P. Farras)

### 1. Structure in the Solid State

This lecture series will cover metallic and ionic lattices, polymorphism, alloys, intermetallic compounds and the Born-Haber cycle. The learning outcomes that will be assessed will include:

- The student being able to describe the packing-of-spheres model.
- The student being able to describe common types of packing in metal lattices (cubic and hexagonal close-packing, simple cubic, body-centred cubic)
- The student being able to describe the most important ionic lattices (NaCl lattice, CsCl lattice, CaF<sub>2</sub> lattice, zinc blende and wurtzite lattice, TiO<sub>2</sub> lattice)
- The student being able to explain the following terms; polymorphism, alloy (substitutional, interstitial), intermetallic compound, metallic radius, unit cell, octahedral and tetrahedral sites in lattices.
- The student being able to draw the Born-Haber cycle and to apply the Born-Haber cycle to calculate lattice energies,  $\Delta_f H^\circ$ ,  $\Delta_a H^\circ$ , dissociation energies, ionization energies or electron affinities.

### 2. Titrations and calculations

These lectures will cover the theory of the titration experiments and the redox reactions that the student will carry out during the practicals. The learning outcomes that will be assessed will include:

- The student being able to solve unseen titration calculation problems
- The student being able balance redox equations
- The student being able to use redox potentials to predict the products of redox reactions

### 3. Molecular Structure & Bonding

The learning outcomes that will be assessed are:

- basic principles (periodic properties of the elements, chemical bonding, oxidation numbers, valence);
- the octet rule, formal charges and drawing Lewis structures;
- the Valence-Shell Electron-Pair Repulsion (VSEPR) theory, including practical applications to derive the some molecular properties (geometry, shape, polarity, isomers), and its limitations;
- the hybridization model and the Valence Bond (VB) theory, including practical applications to derive the molecular geometry, and their limitations;

- Linear Combination of Atomic Orbitals (LCAO) and the Molecular Orbitals (MOs) theory;
- application of the MOs theory to sketch diagrams for simple homonuclear and heteronuclear diatomic molecules and to predict their bond orders and magnetic properties.

#### 4. Comparative Chemistry of the Elements

This lecture series will give an overview of the properties and reactions of the elements of group 1, 2, 13 – 18. The learning outcomes that will be assessed will include:

- The student understanding trends in physical and chemical properties in the main groups of the Periodic Table.
- The student being familiar with the physical and chemical properties of selected main group elements.

#### 5. Co-ordination Compounds

The reactions of transition metal compounds with ligands, the properties of the molecules formed and the theories used to explain these phenomena will be explored. The student will endeavour to be able to:

- Give valence shell electron configurations for coordination compounds of the transition metals and their ions
- Draw molecular structures for common ligands and the coordination compounds they form with the transition metals, to include isomers
- Use chemical equations to represent the reactions involved in the formation of transition metal coordination compounds
- Give scientific accounts, at the phenomenological level, of magnetism and colour and their measurement using Gouy balance and spectrometer
- Use crystal field theory to explain the origin of colour and magnetism in transition metal compounds and to account for measured magnetic moments and maximal wavelengths of absorption.

#### Practicals

The Inorganic Practical Course will take place over a 5 week period (4 hrs per week). There will be a tutorial at the end of each practical session. 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. There will be an MCQ examination at the end of the practical course.

The principal objectives of the CH204 laboratory course 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. The experiments are to be done in cyclic order (by each individual student); for example, if you begin with experiment number 3, then the next week you will do #4, followed by #5 etc. For some experiments students may work in pairs. To derive full benefit from the course the student should, before coming to the laboratory, read details of the experiment to be performed.

The experiments include the following:

1. Complexometric Titrations using EDTA
  - (a) Determining the Hardness of Water.
  - (b) Separation of Zinc and Magnesium on an Anion Exchange Resin.

2. (a) Gravimetric Determination of Nickel.  
(b) Application of Spot Tests.
3. Introduction to Molecular Modelling.
4. Oxidation States of the First Transition Series.
5. Preparation and Analysis of an Iron Oxalate Complex.

