University of Glasgow | School of Chemistry

2020-2021

Module Outlines

Chemistry-4H & -4/5M

Module Outlines for Chemistry Lecture Courses of:

Chemistry (CHEM)
Chemistry with Medicinal Chemistry (CMC)
Chemical Physics (CP)
Chemistry & Maths (C&M)

Please note:

This handbook contains all the Module Outlines for all the final year lecture course modules. These are also posted on Moodle for each lecture module. If there are any updates to this published module outline, this will be posted on the Level 4 Moodle, showing the date, to indicate that there has been an update.

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Recommended Reading Material

Unless indicated otherwise in the Module Outlines for individual course modules, the following essential purchases will cover most of the material given in Level-4.

(a) **ESSENTIAL PURCHASES. Level-4 Students will already have most of these books.**

- **Organic Chemistry**, J Clayden, N Greeves, S Warren and P Wothers, OUP (2nd Edition)*
- **Inorganic Chemistry**, Weller, Overton, Rourke, Armstrong, OUP (7th Edition)*
- **Physical Chemistry**, Atkins OUP (11th Edition)*.

  *The newest editions of the OUP chemistry textbooks can be found in the UoG library. Older versions are still very helpful and useful and can also be used (except if there is a specific direction to the newest edition.
- **Molecular models**, table molecular model kit such as Organic/Inorganic Orbit kit, Orbit Molecular Building System, Cochranes of Oxford Ltd, Leafield, Oxford OX8 5NT.
- **Spectroscopic Methods in Organic Chemistry**, D H Williams and I Fleming, McGraw-Hill, 5th Edition Revised.

Overview of Required Chemistry Courses & Modules for Degree Progamme

On the following page is a **Course Information Table** that shows, for each of the Courses (eg Organic, Inorganic, etc), the lecture modules and associated lecturer. Furthermore, as indicated by a “Y”, it shows which courses/modules must be taken by each student cohort (eg 4H-CMC or 5M-CHEM).

BSci Students (4H-CHEM & 4H-CMC & 4H-C&P & 4H-CP):

The Chem-4H class takes modules 1-4 of all the Organic (o), Inorganic (i), and Physical (p) courses. The CMC-4H class also takes modules 1-4 of the Organic course but takes only modules 1&4 of the Inorganic and Physical courses. Furthermore, the CMC-4H students take all 4 modules of the Medicinal Chemistry (M) course. The Special Topics (S1-S6) course covers a range of topical subjects in modern chemistry and all six modules are compulsory for all 4H-Chem and 4H-CMC students. The 4H-C&M students will select options from the modules indicated with Y°, with discussion and guidance from the C&M class head. The 4H-CP students take Modules 2-4 of the Inorganic (i) course and modules 1-4 of the Physical (p) course, as well as Modules 3-6 of the Special Topics (S/ST) course. All modules are taught in common with the MSci Class, but will be examined at a higher level for the Masters students.

MSci Students (5M-CHEM & 5M-CMC & 4/5M-C&M & 5M-CP):

The Chem-4/5M class takes all the Organic (o), Inorganic (i), and Physical (p) modules. The CMC-4/5M class takes all the Organic, and Medicinal Chem (M) modules and subset (1 & 4-6) of the Inorganic and Physical modules. The Special Topics (S1-S6) courses cover a range of topical subjects in modern chemistry and are compulsory for all 4/5M-Chem and 4/5M-CMC students. The 4/5M-C&M students will select modules with the guidance of their C&M Class Head and this will be confirmed at the start of term. The 5M-CP students will take modules 2,3 & 5 of the Inorganic course and all modules of the Physical course, and modules 3-6 of the Special topics course. The o/i/p modules listed as “5m” or “6m” are Masters level only. All other modules are taught in common with the BSc Class, but will be examined at a higher level for the Masters students.

4M/5M Course Lecturers & Modules (20-21)

v18 (05 Sept 20)

Org	Organic Chem Module	Lecturer	Chem		CMC		CP	
			Chem-4H	Chem-4M	CMC-4H	CMC-4M	CP-4H	CP-5M
o1	Pericyclic Reactions	Dr Sutherland	Y	Y	Y	Y		
o2	Heterocyclic Chemistry	Dr Boyer	Y	Y	Y	Y		
o3	Advanced Organic Synthesis	Dr Prunet	Y	Y	Y	Y		
o4	Polymer Chemistry	Dr Schmidt	Y	Y	Y	Y		
o5m	Asymmetric Synthesis	Prof Clark		Y		Y		
o6m	Organic Materials	Dr Draper		Y		Y		

Inorg	Inorganic Chem Module	Lecturer	Chem		CMC		CP	
			Chem-4H	Chem-4M	CMC-4H	CMC-4M	CP-4H	CP-5M
i1	Metals in Medicine	Prof Cronin	Y	Y	Y	Y		
*i2	*Inorganic Mechanisms	Dr Moiras	Y	Y			Y	Y
*i3	*Industrial Catalysis Chemistry	Prof Jackson	Y	Y			Y	Y
i4	Applied Coordination Chemistry	Dr Sproules	Y	Y	Y	Y	Y	
i5m	Inorganic Materials Design	Prof Gregory		Y		Y		Y
i6m	Chemistry of the f-block	Dr Price		Y		Y		

Phys	Physical Chemistry Module	Lecturer	Chem		CMC		CP	
			Chem-4H	Chem-4M	CMC-4H	CMC-4M	CP-4H	CP-5M
p1	Macromolecules and Colloids	Dr Magennis	Y	Y	Y	Y	Y	Y
*p2	*Surface Chemistry	Prof Lennon	Y	Y			Y	Y
*p3	*Advanced Chemical Thermodynamics	Dr Hedley	Y	Y			Y	Y
p4	Modern NMR Spectroscopy	Dr Odedra	Y	Y	Y	Y	Y	Y
p5m	Statistical Mechanics & Reaction Dynamics	Dr Docherty		Y		Y		Y
p6m	Theoretical & Computational Chemistry	Dr Senn		Y		Y		Y

CMC	Chem with Medicinal Chemistry Module	Lecturer	Chem		CMC		CP	
			Chem-4H	Chem-4M	CMC-4H	CMC-4M	CP-4H	CP-5M
M1-o	#Biopolymers Chemistry and Synthesis	Dr Jamieson			Y	Y		
M2cmc	#Industrial Medicinal Chemistry	Dr Humphreys GSK & Dr Scott AZ			Y	Y		
M3-o	#Medicinal Chemistry of Cancer	Dr Watts			Y	Y		
M4-o	#Chemical Biology	Prof Hartley			Y	Y		

