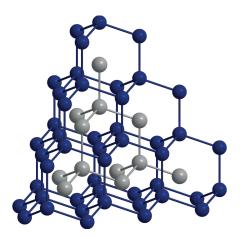


# **Yusuf Hamied Department of Chemistry**

# IB Chemistry: A Guide to the Course



# Academic Year 2023/2024



The Department of Chemistry endeavours to develop an inclusive, supportive and intellectually stimulating environment for our undergraduate community.

Athena SWAN is an ongoing program to address the underrepresentation of women in the sciences. The Silver Award recognises the progress that the Department has made in recent years, and the actions that benefit not only our female students, but all our undergraduate chemists.

Information about activities and profiles will appear inside the front cover of your lecture handouts.

#### IB Chemistry 2023/24

#### Chemistry A lectures are at 12:00 in the Wolfson Lecture Theatre

Chemistry B lectures are at 09:00 in the Wolfson Lecture Theatre; the lectures will start promptly at 09:00

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	6/10 Fr					19/1	Fr		
	7/10 Sa	SCA	SGS			20/1		JWRM	SRB
	9/10 Mo					22/1			
	10/10 Tu	SCA	SGS			23/1	Tu	JWRM	SRB
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2	12/10 Th	SCA	SGS		2	25/1		JWRM	SRB
	13/10 Fr					26/1			
	14/10 Sa	SCA	SGS			27/1	Sa	JWRM	SRB
	16/10 Mo					29/1			
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4	26/10 Th	SCA	NB		4	8/2	Th	JWRM	PDB
	27/10 Fr					9/2	Fr		
	28/10 Sa	SCA	NB			10/2	Sa	JWRM	PDB
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	3/11 Fr					16/2			
	4/11 Sa	SCA	PDW			17/2	Sa	JHK	PDB
	6/11 Mo					19/2			
	7/11 Tu	SC	PDW			20/2	Tu	JHK	PDB
	8/11 We			ļ		21/2			
6	9/11 Th	SC	PDW		6	22/2	Th	JHK	PDB
	10/11 Fr					23/2	Fr		
	11/11 Sa	SC	PDW			24/2	Sa	JHK	PDB
	13/11 Mo					26/2	Mo		
	14/11 Tu	SC	PDW			27/2	Tu	JHK	RJL
	15/11 We			ļ		28/2			
7	16/11 Th	OAMP	JMG		7	29/2	Th -	JHK	RJL
	17/11 Fr	<b></b>				1/3	Fr		<b>.</b>
	18/11 Sa	ΟΑΜΡ	JMG			2/3	Sa	JHK	RJL
	20/11 Mo					4/3	Mo		
	21/11 Tu	OAMP	JMG			5/3	Tu	JHK	RJL
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8	23/11 Th	JWRM	JMG		8	7/3	Th	JHK	RJL
	24/11 Fr					8/3	Fr		
	25/11 Sa	JWRM	JMG			9/3	Sa	JHK	RJL
	27/11 Mo					11/3	Mo		
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	Easter					
			А	В		
0	24/4	We	S11+	CAH <sup>+</sup>		
1	25/4	Th	SIJ	CAH		
	26/4	Fr				
	27/4	Sa	SJJ	CAH		
	29/4	Мо				
	30/4	Tu	SIJ	CAH		
	1/5	We				
2	2/5	Th	SIJ	CAH		
	3/5	Fr				
	4/5	Sa	SIJ	CAH		
	6/5	Мо				
	7/5	Tu	SIJ	CAH		
	8/5	We				
3	9/5		SIJ	CAH		
	10/5	Fr				
	11/5	Sa	SIJ	CAH		
	13/5					
	14/5	Tu	SIJ	CAH		
	15/5	We				
4	16/5	Th	SIJ	CAH		
	17/5	Fr				
	18/5	Sa		SGS*		
	20/5			SRB‡		
	21/5	Tu		SGS*		
	22/5	We		SRB/RJL‡		

<sup>+</sup>Note that the first lecture in the Easter Term is given on Wednesday

\* Organic revision lectures 9:00 am ‡Inorganic revision lectures; both at 12:00

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#### Introduction

The second-year courses build on the topics studied in the first year and explore these chemical ideas and principles in more depth. A broad range of topics is covered and the connections between these different topics are emphasised, as is the way in which one idea grows from another and can be developed to aid our understanding of chemistry as a whole. The courses lay a firm foundation of chemical principles which inform both more advanced study of chemistry and also related areas such as Biochemistry, Physics, Molecular Biology, Materials Science and Earth Sciences.

Two courses are offered in the second year: Chemistry A and Chemistry B; students may take either or both of them. Chemistry A focusses mainly on the theories which are used to understand and probe chemical bonding, structures and reactions. It starts out with a discussion of quantum mechanics which is the fundamental theory used by chemists to understand the microscopic nature of matter and molecules. The course goes on to use these ideas to discuss chemical bonding, the way in which microscopic properties influence those of bulk matter, and how all of these ideas can be used together to understand the properties and chemistry of solid materials. The underlying theme which runs through the course is endeavouring to understand the microscopic nature of molecules, matter and reactions.

Chemistry B focusses mainly on how chemists find out about and rationalise the enormous range of chemical structures and reactions that are known; a wide range is covered, from the familiar world of carbon-based chemistry, through the huge diversity of compounds and structures that are the domain of inorganic chemistry, and finally to the important topic of biological chemistry, in which we look at the chemistry of life. Despite the huge range that the course will cover, we will find that we can begin to make sense of it all by using a relatively small number of key concepts in chemical bonding and reactivity. As the discussion develops, the central role taken by electronic structure and the three-dimensional shape of molecules becomes apparent; it is these properties that influence their reactivity and other properties.

If you are planning on continuing with chemistry in the third, and possibly fourth, year, the best choice is to take both Chemistry A and B in the second year. By doing this, you will have the best coverage of chemistry, and be able to choose from the full range of specialist courses on offer in the final years. A route is provided within Part II Chemistry for those who have only taken Chemistry B in Part IB, but it is important to realise that by taking this route you will have a more restricted range of options. If you have only taken Chemistry A it may be possible to continue with Part II, but you will need to undertake some directed study over the preceding vacation.

