Liverpool John Moores University

Title: CORE CHEMISTRY
Status: Definitive
Code: **6007CHACAP** (113197)
Version Start Date: 01-08-2011

Owning School/Faculty: Pharmacy & Biomolecular Sciences
Teaching School/Faculty: Pharmacy & Biomolecular Sciences

Team	Leader
Barry Nicholls	Y
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Academic Level: FHEQ6 **Credit Value:** 24.00 **Total Delivered Hours:** 48.00

Total Learning Hours: 240 **Private Study:** 192

Delivery Options
Course typically offered: Standard Year Long

Component	Contact Hours
Lecture	39.000
Practical	6.000

Grading Basis: 40 %

Assessment Details

Category	Short Description	Description	Weighting (%)	Exam Duration
Exam	AS1	Examination	75.0	3.00
Essay	AS2	Coursework - written assignments	12.5	
Essay	AS3	Coursework - written assignments	12.5	

Aims

To develop knowledge of the main branches of Chemistry to BSc level with Core Inorganic, Organic and Physical principles and applications.

Learning Outcomes

After completing the module the student should be able to:

1 discuss the basic axioms of quantum mechanics and be able to apply the knowledge to simple molecular problems.
2 discuss the basic principles of microwave, ir, uv/visible and photoelectron spectroscopy and use the spectral data to determine fundamental molecular parameters.
3 discuss the basic principles, interpretation of spectra and basic spectrometer design of photoelectron spectroscopy
4 discuss the factors which govern the electronic and molecular structure of transition metal cluster complexes, together with their synthesis and catalytic properties.
5 discuss the basic principles underlying homogeneous and heterogeneous catalysis
6 apply the principles of static stereochemistry to selected chemical reactions in order to predict their stereochemical outcome.
7 discuss the effects of symmetry in organic synthesis.
8 compare and contrast the chemistry of heterocycles containing one heteroatom with those containing two or more heteroatoms.
9 recognize the importance of enols, enoates and enamines in organic reactions.

Learning Outcomes of Assessments

The assessment item list is assessed via the learning outcomes listed:

EXAM	1	2	3	4	5	6	7	8	9
CW	1	2	3	4					
CW	5	6	7	8	9				

Outline Syllabus

(1) Application of spectroscopy to determine molecular parameters.
Quantum Mechanics and Spectroscopy: The postulates of quantum mechanics - observables and equivalent operators - the interpretation of the wave function. Application of the basic principles to the solution of the particle in a 1-D potential well.
- application to the electronic energy levels of linear conjugated dienes.
The rotational energy levels of a diatomic molecule. Reduced mass, selection rules and construction of a theoretical spectrum. Calculation of the bondlength from the line spacing. Limitations of the rigid rotor model; centrifugation distortion - determination of the structure constants B and D from the microwave spectrum..
The vibrational energy levels of a diatomic molecule. The SHO model, selection rules, zero-point energy and calculation of the force constant of a molecule. Fundamental, 1st and 2nd overtones; limitations of the SHO model - extension to AHO. Calculation of the dissociation energy from the fundamental and lst overtone.

The wavefunctions for an AHO.
Rotational fine structure - calculation of the bond lengths in the v=0 and v=1 states.
Modes of vibration in vibration in simple polyatomic molecules..
The electronic energy levels of molecules. The Franck-Condon principle, vibrational fine structure and vibrational overlap between the ground and excited states. The mechanism of photodissociation, fluorescence, phosphoresence and laser action. Calculation of dissociation energies from uv/visible spectral data.

(2) Photoelectron spectroscopy:
The photoionisation process and line resolution. Photon sources in UV pes. Detailed analysis of photoelectron spectra, particularly of Cl2, N2, NO, HBr, Ar, Hg and molecules with localised orbitals. Photon sources in xpes. Spectra of simple structural molecules such as NaN3, B5H9, CH3CH2COOCF2CF3, ClF3. Instrumentation in PES, including retarding grid and deflection analysers.

