# STAGE 4: MODULES

**Autumn Term:** Monday 21 Sept 2009 – Friday 11 Dec 2009
**Spring Term:** Monday 4 Jan 2010 – Friday 19 March 2010
**Summer Term:** Monday 19 April 2010 – Friday 11 June 2010

**Semester 1:** Monday 21 Sept 2009 – Friday 22 Jan 2010
**Semester 2:** Monday 25 Jan 2010 – Friday 11 June 2010

| RESEARCH PROJECT IN INDUSTRY | **CHY8310**<br>80 credits<br>[40 ECS credits]<br>semester 1 & 2 |
|---|---|
| Module Leader | Dr JG Knight |
| Staff | Various |
| Prerequisites | Stage 2 of an MChem programme |
| Aims | To provide students with research experience in an industrial context |
| Timetabled sessions | Full-time employment over both Semesters 1 & 2 involving laboratory work in an industrial company. |
| Assessment | Assessment of project work (30%), final report (30%), presentation (15%) and viva (25%) |

The project provides Stage 3 students with an opportunity to work in an industrial setting on a project with industrial relevance.

Assessment of the practical work performed during the project will be carried out by the project supervisor. In addition, students will be expected to submit a final written report summarising the context and results. After submission of the report, students will make a presentation (15 minutes) on their work to an audience consisting of at least the industrial supervisor and a member of academic staff. The report will be marked by the supervisor and another member of academic staff, who will then together conduct an oral examination (45 minutes) of the candidate.

The resit will be re-submission of the report, and viva.

**Coursework**

| **Type** | **Duration** | **Date set** | **Deadline** | **Feedback** |
|---|---|---|---|---|
| Report | | Induction week | 7 May | By 26 June |
| Presentation | 15 min | Induction week | 17-28 May | By 26 June |
| Oral | 40 min | Induction week | 17-28 May | By 26 June |

| RESEARCH PROJECT ABROAD | **CHY8311**<br>80 credits<br>[40 ECTS credits]<br>semester 1 & 2 |
|---|---|
| Module Leader | Dr JG Knight |
| Staff | Various |
| Prerequisites | Stage 2 of an MChem programme<br>An MChem placement in a university in North America or France or Spain or Germany |
| Aims | To provide students with research experience in an university in another country |
| Timetabled sessions | Students undertake a project while on placement. Assessment is based on written reports, project work and presentations. |
| Assessment | Assessment of project work (50%) and final report (50%) |

Most of the module involves practical work within the research laboratories at the host institution but also includes time for experimental design and some background work. Private study includes time for background reading, project planning and writing and preparing reports and presentations

Assessment of the practical work performed during the project will be carried out by the project supervisor. In addition, students will be expected to submit a final written report summarising the context and results.
The resit will be re-submission of the report, and viva.

**Coursework**

| **Type** | **Date set** | **Deadline** | **Feedback** |
|---|---|---|---|
| Report | Induction week | 7 May | By 26 June |

| RESEARCH PREPARATION | **CHY8410**<br>10 credits<br>[5 ECTS credits]<br>semester 1 |
|---|---|

| | |
|---|---|
| Module Leader | Dr C Bleasdale |
| Staff | Dr C Bleasdale, , Dr IR Hardcastle and Dr JG Knight.<br>External speakers from industry and academia |
| Pre-requisites | A BSc or equivalent in Chemistry or a related subject |
| Aims | To prepare students for their research project; to introduce and consolidate key skills to enhance performance in the research project |
| Timetabled sessions | Lectures and seminars 24h, PC work 3h |
| Assessment | Written coursework (100%) |

**Intended Learning Outcomes**

At the end of this course, students should be able to:

- understand research methods, process and tools
- search and locate sources of chemical information
- formulate strategies for finding information
- interpret primary literature and plan future work on the basis of this interpretation
- find and abstract information from primary research sources
- communicate the essence of the information in written and oral form
- formulate a project plan effectively
- assimilate information presented in research seminars and construct abstracts
- perform a risk assessment for a practical experiment

**Workshops**

Workshops will cover the following areas:

- Research seminars and seminar reports
- Scientific ethics
- Searching the Scientific Literature: primary and secondary sources
- Abstracting information and writing reports
- Databases
- Citations and Endnote
- Project plans
- Safety and risk assessments

A schedule for the delivery of workshops is below, please check noticeboards for further information.

