

UNIVERSITY OF OXFORD



Department of Chemistry
Undergraduate Course Handbook
Academic Year 2017 - 2018

<http://www.chem.ox.ac.uk>

APPENDIX D

Syllabus for Prelims 2017-18

SUBJECT 1, Chemistry 1: Inorganic

Aims: The aim of the first year inorganic chemistry course is to lay foundations in the areas of atomic structure, bonding and the structures of molecules and solids, and chemical reactivity. These areas and their importance will be illustrated by a wide-ranging descriptive chemistry of the elements.

Atomic Structure and Periodic Trends

The Bohr model, wave properties of electrons, the Born Interpretation: probability densities. The Schrödinger equation and the H atom. The quantum numbers n , l , m , their values and interpretation (hence $2s$, $3d$, $4f$, etc.) Shapes and energies of orbitals. Radial wavefunction and the radial distribution function. Polyelectronic atoms: Orbital approximation, spherical average of electron repulsion. Helium and the Pauli Exclusion Principle: electron spin, antisymmetry. Screening and penetration, effective nuclear charge. Structure of the Periodic Table: s -, p -, d -, f -blocks. Trends in ionisation energies, electron affinities, ionic radii, $3d$ and $4f$ contractions.

Ionic Model, Pre-Transition Metal and Solid State Chemistry

General atomic and chemical properties of elements of Groups 1,2, within the framework of the Periodic Table. Elements, halides, hydrides, oxides. Born-Haber cycles, Born-Landé and Kapustinskii equation. Hess's Law cycles. Trends in the stability of binary compounds. Structures of ionic solids based on closed packing and filling of interstitial holes. Close packing, unit cells, space efficiency. Fractional coordinates, plan views and projections. Location, number and size of octahedral and tetrahedral interstitial holes. Common AB and AB₂ structures. Factors affecting structure: relative sizes, charges, ionicity, van der Waals, the NiAs class of compounds. Chemistry in aqueous solution, trends in solubility of compounds, complex formation, nature of ligands and driving force. Chemistry in non-aqueous solution, metals in liquid ammonia, unusual oxidation states, organometallic chemistry (e.g. methyl lithium).

Shapes, Symmetry and Molecular Orbital Theory

Lewis structures, VSEPR rules. Symmetry of molecules, symmetry elements, point group determination. Molecular orbital theory: H₂⁺, H₂, homonuclear diatomics, s/p mixing, bond strength and bond order, paramagnetism. Heteronuclear diatomics, HF and CO. 3-centre/2-electron, 4-centre/2-electron bonds: H₃⁺, H₃⁻, HF₂⁻, B₂H₆.

Acids, Bases and Solution Equilibria

Definitions (Brønsted, Lewis), pK_a , trends in acid strength, Pauling's rules for oxy-acids. Buffers. Redox potentials, Nernst equation, pH dependence, Latimer diagrams, Frost diagrams - construction and interpretation. Calculation of equilibrium constants from redox potentials.

Non-Metal Chemistry

General atomic and chemical properties of elements of Groups 13,14,15,16,17 within the framework of the Periodic Table. Elements, halides, hydrides, oxides, oxoacids. Structure, bonding, trends in stability, acid/base properties and reactivity patterns.

Transition Metal Chemistry

Transition elements and the Periodic Table. Survey of atomic properties, oxidation states, energetics and coordination environments. Key ideas of coordination chemistry. Introduction to ligand fields.

SUBJECT 2, Chemistry 2: Organic

A knowledge of the dynamic and evolving science of Organic Chemistry is central to the discovery, understanding and development of many important breakthroughs in biology, medicine, and materials science. This course will provide an introduction of the concepts and fundamental reactions of Organic Chemistry, show how these discoveries are supported experimentally, and how this knowledge can be used in a problem-solving and predictive capacity.

Aims: The course is designed to introduce and develop the fundamental concepts of organic chemistry; to show some of the key experimental evidence which supports these concepts; to apply these data and concepts to chemical problem solving.

Introduction to Organic Chemistry

Lewis bonding, bond polarisation. Lewis acids. Structures and isomers. Stereochemistry. Enantiomers: chirality, stereogenicity. Molecular orbital theory hybridisation. Functional groups: carbonyls, imines, oximes, nitriles. Lewis acids and bases. Curly arrows and mechanism. Resonance.