(3) Synthesis, structure and catalytic properties of transition metal binary carbonly cluster complexes/transition metal complexes.

(4) Homogeneous catalysis:
General aspects of catalysis. Comparison and contrast with heterogeneous catalysis. General mechanism using the 16/18 electron rule - catalysis activation, substrate coordination, substrate oxidative addition, insertion and reductive elimination steps. Detailed rationalisation of alkene isomerisation using hydrido- and non-hydrido-catalysis, alkene hydroformulation, alkene hydrogenation (including asymmetric hydrogenation). Potential of cluster complexes as catalysts. Supported homogeneous catalysis using oxide and organic polymer supports.

(5) Stereochemistry:
Conformational analysis, gauche interactions. Conformationally rigid systems, cyclohexanes, decalins, steroids. Conformation and reactivity w.r.t. hydrolysis, esterification, oxidation and elimination reactions including unimolecular and bimolecular systems. Additions to alkenes via epi-cationic intermediates, organomercury, -sulphur, and -selenium reagents. Neighbouring group effects involving halo-, alkenyl- and aryl-substituents. Conformational control over configuration, Cram's rule, Felkin-Anh approach. Physical determination of conformation; 1H NMR coupling constants, optical rotary dispersion.

(6) Symmetry controlled reactions:
Pericyclic vs stepwise reactions. Electrocyclic ring closures/openings, cheleotropic reactions, [2+4] and [2+2] cycloadditional reactions, 1,3-dipolar cycloadditions, H and C sigmatropic shifts, the Cope, Oxy-Cope, Claisen and Claisen-Ireland rearrangements. Frontier orbital approach, disrotatory vs conrotatory ring closure, suprafacial vs antarafacial addition, thermal vs photochemical reactions, secondary orbital interactions.

(7) Hererocyclic chemistry:
Heterocycles containing two or more heteroatoms: Introduction including importance and nomenclature. Revision of structures and chemistry of pyridine and pyrolle. Chemistry of diazines including (i) electrophilic attack at N and C (ii) nucleophilic substitution (iii) free radical substitution (iv) oxidation and reduction.

Chemistry of the 1,3-azoles (imidazole, oxazole and thiazole) - as for diazines except (i) is electrophilic substitution. N.B. (a) the emphasis is predicting the reactivity of these systems from a knowledge of benzene, pyridine and pyrrole chemistry. (b) synthesis and physical properties are dealt with briefly. (c) Important examples of these heterocyclic systems are stressed.

(8) Enols:
Enols, Enolate anions, Enamines and their reactions: Base-catalysed enolate reactions, regioselectivity: Kinetic and thermodynamic control. Enolate trapping. Reactions of enolates: halogenation, alkylation. Malonic ester and ethyl acetoacetate for forming new C-C bonds. Enolate anions as ambient nucleophiles. . The aldol reaction, Michael addition and Robinson annulation. Enamines: their formation and reactions
Introduction to the disconnection approach. Retrosynthesis and disconnections of target molecules in relation to enolate alkylation, the Diels-Alder and Wittig reactions.

Learning Activities

Lectures and practicals. Dedicated Computer Assisited Learning Software (ChemiCAL)

References

Course Material	Book
Author	P W Atkins and J de Paula
Publishing Year	2002
Title	Physical Chemistry
Subtitle	
Edition	7th
Publisher	Oxford University Press
ISBN	0-19-879285-9

Course Material	Book
Author	J Mailtland Jr.
Publishing Year	0
Title	Organic Chemistry
Subtitle	
Edition	3rd
Publisher	W W Norton, NY
ISBN	0-393-92408-4

Course Material	Book
Author	TWG Solomons

Publishing Year	0
Title	Organic Chemistry
Subtitle	
Edition	8th
Publisher	John Wiley, NY
ISBN	0-471-44890-7

Course Material	Book
Author	B S Nicholls
Publishing Year	2008
Title	ChemiCAL Software
Subtitle	
Edition	
Publisher	LJMU
ISBN	

Notes

Standard chemistry module supporting the pharmaceutical sciences