**Research Seminars**
**(These will be held on Tuesdays at 4.15pm in Bedson Lecture Theatre 3)**

| | |
|---|---|
| 29 September | Dr Rachel O'Reilly, Warwick University |
| 6 October | Prof Neil Hunter, Sheffield University |
| 13 October | Dr Darren Dixon, Oxford University |
| 20 October | Prof Ole Hindergard, Copenhagen |
| 27 October | Prof Martin Schroder, Nottingham University |
| 6 November | Dr Scott Denmark, University of Illinois |
| 10 November | Prof Barry Potter, Bath University (PROVISIONAL) |
| 17 November | Prof Martin Wills, Warwick University |
| 24 November | Prof Paul Raithby, Bath University |
| 1 December | Prof Dave Garner, Nottingham university |
| 8 December | Prof Rab Mulvey, Strathclyde University |

**Coursework**

A programme of coursework deadlines will be distributed in the first workshop.  Feedback will be provided within 4 weeks.

| RESEARCH PROJECT | **CHY8411**<br>60 credits<br>[40 ECTS credits]<br>semester 1 & 2 |
|---|---|
| Module Leader | Dr JG Knight |
| Staff | Various |
| Prerequisites | CHY3001 |
| Aims | To provide students with a research project in a modern area of chemistry; to give students the experience of working in a research environment |
| Timetabled sessions | Laboratory work: half time during Semesters 1 & 2 |
| Assessment | Assessment of project work (30%)<br>Report (30%)<br>Oral examination (25%)<br>Presentation (15%) |

The project provides Stage 4 students with an opportunity to work in an active research environment on a project relevant to their areas of interest. Students indicate their preferences for projects at the beginning of Semester 1.

Assessment of the practical work performed during the project will be carried out by the project supervisor. Students will be expected to submit a final written report, at the end of the module. Students will deliver a final presentation (15 minutes, plus 5 minutes of questions), summarising their work, to an audience consisting of their peers and members of staff. Academic staff assess the final project report and conduct an oral examination (30 minutes) of the candidate.

**Coursework**

| **Type** | **Date set** | **Deadline** | **Feedback** |
|---|---|---|---|
| Project | Induction week | | By 26 June |
| Report | Induction week | 5 pm Fri Week 44 | By 26 June |
| Presentation | Induction week | Thurs week 45 | By 26 June |
| Oral Exam | Induction week | Mon–Wed week 46 | By 26 June |

| RESEARCH PROJECT | **CHY8412**<br>40 credits<br>[20 ECTS credits]<br>semester 1 & 2 |
|---|---|
| Module Leader | Dr JG Knight |
| Staff | Various |
| Prerequisites | A placement in industry or at another university at stage 3 |
| Aims | To provide students with a research project in a modern area of chemistry; to give students the experience of working in a research environment |
| Timetabled sessions | Laboratory work: full time |
| Assessment | Assessment of project work (30%)<br>Report (30%)<br>Oral examination (25%)<br>Presentation (15%) |

The project provides Stage 4 students with an opportunity to work in an active research environment on a project relevant to their areas of interest. Students indicate their preferences for projects at the beginning of Semester 1.

Assessment of the practical work performed during the project will be carried out by the project supervisor. Students will be expected to submit a final written report, at the end of the module. Students will deliver a final presentation (15 minutes, plus 5 minutes of questions), summarising their work, to an audience consisting of their peers and members of staff. Academic staff assess the final project report and conduct an oral examination (40 minutes) of the candidate.

**Coursework**

| **Type** | **Date set** | **Deadline** | **Feedback** |
|---|---|---|---|
| Project | Induction week | | By 26 June |
| Report | Induction week | 22 May | By 26 June |
| Presentation | Induction week | 28 May | By 26 June |
| Oral Exam | Induction week | 4 June | By 26 June |

| ORGANIC SYNTHESIS FOR DRUG TARGETS | **CHY8420**<br>10 credits<br>[5 ECTS credits]<br>semester 2 |
|---|---|
| Module Leader | Dr JG Knight |
| Lecturers | Dr JG Knight and Professor M North |
| Prerequisites | CHY3101 |
| Aims | To familiarise students with the key strategies for the stereocontrolled synthesis of drug targets; to provide practise in identifying and applying such strategies; to exemplify the principles in the context of the synthesis of drug targets |
| Timetabled sessions | Lectures and seminars 24 h |
| Assessment | Exam 2h at the end of semester 1 (100%) |