Introduction to Organic Spectroscopy

Introduction to spectroscopy. Nuclear spin and resonance. The chemical shift. Factors that influence carbon chemical shifts. Spin-spin coupling. Multiplet patterns for carbon-hydrogen couplings. Correlating carbon chemical shifts with organic structures

Orbitals and Mechanisms

Acids and bases: resonance and inductive effects. Thermodynamics and kinetics. Hammond postulate. FMO interactions. Conjugation; vinylogy. Reactions: curly arrow rules, formal charges, mechanism and structure as a consequence of FMO interactions. Solvent effects, reactive intermediates: C⁻, C[•], C⁺. A unified approach to mechanism. Neutralisation and ionisation, S_N1. 1,2-Addition to C=O and β-elimination (E1cB, E2). S_N2. Electrophilic addition with H⁺ & regiochemistry. E1. Electrophiles and stereospecificity. Attack by carbenes, dienes = pericyclic.

Substitution and Elimination at Saturated Carbons

Substitution and Elimination at Saturated Carbons. Substitution reactions and mechanisms. Synthetically useful variants of eliminations.

Core Carbonyl Chemistry

Nucleophilic addition to C=O, reversible and irreversible. Nucleophilic substitution of C=O, (acetals; imines, oximes and hydrazones; enamines, Wittig and Horner-Emmons reactions, Wolff-Kishner reaction). Nucleophilic substitution at C=O, (acid chlorides; anhydrides; esters; amides). Simple IR stretch of C=O groups. Chemistry of carboxylic acids. Keto-enol tautomerism: α -racemisation in acid or base. pKa of simple FGs including malonates. Reactions of enolates. Alkylation, Claisen condensation, halogenation of ketones. The haloform, Reformatsky and Darzens reactions. Condensation reactions with carbonyl groups. The aldol reaction. Conjugate additions.

Chemistry of C–C π -Bonds

Alkene and alkyne chemistry: influence of orbitals on reactivity. Overview of types of reaction. Alkene reactivity: electrophilic addition, pericyclic addition, free radical addition, catalytic hydrogenation. Allylic bromination. Alkyne reactivity: electrophilic addition, hydration to ketones, alkylation of terminal alkynes, reduction. Conjugation/delocalisation in non-aromatic systems: conjugated alkenes and alkynes, allenes. Modifications to reactivity, conjugate addition reactions. Structure and Reactivity of Aromatic compounds. Electrophilic aromatic substitution. Mechanism. Reactions: halogenation, nitration, sulfonation, Friedel-Crafts alkylation/acylation, formation of azo dyes (coupling with diazonium salts). Directing effects. Nucleophilic aromatic substitution.

Introduction to Biological Chemistry.

Introduction, context and structure of a cell, highlighting molecules that are important in biology. Amino acid structure, chemistry and synthesis. Peptide structure, conformation and simple synthesis. Primary protein structure and sequencing, secondary, tertiary and quaternary protein structure. Introduction to the importance of enzymes in catalysing the diverse chemical reactions of life; how enzyme active sites enable catalysis including through the use of cofactors; how enzymes achieve specificity in catalysis; introduction to transition state stabilisation and the thermodynamics of enzyme-catalysed reactions; a simple enzyme mechanism to illustrate how the conformation of amino acid side chains enables efficient catalysis. The chemical structure and fundamental properties of nucleic acids and their building blocks; the nucleobases that occur in DNA and RNA, their physical properties, the ribose and deoxyribose sugars, nucleosides, nucleotides, and single stranded nucleic acids. The chemical structure of double stranded DNA, A, B, and Z-DNA structures, how the structure of the double helix was determined. Chargaff's rules. Watson-Crick A.T and G.C base pairs, the importance of base stacking and hydrogen bonding in stabilising the double helix. Replication, involvement of dNTPs and the importance of enzymatic control to ensure a high level of efficiency and accuracy. Base mispairing and the structures and physical properties of mispaired bases.

