

## STAGE 2: YEAR OVERVIEW, DEADLINES AND 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

Sy+ Week and date w/c	Laboratory Classes	Deadline for Lab Reports	Exams
10   21 Sept	<b>Induction week</b>		
11   28 Sept	<b>CHY2301</b> Inorganic Practical		
12   5 Oct			
13   12 Oct			
14   19 Oct			
15   26 Oct			
16   2 Nov		<b>CHY2301</b> 12 noon Fri 6 Nov	
17   9 Nov	<b>CHY2401</b> Structural Chemistry		
18   16 Nov			
19   23 Nov			
20   30 Nov			
21   7 Dec			
<b>Vacation</b>			
25   4 Jan		<b>CHY2401</b> 12 noon Mon 4 Jan	
26   11 Jan			Examinations
27   18 Jan			Examinations
28   25 Jan	<b>CHY2101</b> Organic Practical		
29   1 Feb			
30   8 Feb			
31   15 Feb			
32   22 Feb			
33   1 Mar		<b>CHY2101</b> 12 noon Fri 5 Mar	
34   8 Mar	<b>CHY2201</b>		
35   15 Mar			
<b>Vacation</b>			
40   19 Apr	Physical Practical		
41   26 Apr			
42   3 May			
43   10 May		<b>CHY2201</b> 12 noon Fri 14 May	
44   17 May			Examinations
45   24 May			Examinations
46   31 May			Examinations
47   7 June			Examinations

Weeks are numbered according to the Syllabus Plus (S+) system. These week numbers will also feature on timetables

<b>GROUP ASSIGNMENT IN CHEMISTRY OR MEDICINAL CHEMISTRY</b>		<b>CHY2001</b> 20 credits [10 ECTS credits] semesters 1 & 2
Module Leader	Dr JG Knight	
Staff	Dr AC Benniston, Dr C Bleasdale, Dr DA Fulton, Professor RA Henderson, Dr JG Knight and Dr AR Pike	
Prerequisites	CHY1101, CHY1201, CHY1301	
Aims	To consider issues of effective communication to independent learners including scope and style of material and style of presentation; to develop a range of transferable skills; to consolidate and extend knowledge of a fundamental aspect of chemistry	
Timetabled sessions	15h Seminars and 40h Group learning	
Assessment	Staff assessment of group work (10%), portfolio & CVs (10%), problem solving (15%), written assignments (reports, poster) (50%) and presentation (15%) which is then moderated by peer assessment	

### Intended Learning Outcomes

At the end of this course, students should:

- understand a fundamental area of chemistry or medicinal chemistry, which was introduced at Stage 1, and which they choose for their group assignment
- appreciate the factors to be considered in communicating chemistry to a non-expert audience
- be able to work as a team in solving chemical problems

### Sessions will include seminars/workshops on:

- Use of the library and electronic databases
- Preparation and evaluation of CV's
- Teamwork
- Meetings skills
- Presentation skills
- Spectroscopic analysis

Much of the timetabled work will involve group activities which will be supported and assessed by group tutors.

Further information about the timetabling of student activities and on the assessment scheme may be found on the Blackboard website (URL below) which is accessed from the main university home page <http://bb.ncl.ac.uk/>

### Coursework

Type	Date set	Deadline	Feedback
Written summary of plans	Induction week	12 noon, Wednesday week 15	Verbal feedback within 2 weeks
Written report/learning pack	Induction week	12 noon, Wednesday week 21	Verbal feedback within 3 weeks
Group problem session	Induction week	Tues or Thurs of week 25	Verbal feedback within 3 weeks
Poster	Induction week	12 noon, Wednesday week 32	Verbal feedback by 1st week of Semester 2

Presentation

Induction week

Tues or Thurs  
of week 35

Written feedback from peers,  
immediately.