**Intended Learning Outcomes**

At the end of this course, students should:

- recognise and be able to comment on different synthetic strategies and methods for stereocontrol when faced with a synthetic scheme
- understand the different classes of 'selectivity' and 'specificity'
- understand and be able to use the Felkin-Anh model, chelation control, and 1,3-allylic strain to predict the stereoselectivity of reactions
- be able to use chair transition state models to explain the stereochemical outcome of reactions when appropriate (such as enolisations and the aldol reaction)
- understand the ideas of topicity, double stereodifferentiation, and chiral amplification
- have an awareness of typical reagents and transformations used in modern organic synthesis
- be able to identify aspects of selectivity and specificity within a given synthetic scheme
- to make a reasoned choice of theoretical model
- to apply this model in order to predict or explain the observed outcome.

**Lectures**

**Stereocontrol In Organic Synthesis ,JGK**

| | |
|---|---|
| 1 | Introduction to synthetic strategy, selectivity and specificity |
| 2 | Regioselectivity |
| 3, 4 | Stereoselectivity |
| 5, 6 | The aldol reaction |
| 7 | Asymmetric synthesis. Use of the chiral pool |
| 8, 9,10 | Chiral auxiliaries |
| 11 | Seminar covering the material in lectures 1-10 |

**Asymmetric Catalysis, MN**

| | |
|---|---|
| 12 | Introduction to catalysis and asymmetric catalysis. Energy diagrams. Temperature dependence of asymmetric induction. Examples of commercial asymmetric catalytic procedures. |
| 13 | Chiral ligands. Ligand design. Ligand-symmetry. Energy diagrams for C1- and C2-symmetric processes. |
| 14 | Metals used in asymmetric catalysis. Role of the metal. What makes a good asymmetric catalyst? |
| 15 | Asymmetric catalysis of reduction reactions. Alkene hydrogenation. Ketone reduction. |
| 16 | Corey oxazaborolidinone? Asymmetric catalysis of oxidation reactions. Sharpless epoxidation. Jacobsen epoxidation and related reactions. |
| 17 | Sharpless bis-hydroxylation and aminohydroxylation. Asymmetric catalysis of carbon-carbon bond forming reactions. Cycloaddition reactions. |
| 18 | Addition of diethylzinc to aldehydes. Addition of silylated nucleophiles to aldehydes. Asymmetric cyanohydrin synthesis. |

19 Organocatalysis. Enamine chemistry. Proline catalysed aldol reactions. Mannich reactions. Aldehyde amination and oxygenation. Michael additions.

20 Use of enzymes as catalysts. Whole cell and isolated enzymes. Need for cofactors. Oxidoreductases. Lipases. Oxynitrilases including Henry reaction.

21 Asymmetric catalysis on compounds which already contain stereocentres. Kinetic resolution. Dynamic kinetic resolution. Desymmetrization of meso compounds. Double stereodifferentiation.

22 Non-linear effects. Autocatalytic asymmetric induction. Absolute asymmetric synthesis.

23, 24 Seminars covering questions on the material in lectures 1-22

**Reading References**

Organic Chemistry, J Clayden, N Greeves, S Warren, P Wothers, Oxford University Press, 2000 IBSN: 0198503466

Principles and Applications of Stereochemistry, M. North, STP, 1998 IBSN: 0751404209

Stereoselectivity in Organic Synthesis, G Procter, Oxford Chemistry Primer, Oxford University Press, 1998 IBSN: 0198559577

| ADVANCED METHODS IN DRUG DISCOVERY | **CHY8421**<br>10 credits<br>[5 ECTS credits]<br>semester 1 |
|---|---|
| Module Leader | Dr IR Hardcastle |
| Lecturers | Dr IR Hardcastle and Dr MA Carroll |
| Prerequisites | CHY3101 |
| Aims | To demonstrate the role of combinational synthesis in drug discovery; to provide students with an understanding of the historical development of combinational methods; to introduce the concepts of solid- phase synthesis and resin- assisted synthesis; to provide students with an understanding of radioisotopes in medical imaging. |
| Timetabled sessions | 24 Lectures and seminars |
| Assessment | Exam 2h at the end of semester 1 (80%), problem seminars (20%) |

**Intended Learning Outcomes**

At the end of this course, students should:

- understand the application of solid-phase methods in the synthesis of peptides, peptide libraries, and small molecule libraries
- appreciate the different combinatorial techniques including split-mix synthesis and multiple parallel synthesis
- be familiar with a range of solid-phase reactions
- be familiar with a range of commonly used radioisotopes and practical aspects relating to their use in a range of applications