Revision and Problem Solving

The course will cover recent Prelims questions

SUBJECT 3, Chemistry 3: Physical

Aims: *The first-year physical chemistry course lays foundations in the key areas of quantum mechanics, physics, thermodynamics and reaction kinetics, upon which the whole of modern physical chemistry is based.*

States of matter and equilibrium Thermodynamics

Le Chatelier's principle. Equations of state. Systems and surroundings. Work and heat. First law. Internal energy. State functions. Expansion work. Reversible and irreversible changes. Heat capacity and enthalpy. Thermochemistry. Standard states. Standard enthalpy changes (transition, reaction, formation). Kirchhoff law. Second law. Direction of change. Entropy. Condition of equilibrium. Entropy changes of phase transition. Temperature and pressure dependence of entropy. Third law. Statistical interpretation. Free energy. A and G. Available work. Temperature and pressure dependence of Gibbs energy. Phase equilibria. Clapeyron and Clausius-Clapeyron equations. One-component phase diagrams. Chemical equilibrium. Thermodynamics of mixtures. Chemical potential. Entropy and enthalpy of mixing. Extent of reaction. Reaction quotient. Condition for equilibrium, equilibrium constant and its temperature dependence; relation to standard Gibbs function.

Electrochemistry

The metal/solution interface. Electrochemical potential. Equilibrium Nernstian electrochemistry. Activity and activity coefficients and their determination. Nernst equation. Cells and half cells. Reference electrodes. Reversibility and irreversibility of cells. Relation of standard potentials to thermodynamic quantities. Conductivity of ionic solutions - liquid junction potentials. Measurement of standard electrode potentials.

States of Matter

Microscopic view of structure and motion in the three states; radial distribution function. Density, mechanical properties, diffusion and viscosity, degrees of freedom, equipartition and heat capacity. Intermediate states of matter: liquid crystals, gels, glasses. Intermolecular forces and pair potentials. Gas imperfection, van der Waals equation, virial expansion. Relationship between potential energy curve and the virial coefficients/internal energy. Single component phase diagrams (e.g., H₂O, CO₂, He); phase coexistence and stability, triple point, critical point, multiple solid phases.

Quantum Mechanics and Spectroscopy

The physical basis of Chemistry: Electromagnetism Coulomb's Law, electrostatic forces and fields Electric energy and potential. Electric dipole moment. Electric current, resistance and conductivity. Magnetic forces – the Lorentz force. Magnetic fields and the Biot-Savart law. Magnetic dipoles and magnetic materials. Waves, the E.M. spectrum. Superposition and diffraction. Refraction (Snell's Law).

Quantum theory of atoms and molecules

Quantum theory. Failures of classical physics. Quantization of electromagnetic radiation. Wave-particle duality. The de Broglie relation. The Schrödinger equation. Solution for particle in a *one*-dimensional square well and results for an *n*-dimensional square well; particle on a ring and the rigid rotor; simple harmonic oscillator; hydrogen atom. Born interpretation. Correspondence principle. Zero point energy. Quantum Tunnelling. Eigenvalue equations. Position, momentum and Hamiltonian operators. Expectation values, uncertainty principle. Atomic spectra: one-electron atoms and alkali metals. Orbitals, energy levels and quantum numbers. Radial and angular distributions. Term and level symbols. Spin-orbit coupling. Penetration and shielding. Selection rules and spectra. Structure of many-electron atoms and the Aufbau principle.

Kinetics**The physical basis of chemistry: Classical mechanics and properties of gases**

Newton's Laws of motion: forces, momentum and acceleration. Work, and kinetic and potential energy. Rotations: angular momentum and moments of inertia. Vibrations: simple harmonic motion. Properties of gases: the perfect gas equation. Kinetic theory of gases, origin of pressure, Maxwell-Boltzmann distribution. Molecular motions and equipartition. Collisions between molecules, mean free path, collision frequency, effusion, diffusion.

Reaction kinetics

Rates of reactions. Order and molecularity. Rate laws and their determination. Experimental measurement of reaction rates. Sequential and reversible reactions, pre-equilibrium, the steady state approximation: applications to unimolecular reactions (Lindemann) and enzyme catalysis. Temperature dependence of reaction rates: Arrhenius Equation, activation energies, elementary collision theory.

SUBJECT 4, Mathematics for Chemistry

Calculators will not be permitted in the Examination but Tables containing standard results from calculus and trigonometry will be provided.