ST	Special Topics Module	Lecturer	Chem		CMC		CP	
			Chem-4H	Chem-4M	CMC-4H	CMC-4M	CP-4H	CP-5M
S1-o	Organometallics in Synthesis	Dr France	Y	Y	Y	Y		
S2-o	Organic Supramolecular Chem	Prof Adams	Y	Y	Y	Y		
S3-i	Molecular Magnetism	Prof Murrie	Y	Y	Y	Y	Y	Y
S4-i	Electrochemistry for a Sustainable Future	Dr Symes	Y	Y	Y	Y	Y	Y
S5-p	Surface Structure & Spectroscopy	Dr Karimullah	Y	Y	Y	Y	Y	Y
S6-p	Dynamics of Molecular Clusters and Fluids	Prof Wynne	Y	Y	Y	Y	Y	Y

Note: this may be subject to change. Please refer to Moodle for most up-to-date information

Code: **o1**

Title: **Pericyclic Reactions**

Lecturer: Dr. Andrew Sutherland

Topics generally covered in this module include:

1. The outcomes of many cycloaddition and rearrangement reactions, understood in terms of frontier orbital interactions.

2. The various types of pericyclic reaction; definition of such terms as “conrotatory”, “suprafacial”, etc; the Woodward-Hoffmann Rules.

3. Diels-Alder cycloadditions, including stereospecificity, regioselectivity, and stereoselectivity, in terms of primary and secondary orbital interactions.

4. Other cycloaddition reactions, including 1,3-dipolar and [2+2] cycloadditions, cheletropic reactions, and the ene reaction. Applications of the Woodward-Hoffmann Rules to cycloaddition reactions under thermal or photochemical conditions.

5. How to predict and rationalise the outcomes of electrocyclic reactions in terms of orbital interactions and/or the Woodward-Hoffmann Rules.

6. How to predict and rationalise the outcomes of [1,n]-, [2,3]- and [3,3]-sigmatropic rearrangements, in terms of primary and secondary orbital interactions and the Woodward-Hoffmann Rules. Rationalise and predict stereoselectivity in [2,3]- and [3,3]-sigmatropic rearrangement reactions in terms of chair-like transition states.

7. The synthetic importance of the above cycloaddition and rearrangement reactions, and how to give disconnections of target compounds corresponding to these reactions.

8. Application of the understanding of the above to examples published in the chemical literature.

Module Outline:

- **Introduction:** Shape of bonding and anti-bonding σ and π orbitals; extended π systems; energy levels; orbital interactions.

- **Diels-Alder Cycloaddition:** The basic reaction and its disconnection; Orbitals involved and their implications for transition state geometry; Stereospecificity with respect to diene and dienophile. Substituted dienes and dienophiles and their orbitals; Orbital energy and its effect on reaction rate; Regioselectivity; Stereoselectivity (*exo/endo*) governed by secondary orbital interactions. Intramolecular reactions. Chiral starting materials.

- **Other Cycloadditions:** 1,3-Dipolar cycloadditions; [2+2] cycloadditions; Woodward-Hoffmann Rules as applied to cycloadditions; synthetic applications; Alder’s ene reaction; cheletropic reactions; comparison with cycloadditions.

- **Electrocyclic Reactions:** Occurrence with 2, 3, 4, etc. electron pairs; direction of equilibrium; con- and dis-rotatory reaction; Woodward-Hoffmann Rules as applied to electrocyclic reactions.

- **Pericyclic Rearrangements:** Prototropic and sigmatropic rearrangements, including Claisen and related rearrangements, and rearrangements involving sulfur or selenium; Orbital involvement; chair-shaped transition states; stereochemical control; synthetic applications including the synthesis of α,β-unsaturated carbonyl compounds and the geometry of enolate formation.

Code: **o2**

Title: **Heterocyclic Chemistry**

Lecturer: Dr. Alistair Boyer

Aims: Heterocycles are crucial components of molecules found across all facets of chemistry. This module aims to provide a rigorous foundation of heterocyclic chemistry. It will cover heterocycle identification and nomenclature, reactivity and synthesis. The module covers all the most commonly encountered heterocycles and will provide the tools for students to design syntheses and predict the properties of any heterocycles that they may encounter in their future career.

Topics generally covered in this module include:

Identification

1. Identification of heterocyclic motifs and the nomenclature of the most commonly encountered heterocycles (i.e. the ones discussed subsequently in this module).

Reactivity

2. How the aromatic bonding is constituted within an aromatic heterocycle and the different ways in which a heteroatom can contribute to aromaticity
3. Identification of electron-rich and electron-poor heterocyclic aromatic systems and explanation of the reactivity of these as electrophiles and nucleophiles.
4. How the electronic configuration of a heterocyclic affects its reactivity in α-positions to the ring.
5. How heterocyclic systems behave under conditions for lithiation; and that some can undergo Diels-Alder cycloadditions.
6. How the inclusion of ring substituents can alter a heterocycle's reactivity.

Synthesis

7. The mechanism for the formation of key heterocycles based upon the most commonly encountered syntheses.
8. The synthesis of substituted or complex heterocyclic compounds based upon pattern matching with the syntheses discussed within the course.

Properties

9. The importance of heterocycles in molecules' function. The role which heterocycles can play in pharmaceutical and materials-chemistry.

Module Outline:

A. Introduction
   a. Course overview
   b. What is a heterocycle? Why are heterocycles important?
   c. Nomenclature: systematic and traditional
B. Aromaticity
   a. Revision
   b. Application to heterocyclic systems: 6-membered rings
C. Reactivity
   a. Reactivity of 6-membered heterocyclic systems
   b. Reactivity of 5-membered heterocyclic systems
D. Synthesis
   a. Selected important synthesis of heterocycles

Code: **o3**

Title: **Advanced Organic Synthesis**

Lecturer: Dr Joëlle Prunet

Aims: To introduce new methods and extend previously encountered strategies for the preparation of organic molecules with a particular focus on alkenes. To illustrate these methods with syntheses of structurally complex molecules.

Topics generally covered in this module include:

1. Analysis of heteroatom containing organic molecules and prediction of the hybridisation of both carbon and heteroatoms.

2. Interpretation of the effect of hybridisation on reactivity.

3. Reagents for the olefination of carbonyl compounds, description of the reaction mechanisms, and application of these reactions to synthesis.

4. Explanation of both the mechanism and the use of metathesis and palladium-catalysed reactions in organic synthesis.

5. Prediction of the olefin geometry of products from a range of olefination reactions.

6. Description of mechanisms for the reactions of allylboranes and allylsilanes, application of these reagents to synthesis and explanation of diastereoselectivity in crotylation reactions.

Module Outline:

- Orbitals, Hybridisation, and Reactivity
- Nitrogen-containing organic molecules – hybridisation, reactivity, use in synthesis.
- Olefination reactions: Wittig (revision) and related, Julia, Peterson, Tebbe/Petasis alkylidenation reactions
- Synthesis of alkenes from alkynes
- Cross-metathesis
- Palladium-catalysed reactions
- Allylating and crotylating reagents for the synthesis of homoallylic alcohols.