<b>TOPICS IN CHEMISTRY</b>		<b>CHY2003</b> 10 credits [5 ECTS credits] semester 1
Module Leader	Dr EM Tuite	
Lecturers	Dr A C Benniston, Professor RA Henderson, and Dr AR Pike	
prerequisites	CHY1101, CHY1201, CHY1301	
Aims	To introduce a series of topics in contemporary inorganic, organic and physical chemistry, reinforcing the chemical principles learnt in stage 1 chemistry	
timetabled sessions	Lectures and Seminars 22h	
Assessment	Exam 2h at end of semester 1 (100%)	

### Intended Learning Outcomes

At the end of this course the students should

#### Redox Reactions, RAH

- understand the factors controlling the rate of electron transfer between metal sites
- to be able to distinguish between inner- and outer-sphere electron transfer mechanisms
- be able to predict the mechanisms and products of certain redox reactions
- appreciate the problems associated with non-complementary electron transfer mechanisms

#### Light-Activated Reactions, ACB

- understand how light affects the reactivity of molecules
- know how excited states are formed and the difference between triplet and singlet states
- understand what is fluorescence and phosphorescence
- know the difference between electron transfer and energy transfer
- understand the general photochemistry of inorganic complexes such as  $[\text{Ru}(\text{bipy})_3]^{2+}$
- understand the photoreactivity of MLCT states of metal complexes

#### Polymers, EMT

- understand what a polymer and a copolymer is and the different levels of structure they can assume
- appreciate the different mechanisms of polymerization and the different possible resultant structures
- know what the different expressions for polymer molar mass ( $M_n$ ,  $M_v$ ,  $M_w$ ,  $M_z$ ) are and how they inter-relate
- appreciate the different aspects of polymer stereochemistry
- know how to describe polymer structure in terms of the parameters of the freely-jointed chain model, e.g. contour length ( $R_c$ ), radius of gyration ( $R_g$ ), root mean square separation ( $R_{rms}$ )

#### Supramolecular Chemistry, ARP

- understand the concepts and principles of supramolecular chemistry as "chemistry beyond the molecule".
- appreciate the development of research in the area including Nobel prize winning work
- recognise the nature of supramolecular interactions
- understand how nature utilises supramolecular assemblies and how they can be mimicked
- be able to design supramolecular components for self-assembly and use in molecular devices.

## Lectures

### Redox Reactions, RAH

- 1 Introduction to electron transfer reactions of inorganic compounds
- 2-3 The outer-sphere and inner-sphere mechanisms
- 4 The role of the bridge in inner-sphere mechanisms
- 5 Electron transfer in bioinorganic chemistry
- 6 Problem solving. Exam revision

### Light-Activated Reactions, ACB

- 1 How light affects the reactivity of molecules
- 2 Excited states and the difference between triplet and singlet states
- 3 Fluorescence and phosphorescence
- 4 Electron transfer and energy transfer
- 5 General photochemistry of inorganic complexes such as  $[\text{Ru}(\text{bipy})_3]^{2+}$
- 6 Photoreactivity of MLCT states of metal complexes
- 6 Problem solving. Exam revision

### Polymers, EMT

- 1 Polymer Characteristics/Radical Chain Polymerization
- 2 Polymer Size/Anionic Polymerization
- 3 Copolymers/Cationic Polymerization
- 4 Polymer Stereochemistry/Ziegler-Natta Catalysis of Polymerization
- 5 Polymer Shape/Step-Growth Polymerization
- 6 Specialised Polymers
- 7 Problem solving. Exam revision

### Supramolecular Chemistry, ARP

- 1 Introduction to Supramolecular Chemistry; definition and development.
- 2 Supramolecular interactions.
- 3 Supramolecular chemistry in nature, and biological mimics.
- 4 Cation, anion and neutral binding molecules.
- 5 Self-assembled complexes and molecular devices.
- 6 Problem solving. Exam revision

## Reading References

R A Henderson, Mechanisms of Reactions at Transition Metal Sites, OUP, 1995, Chapter 6  
ISBN: 0198557469

C E Wayne & R P Wayne, Photochemistry, OUP, 1996 ISBN: 0198558864

D Walton and P Lorimer, Polymers, OUP, 2000, ISBN: 019850389X

P D Beer, P A Gale & D K Smith Supramolecular Chemistry, OUP, 1999, ISBN: 0198504470