**Lectures**

**Combinatorial chemistry in Drug Discovery, IRH**

1 Introduction to Drug Discovery
2 Origins of solid-phase synthesis
3 Peptide libraries (1)
4 Peptide libraries (2)
5 Small-molecule combinatorial libraries
6 Small-molecule combinatorial synthesis (synthesis strategies)
7 Solid-phase synthesis (resins and linkers)Solid-phase reactions (1)
8 Solid-phase reactions (2)
9 Solid-phase-assisted solution-phase synthesis
10 Examples from combinatorial drug discovery
11 'Magic-microwaves'
12 Drug discovery technology
13 Recent examples and advances
14 Seminar

**Radioisotopes in Drug Discovery, MAC**

1 Introduction to radioactivity
2 Tritium, and $^{14}$Carbon
3 Positron Emision Tomography (PET)
4 Compounds containing $^{11}$C (1)
5 Compounds containing $^{11}$C (2)
6 Compounds containing $^{18}$F (1)
7 Compounds containing $^{18}$F (2)
8 Other isotopes.
9 Seminar + Assignment 2

**Reading References**


Combinatorial Chemistry, NK Terrett, Oxford, 1998 IBSN: 0198502192

Solid Supported and Parallel Synthesis of Small – Molecular Weight Compound, D Obrecht and JM Villalgordo, Perganon, 1998 IBSN: 0080432573

Medicinal Chemistry Principles and Practice, FD King The Royal Society of Chemistry 2002 IBSN: 0854046131

Radiopharmaceuticals: Radiochemistry and Applications, Eds. M. J. Welch and C. S. Redvanly, Wiley, 2003 ISBN: 0471495603

| FURTHER ORGANIC CHEMISTRY | **CHY8422**<br>10 credits<br>[5 ECTS credits]<br>Semesters 1 |
|---|---|
| Module Leader | Dr MJ Hall |
| Lecturers | Dr MJ Hall and Dr J Knight |
| Pre-requisites | CHY3101 |
| Aims | To introduce and develop the concepts of thermal and photochemical pericyclic reactions and Frontier Molecular Orbital (FMO) theory; to describe the methods used to determine the mechanisms of such reactions; to discuss radical chemistry; to explore reactions involving radicals and ions in cyclisation reactions |
| Assessment | 2 h Examination at the end of Semester 1 (100%) |

**Intended Learning Outcomes**

At the end of this course, students should:

- be able to construct simple π-molecular orbitals for linear, conjugated systems
- know the basic types of pericyclic reactions
- understand and apply FMO theory and the Woodward-Hoffmann rules to thermal and photochemical pericyclic reactions
- have knowledge of the methods used to generate stable and transient radicals species
- understand radical chain reactions; initiation, propagation and termination steps
- understand the usefulness of radical reactions and apply concepts to synthetic problems
- be able to predict the outcome of radical ring closing reactions using Baldwin's rules

**Lectures**

**Pericyclic reactions and Frontier Molecular Orbital Theory (FMO), JK**

1-3 Molecular Orbitals and revision of the application of Frontier MO theory to ionic (and radical) processes and relevance to Hard and Soft Acid and Base theory. Construction of basic FMO's for linear conjugated π-systems. Introduction to pericyclic reactions.

4-6 Cycloaddition reactions. The Diels-Alder reaction: mechanism, Frontier-Orbital analysis, stereospecificity. The effect of substituents on FMO energies and coefficients. Stereoselectivity and regioselectivity in Diels-Alder reactions. Cheletropic reactions and 1,3-dipolar cycloadditions. Photochemical cycloaddition reactions. The Woodward-Hoffmann rules.

7-8 Electrocyclic reactions.

9-10 Sigmatropic reactions. Group transfer reactions.

**Radical Reactions, MJH**

1, 2 Introduction to free radicals: generation of radicals (thermal, photochemical, electrochemical), properties and reactivity, SOMO, hard vs. soft.

3, 4 Stoichiometric radical processes: removal of functional groups and other applications in synthesis.

5-7 Kinetics of radical reactions: chain reactions, polymerisation, the use of tin centred radicals, applications in synthesis, alternatives for tin.