### Tutorials

Tuesdays and Thursdays, 5 - 6 pm during week 2 - 6

Solid state chemistry	Dr Erxleben	Tuesday, September 13 and Thursday September 15 *)
Titration calculations and redox equations	Dr Ronconi	Tuesday, September 20 and Thursday September 22 *)
Molecular structure and bonding	Dr Ronconi	Tuesday, September 27 and Thursday September 29 *)
Comparative chemistry	Dr Erxleben	Tuesday, October 4 and Thursday October 6 *)
Coordination chemistry	Dr Farras	Tuesday, October 11 and Thursday October 13 *)

\*) parallel sessions

## Physical Chemistry I: CH203

Staff: Dr. David Cheung (Module Co-ordinator), Prof. Henry Curran, Prof. Donal Leech, Prof. Alan Ryder

**Text Book:** "Elements of Physical Chemistry", 4<sup>th</sup> or 5<sup>th</sup> Edition, by Atkins and De Paula, available in the library and in the university book shop, price €39.95. This text is also the prescribed text for third year physical chemistry.

### Thermodynamics (6 h, DC): Chapters 1–4 of textbook

Students will understand that:

- The kinetic model of gases expresses the properties of a perfect gas in terms of a collection of mass points in ceaseless random motion
- Real gas properties deviate from that of a perfect gas because of molecular interactions
- Maximum expansion work is achieved in a reversible change
- The 1<sup>st</sup> law of thermodynamics states that the internal energy of an isolated system is constant
- The standard enthalpy of a process is the sum of the standard enthalpies of the individual processes into which it may be regarded as divided
- A spontaneous change is a change that has a tendency to occur without work having to be done to bring it about
- The 2<sup>nd</sup> law of thermodynamics states that entropy of an isolated system tends to increase
- The 3<sup>rd</sup> law of thermodynamics states that the entropies of all perfectly crystalline substances are the same at T=0 (and may be taken to be zero)

### Spectroscopy (3 h, AR): Chapter 19 and 20 of textbook

Students will understand that:

- Energy is quantised, with transitions allowed between energy states
- The Beer-Lambert law relates intensity of absorption of radiation to concentration of the absorbing species
- The Franck-Condon principle states that because nuclei are much more massive than electrons an electronic transition takes place faster than the nuclei can respond.
- A selection rule is a statement about when the transition dipole is non-zero.
- A gross selection rule specifies the general features a molecule must have if it is to have a spectrum of a given kind. The gross selection rule for MIR absorption is that there must be a change in dipole moment during the motion for the vibration to be IR active. For Raman spectroscopy there must be a change in polarizability for the molecule/vibration to be Raman active
- A specific selection rule is a statement about which changes in quantum number may occur in a transition. The specific selection rule for vibrational spectroscopy is  $\Delta v = \pm 1$ .
- The vibrational energy levels of a molecule are given by:

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

- $\mu$  = effective or reduced mass, for a diatomic AB,  $\mu = m_A m_B / (m_A + m_B)$
- The number of vibrational modes for a non-linear molecule is  $3N-6$ , for a linear molecule it is  $3N-5$  where N is the number of atoms in the molecule.
- Fluorescence is the spontaneous emission of light from molecules where the transitions occurs from states of the same multiplicity.
- Phosphorescence is the spontaneous emission of light from molecules where the transitions occurs from states of the different spin multiplicity.