<b>ORGANIC CHEMISTRY</b>		<b>CHY2101</b> 20 credits [10 ECTS credits] semester 1 & 2
Module Leader	Dr DA Fulton	
Lecturers	Dr DA Fulton, Dr MJ Hall, and Professor M North	
Prerequisites	CHY1101	
Aims	To provide a thorough understanding of the influence of conformational and stereoelectronic effects on the reactivity of organic compounds; to show how mechanisms of some organic reactions have been investigated and to present the currently accepted mechanisms of these reactions; to provide an understanding of mechanistic and synthetic chemistry; to consider the chemistry of aromatic and heteroaromatic systems and to develop experimental technique through practical sessions	
Timetabled sessions	Lectures 34h, Seminars 3h, Tutorials 8h, 2h lab Intro Practicals 9h per week for 5 weeks	
Assessment	In course assessment for practical work (25%) 1½ h exam at end of Semester 1 (30%) 1½ h exam at end of Semester 2 (30%) In-course assessment (15%)	

### Intended Learning Outcomes

At the end of this course, students should

- understand basic principles of organic chemistry
- understand analysis of molecules and how conformation affects reactivity
- know the mechanistic rationale of substitution and elimination reactions
- understand aromaticity and the chemistry of aromatic systems
- know the different aromatic substitution processes and their application to heteroaromatic systems
- know the main syntheses of heteroaromatic ring systems and be able to relate these to key concepts of carbonyl chemistry

### Lectures

#### Aromatic Chemistry including Rearrangements, DAF

- 1 The definitions of aromaticity
- 2 Electrophilic aromatic substitution
- 3 Electrophilic aromatic substitution reactions of substituted benzenes
- 4 Synthesis of substituted benzenes; the reactions of benzene diazonium salts
- 5 Nucleophilic aromatic substitution; the chemistry of benzyne
- 6 Aromatic oxidations and reductions
- 7, 8 Rearrangement reactions
- 9 Mid semester test
- 10 Revision Seminar

#### Heteroaromatic Chemistry, MJH

- 1 Aromatic systems containing heteroatoms; introduction and overview
- 2–4 Membered heteroaromatics containing one heteroatom; pyrroles, furans and thiophenes
- 5, 6 Membered heteroaromatics containing one heteroatom; pyridines
- 7 Fused heteroaromatics; indoles and quinolines
- 8 Heteroaromatics containing more than one heteroatom
- 9 Revision Seminar

#### Stereochemistry and Mechanism, MN & DAF

- 1 Stereochemistry. Revision of basic concepts.

- 2 Conformations of acyclic compounds.
- 3 Conformations of 3–6 membered rings
- 4 Higher energy conformations of cyclohexanes
- 5 Stereocentres at atoms other than carbon. Chiral molecules which do not contain a stereocentre.
- 6 Topism
- 7 Intermolecular substitution reactions
- 8 Stereochemistry of  $S_N2$  and  $S_N1$
- 9 Mid semester test
- 10, 11 Nucleophilic substitution reactions in more detail
- 12, 13 Elimination reactions in more detail
- 14 Investigating reaction mechanisms
- 15 Hammett relationships
- 16, 17 Mechanisms of ester hydrolysis
- 18 Revision Seminar

### Laboratory Course

Course organiser Dr DA Fulton

Students do experiments dealing with the following transformations:

- 1 Stereoselective formation of a diol diastereoisomer and its conversion into an acetal
- 2 Electrophilic aromatic substitution
- 3 Amide bond formation
- 4 Aldol reaction
- 5 Investigations into  $S_N1$  and  $S_N2$  reactions

### Coursework

Type	Date set	Deadline	Feedback
Practical assessment	Weekly	By Friday of Week 33	Friday of Week 39
Mid term assessments	Week 16 and Week 33	During timetabled sessions	Scripts returned written and oral feedback by Semester 1 by week 20 Semester 2 by week 39

#### Reading References

Organic Chemistry, J Clayden, N Greeves, S Warren, P Wothers, Oxford University Press, 2001  
ISBN:0198503466

Principles and Applications of Stereochemistry, M North, Nelson Thornes, 1998  
ISBN: 0751404209

Aromatic Heterocyclic Chemistry (Oxford Chemistry Primers), D T Davis, Oxford University Press, 1992 ISBN : 0198556608