8 Ring closing reactions: predicting ring closure with Baldwin's rules and cascade processes.

9, 10 Modern advances in radical chemistry

**Reading references**

Organic Chemistry, J Clayden, N Greeves, S Warren and P Wothers, Oxford University Press, 2000, ISBN: 9780198503466

**Pericylics and FMO**
Pericyclic Reactions (Oxford Chemistry Primers), I. Fleming, Oxford University Press, 1999, ISBN: 9780198503071

Frontier Orbitals and Organic Chemical Reactions, I. Fleming, Wiley, 1978, ISBN: 9780471018193

Frontier Orbitals a Practical Manual, N.T. Anh, Wiley, 2007, ISBN: 9780471973584

**Radicals**
Radical Reactions in Organic Synthesis (Oxford Chemistry Masters), S. Z. Zard, Oxford University Press, 2003, ISBN: 9780198502400

Radical Chemistry: The Fundamentals (Oxford Chemistry Primers), J. Perkins, Oxford University Press, 2000, ISBN: 9780198792891

Radicals in Organic Synthesis: Formation of Carbon-Carbon Bonds, B. Geise, Pergamon, 1986, ISBN: 9780080324944

| ADVANCED TOPICS IN CONTEMPORARY PHYSICAL CHEMISTRY | | **CHY8423**<br>10 credits<br>[5 ECTS credits]<br>semester 2 |
|---|---|---|
| Module Leader | Professor A Harriman | |
| Lecturers | Professor A Harriman, Dr BR Horrocks and Professor KM Thomas | |
| Prerequisites | CHY2201 & CHY3201 | |
| Aims | To describe modern advances in advanced physical chemistry by reference to selected topics built around the design of chemical sensors. Included are the basic principles underlying the concepts of modern computational chemistry, porous nanostructures, electron transfer processes and aspects of modern theoretical chemistry.. | |
| Timetabled sessions | Lectures 24h (8h per course) | |
| Assessment | 2h exam at the end of Semester 1 (100%) | |

**Intended Learning Outcomes**

At the end of this course, students should:

- have developed an in-depth understanding of the principles of theoretical chemistry and the ability to use contemporary software
- be able to appreciate the power and limitations of modern computational chemistry
- understand the mechanisms and principles by which porous material operate
- appreciate the significance of molecular sieving and storage in terms of industrial needs
- be able to develop mathematical models explaining the conductivity of electrons along a molecular axis
- be able to design and test molecular-scale wires

**Lectures**

**Computational Chemistry. BRH**

1 Review of quantum chemistry; many-electron wave-functions
2 Hartree-Fock theory
3 Semi-empirical methods
4 Electron correlation
5 Density functional methods
6 Molecular mechanics
7 Simulation of condensed phases: molecular dynamics
8 Monte Carlo methods

**Porous Materials. KMT**

1 Comparison of rigid adsorbents and porous metal organic framework (MOF) materials
2 Underlying principles of design strategies for MOF's – template interactions
3 Framework dimensionality and flexibility
4 Relationships between structure and adsorption characteristics
5 Structural changes during adsorption
6 Kinetic trapping and gating effects
7 Pore cavity and window interaction, vapochromic effects
8 Quantum molecular sieving

**Molecular Conductivity. AHa**

1 Review of the underlying concepts of electronic coupling in molecules
2 Tunneling probability
3 Super-exchange interactions and McConnell's theorem
4 Bridge-mediated electron exchange
5 Interaction between bridge components

6 Single-molecule physics
7 Experimental methods
8 The molecular computer

**Reading References**

In each of the courses, literature references and appropriate web sites will be given to students. Because of the contemporary nature of the courses in this module, the main references will often be to articles in the primary chemical literature. Important books include:

Introduction to Computational Chemistry; F. H. Jensen; Wiley, 2002 IBSN: 0471984256

A Laboratory Book of Computational Organic Chemistry; WJ Hehre, AJ Shusterman, WW Huang, Wavefunction Inc, 1996. IBSN: 0964349558

Molecular Modeling and Bonding; E Moore; RSC; 2002 IBSN: 0854046755

Computational Chemistry; GH Grant, WG Richards; Oxford Chemistry Primer; 1995 IBSN: 019855740X

Chemical Modeling: From Atoms to Liquids; A Hinchliffe; Wiley; 1999 IBSN: 0471999040

Molecular Quantum Mechanics; P Atkins, R. Friedman; Oxford, 2006 IBSN: 0199274983

Charge and Energy Transfer Dynamics in Molecular Systems; V May. O. Kuhn; Wiley-VCH; 2000 IBSN: 3527296085