Within IB Natural Sciences there are many courses which complement the two chemistry courses. Physics, Materials Science, and Mathematics are commonly taken alongside Chemistry A. Any of the biological courses with a more 'molecular' slant sit well with Chemistry B, and those with interests in Earth Sciences will find useful content in both Chemistry A and B.

The individual lecture courses in Chemistry A and Chemistry B are outlined below, and a complete timetable is given on the inside of the cover page.

## 2 Outline of the courses

Chemistry A and Chemistry B are outlined below: follow the tables vertically down the page. The number of lectures in each course is given in the bracket. A complete timetable is given on the reverse of the front cover.

Chemistry A	Chemistry B				
Michaelmas Term	Michaelmas Term				
Introduction to quantum mechanics (14)	Aromatic and enolate chemistry (6)				
Molecular spectroscopy (7)	Conjugate addition and chirality (5)				
	Introduction to stereochemistry (7)				
Symmetry and bonding I (3)	Shape and organic reactivity (6)				
Lent Term	Lent Term				
Symmetry and bonding II (11) Molecular energy levels and	Structure, bonding and reactivity of transition metal complexes (17)				
thermodynamics (13)	Structure, bonding and the p-block elements (7)				
Easter Term	Easter Term				
Electronic structure and properties of solids (11)	Introduction to chemical biology (11)				

3

#### Lecture synopses for Course A

#### Introduction to quantum mechanics: 14 lectures

#### Prof. Stuart Althorpe

The principles of Quantum Mechanics underlie all of chemistry at the molecular level, and provide a foundation on which the subsequent courses in Chemistry A are built. This course will introduce the fundamental ideas of quantum mechanics, and show how they may be applied to some simple but important examples: the harmonic oscillator, the rigid rotor and the hydrogen atom.

From there we shall move on to many-electron atoms and the consequences of electron spin, and finally show how the variation principle leads to an understanding of chemical bonding.

Mathematically, all that is required is some fluency with Part IA Mathematics (course A). The practical course in the Michaelmas Term contains a set of computer-based exercises designed to illustrate the contents of this course.

#### Molecular spectroscopy: 7 lectures

#### Prof. Stuart Clarke and Dr Lekan Popoola

Spectroscopy provides us with some of the best evidence for the quantization of energy. This course is integrated with the Quantum Mechanics course and illustrates how the key ideas may be used to understand the appearance of spectra and allow us to determine fundamental molecular parameters. The course also provides the background for the laboratory sessions where you will be able to put the theory into practice.

We shall start with the rotational spectra of diatomic molecules and its applications from microwave spectroscopy in the labs, which allows us to determine bond lengths in simple molecules, to radio astronomy which allows us to determine the composition of heavenly bodies. We shall then examine vibrational spectroscopy using both the harmonic oscillator and Morse oscillator as models. Finally, we shall touch on the electronic spectroscopy of atoms and simple molecules.

#### Symmetry and bonding: 14 lectures

#### Dr John Morgan

Humans seem to have an innate ability to recognise and appreciate the symmetry of objects, and chemists seem to be especially fascinated by molecules or other structures which display high or unusual symmetry. In this course we will show how *Group Theory* provides a formal framework for describing the symmetry of molecules and how this theory can be used as a powerful tool for predicting the properties and behaviour of molecules. In particular we will look at how symmetry helps us to construct molecular orbital (MO) diagrams and then how these can be used to understand key properties such as shape or stability.

We will also see how symmetry helps us to understand the vibrations of molecules via a normal mode analysis. Finally, we will look at how we can actually calculate the energies and form of the MOs in simple molecules using the Hückel approach. The application of symmetry to such calculations results in considerable simplification.

This course will take a relatively informal approach to Group Theory with the emphasis being on developing a practical set of tools which can be applied with ease.

**Introducing Group Theory** Symmetry elements and symmetry operations. Point groups. Character tables. Representations. Direct products.

**Applications** Vanishing integrals. Symmetry orbitals and molecular orbitals. Transition metal complexes. Hückel MO calculations. Normal mode analysis and vibrational spectroscopy. Dipole moments and chirality. Infinite groups and the symmetry of electronic states.

#### Molecular energy levels and thermodynamics: 13 lectures

#### Prof. James Keeler

Quantum mechanics provides us with a detailed description of the energy levels of single atoms and molecules, but when we are doing chemistry we deal not with one molecule at a time but vast numbers. The question is, then, how are the properties of bulk matter related to the energy levels of the molecules of which it is composed? The methods of *statistical thermodynamics*, which are introduced in this course, make this connection. In particular, we will see how the thermodynamic properties of matter (internal energy, entropy, Gibbs energy etc.) can be calculated from a knowledge of the molecular energy levels. As you will have seen in the earlier courses, these energy levels can be predicted by quantum mechanics and determined experimentally from spectroscopy. We will also investigate the Boltzmann distribution which is used to understand many molecular phenomena.

The course closes with a number of applications of the ideas developed in the earlier part. We will look at how it is possible to understand the temperature variation of heat capacities, and how it is possible to predict the values of equilibrium constants simply from spectroscopic data. Statistical thermodynamics can also be used to predict the values of reaction rate constants using transition state theory. We will look at how this is developed and the interpretation of the parameters involved.

**Topics** Review of thermodynamic ideas: the Second Law, internal energy, the Gibbs and Helmholtz functions. Microstates and macrostates: the canonical distribution function, the partition function and thermodynamics quantities.

Evaluation of the partition function: translation, rotation and vibration.

Internal energy and heat capacities; temperature variation. Calculation of absolute entropies.

Chemical equilibrium and the prediction of equilibrium constants.

Transition state theory: concept of a potential energy surface and the transition state; formulation in terms of partition functions; comparison with collision theory. Thermodynamic formulation.

The Boltzmann distribution; applications in spectroscopy. Density of states.

#### Electronic structure and properties of solids: 11 lectures

#### Prof. Stephen Jenkins

The objective of this course is to introduce the concepts of structure and bonding that are required to explain the behaviour of electrons in solids. The course is designed in such as way that it builds upon the material presented in all of the preceding courses in Chemistry A. At the heart of the course lie two contrasting models for the behaviour of electrons in solids – the free electron and the LCAO models.