Code: **o4**

Title: **Polymer Chemistry**

Lecturer: Dr B Schmidt

Aims: Polymers are important materials in everyday life. This module aims for a basic introduction into polymer chemistry. After an introduction into the field, the foundations of polymer synthesis will be discussed based on three basic polymerisation methods (step growth, free radical and anionic). Finally, the basics of the main analytical method for polymers, size exclusion chromatography, will be introduced and polymer properties discussed.

Topics generally covered in this module include:

1. The importance of polymer chemistry in the chemical sciences and nomenclature of the subject.
2. Polymer structure and isomerism discussed with examples.
3. Collection of common polymers.
4. Description of basic polymerisation mechanisms and their differences: Step-growth polymerisation and chain-growth polymerisation.
5. Polymerisation methods (polycondensation, free radical polymerization and anionic polymerization) and their effect on molecular mass.
6. Discussion on polymerisation kinetics with respect to the polymerisation method.
7. Explanation of the size-exclusion chromatography method and the underlying separation mechanism.
8. Application of polymers in the real world, i.e. commodity polymers, technical polymers and functional polymers.

Module Outline:

- Introduction
  - Definition and common Polymers
  - Polymer Structure
  - Nomenclature
  - Molecular Mass Averages
- Polymer Synthesis
  - Step Growth Polymerisation
  - Free Radical Polymerisation
  - Anionic Polymerisation
- Polymer Properties
  - Size Exclusion Chromatography
  - Examples

Recommended Reading (online via the library):
Polymer Chemistry- Koltzenburg, Maskos and Nuyken, *Springer*

Code: **o5m**

Title: **Asymmetric Synthesis**

Lecturer: Prof Stephen Clark

Aims: To introduce some of the most important asymmetric reactions available to the organic chemist. To discuss in detail asymmetric oxidation reactions (epoxidation, dihydroxylation and aminohydroxylation of alkenes), reduction reactions (hydrogenation of C=C and C=O bond, transfer hydrogenation and hydroboration), and asymmetric C-C bond forming reactions using chiral auxiliaries, chiral Lewis acids and organocatalysts.

Topics generally covered in this module include:

1. The importance of asymmetric reactions in organic synthesis and the fundamental concepts and nomenclature of the subject.
2. Description of the Sharpless asymmetric epoxidation of allylic alcohols, including kinetic resolution of secondary allylic alcohols.
3. Description of the direct Jacobsen-Katsuki asymmetric epoxidation of simple unfunctionalised alkenes.
4. Description of the Sharpless asymmetric dihydroxylation and aminohydroxylation reactions and their use in synthesis, and use the mneumonic to predict the stereoselectivity of these reactions.
5. Description of the asymmetric hydrogenation and transfer hydrogenation catalysed by Ru and Rh complexes as well as Corey's oxazaborolidine reduction of carbonyl compounds.
6. Organocatalysis as an alternative to metal-based methods, the application of organocatalysts in asymmetric C-C bond-forming reactions, and the major design features of the catalysts.
7. Description of the asymmetric aldol reactions and explanation of the factors that can be used to control enolate geometry and stereochemical (relative and absolute) outcome of the reactions with reference to Zimmerman-Traxler transition states and chiral Lewis Base catalysis. Explanation of how asymmetric aldol reactions, in which either chiral auxiliaries or chiral Lewis acids are employed, can be used to deliver products with high levels of stereocontrol.

Module Outline:

- A brief illustration of the importance of asymmetric synthesis to a wide range of areas. The basic nomenclature and principles of asymmetric synthesis will then be revised.
- Enantioselective reactions controlled by chiral reagents; asymmetric oxidation reactions, such as the Sharpless asymmetric epoxidation, dihydroxylation and aminohydroxylation; a brief discussion of kinetic resolution; the Jacobsen-Katsuki asymmetric oxidation; Corey's method for the asymmetric reduction of carbonyl compounds. For all the above reactions, examples of their use in the syntheses of important molecules will conclude each discussion.
- Iminium based organocatalysis and their applications in synthesis; the design features of organocatalysts.
- Diastereoselective asymmetric reactions using chiral auxiliaries; Evans' auxiliary in asymmetric aldol reactions and alkylation reactions; Enolate stereochemistry and its effect on the outcome of aldol reactions; Chiral Lewis Base catalysis; asymmetric Mukaiyama aldol reaction using chiral Lewis Acid catalysts.

Code: **o6m**

Title: **Organic Materials**

Lecturer: Dr Emily Draper

Aims: An introduction into the chemistry behind the design, synthesis and processing of organic based materials. Understanding how the state-of-the-art organic materials work and how to design materials for our future.

Topics generally covered in this module include:

1. Structural and performance characterisation techniques for organic materials.
2. General processing techniques.
3. Design principles and considerations when designing new materials.
4. State-of-the-art organic materials.

Module Outline:

- Introduction to organic materials chemistry
- Structural characterisation
- Performance characterisation
- Thin films and coatings
- Porous materials
- Organic electronics
- Gels and biomaterials
- ‘Smart’ materials

Code: **i1**

Title: **Metals in Medicine**

Lecturer: Prof. L Cronin

Aims: To discuss the increasingly important role played by metallo-organic compounds, in particular those of certain transition metals, in both diagnostic and therapeutic medicine. To introduce some of the more important medical applications of transition metals, and to explore the underlying chemistry that makes a particular element useful in a particular application.

Topics generally covered in this module include:

1. The reasons why the given properties for a particular metal ion make it useful for use in medical applications.

2. The concepts behind the use of radiopharmaceuticals and imaging.

3. Why regulation of metal ions *In Vivo* is vital for life.

4. Why certain types of metal complexes can be used to treat cancer and discuss the mode of action for platinum drugs in cancer chemo-therapy.

5. How ions are regulated entering cells and of the methods of transport through the cell membrane

Module Outline:

- **Introduction**: The roles of the metallic elements in biology are briefly considered to provide a context for, and contrast to, the uses of transition metal compounds in medicine;
- **Cell membranes and ion pumps**: The concentration of ions, and establishing gradients in ion concentration are crucial for cell function. This section describes the basic processes and explains the concept of membrane potential;
- **Radiopharmaceuticals and Imaging**: The nuclear properties of radioisotopes used in medical applications are reviewed and the applications for which they are suited are considered. The use of non-radioactive paramagnetic metal ions as contrast agents in Magnetic Resonance Imaging (MRI) will be included;
- **Regulation of Metal Ions *In Vivo***: This section will consider the treatment of two contrasting ailments; human deficiencies of certain metals and the use of sequestering agents to remove excess or unwanted metals from patients.
- **Cancer Therapy**: The use of platinum complexes in the treatment of certain cancers is well establish and models for the mechanism of active are well developed. A variety of other metallo-organic systems also show anti-tumor activity and are finding their way to clinical trials. These will also be considered.