#### Further Reading

Organic Chemistry, J McMurray, Pacific Grove, 1995 ISBN : 0534238327

Designing Organic Syntheses, S. Warren, Wiley, 1978 ISBN: 0471996122  
Heterocyclic Chemistry, J A Joule, K Mills, Blackwell Science, 2000 ISBN 063205453

<b>BIOACTIVE NATURAL PRODUCTS</b>		<b>CHY2102</b> 10 credits [5 ECTS credits] semester 2
Module Leader	Professor B T Golding	

Lecturers	Dr MA Carroll and Professor BT Golding
Prerequisites	CHY1101, SFY0005 or Grade A or B at Chemistry A Level
Aims	To equip students with the knowledge of natural products from a range of plants including those in the sea known or believed to have medicinal properties; to introduce extraction techniques and how these will influence chemical composition of the extract, compound classes of active constituents, the biosynthesis of some key compound classes, medicines that have been derived from extracts and to equip students with a basic understanding of how these preparations are believed to work; to place plant natural products in the wider context of bioactive compounds
Timetabled sessions	Lectures and seminars 20h
Assessment	2h exam at the end of semester 2 (75%) Assignment report (25%)

### Intended Learning Outcomes

At the end of this course, students should:

- understand plant medicine and regional variations
- be familiar with a range of medicinal plants and their uses
- be aware of methods for the preparation of plant extracts and how they affect chemical composition
- know the structures and functions of phenolics, flavonoids, terpenes, steroids, vitamins, alkaloids and glycosides
- understand the biosynthesis and synthesis of selected bioactive compounds
- appreciate the mode of action of selected bioactive natural products

### Lectures

#### Introduction to Medicinal Plants and Key Natural Products, MAC

- 1 The origins of plant medicine and examples of medicinal plants
- 2 Methods of extraction. Screening plants for biological activity
- 3 Isolation, purification, identification techniques for natural products
- 4, 5 Natural Products of marine origin
- 6 Glycosides/polysaccharides – nomenclature, structures
- 7 Phenolics coumarins and lignans; flavonoids and anthocyanins
- 8 Terpenoids: essential oils, 'isoprene rule', flavours and fragrances, taxol, biosynthesis
- 9 Steroids, steroid biosynthesis
- 10 Revision Seminar

#### Vitamins and Alkaloids BTG

- 1 Vitamins and coenzymes 1: general survey of vitamins; historical aspects of vitamin discovery
- 2 Vitamins and coenzymes: vitamin A (retinal) in the visual process, vitamin B<sub>1</sub> (thiamine), vitamin C (ascorbic acid)
- 3 Vitamins and coenzymes 3: Vitamin B<sub>1</sub> (thiamine), vitamin C (ascorbic acid), vitamin D and vitamin K
- 4 Alkaloids 1: history, isolation and structure determination
- 5 Alkaloids 2: morphine: biosynthesis, medicinal applications, mode of action
- 6 Alkaloids 3: quinine; comparison with artemisinin as an anti-malarial agent
- 7 Alkaloids 4: cocaine, LSD, galanthamine
- 8 GM plants
- 9 Revision Seminar
- 10 Answering exam questions seminar

**Assignment**

Given the Latin name for a particular plant early in the semester, each student will investigate what is known about the plant, its activity, its constituents etc, and prepare a 4 pages report which should be word processed and should include diagrams and/or pictures, charts etc. The focus should be the natural products present and their biological activity. This task has been scheduled for the week 31 (beginning ??) and the deadline for submission of the assignment, to the School Office, is 12 noon on Friday ??, week 34.