Free electron theory is used as a starting point because it is simple and it permits the introduction of essential concepts such as wavevectors, travelling waves and the Fermi surface. However, this theory does not take account of the presence of atoms and orbitals and offers no structural predictions. LCAO theory is used to show how atomic orbitals may be used as a basis for constructing wavefunctions appropriate for solids. This theory is used to explain the bonding and energy bands in a wide variety of solids.

The last part of the course focuses on semi-conductors and doped semi-conductors which are exceptionally important as they are used to create the basic building blocks of all modern electronic devices.

Topics Introduction to the description of crystalline materials: lattices; unit cells; space filling.

The free-electron theory of solids: plane waves; the reciprocal lattice; wavevectors.

The Fermi–Dirac distribution: the Fermi level; the Fermi energy; the Fermi surface.

Electrical conductivity and other physical properties.

Tight-binding model for solids: bands; band gaps; band structure.

Semiconductors: doping; electrical properties; spectroscopic properties.

Electronic devices: the p-n junction; transistors.

### 4 — Recommended books for Chemistry A

These recommended books should be in your College Library. They can also be consulted in the Departmental Library, and some are available on short loans. The designations in brackets [...] are the class marks used to identify the books in the Chemistry Department Library, and you should find these texts shelved separately as the *Blue Book* collection in Unit 17, on the right hand side as you enter the library.

#### **Reading Lists Online (RLO)**

The link below gives access to the online reading lists for all the Chemistry courses. They have been compiled to follow the structure of the Course Guides. Each one includes a record of the borrowable items held in the Cambridge University Libraries' collections (including the Chemistry Library) and those accessible as eBook titles.

www-library.ch.cam.ac.uk/reading-lists-online-rlo

#### Quantum mechanics

Green N.J.B. *Quantum Mechanics 1: Foundations*, Oxford Chemistry Primers, 1997. [QC174.12.G74] For reference: McQuarrie, D.A, and Simon, J.D, *Physical Chemistry: A Molecular Approach*, University Science Books, 1997. [QD453.M37] For reference: Atkins P.W. & Friedman R.S. *Molecular Quantum Mechanics*, any edition, OUP. [QD462.A85]

Steiner E. The Chemistry Maths Book, OUP, 1996. [QA37.3.S74]

Green, N.J.B. *Quantum mechanics 2: The toolkit*, Oxford Chemistry Primers, 1998, [QC174.12.G74 1998]

#### Molecular spectroscopy

Banwell, C. and McCash, E., *Fundamentals of Molecular Spectroscopy*, 4th edition, McGraw Hill [QD96.M65.B36]

For reference: McQuarrie, D.A, and Simon, J.D, *Physical Chemistry: A Molecular Approach*, University Science Books, 1997. [QD453.M37]

#### Symmetry and bonding

Vincent A. *Molecular Symmetry and Group Theory*, 2nd edition, Wiley, 2001. [QD461.V56] For reference: Cotton F.A. *Chemical Applications of Group Theory*, Wiley, 3rd Edn, 1990. [QD461.C68] For reference: McQuarrie, D.A, and Simon, J.D, *Physical Chemistry: A Molecular Approach*, University Science Books, 1997. [QD453.M37]

#### Molecular energy levels and thermodynamics

Maczek A.O.S *Statistical Thermodynamics* (Oxford Chemistry Primers 58), OUP 1998. [QD504.M33] 2nd Edn. (2017) available. Gasser R.P.H. and Richards W. G. *An Introduction to Statistical Thermodynamics*, World Scientific, 1995. [QC311.5.G37]

#### Electronic structure and properties of solids

Smart, L. and Moore, E., Solid State Chemistry, 4th Edn, Chapman and Hall, 2012 [QD478.S63]
West, A.R., Basic Solid State Chemistry, Wiley, 2nd Edn,, 1999 [QD478.W47]
Cox P.A. The Electronic Structure and Chemistry of Solids, Oxford Science Publication, 1992.
[QD478.C69]
For reference: Singleton J., Band Theory and Electronic Properties of Solids, OUP 2001.

[QC176.8.E4.S56]

For reference: Elliott S. R. Physics and Chemistry of Solids, Wiley 1998. [QC176.5.E45]

## 5 Lecture synopses for Course B

#### Aromatic and enolate chemistry: 6 lectures

#### Dr Stephanie Smith

This course is divided into two sections. The first looks at the structure and reactivity of the benzene ring and explores the attack of electrophiles as the key reaction. In the second part we look at the formation and reactions of enols and enolates – these are nucleophilic species that allow the synthetic chemist to construct a wide range of new bonds adjacent to the carbonyl group.

#### **Topics Electrophilic aromatic substitution**

Aromaticity and aromatic compounds

- Electrophilic aromatic substitution
- Reactions on substituted benzene derivatives
- Substituent effects and multi-step reactions

#### Enols and enloates

Carbonyl-enol tautomerism

Acid and base catalysed enolisation

Electrophilic addition to enols and enolates

Stable enolate synthetic equivalents

Alkylation issues and solutions

Alternative enolate functionalities

#### Nucleophilic attack on $\pi$ systems: 5 lectures

#### Dr Nick Bampos

The conjugation of alkenes with electron-withdrawing groups makes them electrophilic and susceptible to attack by nucleophiles. Conjugate addition, an important type of reaction involving nucleophilic addition to the remote end of an alkene conjugated with an electron–withdrawing group, is discussed in detail. If the electron-withdrawing group in question is a carbonyl, the nucleophile can react either at the alkene (conjugate addition) or at the carbonyl (direct addition). Factors influencing the selectivity between these two modes of addition (the regioselectivity of nucleophilic addition) are examined. Both direct addition and conjugate addition can create chiral carbon centres (carbon centres with four different substituents attached).

A basic introduction to chirality is given, with a focus upon compounds containing one chiral carbon centre. The Cahn–Ingold–Prelog system for labelling the configuration of chiral carbon centres and alkene geometries is described.

Nucleophilic substitution at conjugated alkenes bearing a leaving group (conjugate substitution) is discussed. A related type of reaction involving nucleophilic substitution on aromatic rings (nucleophilic aromatic substitution) is examined.

**Topics** Conjugate addition with  $\alpha$ ,  $\beta$ -unsaturated carbonyls.

Direct addition versus conjugate addition.