Code: **i2**

Title: **Inorganic Mechanisms**

Lecturer: Dr Haralampos N. Miras

Aims: To describe and place in context, the factors that are important in determining reaction pathways and mechanisms of metal-centred co-ordination compounds in solution. To demonstrate how kinetic and non-kinetic evidence can be used to derive or to substantiate a reaction mechanism. To give examples taken from both main group and transition element chemistry. To make use of ideas and concepts presented in previous years, particularly in the areas of kinetics, ligand field theory and acid/base relationships.

Topics generally covered in this module include:

1. Revision of some fundamentals including, dissolution of salts, metal ions in solution, solvation, solvation numbers and their determination, thermochemistry.

2. Kinetics *vs.* thermodynamics.

3. Solvent exchange.

4. Complex formation, the Eigen-Wilkins mechanism.

5. Substitution at complex ions.

6. Substitution at non-metal centres.

7. Outer sphere and inner sphere electron transfer reactions.

8. An introduction to Marcus-Hush theory.

Code: **i3**

Title: **Industrial Catalytic Chemistry**

Lecturer: Prof. S David Jackson

Aims: To provide an introduction to large-scale industrial processes and the links between them.

Topics generally covered in this module include:

1. The interlinks between a number of large scale industrial processes. (lectures 1-8)

2. Definition of the difference in process requirements of endothermic and exothermic equilibrium limited reactions. (lectures 1-8)

3. Different catalytic processes and comparison/contrast of the catalysts and methodologies used in these processes. (lectures 1-8)

4. Catalytic cycles, including the rate determining steps and specific promotors, used in different processes.

5. An explanation of the roles of catalysts in multi-step processes and how they link to generate the overall process.

Module Outline:

This module is intended to give students an understanding of large petrochemical processes and how they link together by one or more processes supplying the feedstock for other processes

Code: **i4**

Title: **Applied Coordination Chemistry**

Lecturer: Dr Stephen Sproules

Aims: To elucidate the electronic structure of coordination complexes of d-block elements using ligand field and MO theory, and advanced experimental techniques; to understand the importance of ligand design in small molecule activation and reactivity.

Topics generally covered in this module include:

1. The concepts of ligand field theory, coordination geometry, formal and physical oxidation states, spin ground state, electronic structure, ligand type and strength.

2. Application of group theory to the construction of molecular orbital diagrams for six-coordinate complexes possessing octahedral, tetragonal and trigonal symmetry.

3. Illustration of the molecular orbitals involved in metal-ligand multiple bonds and summarisation of the concept of the "oxo wall".

4. The role of ligand design and the desired electronic structure for complexes that activate small molecules such as O_2, N_2, and H_2.

5. Description of the basic principles of electrochemistry, magnetometry, electron paramagnetic resonance and Mössbauer spectroscopy, and their application to determining the electronic structure of coordination complexes.

6. The concept of radical ligands, and the use of experimental data to diagnose electronic structure of complexes with redox-active ligands.

7. The properties of transition metal dithiolene complexes and their applications.

Code: **i5m**

Title: **Inorganic Materials Design**

Lecturer(s): Prof. Duncan Gregory

Aims: To provide an introduction and insight into some of the topics at the forefront of contemporary inorganic solid state and materials chemistry research. The focus of this module is on the link between synthesis, structure and properties and the underpinning concept of materials design. Examples from various areas will illustrate how the concept can lead to both new and improved materials from all parts of the periodic table.

Topics generally covered in this module include:

1. Descriptions of the structures of important binary and ternary oxides and non-oxides

2. Explanation of the principles of synthesis in the solid state and evaluations of the applicability of various synthesis routes to inorganic solids.

3. Some of the important physical properties in solid state materials and how these properties are interconnected with structure and bonding.

4. How the structure within key materials families, such as Perovskites, relate to properties such as ferroelectricity and colossal magnetoresistance.

5. Explanation of the basic functionality of fast ionic conducting materials and their application as electrodes in rechargeable batteries.

6. Description of the effects of size and morphology on materials functionality and assessment of how these effects impact on the structures and properties of inorganic nanomaterials.

Module Outline:

- The major binary and ternary structure types and how to describe them;
- Principles of high temperature solid state synthesis;
- Synthesis design and special synthesis methods;
- Structure-property relationships and simple electronic structure approaches;
- The synthetic, crystal and materials chemistry of Perovskites;
- Perovskite materials as a basis for ferroelectrics and advanced magnetic materials;
- Fast Li^+ ion conductors and intercalation materials in lithium batteries;
- Inorganic nanoparticles, nanotubes and nanowires; synthesis, structures and properties of chalcogenides and other nanomaterials.

Recommended Reading (in library):

Inorganic Materials Chemistry- Weller, *Oxford Primer*
Solid state chemistry, An Introduction – Smart and Moore, *Chapman and Hall*

Code: **i6m**

Title: **Chemistry of the f-block**

Lecturer: Dr. Daniel Price

Aims: The chemistry of the f-block elements is introduced. This module will examine both chemical and physical properties of these elements and their compounds, with an emphasis on the relationship between properties and underlying electronic structure.

Topics generally covered in this module include:

1. The names, symbols and positions in the periodic table of f-block elements
2. Description of the shape and extent of 4f and 5f orbitals
3. Explanation of the origin of the lanthanide contraction.
4. Description of the coordination geometries of lanthanide and actinide ions.
5. Description of the trends in redox chemistry in the f-block elements
6. Description and explanation of the differences and similarities between the chemistry of the lanthanides, the actinides and the d-block transition metal elements.
7. Discussion of the limitations of coupling schemes and the influence of relativistic effects in describing the electronic structures of these elements.
8. Correlation of electronic, magnetic and optical properties with the electronic structures of the 4f elements.
9. Description of the uses of lanthanides and actinides in the nuclear industry.
10. Assessment of the likely decay mechanisms for given actinide isotopes.
11. Description of the basic chemistry of more stable actinides: Thorium to Americium.

Module Outline:

- Occurrence, isolation and current applications of lanthanide elements;
- The nature of f-orbitals, and the electronic structures of lanthanide atoms and ions;
- The lanthanide contraction and coordination chemistry (including coordination numbers and stereochemistry);
- Properties of the elements and binary compounds;
- Electronic properties of lanthanides, coupling schemes and electronic and magnetic materials;
- Spectral properties of lanthanides, and optical materials
- Occurrence and discovery (and synthesis) of the actinides;
- Nuclear properties of actinides; isotope stability and decay mechanisms;
- Lanthanides and actinides in the nuclear industry;
- Reaction chemistry of actinides.