**Coursework**

Type	Date set	Deadline	Feedback
Assignment	Week 31	12 noon Friday Week 34	Scripts returned, written and oral feedback by Week 40

**Reading References**

An Introduction to Enzyme and Coenzyme Chemistry. T Bugg, Blackwell Science, 2<sup>nd</sup> edition, 2004 ISBN: 0865427933

Medicinal Natural Products: A Biosynthetic Approach. P. M. Dewick, Wiley, 2<sup>nd</sup> edition, 2001 ISBN: 0471496413

<b>MEDICINAL CHEMISTRY AND DRUG DESIGN</b>		<b>CHY2103</b> 10 credits [5 ECTS credits] semester 1
Module Leader	Dr C Cano	
lecturers	Dr C Cano and Professor RJ Griffin	
prerequisites	CHY1101	
aims	To equip students with knowledge and understanding of drug-receptor interactions, enzyme chemistry and the principles of drug design and action	
timetabled sessions	Lectures and seminars 22h	
assessment	Exam 2h at the end of semester 1 (100%)	

### Intended Learning Outcomes

At the end of this course, students should:

- understand drug-receptor interactions and theories
- understand the principles of enzyme mechanism and knowledge of some specific examples
- be familiar with quantitative structure activity relationships
- understand how enzyme inhibitors work
- know how some drugs have been designed

### Lectures

#### Principles of Medicinal Chemistry and Enzyme Action, CC

- 1.3 Principles of medicinal chemistry. Forces in biological systems, drug-receptor theories  
 4-7 Enzyme action. Type of catalysis, characteristics of enzymes, vitamins and coenzymes, enzyme kinetics v enzyme inhibition  
 8 Physicochemical properties of drugs  
 9-10 Structures - activity relationships (SARs) and quantitative SARs (QSARs)

#### Drug Design, RJG

- 1 Introduction and historical overview  
 2-4 Approaches to drug discovery and development  
 5-7 Enzymes as drug targets  
 8 Competitive enzyme inhibitors - ACE inhibitors  
 9 Competitive enzyme inhibitors - HMG-CoA reductase inhibitors  
 10 Affinity label inhibitors - aspirin and orlistat  
 11 Mechanism-based inhibitors - chloramphenicol  
 12 Receptor drug targets - serotonin (5-HT)  
 13 The development of sumatriptan  
 14 Revision seminar  
 (10 lectures/seminars selected from the above)

#### Reading references

The Organic Chemistry of Drug Design and Drug Action, RB Silverman, Academic Press, 2004  
 ISBN: 0126437300  
 Instant Notes in Medicinal Chemistry, G Patrick, BIOS Springer 2005 ISBN: 1859962076  
 An Introduction to Enzyme and Coenzyme Chemistry, T Bugg, Blackwell Science. 2004  
 ISBN: 0865427933

<b>PHYSICAL CHEMISTRY</b>		<b>CHY2201</b> 20 credits [10 ECTS credits] semester 2
Module Leader	Dr BR Horrocks	
Lecturers	Professor A Harriman, Dr B R Horrocks and Dr E M Tuite	
Prerequisites	CHY1201	
Aims	To give students an appreciation of intermediary thermodynamics; introduce the principles of time-dependent chemistry; explain the significance and application of quantum concepts as a major tool in modern chemistry; develop experimental techniques through practical work.	
Timetabled sessions	Lectures 33h, Calculation classes 10h Practicals 9h per week for 5 weeks	
Assessment	Exam 3h at end of semester 2 (50%) Coursework associated with calculation classes (25%) In course assessment for practical work (25%)	

### Intended Learning Outcomes

At the end of this course, students should:

- understand the energetics of solutions, interfaces, polymers, colloids and self-assembling systems
- appreciate the significance of energy quantization in chemistry and its link to spectroscopic transitions
- be able to explain the concept of molecular potential energy curves
- appreciate the important factors in molecular kinetics
- be able to carry out calculations using the theories developed in all the areas detailed below

### Lectures

#### Applied Quantum Chemistry, AHa

- 1 Quantized energy levels – translation, rotation, vibration etc
- 2 Electromagnetic radiation – interaction with molecules
- 3 Harmonic model for molecular vibrational motion
- 4 Vibrational – rotational spectra of diatomic molecules
- 5 Anharmonic model for vibrational motion
- 6 Particle-in-a-box model
- 7 Multi-dimensional particle-in-a-box models
- 8 Electronic absorption spectra of conjugated molecules
- 9 Tunneling
- 10 Decay of electronically excited states – fluorescence, phosphorescence
- 11 Revision seminar