Conjugate addition with other electron-deficient alkenes.

Introduction to chirality.

Labelling chiral centres: the Cahn–Ingold–Prelog rules.

Conjugate substitution.

Nucleophilic aromatic substitution.

#### Introduction to stereochemistry: 7 lectures

#### Prof. Peter Wothers

Molecular shape and reactivity is the foundation of organic chemistry. We need to be able to understand the critical, and often subtle, interactions between the shape of a molecule and its reactions. In three dimensions, molecules have more flexible shapes than two-dimensional structures with rigid  $\pi$  systems. In this course we will look at the different conformations that molecules can adopt and how stereochemistry plays an important role in determining reactivity.

Topics Introduction to Chirality.

Stereochemistry with two or more chiral centres. Resolution of enantiomers by forming diastereoisomers. Elimination reactions. Conformational analysis of chains and rings. Cyclisation reactions.

#### Shape and organic reactivity: 6 lectures

#### Prof. Jonathan Goodman

The final part of the course will combine the concepts of two- and three-dimensional shape, stereochemistry and NMR and apply these to the analysis a variety of reactions. These ideas can then be applied to some unfamiliar systems to work out how they might react.

#### Topics Alkynes and alkenes.

Bases and nucleophiles. Kinetic and thermodynamic control. Imines, oximes, and hydrazones. Beckmann rearrangement. Acetals and aldols. Stereoselective reactions on chiral molecules.

#### Structure, bonding and reactivity of transition metal complexes: 17 lectures

#### Prof. Sally Boss and Prof. Paul Barker

This seventeen-lecture course will introduce students to the rich and varied chemistry of transition metal complexes. The periodic properties of the metals and the types of molecule which metals will coordinate to (the ligands) will be described. The bonding in the resulting metal-ligand complexes will be modelled using both Molecular Orbital Theory and Crystal Field Theory which differ in their sophistication but share the same common symmetry arguments.

The course will focus on the on the role of d-orbitals and d-electrons in transition metal chemistry and the physical and spectroscopic consequences that result from the d orbitals losing their degeneracy on forming complexes with ligands. These include preferred geometries, oxidation states, high spin and low spin complexes and the magnetic and spectroscopic properties of complexed transition metal ions.

A consideration of ionic vs covalent bonding in transition metal complexes will be presented. Complexes which offer more covalency influence the chemical nature of the attached ligands more and it is these metal complexes which tend to be active catalytically. The key reaction types for more covalent metal complexes will be discussed in detail and their catalytic reactivity will be explained.

**Topics** The common structural geometries and stereochemistries of 1st-row transition metal complexes

Bonding models for transition metal compounds – Molecular Orbital Theory and Crystal Field Theory

Thermodynamic and electronic properties of transition metal chemistry – predicting structure, chemical behaviour and rationalising experimental results using bonding theories

The spectrum of ionic-covalent bonding in transition metal complexes and comparison of 3d, 4d and 5d metals

Key reaction types of transition metal complexes

Transition metal complexes as catalysts

#### Structure, bonding and the p-block elements: 7 Lectures

#### Dr Robert Less

This course describes the synthesis, structures and bonding for p-block species such as the borazines, phosphazenes and thiazenes (B/N, P/N and S/N systems). Emphasis is placed on synthetic methodologies, chemical reactivity and understanding how the main group elements bond in the resulting compounds. A range of arguments have been proposed to rationalize the structure and bonding principles underpinning these systems. Whilst  $p\pi$ – $p\pi$  bonding in borazines is generally accepted, the bonding in phosphazenes has proved more contentious and it is only recently that covalent bonding models have given way to a combination of more ionic perspectives and negative hyperconjugation. These ideas will be discussed and also applied to sulfur-containing systems. Methods for characterising main group systems will be explored. Students will be expected to extend structure, bonding and analytical concepts to related systems, such as boroxane and siloxane (B/O, Si/O) derivatives.

**Topics** There are many thousands of inorganic compounds composed primarily of p-block elements. Rather than survey all of them, selected N-containing system are focused on in order to exemplify concepts in synthesis, structure and reactivity: Borazanes and borazines; adduct formation; the importance of  $p\pi$ – $p\pi$  bonding in inorganics; substitution by addition elimination reactions; comparisons with organic aromatics. Phosphazanes and phosphazenes; ionic approaches to bonding; reactivity and substitution patterns. The thiazenes; stabilization of weak S/N bonds; insertion reactions. Characterisation of main group inorganic systems; X-ray diffraction and multinuclear NMR spectroscopy.

#### Introduction to chemical biology: 11 lectures

#### Prof. Chris Hunter

This course introduces the chemistry of biopolymers, exploring their structure, function and chemistry. The basic chemical concepts that govern non-covalent interactions will be illustrated by reference to the three-dimensional structures of the two most important classes of biomolecules, nucleic acids and proteins. Intermolecular interactions of organic molecules with DNA and proteins will be discussed along with the principles of drug design.

Basic physical organic chemical concepts such as general acid and general base catalysis, transition state theory, free energy profiles, isotope effects etc. will be illustrated by reference to enzyme chemistry. The chemical mechanisms of proteases and other enzymes will be discussed along with the principles of enzyme inhibition and its role in medicine.

This course looks forward to Part II and Part III courses when some of the most exciting recent advances in biological chemistry and chemical biology will be discussed. The approach throughout the course will be based on structure and mechanism – we will not assume any previous biochemical knowledge.

1–6 Non-covalent interactions: van der Waals forces, electrostatics, hydrogen bonding, aromatic interactions, functional group properties, desolvation, hydrophobic effect, entropic effects, cooperativity.

Nucleic acid structure: chemistry of heterocycles, sugars, phosphate esters, the double helix.

Protein structure: chemistry of amino acids, peptides, secondary, tertiary and quaternary structures.

Interactions with small molecules and drug design.

7–11 Thermodynamic and kinetic concepts relevant to biological chemistry including transition state theory, kinetic isotope effects, free energy diagrams. General acid catalysis, general base catalysis, electrophilic catalysis by metal ions, nucleophilic catalysis.

The mechanisms of serine proteases, metalloproteases and other types of proteases.

Enzyme inhibition and its role in medicinal chemistry.