Nanoporous Materials: Science and Engineering; GQ Lu, XS Zhao; Series in Chemical Engineering, Vol 4; ICP; 2004 IBSN: 1860942105

Molecular Sieves: Principles of Synthesis and Identification; R Szostak; Springer; 1998 IBSN: 0751404802

| CATALYST APPLICATION AND DESIGN | **CHY8424**<br>10 credits<br>[5 ECTS credits]<br>semester 1 |
|---|---|
| Module leader(s) | Dr S Doherty |
| Staff | Dr S Doherty, Dr R J Errington |
| Pre-requisites | None |
| Aims | This course aims to provide a fundamental understanding of important catalytic reactions, using selected processes to illustrate catalyst development and optimization and show how catalysis is essential for 'green chemistry' and sustainable processing. Key principles of transition metal chemistry and stereochemistry are revised and built upon to show how this knowledge can be used to design Lewis acid based catalysts for important chemical transformations. An overview of heterogeneous catalysis is provided and examples are selected to illustrate how molecular studies have provided mechanistic understanding and improved catalysts. |
| Timetabled sessions | 22 Lectures, 2 Seminars |
| Assessment | 2h Examination at end of Semester 1 (100%) |

**Intended Learning Outcomes:** At the end of this course, students should be able to:
At the end of this course, students should:

- understand the general principles of homogeneous and heterogeneous catalysis and appreciate current and emerging challenges
- appreciate the relationship between fundamental organometallic chemistry and developments in homogeneous catalysis
- have a knowledge of recent major developments in catalysis with potential importance to the chemical industry
- know the broad classes of catalysts that are active for different types of reaction
- understand, by consideration of specific examples, how catalytic processes are designed and optimized

**Lectures**
**Homogeneous Catalysis, SD**

1-2 Background and revision of the basic principles including: bonding, reaction types and mechanisms and the fundamentals of homogeneous catalysis.
3-4 Important palladium catalyzed transformations including carbonylations, the Heck reaction, cross couplings (Suzuki and Negishi) and aminations
5-6 Synthesis of carbo- and heterocycles including rhodium and palladium-catalyzed cycloisomerisations, alkyne trimerisation and the Pauson-Khand reaction
7-8 Hydrogenation- Basic principles, substrate specific catalysis, asymmetric hydrogenation, transfer hydrogenation, kinetic resolution, a discussion on the mechanisms and examples of industrial processes
9 Hydroformylation- the oxo process. selectivity in hydroformylation, catalyst design, mechanism and applications
10 Miscellaneous rhodium catalyzed reactions
11 C-H Activation chemistry
12 Seminar

**Heterogeneous Catalysis and Related Chemistry, RJE**

1-3 Introduction to industrial heterogeneous catalysis: ammonia and methanol synthesis; hydrocarbon cracking and reforming; the Fischer-Tropsch process.
4 Alkene transformations; oxidation, hydration, metathesis, polymerisation.
5 The nature of heterogeneous catalysts: preparation, characterisation and use.
6-7 Alkene polymerization and metathesis: from Ziegler-Natta to Chauvin, Schrock and Grubbs.

8–11 The design of modern catalysts for green chemistry.
12 Seminar

**Reading References**

Homogeneous Catalysis: Understanding the Art, Kluwer Academic Publishers, 2004, Ed. PW van Leeuwen, ISBN: 14020-19998
Applied Homogeneous Catalysis with Organometallic Compounds, VCH-Wiley 2004, Ed. B Cornils and W Herrmann, ISBN: 35273-04347

| FURTHER INORGANIC CHEMISTRY | **CHY8425**<br>10 credits<br>[5 ECTS credits]<br>semester 2 |
|---|---|
| Module Leader | Dr KJ Izod |
| Lecturers | Professor A Houlton, Dr RJ Errington and Dr KJ Izod |
| Prerequisites | CHY3101 & CHY3301 |
| Aims | To present a series of short courses on advanced topics in contemporary inorganic chemistry; to show how fundamental aspects of inorganic chemistry are being used to develop new concepts in chemistry and how they are applied in modern chemical industry |
| Timetabled sessions | Lectures and seminars 24 h (8 h per course) |
| Assessment | 2h Exam at end of Semester 2 (100%) |

**Intended Learning Outcomes**

At the end of this course, students should:

