
Web Site

Up to date information, news and other teaching related material can be found on the teaching web site:

www-teach.ch.cam.ac.uk

In common with other IA NST courses, we will also be using *CamTools*

camtools.caret.cam.ac.uk

Synopses of the Lecture Courses

All lectures take place in the Bristol–Myers Squibb Lecture Theatre in the Department of Chemistry, Lensfield Road. Access to the Department is via the entrance which faces the Scott Polar Institute and the Catholic Church – please do not use the car park entrance. A complete lecture time-table is given on the inside cover of the booklet.

MICHAELMAS TERM

Shapes and Structures of Molecules: 19 lectures

Dr Peter Wothers

The aim of this course is to answer two questions: ‘How do we find out the shapes and structures of molecules’ and ‘Why do molecules have the shapes, structures and properties they do’.

Chemists use different kinds of spectroscopy to answer the first question, and the course will consider two of these in some detail: nuclear magnetic resonance (NMR) and infra-red (IR). The aim is to give you an understanding of the basis of the technique and then to go on to use this understanding to interpret spectra in terms of molecular structures.

The second question is answered by introducing elementary quantum mechanics which is the basis of the modern description of chemical bonding. The aim is to give you an understanding of how the idea of a wavefunction arises in quantum mechanics and the significance of such functions in understanding the behaviour of electrons in atoms and molecules.

We then go on to consider how such wavefunctions can be constructed for a range of molecules of different complexities and what the consequences are in terms of shape and reactivity of the occupancy of these electronic wavefunctions. The aim is to enable you to understand and rationalise key aspects of molecular structure.

Topics Introduction to molecular structure, spectroscopy and the electromagnetic spectrum. Illustration of the basic information derivable from different techniques. NMR spectroscopy as a tool for identifying atom type. Chemical shifts and coupling illustrated for different nuclei. Infra-red spectroscopy as a tool for determining bond type. Relation of vibrational frequency to bond strength and atomic mass. Structural problems solved by joint application of NMR and IR spectroscopy.

Quantum mechanics: energy levels and wavefunctions; interpretation of the wavefunction. Electrons in atoms: the shapes and energies of orbitals. Multi-electron atoms: shielding and penetration. Electrons in molecules, bonding and antibonding orbitals, bonding in diatomic molecules, bond polarity and strength, magnetic properties. Extension to larger systems, hybrid orbitals and conjugation.

Reactions and Mechanisms in Organic Chemistry: 14 Lectures spanning the Michaelmas and Lent Terms

Dr Bill Nolan

The principle aim of this course is to develop an understanding of organic reactions using the concepts of mechanism and ‘curly arrows’. Organic chemistry is made up of a great diversity of structures and functional groups, which can undergo a wide variety of chemical reactions. Some unifying concepts will be introduced to provide a rationale that will enable you to explain and predict a variety of reactions that proceed by different mechanisms. This will also provide a logic as to how molecules can be synthesised.

Topics Why molecules react – the role of energy, orientation and orbital occupancy. Reaction mechanisms – bond forming and breaking, and how these are described using curly arrows. Nucleophilic substitution at saturated carbon atom. Electrophilic attack on π bonds. Addition and substitution at the carbonyl group. Organic synthesis.

LENT TERM

Reactions and Mechanisms in Organic Chemistry, continued

Energetics and Equilibria: 9 Lectures

Dr James Keeler

In the physical and chemical world some things ‘happen naturally’ and some do not. A cup filled with hot tea warms up and the tea cools off, petrol burns to carbon dioxide and water, gases mix and fill the space available to them – but the reverse of these events are never observed to happen ‘naturally’. Water and carbon dioxide do not spontaneously form hydrocarbons, and your tea never gets hotter at the expense of a cooler cup.

It turns out that there is one universal law which described why some things happen spontaneously and some do not – the Second Law of Thermodynamics. In these lectures we will investigate where this law comes from and how it is connected with a quantity called entropy. We will go on to see that entropy has a strong connection with the microscopic nature of matter.

The Second Law is very fundamental, but it also leads on to very practical relationships that can be used to describe chemical equilibrium and how this is affected by factors such as temperature and pressure. In the second part of the course the idea of Gibbs energy (sometimes called free energy) will be introduced, and we will go on to see how this is a very convenient description of chemical equilibrium.

It will enable us, for example, to put familiar ideas such as Le Chatelier's Principle on a firm and quantitative footing and to understand the equilibria between phases. The course will close with a discussion of electrochemical cells and their applications.

Topics Natural processes, the Second Law of Thermodynamics and the concept of entropy; reversible and irreversible processes, equilibrium. Entropy seen in terms of the microscopic properties of matter. Practical formulation for chemistry in terms of the Gibbs energy. How to describe chemical equilibrium and how it is influenced by pressure and temperature; the central equation $\Delta_r G^\circ = -RT \ln K$. Electrochemical cells: description in terms of the Nernst equation and applications.