Recommended Reading (in library):

Inorganic Chemistry and Atkins, Overton, Rourke, Weller, Armstrong, OUP, 5th Edition, 2010. Advanced Inorganic Chemistry, F A Cotton and G Wilkinson, John Wiley, 6th Edition.
Chemistry of the Elements, N N Greenwood and A Earnshaw, Pergamon, 2nd Edition.

Code: **p1**

Title: **Macromolecules and Colloids**

Lecturer: Dr. Steven Magennis

Aims: To provide an overview of the size and structure of macromolecules (with a focus on biomacromolecules) and self-assembled aggregates (colloids, micelles and vesicles), and to examine common methods used to study them.

Topics generally covered in this module include:

1. Explanation of the different levels of macromolecular structure.

2. Calculation of the length of a random coil structure from radius of gyration measurements.

3. Explanation of the solution properties of colloids, particularly related to their attraction/repulsion. Explanation of the difference between colloids, micelles and vesicles.

4. The difference between number average and weight average calculations that are used to obtain mean molar masses for mono- and poly-dispersed molecules.

5. The use of mass spectrometry to determine the mass of a macromolecule.

6. Application of the principles of static light scattering to determine the radius of gyration of a macromolecule.

7. Explanation of how and why the polarization properties of fluorescence light are measured.

8. Explanation of the process of FRET and how it is used it to measure nanoscale distances.

9. Description of the differences between ensemble and single-molecule methods and explanation of how the techniques of confocal and TIRF microscopy allow detection of single molecules and particles.

Module Outline:

- The hierarchy of structure in macromolecules and simple polymer models to estimate their size.
- Self-assembled colloids, micelles and vesicles.
- Determination of molecular mass of macromolecules
- Use of light scattering to determine radius of gyration and shape of macromolecules and colloids.
- Fluorescence spectroscopy for structure determination
- Single-molecule methods to probe macromolecules and colloids

Code: **p2**

Title: **Surface Chemistry**

Lecturer: Professor David Lennon

Aims: To recognise fundamental concepts of heterogeneous catalysis through the study of the chemistry and kinetics of reactions occurring at the catalyst surface. Particular emphasis will be given to the importance of mechanism and the identification of the adsorption complexes active in the catalytic sequence.

Topics generally covered in this module include:

1. The significance of economic and industrial factors in modern heterogeneous catalysis.

2. The connections and constraints on chemisorption and catalysis by metals.

3. The derivation and development of the Langmuir-Hinshelwood kinetic expressions for simple hydrogenation reactions.

4. The discussion of the Horiuti-Polanyi mechanism for the gas phase hydrogenation of alkenes and establishment of the link between reaction kinetics and reaction mechanism.

5. The importance of a multi-technique approach for the elucidation of reaction mechanisms.

6. The discussion of how the kinetic isotope effect can provide mechanistic insight for heterogeneously catalysed reaction systems.

7. The derivation and development of structure/activity relationships in heterogeneous catalysis.

Module Outline:

- Reaction mechanisms active at the gas-solid interface;
- Application of reaction kinetics to assist in the determination of reaction mechanisms in industrially relevant reactions;
- Kinetic isotope effects;
- Structure/Activity relationships

Background reading:

P. Atkins and J. de Paula, *Atkins's Physical Chemistry*, Oxford University Press, 9th Edition (2010) ISBN: 978-0-19-954337-3.

Code: **p3**

Title: **Advanced Chemical Thermodynamics**

Lecturer: Dr Gordon Hedley

Aims: To build on thermodynamic concepts that have been introduced in 1st to 3rd year. In this course we will explore advanced thermodynamic theories, including how thermodynamic laws govern ideal energy cycles, the breakdown of ideally, and how advanced thermodynamic concepts control atomic and molecular diffusion. Special emphasis will be given to the applications of each area examined: how does advanced chemical thermodynamics impact upon problems and processes in the world around us, scientific research and societal problems?

Topics generally covered in this module include:

1. Chemical potentials. We will look at what they are, how we define and derive them, and what they are useful for.

2. The Debye–Hückel law. Beginning our examination of ideality, we will look at what happens in dilute solutions, where deviation from expected behaviour occurs, including usage of the Debye–Hückel equation in applied systems.

3. (A)diabatic processes. Continuing investigations of ideality, we will study what happens in systems where it only does work, without transferring heat or mass, and how this compares with systems that do.

4. Carnot & Stirling Cycles. We will build ideal and realistic cycles that do work, examining how they operate, why true ideallity can never be reached, and what real-world applications these can be used for.

5. Maxwell-Boltzmann Distributions. We will examine and understand the statistical laws that underpin how elements are organised according to statistical distribution, and how this can be used in applied contexts.

6. Fickian Diffusion. Finally, we will examine the laws that govern and the processes that result from statistical redistribution. We will explore practical examples of where these laws play an important role.

Module Outline:

- The concept of chemical potentials and their usage in real systems
- Examining the breakdown of ideality in dilute solutions
- Examining ideality in closed systems and how we can never quite reach it, but build systems that are close
- Looking at how statistical distributions can be used to describe a large collection of nominally independent actors. Those overarching distributions have implications in many areas of chemistry
- Those statistical distributions also play a role in allowing things to physically move – atoms, molecules, heat, excited states. This is called diffusion, and we shall examine the laws that control it and how it can be used in applied systems.

Code: **p4**

Title: **Modern NMR Spectroscopy**

Lecturer: Dr Smita Odedra

Aims: To review the physical basis of NMR spectroscopy and the interactions which determine the appearance of NMR spectra of both liquids and solids. To introduce the vector model of NMR and use it to describe experiments in order to measure longitudinal and transverse relaxation. To introduce methods for enhancing the sensitivity and resolution of NMR spectra of solids. To introduce the concept of coherence selection and define the rules of phase cycling.

Topics generally covered in this module include:

1. A review of the physical basis of NMR spectroscopy and related techniques such as MRI.

2. Explanation of key points relating to instrumentation, signal acquisition and signal processing.

3. Description of the origin and influence of the major interactions that determine the appearance of NMR spectra, such as the chemical shift, J-couplings, the dipolar interaction and quadrupolar couplings; distinguishing between the effects of these in solution-state and solid-state NMR.

4. Description of the vector model of NMR and its application to explain experiments, including those used to measure transverse and longitudinal relaxation; Manipulation of experimental data to calculate relaxation rate constants.

5. Description of methods commonly used to obtain high-resolution NMR spectra of solids with high sensitivity and resolution.

6. The importance of coherence selection and application of the rules of phase cycling to select particular changes in coherence order within a pulse sequence.