**Chemical Equilibrium** (3 h, AR): Chapter 7 of textbook.

Students will understand that:

- The reaction Gibbs energy is the slope of a plot of Gibbs energy against composition
- The condition of chemical equilibrium at constant pressure and temperature is  $\Delta_r G = 0$ .
- The equilibrium constant is the value of the reaction quotient at equilibrium.
- A compound is thermodynamically stable with respect to its elements if  $\Delta_f G^\ominus < 0$ .
- The equilibrium constant of a reaction is independent of the presence of catalysts and independent of the pressure.
- The standard reaction Gibbs Energy  $\Delta_r G^\ominus$  can be calculated from Standard Gibbs energies of formation ( $\Delta_f G^\ominus$ ) of the reaction components.
- The variation of the equilibrium constant with temperature is expressed by the van't Hoff equation.
- The equilibrium constant  $K$  increases with temperature if  $\Delta_r H^\ominus > 0$  (an endothermic reaction) and decreases with temperature if  $\Delta_r H^\ominus < 0$  (an exothermic reaction).
- When a system at equilibrium is compressed, the composition of a gas-phase equilibrium adjusts so as to reduce the number of molecules in the gas phase.

**Transitions and phases** (3 h, HC): Chapter 5 of textbook

Students will understand that:

- A substance has a tendency to change into the phase with the lowest molar Gibbs energy
- How the molar Gibbs energy of a substance varies with pressure and temperature
- The transition temperature between two phases is the temperature, at a given pressure, at which the molar Gibbs energy of the two phases are equal
- The Clapeyron equation, and the Clausius-Clapeyron approximate equation, provide a way to predict the location of phase boundaries
- The vapour pressure of a liquid is the pressure of the vapour in equilibrium with the liquid

**Chemical kinetics** (3 h, HC): Chapter 10 of textbook

Students will understand that:

- The rates of chemical reactions can be measured by using techniques that monitor the concentration of species in a reaction mixture
- A rate law is an expression for the reaction rate in terms of the concentrations of the species that occur in the overall chemical reaction
- An integrated rate law is an expression for the rate of reaction as a function of time
- The half-life of a 1<sup>st</sup> order process is the time taken for the concentration of a species to fall to half its initial value
- The temperature dependence of the rate constant of a reaction typically follows the Arrhenius law

**Ionics and electrochemistry** (6 h, DL): Chapter 9 and 18 of textbook

Students will understand that:

- The molar conductivity of a strong electrolyte follows the Kohlrausch law
- Protons migrate by the Grotthuss mechanism in aqueous solutions
- Conductivity measurements can be used to predict values of equilibrium constants for processes that produce or consume ions, such as acid dissociation
- A galvanic cell is an electrochemical cell in which spontaneous chemical reactions produce a potential difference
- An electrolytic cell is an electrochemical cell in which an external source of current is used to drive a non-spontaneous chemical reaction

- Cell potentials are related to the reaction Gibbs energy, and standard cell potentials can be used to predict thermodynamic functions (Gibbs energy, entropy, enthalpy and equilibrium constant) of processes
- The cell potential is related to concentration of species by the Nernst equation
- To induce electrolysis, the applied potential difference must exceed the cell potential at least by the cell overpotential
- Cell overpotential is the sum of the overpotentials at the anode and the cathode, and of the ohmic ( $iR$ ) drop.

**Practicals** (4 hr per week, over a 6 week period)

The Physical Chemistry Practical Course will take place over a 6 week period (4 hrs per week), commencing with a library training session. There will be a tutorial at the end of most practical sessions. 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. There will be an MCQ examination at the end of the practical course.

The principal objectives of the CH203 laboratory course are:

- To provide an appreciation of the scientific method in the observation, recording and interpretation of laboratory data.
- To illustrate applications of the chemical principles dealt with in the lecture course.
- To familiarise the students 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. Attendance and performance at each laboratory class will be assessed on a weekly basis and part of the marks will be awarded for this continual assessment.

The experiments are to be done in cyclic order (by each individual student); for example, if you begin with experiment number 3, then the next week do #4, followed by #5 *etc.* For some experiments students may work in pairs. To derive full benefit from the course the student should, before coming to the laboratory, read details of the experiment to be performed.