Syllabus

Linear equations and determinants. Vector algebra and calculus, and applications to mechanics. Plane polar, spherical polar and cylindrical polar coordinates. Inverse functions. Hyperbolic functions. Limits and their determination. Elementary calculus of one and of two variables. Taylor series and L'Hopital's rule. Integration, integration by parts. Transformation of coordinates. Theory of errors. Multiple Integrals in two and three dimensions. Complex Numbers. Argand diagram, Euler equation, de Moivre's theorem. Solutions of the equation $z^m = a + ib$

First Order Differential Equations, exact, separable, linear, homogeneous. Second order Linear Differential Equations, linear homogeneous differential equations, equation of harmonic motion, damping terms. Second order linear inhomogeneous differential equations. Matrix addition and multiplication. Inverse matrices. Orthogonal matrices. Eigenvalues and eigenvectors. Properties of symmetric and of Hermitian matrices.

APPENDIX E1

Syllabus for Part IA 2017-18

INORGANIC CHEMISTRY

The content of the Part IA Examination in Inorganic Chemistry will be based on the content of the lectures delivered to 2nd year students. Candidates will also be expected to be familiar with material covered in the 1st year course. In some questions it may be necessary to make use of simple symmetry arguments at the level covered in the Symmetry I and Symmetry II General Chemistry course. Candidates will be expected to be familiar with the content of the 1st and 2nd year practical courses.

Transition Metal Chemistry

Atomic properties. Relative energies of *s* and *d* orbitals. Electronic configurations. Ionisation energies. Δ_{eff} . The relative stability of oxidation states. The stability of the half-filled shell. Sublimation energies of the elements. Heats of formation of cations. Trends in stability of binary compounds. Rationalisation of electrode potentials. Ligand field splittings: high and low spin complexes, spin-pairing energies; LFSE effects in lattice energies, heats of formation, hydration energies, etc.; site preference energies in spinels. Dependence on ligand type, oxidation state, and transition metal series. The Jahn-Teller effect and its consequences. Stability of oxidation states in the 1st transition series. Trends in reduction potentials for $M^{3+}/M^{2+}(aq)$. Oxidation state (Frost) diagrams. The effect of pH and of ligands on redox potentials. Factors and ligands stabilising high and low oxidation states (eg π acceptor ligands versus π donor ligands). Role of entropy. Main differences between the 1st and the 2nd and 3rd transition series. Main differences between the 1st and the 2nd and 3rd transition series: stability of oxidation states; trends in covalence; metal-metal bonding. High coordination numbers. π bonding effects with ligands. Comparative survey of the chemistry of transition metal groups, e.g. titanium, zirconium and hafnium; chromium, molybdenum and tungsten, nickel, palladium and platinum.

Lanthanides & Actinides

Lanthanides: Occurrence of the elements; electronic properties: the nature of *f*-electrons; periodicity in the *f*-block. Extraction and separation. Properties of the metals. The predominance of the 3+ oxidation state. Structural chemistry of the lanthanide compounds. Aqueous chemistry, complex formation, nature of ligands, redox chemistry. Examination of binary halides, hydrides, oxides and borides: structures and electronic properties. Organometallic chemistry. Comparisons/contrasts with transition metals. Actinides: Occurrence and properties of the metals. Periodicity and general chemistry of the actinides including comparisons with lanthanides and transition series: oxidation states; aqueous chemistry; coordination stereochemistry. Focus on uranium chemistry: halides, hydrides, oxides, aqueous chemistry (especially of the uranyl ion), organometallic chemistry.

Coordination Chemistry

Thermodynamics and kinetics of complex formation: monodentate vs polydentate ligands, including acyclic and macrocyclic examples. Isomerism. Thermodynamics of complex formation: stability constants. Factors affecting the magnitude of stability constants – Irving Williams series, chelate effect, class a and class b classification, requirements of ligands. Macrocyclic Ligand Complexes: biological importance, macrocyclic effect. Macrocyclic ligand syntheses – template and non-template syntheses. Template effect: thermodynamic and kinetic contributions. Occurrence of common geometries: the role of metal electronic configuration and ligand in determining the stereochemistry in d^6 , d^{10} ions.