7. Application of the theory and techniques introduced during this course to related exercises.

In addition to the resources available on Moodle, these textbooks are recommended for further reading:

- P. J. Hore, *Nuclear Magnetic Resonance*, Oxford Chemistry Primers No. 32, Oxford University Press, Oxford, 1995. ISBN: 978-0198556824
- P. J. Hore, J. A. Jones and S. Wimperis, *NMR: The Toolkit*, Oxford Chemistry Primers, Oxford University Press, Oxford, 2015. ISBN: 978-0198703426
- J. Keeler, *Understanding NMR Spectroscopy*, Wiley, Chichester, 2005. ISBN: 978-0470017876
- M. H. Levitt, *Spin Dynamics: Basics of Nuclear Magnetic Resonance*, Wiley, Chichester, 2001. ISBN: 978-047148922
- D. Apperley, R. K. Harris and P. Hodgkinson, *Solid-State NMR: Basic Principles and Practice*, Momentum, New York, 2012. ISBN: 978-1606503508
- M. Duer*, Introduction to Solid-State NMR Spectroscopy*, Wiley, Chichester, 2010. ISBN: 978-8126525706

Code: **p5m**

Title: **Statistical Mechanics & Reaction Dynamics**

Lecturer: Dr. Frances Docherty

Aims: To build upon existing knowledge of classical thermodynamics, spectroscopy and quantum mechanics such that an understanding of the statistical behaviour of bulk samples is developed. Quantitative methods for describing reaction dynamics and how this relates to kinetics and transition states will also be described.

Topics generally covered in this module include:

1. Definition of the Boltzmann distribution through concepts such as instantaneous configurations and employ the Boltzmann law for a system of particles.

2. Derivation and application of the equations that define the molecular partition function with respect to populations and internal energy.

3. How to differentiate between the molecular and canonical partition functions and use them in obtaining thermodynamic information (including some derivations).

4. Demonstration of how statistical thermodynamics can be applied to gain insight into a number of physical, chemical, and biological processes.

5. The expression, derivation and application of quantitative theories for the dynamics of a reaction, including collision theory, transition state theory, and potential energy surfaces.

Code: **p6m**

Title: **Theoretical & Computational Chemistry**

Lecturer: Dr. Hans Senn

Aims: To introduce basic elements of quantum chemistry and molecular electronic structure theory, including computational aspects.

Topics generally covered in this module include:

1. How to formulate the connection between classical and quantum mechanics using the correspondence principle.

2. Application of the postulates of quantum mechanics.

3. Explanation of the properties of (electronic) wavefunctions. Description of the construction of Slater determinants.

4. Description of the molecular Schrödinger equation.

5. Description and application of the variation principle for the ground state.

6. Description of the Born–Oppenheimer approximation and of the concept of potential-energy surfaces.

7. Description of the principles of the self-consistent field (SCF) method and Hartree–Fock theory.

8. Explanation of the phenomenon of electron correlation and its consequences on solving the Schrödinger equation.

9. Description of the principles of approximate methods to recover the correlation energy.

10. Description of the principles and features of density functional theory.

Module Outline:

- Classical and quantum mechanics: From Newton to Hamilton to Schrödinger.
- The Schrödinger equation. Motivation from classical wave equation; correspondence principle.
- Properties of the wavefunction. Born interpretation.
- Postulates of quantum mechanics.
- Mathematical background: Operators, eigenvalue problems, Hermiticity, orthonormality.
- The variation principle.
- Wavefunctions for multielectron systems. Pauli principle and amtisymmetry; fermions and bosons. Slater determinants.
- The molecular Schrödinger equation.
- Separation of nuclear and electronic motion; Born–Oppenheimer approximation. Potential energy surfaces.
- Self-consistent field method, Hartree–Fock theory.
- Electron correlation. Approximate methods beyond Hartree–Fock.
- Density-functional theory

Code: **m1-o**

Title: **Biopolymer chemistry and synthesis**

Lecturer: Dr Andrew Jamieson

Aims: To introduce biopolymers, namely nucleic acids, peptides/proteins and carbohydrates. Their properties, chemistry and approaches for synthesis will be discussed.

Topics generally covered in this module include:

1. Explanation of the structure of nucleic acids, peptide/proteins and carbohydrates.

2. How to derive, explain and predict the physical and chemical properties of these biopolymers from the presence of their characteristic functional groups.

3. Explanation of the structures, names and abbreviated names of amino acids as well as explanation of their properties.

4. Explanation of the structure, properties, introduction and cleavage of the protecting groups commonly used in peptide, nucleic acid and carbohydrate synthesis.

5. Explanation of the structure of coupling reagents and conditions commonly used in peptide, nucleic acid and carbohydrate synthesis.

6. Classification and explanation of the different methods for peptide, nucleic acid and carbohydrate synthesis (solution, solid-phase, enzymatic).

7. How to devise the step-wise synthesis of a peptide, nucleic acid or disaccharide.

8. Explanation of the structure, properties and application of biomimetic polymers.

Module Outline:

- Revision of nucleic acid, peptide/protein and carbohydrate structure and introduction to their chemical properties.
- Introduction of protecting groups and their use in peptide synthesis.
- Explanation of the different approaches to solid phase peptide synthesis.
- Introduction to protecting groups and the synthesis of nucleic acids.
- Explanation of the different approaches to disaccharide synthesis.
- Introduction to biomimetic polymers.

Code: **m2-o**

Title: **Industrial Medicinal Chemistry**

Lecturers: Dr. Jamie Scott (AstraZeneca), Dr. Phil Humphreys (GlaxoSmithKline)

Aims: To establish an appreciation of modern drug identification approaches and the multiparameter nature of optimisation in modern drug discovery research. In particular, the central importance of control of lipophilicity in generating high quality candidates. This will be illustrated by recent examples of pharmaceutical research programs.

Topics generally covered in this module include:

1. Definition of lipophilicity and how it is measured, differentiating between logP and logD and explanation of changes to a structure that will modulate its lipophilicity.

2. Description of some of the factors that need to be optimised in drug discovery (e.g. potency/solubility/metabolism/plasma-protein-binding/toxicity) and how these factors are correlated with lipophilicity.

3. Definition of terms such as Ligand Efficiency (LE), Ligand Lipophilicity Efficiency (LLE) and how to calculate these when provided with the appropriate data.

4. Explanation of basic pharmacokinetic principles (ADME), description of metabolic processes and how changes to a structure can be applied to modulate its metabolism.

5. Discussion of the importance of hERG as an anti-target and how changes to a structure can be applied to modulate its hERG liabilities.

6. Description of how to use fragment-based drug design strategies to identify and optimize potential drug molecules.

7. Explanation of molecular interactions that drugs typically make with their protein targets and strategies for optimizing these interactions.