The experiments include the following:

1. The Clausius-Clapeyron Equation
2. The Beer-Lambert Law; Quantitative Analysis
3. Molar Conductance of Weak and Strong Electrolytes
4. Conductometric Titration of an Acid Mixture
5. Chemical Kinetics; Fading of Phenolphthalein
6. The Nernst Equation; Electrochemical Cells

## Organic Chemistry I – CH202

**Staff:** Dr. Patrick O'Leary, Prof Paul Murphy, Prof. Olivier Thomas, Prof Peter Crowley, Dr Fabien Cougnon

**Textbook:** *Organic Chemistry, 8<sup>th</sup> edition, John E. McMurry international edition. Available in the Library and the university bookshop. This text is also the prescribed text for third year Organic chemistry.*

### Dr O'Leary

Carboxylic Acids [From Mc Murry Chapters 20 and 21]

Students will understand and be able to apply

- Naming conventions, synthesis strategies for, and basic reactions of, carboxylic acids and their derivatives (esters, amides, anhydrides, acid chlorides).
- Reaction mechanisms associated with these reactions (both reversible and irreversible)

Structure and reactions of hydrocarbons: Alkanes Alkenes and Alkynes [From Mc Murry Chapters 3, 4, 7, 8 and 9]

Students will understand and be able to apply

- Naming conventions and synthesis strategies for alkanes, alkenes and alkynes.
- Reactions of alkanes such as halogenation
- Bayer strain theory
- Reactions of alkenes such as, addition of X<sub>2</sub> or HX, diol formation, epoxidation polymerisation and ozonolysis
- Application and reasoning behind Markovnikov and anti-Markovnikov addition, regio- and stereo-selectivity
- Use of the acidity of alkynes
- Hybridisation and isomers
- Reaction mechanisms associated with these reactions

### TBC

Aldehydes, ketones (Mc Murry Chapters 19, 22-23)

Students will gain an understanding of

- Valency, bonding, and how to draw molecules
- How to draw reaction mechanisms using curly arrows
- The ability to suggest how a given molecule might be synthesised using any of the reactions covered
- The ability to draw the structure of the product that would be formed from a given molecule using any of the reactions covered

Alcohols (McMurry Chapter 17)

Students will understand and be able to apply

- IUPAC nomenclature of alcohols
- The importance of functional groups for the reactivity and physical properties of molecules
- Physical and chemical properties of alcohols
- Synthesis of alcohols (e.g. from alkenes, alkyl halides, redox reactions)
- The synthetic utility of Grignard reagents
- Reactions of alcohols (e.g. acid/base chemistry, redox behaviour, elimination reactions)
- Selectivity in organic reactions, as demonstrated by Markovnikov's rule and Zaitsev's rule as well as an understanding of the underlying chemical principles

Aldehydes and Ketones (McMurry Chapters 19, 22–23)

Students will understand and be able to apply

- IUPAC nomenclature of aldehydes and ketones
- Physical and chemical properties of aldehydes and ketones
- Synthesis of aldehydes and ketones (e.g. from alkenes, via Friedel Crafts acylation)
- Reactivity of aldehydes and ketones (both on the electrophilic carbonyl carbon, and on the acidic alpha-hydrogen via enolate chemistry): e.g. nucleophilic addition (acetal/ketal formation, imine/enamine formation, reduction), conjugate addition, enolate chemistry (alpha-halogenation, the Aldol reaction, the Mannich reaction)
- The difference between intermolecular and intramolecular reactions
- Kinetic vs. thermodynamic control

### **Prof. Murphy**

Stereochemistry (Mc Murry Chapter 4)

Introduction to natural product chemistry (Mc Murry Chapters 24, 25)

Substitution reactions of alkyl halides ( $S_N2$  and  $S_N1$ ) (Mc Murry Chapter 11)