- understand the fundamental chemistry of the f-block elements
- be aware of the ways in which inorganic compounds can be designed to give rise to commercially important new materials
- be aware of the application of some of the less common spectroscopic and structural methods used for materials analysis

**Module Content**

This module will comprise 3 courses (of 8 lectures each)

**Lectures**

**Lanthanide Chemistry. KJI**

1 The f-orbitals – consequences for lanthanide chemistry
2 Occurrence, isolation and separation of the elements
3 Coordination chemistry – stability, oxidation states, geometries
4 Organometallics
5 Spectroscopy and magnetism
6 Lanthanides in organic synthesis
7 Lanthanides in catalysis
8 Lanthanides in medicine

**Inorganic Materials. RJE**

1 Introduction
2 Ceramics, Sol-Gel Process
3 Metal alkoxides
4 Electroceramic thin films, silica materials, Porosity, Zeolites
5 Micelles, Liquid Crystals, Mesoporous solids
6 Compound semiconductors
7 Quantum dots
8 Langmuir Blodgett films, Self-Assembly monolayers

**Structural Methods in Materials Chemistry. AHo**

1 Introduction
2 X-ray Photoelectron Spectroscopy
3,4 γ-ray Spectroscopy
5, 6 Scanning Probe Microscopy
7,8 Case Studies

| **Reading References** |
|---|

In each of the courses references will be given to the students. Because of the contemporary nature of the courses in this module the references will often be to articles in the primary chemical literature

| FUNCTIONAL MOLECULES | **CHY8426**<br>10 credits<br>[5 ECTS credits]<br>semester 2 |
|---|---|
| Module Leader | Professor A Harriman |
| Staff | Dr AC Benniston and Professor A Harriman |
| Prerequisites | Stage 3 Chemistry modules |
| Aims | To introduce the basic principles involved in the design, synthesis and application of molecular systems used for a variety of purposes and to develop new materials. |
| Timetabled sessions | Lectures 24h, 2 lectures per week. |
| Assessment | 2 Assignments (50%)<br>Each assignment will involve the design of selected prototypes and a consideration of their synthesis and testing. Students will be given considerable flexibility in their choice of topic for the assignments.<br>1h 45m Exam at the end of Semester 2 (50%)<br>The exam will cover all aspects of the course, and will assess the ability of the students to discriminate between various theoretical approaches. |

**Intended Learning Outcomes**

At the end of this course, students should be able:

- to understand the basic principles of designing molecular systems for predetermined applications
- to explain how to synthesize a suitable molecule that is fully compatible with the intended application
- to demonstrate how to evaluate and test the molecule under operating conditions

**Lectures**

1. **Design of luminescent sensors for analytical protocols**:*
Fluorescence spectroscopy is one of the most sensitive spectroscopic tools available to the modern chemist – it can detect single molecules. By equipping a fluorescent reagent with an ancillary binding pocket, it becomes possible to design chemical sensors that will recognise and quantify a tremendous range of substrates under different conditions. The only real skill involved in the design element is linking the recognition event to a substantial change in fluorescence yield. Related systems, such as the *in situ* measurement of oxygen levels, are based on phosphorescence.

2. **Novel anti-cancer drugs for eradication of tumours**:*
Photodynamic therapy offers an alternative treatment for many types of cancer, provided the target is accessible to an optical fibre. The technique works by injecting a suitable drug into the tumour, followed by illumination with laser light. The tumour is literally burned out and all cancerous cells are killed during the process. Much is known about the chemical processes and intermediates involved in PDT and several reagents are on the market. The field is ripe for the design of vastly improved reagents and this course will set out to formulate the perfect PDT reagent.

3. **A new generation of conducting polymers and light-emitting diodes**:
We have grown used to the idea of light-emitting diodes (LED's) as warning elements and as switches. Mostly, LED's are made from organic polymers that are able to conduct electricity and convert electric charge into optical energy. New materials are becoming available that offer a wide range of colours and that are highly efficient. Here, we introduce the basic theory by which LED's operate and set out to design improved materials with novel properties. The most important feature is to improve the efficacy with which electrical charge is converted into light.

4. **Storing sunlight as chemical fuel**:*

The world as we know it will terminate in less than 50 years unless we solve the problem of using and storing solar energy. This is a major issue that will dominate chemistry for the next few decades… but we need to start now. The key concepts are the oxidation of water to molecular oxygen and the reduction of carbon dioxide to chemical fuels. The only energy input is drawn from sunlight. The rewards will be tremendous but the challenges are formidable. Here, we focus on the underlying chemistry associated with the two key processes and with the general principle of electron transfer.