#### 6 -

#### **Recommended books for Chemistry B**

These recommended books should be in your College Library. They can also be consulted in the Departmental Library, and some are available on short-term loan. The designations in brackets [...] are the class marks used to identify the books in the Chemistry Department Library, and you should find these texts shelved separately as the *Blue Book* collection in Unit 17, on the right hand side as you enter the library.

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borrowable items held in the Cambridge University Libraries' collections (including the Chemistry Library) and those accessible as eBook titles.

www-library.ch.cam.ac.uk/reading-lists-online-rlo

Organic chemistry

#### General organic chemistry

There are a variety of good texts which all cover the first term's material:

Clayden J., Greeves N., Warren S. and Wothers P. *Organic Chemistry*, OUP, 2001.[QD251.O74] Clayden J., Greeves N. and Warren S. *Organic Chemistry*, 2nd Edn, OUP 2012. (Either edition is acceptable) [QD251.O74]

Carey F. A. and Sundberg R. J., *Advanced Organic Chemistry*, 5th Edn, Springer 2007. [QD251.C37] Sainsbury M., *Aromatic Chemistry*, Oxford Chemistry Primer No. 4, OUP. [QD331.S25] McMurry J., *Organic Chemistry*, 9th Edn, Brooks/Cole 2016.[QD251.M36]

Vollhardt K. P. C. and Schore N. E., Organic Chemistry, 7th Edn, Freeman 2014. [QD251.V65] Smith, M. B. and March, J. Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th Edn, Wiley, 2013. [QD251.M37]

#### Structure determination

Williams D. H. & Fleming I. Spectroscopic Methods in Organic Chemistry McGraw Hill 6th edition, 2007. [QD272.S6.W55] Organic Structure Analysis, 2nd Edition Phillip Crews, Jaime Rodriguez and Marcel Jaspars. Oxford

*Organic Structure Analysis*, 2nd Edition Phillip Crews, Jaime Rodriguez and Marcel Jaspars. Oxford University Press, 2010. [QD272.S6.C74]

#### General inorganic chemistry

Cotton, F. A., Wilkinson, G., Murillo, C. A. and Bochmann , M., *Advanced Inorganic Chemistry* 6th Ed., Wiley (1999). [QD151.C68] Shriver and Atkins *Inorganic Chemistry*, latest editions. [QD151.S57] Greenwood N. N. Earnshaw, A. *Chemistry of the Elements*, 2nd Edition. [QD466.G74] Douglas, B., McDaniel, D. and Alexander, J., *Concepts and Models of Inorganic Chemistry*, 3rd Edition. Wiley. [QD475.D68]

#### Co-ordination chemistry

M.J. Winter *d–Block Chemistry*, Oxford Chemistry Primer 27, OUP. [QD172.T6.W56] 2nd Edn, (2015) available.

J. McCleverty *Chemistry of the First-Row Transition Metals*, Oxford Chemistry Primer 71, OUP. [QD172.T6.M33]

J. Keeler & P. Wothers Chemical Structure and Reactivity (Chapter. 15) 2nd Ed. [QD471.K44]

#### Organometallic chemistry

Spessard, G.O. and Miessler, G.L., *Organometallic Chemistry*, Prentice Hall (1997). [QD411.S64] Elschenbroich, C., *Organometallics*, Wiley-VCH 3nd Ed. (2005). [QD411.E47] Bochmann M. *Organometallics Volumes 1 and 2*, OUP Primers (1994). [QD411.8.T73.B63] Crabtree R.H. *The Organometallic Chemistry of the Transition Metals*. 6th Ed. 2014. [QD411.8.T73.C73].

#### Structure, Bonding and the p-Block Elements

F.A. Cotton, G. Wilkinson, C.A. Murillo & M. Bochmann, *Advanced Inorganic Chemistry*, John Wiley & Sons, 6th Ed, 1999. [QD151.C68]

C.E. Housecroft & A.G. Sharpe *Inorganic Chemistry*, Pearson Eduction, 5th Ed. 2018. [QD151.H68] N.N. Greenwood & A. Earnshaw *Chemistry of the Elements*, Pergamon Press, 2nd Ed. 1997. [QD466.G74]

J.E. Huheey Inorganic Chemistry, Prentice Hall, 4th Ed 1997.[QD151.H84]

N.C. Norman, *Periodicity in the s– and p–Block Elements*, Oxford Primer, 2nd Ed. 1997. [QD466.N67] T. Chivers & I. Manners *Inorganic Rings and Polymers of the p-Block Elements*, RSC publications, 1st Ed. 2009. [QD196.C45]

#### Introduction to chemical biology

A. R. Fersht, *Structure and Mechanism in Protein Science: A Guide to Enzyme Catalysis and Protein Folding*, 3rd edition, W. H. Freeman, 1998. [QD431.25.S85]

C. M. Dobson, J. A. Gerard & A.J. Pratt, *Foundations of Chemical Biology*, Oxford Chemistry Primers, OUP, 2001. [QD415.D63]

E.V.Anslyn & D.A. Doughterty, *Modern Physical Organic Chemistry*, University Science Books, 2006. [QD476.A57]

#### Practical work

On Wednesday 4th October there are separate introductory talks for Chemistry A and Chemistry B concerning the associated practical course. It is essential that you attend the talk or talks relevant to the course you are taking.

- For Chemistry B the talk is at 10:00 in the Bristol–Myers Squibb Lecture Theatre
- For Chemistry A the talk is at 11:00 in the Bristol–Myers Squibb Lecture Theatre

The practical work in chemistry fulfils two important roles: the first is to illustrate the material presented in the lectures so as to help you understand the concepts and gain familiarity in using them; the second is to develop the skills you will need as an experimental scientist. As chemistry is above all an experimentally based science, it is absolutely essential that you become adept at both performing and interpreting experiments. Chemistry is such a diverse subject that the range of skills needed is quite large; you need confidence in handling the apparatus and reagents used in preparative work, in the use of spectrometers and other instruments to make measurements of physical quantities and in using computers both to analyse data and calculate molecular properties.

When you register you will be assigned a day on which you should attend and complete the practical work; you will be given separate days for Chemistry A and Chemistry B. For Chemistry A the class will be divided into two groups, Group 1 and Group 2. Each Group will complete the same set of experiments and computer-based exercises, but in a different order; the detailed time table is given below.