Kinetics of Chemical Reactions: 6 Lectures

Prof. John Pyle

In this course we will investigate how it is possible to determine the mechanism of a reaction and some of the factors that influence it. The main tool will be the study of the kinetics of the reaction, that is how fast it proceeds and how this rate is affected by temperature, concentration and other factors such as solvent type.

We will begin with the simplest reactions, 'elementary reactions', which take place as a result of a single molecular encounter. Two theories for describing such processes will be discussed, and in the course of the discussion the key ideas of activation energy and the reaction energy profile will be introduced. We will then go on to describe how a reaction mechanism can be thought of as a series of elementary steps, and how the kinetics of such a scheme can be analysed using the steady state hypothesis and other tools.

Examples from many different areas of chemistry will be given, from conventional organic reactions, enzyme kinetics through to atmospheric chemistry. We will also consider how the raw data of chemical kinetics, that is the measurement of concentration as a function of time, can be obtained and how such data can be interpreted in terms of rate laws. As chemical reactions cover a vast range of timescales, considerable ingenuity is needed in their measurement.

Topics What do we mean by rate of reaction, rate constants and rate laws? Theories about reaction rates: potential energy profiles, reaction coordinates and collisions. Experimental determination of rate laws: fitting data to rate laws, obtaining data for different timescales. Complex reactions and reaction mechanisms: rate determining steps, pre-equilibrium hypothesis, steady-state approximation and their applications. Chain reactions.

EASTER TERM

Chemistry of the Elements: 12 Lectures

Dr Nick Bampos

With over one hundred elements to use, the number and types of different inorganic compounds are truly limitless. From ceramics which conduct electricity as well as a metal to compounds which spontaneously ignite in air, chemists can create substances for almost any application. In order to understand the compounds, we need to look at the structures and properties of the elements themselves and how they bond with each other. Crucial to this is an understanding of the periodic table. The lectures draw on ideas from all the previous parts of the course.

Topics Why are most of the elements metals? Why are others semiconductors and others non-metals? What exactly is a metal anyway? These are some of the questions answered in the first part of

the course which looks at the properties of the elements and how they relate to their positions in the periodic table and ultimately their electronic structures.

The second part of the course explores the different types of bonding possible between the elements, from pure covalent to pure electrostatic and examines the advantages and limitations of each model. Once the nature of the bonding itself is understood, it is possible to appreciate the different reactions the compounds undergo.

Recommended books for Part IA Chemistry

Before buying any books for yourself, we recommend that you borrow them from a library so you can see whether or not you like the style. These recommended books should all be in your College Library; if they are not, please suggest that they be obtained.

General texts

Keeler J. and Wothers P. *Why chemical reactions happen*, Oxford, 2003.

Keeler J. and Wothers P. *Chemical structure and reactivity: an integrated approach*, Oxford, 2008.

Physical chemistry

Atkins P.W. *The Elements of Physical Chemistry*, any edition, OUP.

Atkins P.W. *Physical Chemistry*, OUP, (any edition).

Organic chemistry

Carey F.A. *Organic Chemistry*, McGraw Hill, 5th Edn, 2003.

Solomons T.W.G. *Organic Chemistry*, Wiley, 7th Edn, 2000.

(earlier editions of both of these texts are perfectly acceptable)

Clayden J., Greeves N., Warren S. and Wothers P. *Organic Chemistry*, OUP, 2000.

Sykes P. *Guidebook to Mechanism in Organic Chemistry*, Longman, 6th Edn, 1986

Warren S. *Chemistry of the Carbonyl Group*, Wiley 1974.

Inorganic chemistry

Wulfsberg, G. *Inorganic Chemistry*, University Science Books.

Mingos, E.M.P. *Essentials of Inorganic Chemistry*, OUP, 1995.

For reference: Cotton F.A. and Wilkinson G. *Advanced Inorganic Chemistry*, Wiley, 5th Edn, 1988.

For reference: Greenwood N.N. and Earnshaw A. *Chemistry of the Elements*, Pergamon, 1984.

Henderson E. *Main Group Chemistry*, Royal Society of Chemistry 2000

Spectroscopy

Williams D.H. and Fleming I. *Spectroscopic Methods in Organic Chemistry*, McGraw Hill, 5th Edn, 1995.

Kinetics

Cox B.G. *Modern Liquid Phase Kinetics*, (Oxford Chemistry Primers 21), OUP, 1994.

Pilling M.J. and Seakins P.W. *Reaction Kinetics*, (Oxford Science Publications), OUP, 1995.

Energetics

Price G.J. *Thermodynamics of Chemical Processes*, (Oxford Chemistry Primers 58), OUP, 1998.

Atkins P.W. *The Second Law*, (Scientific American Library) Freeman, 1994 (an excellent account of the history, background and applications of the Second Law)