8. Description of the factors important in designing and synthesising drugs with the lowest odds of toxicity and promiscuity.

Module Outline:

- Introduction to Medicinal Chemistry concepts
- The importance of lipophilicity
- Balancing multiple opposing parameters (e.g. potency/solubility/metabolism/plasma-protein-binding/toxicity) in order to identify high quality candidates
- hERG as an example of an anti-target
- **Case studies**

Code: **m3-o**

Title: **Medicinal Chemistry of Cancer**

Lecturer: Dr. Ciorsdaidh Watts

Aims: To introduce the different types of anticancer drugs, their design, synthesis and mode of action, together with new ways of discovering and optimising drug candidates.

Topics generally covered in this module include:

1. Explanation of abnormal cell growth, its causes and possible treatments.
2. Classification of different types of targets and potential targets for anticancer therapies, and different types of anticancer drugs and potential anticancer drugs.
3. Explanation of the synthesis (or partial synthesis) of different types of anticancer drugs and potential anticancer drugs, and their mechanisms of action and pharmacology.
4. Discussion of design syntheses of novel compounds structurally related to known anticancer compounds.
5. Evaluation of chemical structures for their potential as anticancer agents.
6. Explanation of chemical genetics, the design of libraries for screening and the role of chemical biology in drug discovery.
7. Discussion of the purpose and use of fragment-based design in drug discovery.
8. Explanation of terms including *ligand efficiency* and pIC_{50} and how to use the associated equations to calculate these.

Module Outline:

- Introduction to cancer biology and therapy
- Past successes (including in depth study of several classes of important anticancer drugs)
- Modern techniques for drug discovery (chemical biology, chemical genetics, library design, privileged structures)
- New opportunities for cancer chemotherapy

Code: **m4-o**

Title: **Chemical Biology**

Lecturers: Prof. Richard Hartley

Aims: To introduce the main concepts of chemical biology and the tools for elucidating biological processes through synthetic chemistry.

Topics generally covered in this module include:

1. The structure of cells and the processes within them.

2. The structures, names and abbreviated names of amino acids and explanation of their roles in proteins including mechanisms for reactions involving them.

3. How to devise and explain the mechanisms involved in the synthesis of peptides, particularly native chemical ligation and removal of the thiol group from cysteine.

4. Explanation of molecular biological tools for incorporating labels, tags and sensors, and manipulating biological processes (e.g. unnatural amino acids, SNAP-tag).

5. Classification and explanation of different ways of identifying, sensing, reporting, quantifying, locating, and determining the temporal control of biological molecules and processes (including monitoring protein biosynthesis and activity-based profiling)

6. Design and explanation of the structures of, syntheses of and mechanisms of sensors, in particular ROS and calcium sensors.

7. Design and explanation of the structures, syntheses and mechanisms involved in bio-orthogonal reactions, tagging, labelling, targeting and pull down technologies.

8. Design and explanation of the structures, syntheses and mechanisms involved in photoactivation (e.g. in photoaffinity labelling, uncaging, and photoswitching) and how it is used to understand biological processes and identify biomolecules.

9. Evaluation of chemical structures for their potential as tags, labels, molecular probes, sensors or functional molecules.

10. How to design structures for and syntheses of novel compounds structurally related to known labels, molecular probes, sensors or functional molecules to behave in similar ways.

11. Discussion of chemical genetics and evaluation of this and of competing techniques

Module Outline:

- Introduction to cell structure and chemical biology, revision of the amino acids and the functional roles they play in proteins
- Bio-orthogonal reactions
- Reporting on biological processes: modes of reporting (light, mass), sensors (irreversible and reversible), spatial resolution (labeling and targeting strategies)
- Activity-based probes and photoaffinity probes
- Chemical genetics and pull down technologies
- Intracellular targeting
- Sensing reactive oxygen species and calcium ions.
- Instructing biological processes: small molecule modulators, temporal external control (photoactivation and photoswitching), internal control (uncaging)

Code: **s1-o**

Title: **Organometallics in Synthesis**

Lecturer: Dr. David France

Aims: To develop a mechanistic understanding of reactions of organic molecules with transition metal complexes, and a working knowledge of transition metal-mediated methods that are of particular importance to organic synthesis.

Topics generally covered in this module include:

1. The recognition and description of fundamental organometallic processes (*e.g.* coordination/dissociation, oxidative addition/reductive elimination, insertion).

2. How to predict the product of organometallic reactions based on fundamental principles.

3. Explanation of the mechanisms of transition metal-mediated reactions in organic chemistry.

4. Identification of specific reaction conditions required for catalytic cycles to be efficient.

5. How to design syntheses of target organic molecules that make use of transition metals.

Module Outline:

Fundamental organometallic processes, including catalytic cycles. Alkene metathesis catalysts. Palladium catalysed reactions including C–C, C–N, and C–O bond formation and C–H activation.

Code: **s2-o**

Title: **Organic Supramolecular Chemistry**

Lecturer: Prof. Dave Adams

Aims: To describe, illustrate and use the basic principles of supramolecular chemistry.

Topics generally covered in this module include:

1. Discussion and use of the fundamental principles of non-covalent interactions.

2. Illustration on how to use the principles of molecular recognition and self-assembly.

3. Illustration of how the principles of supramolecular chemistry can be used in the development of enzyme models and mimics.

4. Illustration of how the principles of supramolecular chemistry can be used to develop self-replicating systems, in the construction of molecular machines and devices.

Module Outline:

- Introduction to organic supramolecular chemistry;
- Host-guest chemistry;
- Self-assembly;
- Biomimetic chemistry (e.g. enzyme models, photosynthetic models and molecular replication);
- Materials chemistry (e.g. supramolecular polymers);
- Biologically inspired molecular devices and machines.

Code: **s3-i**

Title: **Molecular Magnetism**

Lecturer: Prof. Mark Murrie

Aims: To provide an overview of molecular magnetism, from the magnetic properties of transition metal ions to those of transition metal complexes, and more complex molecular systems such as single-molecule magnets.

Topics generally covered in this module include:

1. Discussion of the magnetic properties of the first row transition metal single-ions and contrasting these properties with those of simple transition metal complexes.

2. Explanation of magnetic properties based upon molecular structure.

3. Prediction of the magnetic properties of large molecular systems.

4. Explanation of the origins of magnetic anisotropy and discussion of the properties of single-molecule magnets.

Module Outline:

- Introduction to magnetic susceptibility: diamagnetism, paramagnetism and the Curie Law;
- Single-ion magnetic properties: spin and orbital contributions;
- Exchange interactions: dimers, superexchange and orbital overlap;
- Spin clusters: exchange coupling and magnetostructural correlations;
- Magnetic anisotropy: from single-ion anisotropy to single-molecule magnets;
- Slow magnetic relaxation and quantum tunnelling in single-molecule magnets.