#### Energetics and interfacial phenomena, BRH

- 1 Review of CHY120 energetics
- 2 Statistical concepts
- 3 Chemical potential and thermodynamics of solutions
- 4 Standard states, activities and electrode potentials
- 5 Interfaces I – adsorption and isotherms
- 6 Interfaces II – electrical double layer
- 7 Polymers
- 8 Colloids
- 9 Calculations
- 10 Revision seminar I
- 11 Revision seminar II

#### Molecules in motion, EMT

- 1 Transport, mobility and conductivity
- 2 Electrophoresis and sedimentation
- 3 Diffusion
- 4 Collision theory
- 5 Medium effects in bimolecular diffusion
- 6 Reversible kinetics
- 7 Activation
- 8 Advanced kinetics
- 9 Relaxation effects
- 10 Fast kinetic reactions
- 11 Revision seminar

### Laboratory Course

Course organizer: Professor A Harriman

Students take a selection from the following experiments:

- 1 Kinetics of hydrolysis
- 2 Stopped flow
- 3 Supramolecular fluorescence
- 4 Calorimetry
- 5 Adsorption on zeolites
- 6 Micelles
- 7 Adsorption of iodine on carbon
- 8 IR rotation-vibration spectra of HCl
- 9 Visible absorption spectrum of iodine

Note The stage 2 laboratory is being updated and further experiments employing the new equipment (flash photolysis, fluorescence lifetime) may be offered.

### Assignments

The assignments associated with the calculation classes consist of calculations based on the lecture material.

### Coursework

Type	Date set	Deadline	Feedback
Calculation Coursework x6	weekly	following week	within 4 weeks
Practical report x4	weekly	within 1 week	within 4 weeks
Oral Feedback Session	after 1 <sup>st</sup> report	n/a	during session

### Reading Reference

Physical Chemistry, PW Atkins and J de Paula, 8<sup>th</sup> edition, Oxford University Press, 2002  
ISBN: 0198700725

Principles of Physical Chemistry, H Kuhn, HD Forsterling, John Wiley, 1999  
ISBN: 0471965413

Molecular Quantum Mechanics, P Atkins, R Friedman, 4<sup>th</sup> edition, Oxford University Press,  
2004 ISBN: 0199274983

Elements of Physical Chemistry, PW Atkins and J de Paula, 4th edition, Oxford University Press,  
2005 ISBN: 0199271836

INORGANIC CHEMISTRY

**CHY2301**  
20 credits  
[10 ECTS credits]  
semester 1 & 2

Module Leader	Dr KJ Izod
Lecturers	Dr RJ Errington and Dr KJ Izod
Prerequisites	CHY1301
Aims	To build on Stage 1 course material and provide the factual basis for an understanding of the electronic and structural properties and reactivities of the main-group elements and the second- and third-row transition elements; to introduce the basic principles of organometallic chemistry; to develop experimental techniques through practical work.
Timetabled sessions	Lectures 35h, tutorials 4h + additional 'sign up' tutorials in term Practicals 9h per week for 5 weeks
Assessment	In course assessment for practical work (30%) 1 <sup>1/2</sup> h exam at end of Semester 1 (35%) 1 <sup>1/2</sup> h exam at end of Semester 2 (35%)

### Intended Learning Outcomes

At the end of this course, students should:

- know the trends in atomic properties within the periodic table and have an understanding of their origin.
- understand ionic (CFSE) and covalent bonding models for transition metal complexes and the relationship between bonding and the spectrochemical series.
- appreciate the general types of compounds formed by transition and main group elements and the bonding involved, including in organometallic compounds.
- understand the basic principles of group theory and how they are applied to the solution of chemical problems

### Lectures

#### Chemical Applications of Symmetry, RJE

- 1 Review of previous material on symmetry elements, symmetry operations and point groups. Introduction to character tables.
- 2, 3 Irreducible and reducible representations. Symmetry analysis of stretching vibrations of small symmetric molecules; normal modes; IR and Raman activity; determination of molecular shape from vibrational spectra.
- 4, 5 Symmetry properties of atomic orbitals and their combination to give molecular orbitals:  $\sigma$  and  $\pi$  orbitals of small symmetric molecules; symmetry analysis of  $d$ -orbitals in transition metal complexes and their consequences for spectroscopy and other properties.