Bonding in Molecules

The orbital approximation, the LCAO approach. The use of symmetry in polyatomic molecules MO treatment of AH_2 (linear and bent), AH_3 (planar and pyramidal), AH_4 (T_d). Walsh diagrams: The shapes of AH_2 molecules, the bonding and shapes of H_3^+ and H_3^- : 3-centre-2-electron and 3-centre-4-electron bonds. Photoelectron spectroscopy and "experimental" MO diagrams, spectra of AH_n molecules. AB_2 molecules from CO_2 to XeF_2 , 12-electron main group octahedral systems: SF_6 as an example. 8-electron main group octahedral systems: $[C(AuPR_3)_6]^{2+}$ as a relative of CH_6^{2+} . Octahedral transition metal systems, σ -bonding, comparison with electrostatic model. MO filling in octahedral complexes: σ -interactions and factors that affect the magnitude of Δ . Molecular orbitals for 4-coordinate geometries: ML_4 (T_d and D_{4h}). First- and second-order Jahn-Teller distortions.

Organometallic Chemistry

General principles: valence electron count, formal oxidation state, number of *d*-electrons. The 18- and 16-electron rules: applications and exceptions. Classification of reactions: addition, dissociation, ligand substitution, migratory insertion, extrusion, oxidative addition, reductive elimination and attack on coordinated ligands. Synthesis, bonding and selected reactions: Transition metal alkyl, alkylidene (carbene), alkylidyne (carbyne) and carbonyl complexes. Hydride, dinitrogen and dihydrogen complexes. Alkene, alkyne and allyl complexes. Cyclopentadienyl, arene and other C_nH_n ($n = 4 - 8$) sandwich and half-sandwich complexes. Synergic bonding and π -complexes: CO as a ligand, alkene complexes, bonding in ferrocene.

Structures and Electronic properties of solids

Diffraction methods Distinction between lattices and structures. Unit cells and Bravais lattices. Fractional coordinates. Miller indices (*hkl*) and $\{hkl\}$. Calculation of d_{hkl} . Derivation of Bragg's Law. Indexing powder diffraction patterns. X-ray powder diffraction: techniques and uses. Consideration of the peak intensity: the structure factor; systematic absences. Use of powder diffraction for following solid state reactions.

Electronic properties of solids

Models of electronic structure: introduction to energy bands in ionic, covalent and metallic solids. Band gaps and their importance in the properties of solids. Free Electron and Tight Binding models (treated somewhat mathematically). Simple Tight Binding pictures for elements such as: Li, Be, transition metals, diamond and Si, solid I₂. Comparison with the molecular picture. Extension of band model to simple ionic compounds: e.g. NaCl and CaO; transition metal oxides: TiO, ReO₃, TiO₂ and VO₂, and sulfides: ZrS₂, NbS₂, MoS₂. Trends in the properties of solids and how they relate to the general chemistry of the transition metals in particular. Brief description of Spectroscopic techniques for studying band structure. Mott-Hubbard insulators and breakdown of the band model. Chemical trends in the Mott-Hubbard transition – competition between bandwidth and interelectron repulsion. Low-dimensional metals and the Peierls distortion with examples – electronically-driven structural distortions. Intrinsic and extrinsic semiconductors; the effect of doping level on the properties.

Structures of solids

Review of important structure types; relationship between crystal structure and electronic structure – electronic structure-directing effects and comparison with molecular systems.

Inorganic NMR

Multinuclear NMR. Review of the fundamentals: chemical shielding (diamagnetic & paramagnetic shielding terms) and scalar spin-spin coupling (multiplets, sequential stick diagrams, coupling constant values, satellites). Structures from NMR data (e.g. ¹⁹F NMR of main group fluorides). Quadrupolar Nuclei. Introduction to NMR in the solid state. Dynamical processes and NMR: (a range of examples including trigonal bipyramidal molecules and organometallic systems).

Non-Metal Chemistry

Survey of group trends. Electronegativity, size and polarisability: implications for "ionic" compounds formed with metals. Covalent bonds: trends in bond strength; formation of multiple bonds; hypervalence. Bonding models for hypervalent compounds. Catenation and polymerisation. Catenated and multiple bonds with Si, P, and S. Polymeric structures formed by Si-O, P-N and S-N compounds. Boranes: structural classification and Wade's rules; aspects of preparation and reactivity. Donor/acceptor properties. Major trends in Lewis acid/base chemistry. HSAB classification. Ligand properties. High oxidation states. Group trends: the "Alternation effect". Formation of polycations. Aspects of xenon chemistry.