The practical sessions in the Michaelmas Term are just the afternoon i.e. 13:45–18:00. The experiments have been devised so that you will be able to complete them in this time, but in contrast to the IA practicals, there will not be time for you to write up your account during the laboratory session.

The arrangements for marking practicals will vary slightly from course to course, but the basic idea is that you should have your experiment marked off either before or during your next practical session in the relevant part of the course. All marking will be done in the class by the senior demonstrators.

The marks you obtain in your practical work will be combined with those from the written papers at the end of the year to give your overall mark in Chemistry A or B.

#### **Chemistry A**

The main aim of the Chemistry A practical course is to help you to understand the concepts presented in the lectures – especially the key ideas in quantum mechanics which lie at the heart of the course. By doing the experiments and computer exercises you will see these key concepts 'in action' and will also see how they can be used in 'real' situations.

In addition, as you do the experiments and exercises you will acquire practical skills, such as the use of spectrometers, handling a vacuum line, and making careful measurements with different kinds of apparatus. You will also learn how computers can be used to great advantage in chemistry, for example for analysing data and plotting graphs (using EXCEL), visualising mathematical functions, such as wavefunctions (using Python in Google CoLab) and calculating molecular orbitals (using ORCA and Avogadro).

The course consists of experiments (E) and computer exercises (C) which approximately alternate according to the following time table:

Michaelmas Term							
Week no.	1	2	3	4	5	6	7
Group 1	С	Е	С	Е	С	Е	
Group 2		С	Е	С	Е	С	Е
Lent Term							
Week no.	. 1	2	2 ;	34	4	5	6

Week no.	1	2	3	4	5	6	
Group 1	С	Е	С	Е	С	Е	
Group 2	Е	С	Е	С	Е	С	

Experiments (E) are held in the Part IB/II Physical Laboratory which is on the first floor of the wing of the building which runs along Lensfield Road; to reach this laboratory turn left on entering the car park end of the building, go through the doors and then up three flights of stairs. Computer exercises are held in the Chemistry UMD (University Managed Desktop) (room G30) which is located by the lift on the ground floor at the car park end of the building nearest to Lensfield Road.

Each session starts are 13:45 pm promptly; it is essential that you are ready to start work at this time as the session will commence with a demonstration. The sessions end at 6 pm, but you may leave earlier if you have completed your work.

You will be given a rough book in which you must record your observations and measurements as you make them. For experiments in the Physical Laboratory the demonstrator will stamp your book and you need to bring it with you when you have an experiment marked off. Your write-up must be presented in the plastic wallets provided.

Write-ups will be marked in the class by the Senior Demonstrator on duty. You must have your write-up of an experiment or exercise marked the next time you do an experiment or computer exercise in the same place. Normally this will be two weeks later. For example, if you are in Group 1 your write-up of the experiment you do in week 2 of the Michaelmas Term will be marked in week 4; likewise if you do a computer exercise in week 5 of the Lent Term, it will be marked in week 7. Senior Demonstrators will be available for marking in week 7 of the Michaelmas Term and weeks 7 & 8 of the Lent Term.

The technical staff in charge of the Physical Chemistry Laboratory are Sarah Mitchell and Tom Wilkins and the member of staff responsible for the Physical practicals is Prof Peter Wothers and for the Computer exercises it is Dr John Morgan.

#### **Chemistry B**

The first aim of the Chemistry B practicals is to teach you the skills needed to synthesise and characterise compounds – this part of the course is entitled Preparative Chemistry. In the first year you have made relatively simple chemical transformations involving one step; the Preparative Chemistry course widens this experience to more complex reactions and experiments in which it is necessary to separate and purify the products. You will also see how to characterise the products of the reactions using spectroscopic tools such as NMR, IR and mass spectrometry. The Preparative Chemistry course will take its examples from across the Periodic Table, from carbon-based organic chemistry through to the diverse chemistry of other non-metallic and metallic elements.

The course will be held in the West end of the ground floor Organic and Inorganic Chemistry Laboratory, whose entrance is on the ground floor by the student pigeon holes. On the day allocated to you, you are required to be in the laboratory and ready to start work at 13:45; the session will commence with a demonstration, and will finish by 18:00. You will attend eight

afternoon sessions during the Michaelmas Term, and eight during the Lent Term. You will be given a rough book in which you must record any measurements as you make them.

Your write-up must be presented in the plastic wallets provided and handed in to the technicians at the start of your next practical session. Your demonstrator will mark your scripts and return them to you the following week. You should keep them in a safe place until after the examinations. There is a penalty if you do not hand in your write-up by the following session.

The technician in charge of the class is Helen Jobson (hcj27@cam.ac.uk) and she is assisted by Simon Chapman and Will Hancock-Smith. The members of staff responsible for the class are Prof Sally Boss and Dr Bill Nolan.

#### End of year arrangements

All practical write-ups must be marked before the end of the Term in which the experiments or exercises were completed. You must not accumulate un-marked practicals throughout the Term and then expect to have them marked in the last few days. There will be restrictions and penalties imposed on marking such practicals in the last week.

Any write-ups returned to you after they have been assessed should be kept in a safe place so that they can be reviewed if required.

Practical marks are subject to moderation and/or scaling by the Examiners in order to maintain comparability between different areas and assessors.

Attendance at practical classes is compulsory; you will lose marks from your final total if you do not complete and hand in the accounts of your practical work. If you are unable to attend a practical on the usual day, for example through illness or other good cause, you may come on another day provided that there is sufficient space and equipment available. If you are unable to make up a missed practical session, you should ask your Director of Studies or Tutor to complete a missed practical form (available at www.ch.cam.ac.uk/teaching/resources) and return it to the Teaching Office (teaching.office@ch.cam.ac.uk); we may be able to award you an average mark for a session that you missed with good cause.

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#### Plagiarism

Plagiarism is defined as submitting as one's own work that which derives in part or in its entirety from the work of others without due acknowledgement. It is both poor scholarship and a breach of academic integrity. The University views plagiarism as a serious matter and, under Discipline Regulation 6, has the power to take disciplinary action against those found guilty of plagiarising the work of others.