#### Bonding and Reactivity in Transition Metal Chemistry, RJE

- 1-3 Transition metals – general considerations and review of Stage 1 material. Trends in atomic properties for the  $d$ -block and their consequences. Binary compounds, redox properties, Lewis acid behaviour.
- 4-9 Bonding models for transition metal complexes.  
Ionic model and the consequences of  $d$ -orbital splitting; covalent model and simple molecular orbital model for octahedral,  $\sigma$ -bonding only,  $ML_6$  complexes.  
 $\pi$ -Bonding and the spectrochemical series.  $\pi$ -Donor ligands; halides and oxo ligands, stabilisation of high oxidation states.  $\pi$ -acid ligands; CO as the prototype, stabilisation of low oxidation states; ligands isoelectronic with CO:  $NO^+$ ,  $CN^-$ ,  $N_2$ ; trivalent phosphorus compounds as ligands.  
Effective atomic number and the 18 electron rule, electron counting and deviations from 18.  
Metal carbonyls: preparation, structure, electron counting; reactivity.  
Metal alkene complexes.
- 10 Trans-effect and trans-influence
- 11 Orbital overlap analysis of metal-metal bonding
- 12 Revision Seminar

#### Selected Topics and Comparative Chemistry, RJE

- 1-3 Higher oxidation states: metal-oxo and organoimido complexes; structural consequences of  $\pi$ -bonding –  $MOL_5$  ( $d^0$ ,  $d^1$ ,  $d^2$ ) and  $MO_2L_4$  ( $d^0$ ) complexes; protonation and aggregation to polyoxometalates.

- 4–5 Lower oxidation states: metal–metal bonding from dinuclear complexes to clusters.  
 6–8 Organometallic chemistry – transition metal alkyls;  $\beta$ -H elimination,  $\alpha$ -H abstraction.  
 Alkenes as ligands:  $C_2H_4$ ,  $C_3H_5$ ,  $C_5H_5$ .  
 9 Revision Seminar

#### Introduction to Main Group Chemistry, KJI

- 1 Review of trends down groups and across periods.  
 2–10 Descriptive chemistry of groups 1,2,13,14,15 and 16 will be used to illustrate concepts including:  
 Electron-deficient compounds (introduction to boranes); discontinuities down the groups and their underlying reasons; the “inert pair effect”; isoelectronic compounds; multiple bonding; hyperconjugation; catenation; rings and cages.  
 11 Revision Seminar

#### Laboratory Course

Course organiser Dr AC Benniston

- 1 Reactions of cobalt ammine complexes
- 2 Preparation of a cobalt 'dioxygen carrier'
- 3 Magnetic properties of transition metal complexes
- 4 Metal–metal bonded cyclopentadienyl carbonyls of molybdenum and tungsten
- 5 Main group chemistry – preparation of tetraphenyltin and mass spectrometry

#### Coursework

Type	Date set	Deadline	Feedback
Practical reports	Each week	following lab session	marked and returned by the following week

#### Reading References

Chemistry of the Elements. NN Greenwood and A Earnshaw, Butterworth Heinemann, 1997, 2<sup>nd</sup> Edition ISBN: 0750633654

Inorganic Chemistry. CE Housecroft and AG Sharpe, Pearson Higher Education, 4<sup>th</sup> edition, 2000 ISBN: 0582310806

Periodicity and the *s* and *p*-Block Elements. NC Norman, OUP, 1997 ISBN: 01982059615

Metal Ligand Bonding. EA Moore, Royal Society of Chemistry, 2004 ISBN: 0854049797

*d*-Block Chemistry. MJ Winter, OUP, 1994 ISBN: 0198556969

Beginning Group Theory for Chemistry. PH Walton, OUP, 1998 ISBN: 019855964X

Introduction to Molecular Symmetry. JS Ogden, OUP, 2001 ISBN: 0198559100

Advanced Inorganic Chemistry. FA Cotton, C Murillo, E Wilkinson, M Bochmann and R Grimes, John Wiley, 1999, 6th edition ISBN: 0471199575

Organometallics, a Concise Introduction. C. Elschenbroich, A. Salzer, 2<sup>nd</sup> edition, VCH, 1992 ISBN: 0895739836