Code: s4-i

Title:	Electrochemistry for a Sustainable Future
Lecturer:	Dr. Mark Symes
Aims:	This module will examine the applications of electrochemistry in a variety of contexts of relevance to sustainable chemical processes. We shall investigate electrochemical methods for water purification, metal extraction and energy (harvesting, storage and conversion). Many of the examples shown are at the cutting edge of scientific and technological research. The emphasis throughout the course will be on the interplay between fundamental concepts and the materials required to perform the tasks of interest.
Topics generally covered in this module include:	
Lecture 1:	*Introduction to Electrochemistry.* Familiarisation with the concepts of electrochemical potential and basic electrochemical processes such as bulk electrolysis and cyclic voltammetry.
Lecture 2:	*Fuel Cells.* Familiarisation with the concepts of the fuel cell and explanation of how fuel cells work and which material properties are desirable when designing such devices.
Lecture 3:	*Electrolysis of Water.* Explanation of why electrolytic production of hydrogen from water is important and comparison of different methods of electrolysis and different materials for this purpose.
Lecture 4:	*Batteries.* Description and explanation of the concepts behind and performance of a selection of battery technologies, including lead-acid batteries, Li-ion batteries and redox flow batteries.
Lecture 5:	*Photo-electrochemistry.* Description and explanation of what a photo-electrochemical cell is and how it works in terms of its materials of construction, and assessment of the relative performance of different cells.
Lecture 6:	*Water Purification.* Explanation of the various electrochemical methods of water purification and discussion of their various merits and demerits.
Lecture 7:	*Metal Extraction.* Explanation of the different electrochemical strategies used to obtain metals from their ores and assessment of these in terms of their relative efficiency and environmental impact.
Lecture 8:	*Electrochemical Fuel Production.* Examination of current research in the direct synthesis of fuels using electrochemistry, looking in particular at the electrochemical reduction of CO_2. Application of the skills and knowledge acquired during the previous seven lectures to assessment of the prospects for this avenue of research.

Suggested Reading:

1. *Electrochemical Methods: Fundamentals and Applications*, 2nd Edition Allen J. Bard and Larry Faulkner (John Wiley and Sons, 2001).
2. *Materials for a Sustainable Future,* Trevor M. Letcher and Janet L. Scott (Eds.) (RSC Publishing, 2012).

Code: **s5-p**

Title: **Surface Structure & Spectroscopy**

Lecturer: Dr A. Karimullah

Aims: To serve as an introduction into surface science, to describe modern spectroscopic techniques of surface analysis and how they can be applied to model systems.

Topics generally covered in this module include:

1. The discussion of why UHV techniques are necessary to study model systems.

2. The nomenclature of surface structure and its use to explain concepts such as surface relaxation and reconstruction.

3. The discussion of low energy electron diffraction and how it can be applied in the determination of surface structure.

4. The description of adsorption at surfaces, and the importance of physisorption and chemisorption.

5. The reasons for the employment of electron based spectroscopic techniques in surface science, highlighting the most commonly used techniques.

6. The explanation of the technique of temperature programmed desorption and its kinetics.

7. The description of vibrational spectroscopy at surfaces and the associated selection rules.

Module Outline:

What is surface science?
- Ultra high vacuum, single crystal surfaces, surface density.
- Techniques generally, electron surface sensitivity.

Electron spectroscopy
- Energy distribution curves
- Auger electron spectroscopy; X-ray photoelectron spectroscopy (chemical shifts, relaxation); UV photoelectron spectroscopy

General adsorption:
- Physisorption; Chemisorption
- Sticking probability
- Langmuir and precursor state adsorption
- Accommodation

Thermal desorption spectroscopy:
- Kinetics of desorption

Surface structure:
- Nomenclature
- 2D Bravais lattices
- Relaxation

Low energy electron diffraction (LEED):
- Electron diffraction
- Ewald sphere construction; Reconstruction
- Matrix notation

Vibrations at surfaces:
- RAIRS, HREELS, SERS, SFG
- Selection rules
- Vibrational relaxation

Code: **s6-p**

Title: **Dynamics of molecular clusters and fluids**

Lecturer: Prof. Klaas Wynne

Aims: To introduce a time-resolved picture of spectroscopy and the molecular world. Various kinds of common spectroscopy will be described in terms of correlations in time, while not so common time-resolved spectroscopies will be introduced. The motions of molecules – vibrations, tumbling, diffusion, and flowing of liquids – will be described as well as ideas related to crystallisation, jamming, supercooling, clustering, supersaturation, *etc*. Finally, it should become clear that the dynamics of molecules is intimately related to those of sand, paint, and car jams on the motorway.

Topics generally covered in this module include:

1. A formal description of time resolved dynamics and time-resolved spectroscopy
2. Description of dynamics in liquids: the types of motions, characteristic timescales, viscosity, and diffusion
3. Description of jamming and glass formation: cooperativity, critical behaviour, jamming, and relaxation.
4. Description of solutions: the effect of solute molecules (including proteins) on the surrounding medium
5. Description of "weird" liquids: room temperature ionic liquids, liquids crystals, liquid proteins, etc.
6. Description of crystal nucleation: supersaturation, etc.

Module Outline:

1. Time-resolved dynamics: seeing the world as it was meant to be, in the time domain
    a. Basic correlation functions, oscillator
    b. Fourier transform basics (not much math)
    c. Damping: homogeneous vs. inhomogeneous
2. Time-resolved spectroscopies
    a. IR, Raman, fluorescence
    b. Ultrafast pump-probe spectroscopy, coherence
3. Dynamics in liquids
    a. "Simple" liquids
    b. Basic motions: vibrations, librations, cage rattling, diffusion
    c. Timescales
    d. Viscosity, Arrhenius behaviour
    e. Diffusion (Stokes-Einstein), rotation (Stokes-Einstein-Debye)
4. Jamming and glasses
    a. Cooperativity, molecular clusters, rattling
    b. Anomalous viscosity *etc*.
    c. Supercooling
    d. Vogel-Fulcher-Tamman, critical divergence
    e. Jamming: cars, sand piles, colloids
    f. VFT for jamming
    g. α-relaxation, β-relaxation
5. Solutions
    a. Viscosity: Jones-Dole
    b. Salt solutions, structure around ions
    c. VFT for solutions
6. Weird liquids
    a. Molten salts: RTILs, magnetic RTILs? Non-protic and protic ionic liquids
    b. Liquid crystals
    c. Liquid protein
7. Crystal nucleation
    a. Solutions, saturation
    b. Nucleation, kinetics, homogenous nucleation theory
    c. Critical density fluctuations enhancing crystal nucleation