Substitution & Elimination Reactions

**Students should be able to:**

- Write simple elimination & substitution reactions including the products from these reactions
- Write basic mechanisms for elimination & substitution reactions
- Relate the rate order of the reactions to the mechanisms
- Describe experimental support for  $S_N1$ ,  $S_N2$ , E1, E2 mechanisms
- Write transition states for elimination & substitution reactions
- Understand factors that affect rates of the various types of elimination & substitution reactions (e.g. leaving group, nucleophile or base)
- Describe and understand the difference between nucleophilicity & basicity
- Describe carbocation rearrangements and understand why they can occur
- Predict when carbocation rearrangements are likely to occur
- Predict the regio-selectivity in elimination reactions
- Understand why structure of the base can lead to changes in regio-selectivity
- Give and understand why elimination reactions can be stereoselective
- Understand and give conditions for where substitution may be preferred to elimination reactions and vice versa (e.g. structure of base/nucleophile, substrate, temperature etc.)
- Identify substitution & elimination reactions in nature

### **Dr. O'Leary**

Aromatic Chemistry and Amines (POL, 6 h)

- An understanding of the electronic structure (incl. delocalisation) of benzene and the rules of aromaticity is expected.
- The student should be able to identify aromatic hydrocarbon structures, and use Hückel rule for aromaticity.
- An understanding of IUPAC naming of aromatic hydrocarbons is expected, and the student should be able to classify common benzenes according to functionality.
- Electrophilic aromatic substitution mechanisms for nitration, sulfonation, halogenation, Friedel-Crafts acylation and alkylation of benzene should be accurately drawn.
- The student should be able to label the parts of an energy profile for substitution of benzene.
- The student should be able to classify substituent directing effects as +R, -R, +I and -I.
- The student should have an understanding of the effect on rate and regioselectivity of weakly inductively and more strongly activating and deactivating resonance substituents on electrophilic substitutions onto substituted benzenes.

- The student should be able to draw accurate resonance structures of substituted benzene intermediates.
- The student should be able to draw mechanisms and products of nucleophilic substitutions onto arenediazonium salts.
- The student should be able to draw mechanisms for azo-dye formation.
- The student should be aware of the synthetic steps required to convert benzene into aniline into azo-dye.
- The student should be able to classify amines into primary, secondary and tertiary.
- The student should be able to draw the products of reactions of secondary amines and tertiary aromatic amines with nitrous acid. Knowledge of identification tests for amines should be demonstrated.
- Knowledge of IUPAC identification of amines is expected.
- The student should revise that amines are derivatives of ammonia (know geometry and electronic structure), and basicity due to the lone pair on the N atom.
- The student should be able to draw resonance structures to show aniline being a weaker base than aliphatic amines.
- The student should be able to write curly arrow mechanisms to rationalise reactions of amines with acids.
- The student should demonstrate knowledge of simple reactions of amines acting as bases and nucleophiles.

Mc Murry, Chapters 15, 16 and 24.

**Practicals** (4 hr per week, over a 6 week period)

The principal objectives of the CH202 laboratory course are:

- To get the students to use the fundamental techniques used by organic chemists such as recrystallisation, distillation, reflux, separation techniques, glassware setup, heating and cooling methods.
- To illustrate some of the fundamental reactions dealt with in the lecture course and to reinforce the background to the chemistry by practical application.
- To familiarise the student with formal report writing, logical progression of reports and clear and concise presentation and analysis of results
- To introduce spectroscopic techniques (UV, IR and MS) for compound identification and to apply this to unknown compounds. This work also reinforces compound naming, functional groups and schematic representation of molecules.

The practicals are to be written up as a separate **Report** and handed up in the lab. Attendance and performance at each laboratory class will be assessed on a weekly basis and part of the marks will be awarded for this continual assessment.

The experiments are to be done on a weekly basis. Each experiment is set up in the lab for only one week and each student does the same experiment on their given day along with all of their labmates. The consequence of this system is that there is ample opportunity for interaction with the staff and demonstrators and should any issues arise the whole class can have it highlighted to then mid lab. There is no possibility of doing the experiment on another week if it is missed. Attendance is thus key to both the lab and the prelab briefing beforehand. This briefing deals with safety issues and failure to attend may lead to exclusion from the lab. To derive full benefit from the course the student should, before coming to the laboratory, read details of the experiment to be performed.