The general university statement on plagiarism, and further general advice on plagiarism and how to avoid it, is given on the University's plagiarism and good academic practice website <a href="https://www.plagiarism.admin.cam.ac.uk/definition">www.plagiarism.admin.cam.ac.uk/definition</a>. Generally the Department follows the advice and policies set out by the University. This section gives further guidance as to how these policies apply to study in the Department of Chemistry.

#### Supervision work and Tripos questions

The majority of questions set as supervision work and in Tripos examinations take the form of problems to be solved. In presenting their solutions to these problems students are not expected to quote the source or authority of the facts, theories and concepts they use to formulate their solutions.

#### Continuously assessed work (principally practical work)

Here the rules against plagiarism are especially relevant as they prohibit copying and colluding. Basing a write-up on data or answers provided by another student is an example of plagiarism (or, more simply, cheating). The following rules apply to all continuously assessed work

- Unless otherwise instructed, you must work alone. Where you are permitted to work in a group, the names of those you have worked with must be stated on your practical write-up.
- The write-up must be entirely your own work. In particular, you may not use spreadsheets or templates prepared by others.
- It is expressly forbidden to invent, falsify or modify data, spectra or observations, or to use data, spectra or samples obtained from other persons unless authorised to do so by a Senior Demonstrator.
- Where data from other sources is quoted in a write-up, the source must be identified.

The following summarizes succinctly the key point:

The Golden Rule: The examiners must be in no doubt as to which parts of your work are your own original work, and which are the rightful property of someone else.

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#### **Examinations**

#### **Chemistry A**

There are two three-hour written papers set for Chemistry A, papers A1 and A2. Each paper will contain five questions of equal weight; candidates are required to answer all five questions.

**Paper A1** will contain two questions relating primarily to the material presented in the lecture course *Introduction to quantum mechanics*, one question relating primarily to the material presented in the lecture course *Molecular spectroscopy* and two questions relating primarily to the material presented in the lecture course *Symmetry and bonding*. Any question may, however, draw on material from the whole of the Chemistry A course.

**Paper A2** will contain three questions relating primarily to the material presented in the lecture course *Molecular energy levels and thermodynamics* and two questions relating primarily to the material presented in the lecture course *Electronic structure and properties of solids*. Any question may, however, draw on material from the whole of the Chemistry A course

#### **Chemistry B**

There are two three-hour written papers set for Chemistry B, papers B1 and B2. Each paper will contain five questions of equal weight; candidates are required to answer all five questions.

**Paper B1** will contain four questions relating primarily to the material presented in Michaelmas Term and one question relating primarily to the material presented in the lecture course *Introduction to chemical biology*. Any question may, however, draw on material from the whole of the Chemistry B course.

**Paper B2** will contain four questions relating primarily to the material presented in Lent Term and one question relating primarily to the material presented in the lecture course *Introduction to chemical biology*. Any question may, however, draw on material from the whole of the Chemistry B course.

The format of the papers is such that you will need to be prepared to answer questions on all of the course. You should also be aware that in the Easter Term there is very little time between

the end of the lectures and the examinations. Please take both of these factors into account when planning your programme of supervisions and revision.

In all of the examinations you will be provided with a Data Book which contains a simple Periodic Table, values of physical constants, certain mathematical formulae and definitions and selected character tables. You will be provided with a copy of the Data Book when you register for the course (accessible on line at <a href="http://www.ch.cam.ac.uk/teaching/data-book">www.ch.cam.ac.uk/teaching/data-book</a>). You may take (unassembled) molecular models into the examinations.

As the course has been altered and revised over the years, not all of the questions on past Tripos papers are directly relevant. However, each lecturer will indicate which, if any questions, are relevant from previous years. A selection of recent past papers are available from the relevant sections of *Moodle* (<u>www.vle.cam.ac.uk</u>), and suggested answers to questions more than five years old are also available.

The marks obtained on the written papers are combined with marks obtained from the assessed practicals: usually 80% of the final mark is for the theory and 20% for the practicals.

The Senior Examiner for Part IB Chemistry A is to be confirmed and for Chemistry B it is Prof Peter Wothers

#### How to approach the examination

As you will have discovered at the end of last year, Cambridge written examinations are very different in style to those you will have become used to at school or college. As you prepare for your second round of tripos examinations, it is a good idea to reflect on your experience from last year, and draw what lessons you can from it. It is absolutely vital that, ahead of the examinations, you familiarize yourself with the style of the questions and spend some time practising some past papers.

Remember that Cambridge examinations are designed to be challenging to even the best students – the average mark for a Chemistry written paper is about 65%, very few students achieve marks of over 80%, but there will be significant numbers with marks below 50%.

All of the questions involve solving a problem of some kind, and to do this successfully you will need both factual information and – most importantly – an understanding of the underlying chemical principles which are being applied in the question. You can expect the questions to be similar in style to those you have done as exercises associated with the lecture course or to past exam questions, but the questions you will be confronted with in your examination will certainly not be the same as those you have seen before. You certainly cannot 'learn' the answers to the questions: you will need to work them out using your understanding of chemical principles.

Many students find the biggest difficulty with a Cambridge examination is that they run out of time. This is a reflection of the difficulty of the questions, which may not only require you to write more than you are used to, but may also need quite a bit of thought before you can start to answer them.

It is for this reason that you need to be very careful about dividing your time equally between the questions on the examination paper. On each Chemistry paper there are five questions to answer, each with equal weight, so 36 minutes should be allocated to each. All those involved in marking examination papers will tell you that the greatest number of marks are achieved earlier in the early stages of answering a question. Therefore, carrying on beyond 36 minutes in the hope that 'the answer' will suddenly pop out, and hence gain you the final few marks, is not a good strategy. Far better to move onto the next question and gain the straightforward marks for this.

Most questions are subdivided into parts, and the approximate division of marks is given at the end of the question. It is important to pay attention to this. If a part receives 10% of the marks, then clearly only a very short answer is expected – not a page of explanation. No matter how much you write, the maximum number of marks will still be 10%.

In setting the questions the examiners will have in mind a particular answer. However, full credit is given for any answer which the examiner deems reasonable, even if it is not the answer that he or she originally had in mind – there is no one right answer.

For many questions, a well-constructed and labelled diagram, accompanied by a few well thought out sentences, is all that is required, and is indeed the best way to structure an answer.