5. **Magnetic resonance imaging of the brain**:*
   Most of us are familiar with the idea of magnetic resonance imaging (MRI), commonly referred to as a "scan". But how does it work and how can the chemist improve the technique? By understanding the technique and introducing enhancement or contrast reagents, it has been possible to reduce the time taken for a scan from several hours to a few minutes. Existing contrast agents, often being based on lanthanides, are expensive and can introduce unwanted side effects. This part of the course looks at designing a viable alternative based on setting up a list of requisites and recognising the chemical principles involved.

6. **How to build a molecular computer**:
   The next generation of ultra-fast super-computers will have all the active components built from organic molecules. The knowledge to design these components is emerging from several key research laboratories around the world, including the Newcastle-based Molecular Photonics Laboratory. What components are necessary and how do we build molecular analogues of a transistor, rectifier, switch, etc.? This fascinating topic is at the forefront of research but involves some relatively simple chemistry. Of course, the successful transformation from the real world to the molecular world demands a high sense of creative imagination.

*NB The * indicates that the material to be covered is suitable for students enrolled on a medicinal chemistry course.*

**Coursework**

| **Type** | **Date set** | **Deadline** | **Feedback** |
|---|---|---|---|
| Assignments | Weeks 31, 35 | Weeks 34, 42 | Within 1 week |

**Reading References**

Chemical Sensors and Biosensors, B R Eggins, Wiley-Blackwell 2002 ISBN: 0471899143

Modern methods of organic synthesis, W Carruthers, I Coldham, Cambridge University Press, 4th edition, 2004 ISBN: 0521778301

Essentials of molecular Photochemistry, A Gilbert, J Baggot, Blackwell Scientific Publications 1990, ISBN: 0632024291

Molecular design and bioorganic catalysis, C S Wilcox, A D Hamilton, Kluwer Academic Pub 1996, ISBN: 0792340248

| ADVANCED PROBLEM SOLVING | **CHY8430**<br>10 credits<br>[40 ECTS credits]<br>semester 2 |
|---|---|

| | |
|---|---|
| Module Leader | Dr JG Knight |
| Staff | Dr JP Goss, Professor RA Henderson and Dr JG Knight |
| Prerequisites | CHY3401, CHY3402 |
| Aims | The module aims to review essential mechanistic principles and structural elucidation and the application of these to advanced chemical problems |
| Timetabled sessions | A 2 week cycle of: receiving a problem exercise (week 1) completing and attending a workshop to go through the answers (week 2) |
| Assessment | Open book 3h exam (100%) |

A range of aspects of modern organic, inorganic and physical chemistry including structure elucidation, synthetic methodology, kinetic analysis and the derivation of reaction mechanism, and the characterisation of molecular properties through molecular orbitals.

This module consists of a series of advanced written problem exercises, designed to test the application of mechanism, reactivity, structure, and spectroscopy

Written examination assesses learning across the taught course material
Written assessment tests students conceptual understanding of primary literature in the subject area

The course involves a series of advanced problem exercises, which will be delivered and completed over the course of the Semester. Formative feedback, based on the answers provided by the students will be given in the workshop sessions on each exercise in order to enhance the performance in the subsequent exercises

Key concepts and supporting examples are delivered by seminars.
Concepts are reinforced and skills practiced during problem solving seminars
Written assignments allow students to access and review representative primary literature adding depth to conceptual understanding

**Reading References**


Spectroscopic Methods in Organic Chemistry, D H Williams & I Fleming, McGraw Hill 1995
ISBN: 0077091477

Organic Chemistry, S Warren, J Clayden, N Greeves, P Wothers OUP 1999
ISBN: 0198503466

Chemical Applications of Molecular Modelling, J.M. Goodman, RSC 1998, ISBN: 0854045791

Practical Strategies for Electronic Structure Calculations, W.J. Hehre, Wavefunction, 1995 ISBN: 0964349515

Computational Chemistry, Grant and Richards, Oxford 1995 ISBN: 019855740X

Computational Organic Chemistry, S.M. Bachrach, Wiley 2007 ISBN: 0471713425

Molecular Symmetry and Group Theory, A. Vincent, Wiley 2005 ISBN: 0471489395

Group Theory for atoms, molecules and solids, B.S. Wherrett, Prentice Hall 1986
ISBN: 0133654613