## Analytical & Environmental Chemistry – CH205

**Staff:** Prof. Alan Ryder (Module Co-ordinator), Prof. Peter Crowley, Prof. Henry Curran, Prof. Donal Leech, Prof. Olivier Thomas.

**Text Books:** “Quantitative Chemical Analysis”, 8<sup>th</sup> Edition, by DC Harris (8+ copies available in library). “Quality Assurance in Analytical Chemistry,” E. Prichard & V. Barwick, Pub. Wiley (2007). “Environmental Chemistry,” C. Baird, Pub. Freeman (1995).

**Blackboard:** All course announcements, content changes, updates, and information will be made via blackboard. All lecture notes, course details etc. will be available here. Students are expected to consult the module page on a regular basis.

**Examination:** Two hour Multiple Choice Question (MCQ) paper with 100 questions.

### Lecture Course Outline:

- 1) Sampling & Electrochemistry (4 lectures, D. Leech)
- 2) Atmospheric Chemistry (4 lectures, H. Curran)
- 3) Water chemistry & treatment, (3 lectures, O. Thomas)
- 4) Atomic & Applied Spectroscopy (6 lectures, A. Ryder)
- 5) Separation Science/Chromatography (3 lectures, O. Thomas)
- 6) Bioanalytical (3 lectures, P. Crowley)

**Sampling** (2 h, DL): E. Prichard & V. Barwick, “Quality Assurance in Analytical Chemistry,” Pub. Wiley (2007). Chapters 3 & 4.

Students will understand:

- The analytical approach for problem solving in chemistry
- How to select a sampling scheme to provide a sample for analysis
- How to report analytical results, using simple statistics

**Electrochemistry** (2 h, DL): D. C. Harris, *Quantitative Chemical Analysis*, Pub. Freeman (2010), 8<sup>th</sup> Edn.: Chapters 13, 14, 16.

Students will understand:

- Basic electrochemical reactions, terminology and conventions
- How to relate chemical amount to electrochemical parameters of potential and current

**Atmospheric Chemistry** (4 h, HC): Chapters 2-4 of *Environmental Chemistry* (C. Baird).

Students will understand that:

- Temperature, pressure and composition of the atmosphere changes as a function of height above sea level
- Photochemical smoke + fog = smog
- Acid rain is formed by the reaction  $\text{CO}_2 + \text{H}_2\text{O} \rightleftharpoons \text{H}_2\text{CO}_3 \rightleftharpoons \text{H}^+ + \text{HCO}_3^-$
- Solar radiation and terrestrial energy balance is important towards global warming
- $\text{CO}_2$  and  $\text{CH}_4$  are the principal greenhouse gases
- Implications of the use of different types of energy, particularly fossil fuels
- Stratospheric ozone content is adversely affected by anthropogenic emissions of chlorofluorocarbons
- Waste disposal is can be primarily by landfill and by incineration with pros and cons for both methods

**Water chemistry and treatment. Atomic Spectroscopy** (3h, OT): Chapters 7–9 of *Environmental Chemistry* (C. Baird).

Students will understand that:

- The origins of drinking water from source (groundwater) to tap
- The many different chemical species that exist and are formed in groundwater
- The origin of these species with respect to the environment
- The redox chemistry and acid-base chemistry of groundwater.
- How groundwater is treated and purified at processing plants
- Pollution and the many origins of its existence (i.e. Groundwater contamination)
- Potential health problems associated with unclean / polluted drinking water
- The chemistry of Toxic Heavy Metals in water (and air).