<b>STRUCTURAL CHEMISTRY</b>		<b>CHY2401</b> 20 credits [10 ECTS credits] semester 1
Module Leader	Dr AC Benniston	
Lecturer	Dr AC Benniston, <b>TBC</b> , Dr RJ Errington and Professor BT Golding	
Prerequisites	CHY1101, CHY1301, CHY1201	

Aims	To introduce the principles of NMR spectroscopy and to familiarise students with the analysis of the NMR spectra of some organic and inorganic compounds; to explain the principles of X-ray diffraction by single crystals and the application of these principles in practical structure determination; to provide students with an appreciation and understanding of all aspects of modern mass spectrometry, building on their knowledge of traditional electron impact mass spectrometry; to provide the necessary background for the interpretation of the vibrational spectra of inorganic and organic molecules
Timetabled sessions	Lectures 32 h, Tutorials 2h Practicals 40h
Assessment	Exam 3h at the end of semester 1 (75%) In course assessment for practical work (25%)

### Intended Learning Outcomes

At the end of this course, students should:

- know and understand NMR spectroscopy, mass spectrometry and vibrational spectroscopy and be able solve problems involving these techniques
- know and understand X-ray crystallography so that they can solve unseen problems

### Lectures

#### Magnetic Resonance Spectroscopy and Organic Compound Identification, ACB

- 1, 2 Revision of NMR spectroscopy
- 3 Chemical shifts and splitting patterns
- 4 Carbon 13 NMR and 20 NMR and their uses
- 5-8 Interpreting NMR spectra and other analytical data in identification of organic compounds

#### Magnetic Resonance Spectroscopy and Inorganic Compound Identification, RJE

- 1, 2 More complex NMR techniques and their uses
- 3, 4 Nuclei with spins  $>1/2$  and their spectra
- 5 Dynamic NMR and interpreting temperature dependent spectra
- 6-8 Identification of inorganic/organometallic compounds by interpretation of NMR spectra and other analytical data

#### Crystallographic Methods, TBC

- 1 Introduction; the basis of crystallographic methods
- 2 Diffraction of X-rays by molecules and crystals: geometry and symmetry
- 3 The intensities of diffracted X-rays
- 4 Crystallography practice: from sample to diffraction pattern
- 5 Crystallography practice: from diffraction pattern to structure
- 6 Results and their significance
- 7 Case studies
- 8 Structural disorder
- 9 Neutron diffraction
- 10 Powder diffraction

#### Mass Spectrometry, BTG

- 1 Revision of the basic principles of EIMS; scope and limitations of EIMS
- 2 Alternative ionisation methods: fundamental principles
- 3 New techniques in MS: practice and applications
- 4 Complete structure determination by MS (primarily organic examples)
- 5 Complete structure determination by MS (primarily inorganic examples)
- 6 Seminar

### Laboratory Course

Course organiser: TBC

- 1 Identification of organic compounds from spectroscopic and other data

- 2 Identification of inorganic compounds from spectroscopic and other data
- 3 X-ray diffraction: Patterson maps; direct analysis; powder patterns
- 4 Molecular modelling; the use of ChemWindow and the Cambridge Structural Database; molecular symmetry
- 5 Mass spectrometry including isotope patterns

### Assignments

There are no formal assignments but the practical course consists of problem-based questions covering taught material on NMR spectroscopy, X-ray, crystallography, mass spectrometry and computer modelling.

### Coursework

Type	Date set	Deadline	Feedback
Practical Reports	Weekly	At Lab session	Within 4 weeks

### Reading References

NMR Spectroscopy, R. J. Abraham, J. Fisher and P. Loftus, Wiley, 1988 ISBN: 0471918946

Physical Chemistry, P. W. Atkins, Oxford University Press, 1988, 6<sup>th</sup> edition  
ISBN: 0198501013

Spectroscopic Methods in Organic Chemistry, D. H. Williams and I. Fleming, McGraw-Hill, 1995, 5<sup>th</sup> edition ISBN: 0077091477

Crystal Structure Determination, W. Clegg, Oxford University Press, 1998 ISBN: 0198559011