If you make a mistake in your answer, simply cross it out and carry on; under no circumstances should you use 'TippEx' or other such products. It may be that you have crossed out the 'right' answer, or at least a valid approach, in which case the Examiner may be inclined to give some credit. On the whole, the examinations are marked in a generous way; there is no negative marking.

Finally, you should try to write as legibly and clearly as you can, simply because this will help the examiner to read and mark what you have written. Use a good quality black or blue pen that makes a medium width line (not a very fine line, which is harder to read). You may draw diagrams in pencil and use colour for these, if it seems helpful. However, the main part of your answers should be written in pen. Do not crowd the page with text and diagrams – rather, leave some space so as to improve legibility.

If you want further advice on how to approach examinations, then you should approach your Director of Studies or supervisor.

#### Criteria for assessment

At the end of the year you will be awarded a mark and a class, separately for Chemistry A and Chemistry B. The Natural Sciences Tripos Committee gives specific guidance on the relationship between marks and classes, and on the expected distribution of candidates amongst the classes.

The final mark will be made up of 20% derived from the marks awarded in the practical course and 80% from the marks achieved in the end of year examination. The marking scheme used in the practical course is not designed to differentiate strongly between candidates, and as a result the spread of marks is quite narrow and the average mark is quite high. Candidates who do not complete the experiments will, therefore, put themselves at a significant disadvantage.

In contrast, the examination is a strong discriminator. In the examination marks are awarded for any reasonable answer – it is not necessary to give the 'expected answer' in order to gain credit. In addition, marking is on the whole quite generous, and there is certainly no negative marking.

# 10 Disclosure of examination marks

The marks which are disclosed (via *CamSIS*) are those for each of the papers, a total mark for the continuously assessed component of the course and the final overall total and class. Please note that the marks from the continuously assessed component may be scaled by the Examiners, and the overall mark may also be subject to scaling, as required by the Natural Sciences Tripos committee. In addition your question-by-question marks should be available via your Director of Studies.

# 11 Chemistry teaching website

You can find up-to-date information on the course and other related matters from the teaching website: www.ch.cam.ac.uk/teaching.

Handouts and other course materials will be posted on *Moodle*: <u>www.vle.cam.ac.uk</u>. If you find that you do not have access to the Chemistry part of Moodle, please email the Teaching Office at teaching.office@ch.cam.ac.uk.

#### 12 Chemistry Consultative Committee

The Chemistry Consultative Committee consists of representatives of students and academic staff. It meets towards the end of each term and is a forum for the discussion of all aspects of the teaching of Chemistry in the Department. Student representatives are elected during the Michaelmas term; comments and suggestions can be passed on to them so that they can be discussed at the meetings.

The minutes of previous meetings may be found on Moodle and the composition of the committee can be found on the teaching website

www.ch.cam.ac.uk/teaching/student-consultative-committee

# 13 Further details of the department

In order to access areas of the Department other than the lecture theatres you will need your University card so that you can pass the turnstiles and various internal doors. You should therefore make it a point to *always* bring your card with you when you come to the Department.

We hope that during the registration process for the practical classes we will be able to collect all of the information we need to make sure that everyone has the appropriate access. If you find that your access rights are different to others in your year group, or access suddenly stops, please contact Mifare Admin (mifareadmin@ch.cam.ac.uk). However, please do not do this until after the first week of term, as it will take some time in order for the whole system to settle down. Please note that undergraduates will *not* be given access to research areas. If you need to meet supervisors and so on, you will need to arrange for them to meet you in a general access area. Make sure you know who they are and how to contact them, so Security can help you locate them if necessary.

Your card will give you access to the building from 08:00–20:00 Monday - Friday and 09:00–14:00 on Saturday.

Outside these times you are not permitted to be in the Department unless some specific arrangement has been made. If you remain in the Department after 20:00 you risk becoming trapped by the security doors and/or the turnstiles.

#### www-library.ch.cam.ac.uk

The Chemistry Library is located in the Centre for Molecular Informatics (CMI) building (first floor, beneath the Cybercafe). You can access it between 09:00 and 20:00 using your University Card. You can apply for evening and weekend access on the recommendation of your DoS only; please visit the 'Access to the library' website: <a href="https://www-library.ch.cam.ac.uk/access-library">www-library.ch.cam.ac.uk/access-library</a> for details.

Books recommended in the Blue Book are either short loan and can be borrowed for four days, or are for reference only. Main loan books can be borrowed for 28 days and are auto-renewed until you return them or someone else requests them from you; short loan books cannot be renewed. You can borrow up to 10 books (incl. max. two short loan books) at a time. All Chemistry books and ebooks are listed on iDiscover, the online catalogue for the libraries of the University: //idiscover.lib.cam.ac.uk There is a dedicated computer in the Library for searching the catalogue. A self-service machine is available for borrowing and returning books.

The Library has four PCs which are hosted on the MCS (Managed Cluster Service) network. Print jobs can be sent from these to a MultiFunctional Device (MFD) situated in the small room next to the Library Office. The MFD offers colour printing, photocopying and free scanning. Online payment for printing and photocopying is made through the Common Balance scheme. You can send print jobs to the MFD from your own desktop, laptop, tablet, or phone; there are instructions for setting this up and information on paying for printing/photocopying at help.uis.cam.ac.uk/service/printing

There are also four docking solutions you can connect your laptop to, consisting of a 27" monitor, VGA and HDMI cables, mouse, and keyboard. Wifi and power points are available throughout the Library.

For comprehensive guidance on the library collections (printed and online), services and much more consult the Chemistry Library website at:

#### www-library.ch.cam.ac.uk

#### 15 Looking ahead: Chemistry in the third year and beyond

If you are intending to specialise in chemistry in the third (and possibly fourth) year the best option is to take both Chemistry A and Chemistry B so as to have the broadest grounding in chemical topics. A route is provided within Part II Chemistry for those who have only taken Chemistry B in Part IB, but it is important to realise that by taking this route you will have a more restricted range of options. If you have only taken Chemistry A it may be possible to continue with Part II, but you will need to undertake some directed study over the preceding vacation.

You should note that in order to proceed to Part III (the fourth year) you need to achieve at least a II.1 in Part II Chemistry.