**Atomic Spectroscopy** (2 L, AR): Chapter 20 of Quantitative Chemical Analysis (8th ed. Harris)

Students will understand:

- The fundamental physics of atomic absorption and emission spectroscopy
- How to apply atomic absorption to quantitative analysis
- The difference between Flame atomic absorption and Graphite Furnace Atomic Absorption
- The Beer-Lambert law and its relationship with atomic absorption
- The origin of colour within transition metal complexes in solution and its relation to atomic absorption

**Applied Spectroscopy & Forensics** (4 L, AR): Chapter 17 & 19 of Quantitative Chemical Analysis (8th ed. Harris).

Students will be expected to have a knowledge of UV-visible, NIR, and MIR spectroscopies and understand:

- How an optical spectrometer operates and the salient features of the components (light sources, spectrometers, detectors) used in their construction.
- The sample holders used for the different spectroscopies depend on the wavelength of light being used and the sample type under investigation.
- UV-visible absorption spectroscopy typically involves the absorption of light in the 190-700 nm range.
- The Beer-Lambert Law can be used for the quantitative analysis of material.
- How Mid Infra-Red (MIR) spectroscopy works involves absorption of light in the 2000-10000 nm range. Molecules absorb light via fundamental vibrations, some overtone & combination modes.
- Attenuated Total Reflectance (ATR) sampling uses the evanescent wave phenomena for robust MIR sampling.
- Optical fibres operate on the principle of Total Internal Reflection (TIR) and are very useful for spectroscopic sampling.
- Near Infra-Red (NIR) spectroscopy involves measuring the absorption of light in the 700-2500 nm range. Molecules absorb light via overtone & combination modes only.
- NIR instrumentation is relatively inexpensive, versatile and portable. One can use simple glass containers for NIR work.

**Separation Science / Chromatography:** (3 L, OT): D. C. Harris, Quantitative Chemical Analysis, Pub. Freeman (2010), 8th Edn.: Chapters 22, 24, and 25.

From this module students will be expected to have a knowledge of the types of separation methods available, including:

- Partitioning
- Electrophoresis
- Basic principles of chromatography

- Paper chromatography
- Thin layer chromatography
- Column chromatography
- Ion chromatography
- Size exclusion chromatography
- Separation using ion-exchange resins

**Bioanalytical** (3 hr., PC): D. C. Harris, Quantitative Chemical Analysis, Pub. Freeman (2010), 8th Edn.: Parts of Chapters 17 & 25.

This aspect of the course focuses on bioanalytical techniques. In particular, you will learn about three methods to study proteins:

- Method 1:
  - Absorption spectroscopy, Beer-Lambert law
  - Bradford assay for quantification of protein concentration (in mg/mL)
- Method 2:
  - Polyacrylamide gel electrophoresis (PAGE) technique for analysing proteins by molecular weight
  - SDS versus Native PAGE and the role of Cysteine will also be studied
- Method 3:
  - Column chromatography and protein purification
  - Ion exchange versus Size exclusion Chromatography

**Practicals** (4 hr per week, over a 5-week period)

All students must undertake the practical element of the module. The Analytical Chemistry Practical Course will take place over a 5-week period (4 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 (30% of the overall module mark).

The principal objectives of the CH205 laboratory course are:

- To provide an appreciation of the scientific method in the observation, recording, and interpretation of laboratory data.
- To illustrate applications of the analytical and chemical principles dealt with in the lecture course.
- To familiarise the students with important techniques fundamental to analytical chemistry.
- To familiarise the students with the use of Excel for the plotting of data and spectra.

The practicals are to be written up as a separate **Report** in a hard-backed notebook and handed up in the lab. at the appropriate time. The experiments are to be done in cyclic order (by each individual student); for example, if you begin with experiment number 3, then the next week do #4, followed by #5 *etc.* For some experiments, students may work in pairs. To derive full benefit from the course the student should, before coming to the laboratory, read details of the experiment to be performed.

The experiments may include the following (these are subject to change, see blackboard for details):

1. Determination of iron using the thiocyanate method – An application of the Beer-Lambert Law.
2. Estimation of Copper and Sulphate in a solution of CuSO<sub>4</sub> using a Cation Exchange Resin.
3. Potentiometric determination of sodium.
4. Experiment in water analysis using the Hach (UV-visible spectroscopy) methodology.
5. Experiments in Mid-IR and Near-IR spectroscopy: Identification of unknown *white powders*.