ORGANIC CHEMISTRY

The course is designed to develop the concepts of organic chemistry introduced in the first year; to show some of the key experimental evidence which supports these concepts; to apply these data and concepts to chemical problem solving; and to demonstrate that the subject is still evolving and that it has a key role to play in modern technological developments in diverse fields, ranging from chemical synthesis to biological science. Questions on the Part IA Examination will be based upon topics covered by both the first and second year lecture courses and in the practical courses.

Topics to be covered are:

Organic Synthesis I

A logical approach to synthesis with a focus on applying concepts from the carbonyl chemistry course. Review of reactions from the 1st year. Retrosynthesis, disconnections, and synthons. Order of events guided by functional group compatibility and selectivity principles; protecting and blocking groups. Carbon-carbon bond formation and functional group interconversion both separately and in combination. Synthesis of mono- and 1,n-difunctionalised molecules.

Organic Spectroscopy

IR spectroscopy. Vibrational transitions as a source of bonding information; characteristic group frequencies; interpretation of spectra. NMR Spectroscopy. Proton NMR spectroscopy. Chemical shifts: factors that influence proton chemical shifts. Spin-spin coupling: proton coupling patterns and resonance multiplicities, coupling to chemically equivalent spins, weak and strong coupling, chemical and magnetic equivalence. Proton spin coupling constants and chemical structure: geminal, vicinal and long-range couplings. Chirality and NMR, chiral solvating agents. Carbon NMR spectroscopy: interpreting carbon chemical shifts. Example proton and carbon spectra.

Mass Spectrometry: Introduction to Mass Spectrometry as an analytical technique in chemical and biochemical analysis. Basic principles, instrumentation and applications; relationship between molecular weight and chemical composition; processes of ion formation and interpretation of a radical cation mass spectrum. Determining location of charge and predicting fragmentation patterns based on product ion stability. Interpreting fragmentation patterns for saturated and unsaturated aliphatic, aromatic and simple heteroatom compounds. Examples. Application of the above spectroscopic techniques to the solution of structural problems.

Aromatic and Heterocyclic Chemistry

What is Aromaticity? Resonance energy; molecular π -orbitals of benzene and cyclobutadiene; Huckel $4n + 2$ rule; aromatic ring currents; examples of non-benzenoid aromatic and anti-aromatic compounds; synthesis and characterisation of cyclobutadiene; homoaromaticity. *Pyrrole, thiophene and furan*. Dipole moments; electrophilic aromatic substitution; deprotonation; comparison with pyridine; indole: reactivity with electrophiles; synthesis of pyrrole, thiophene and furan; Fischer indole synthesis. *Pyridine and related compounds*. Reactivity towards electrophiles; activation via N-oxide formation; pyridones; nucleophilic substitution; reduction of pyridinium salts; reactivity of methyl pyridines; synthesis of pyridine derivatives. *Benzene, benzyne and nano-graphenes*. Synthesis of the benzene ring: from acetophenone and from cyclopentadienones. Benzyne: synthesis and reactivity of ortho and para-benzyne.

Organic Synthesis Problem Solving

Problem-solving lectures relating to the 1st year course 'Introduction to Organic Synthesis'.

Conformational Analysis and Ring Chemistry

This course examines the factors that control conformation and reactivity in organic molecules, covering stereoelectronic, steric, and electronic effects. The conformation of acyclic and cyclic molecules is discussed, and the concept of strain. Using this understanding, we analyze how conformational and stereoelectronic effects influence the reactivity and selectivity of reactions of cyclic and acyclic organic molecules, focusing particularly on reactions of C=O and C=C functional groups. The course also covers methods for ring synthesis.

Physical Organic Chemistry

Structure and reactivity in organic chemical reactions. Kinetics, thermodynamics, transition states, intermediates. Rate equations and kinetics, kinetic isotope effects, solvent effects, linear free energy relationships, elucidating reaction mechanism. Catalysis of organic reactions.

Rearrangements and Reactive Intermediates

Structure, reactivity and rearrangement reactions of carbocations and carbanions. Neutral reactive intermediates including carbenes, nitrenes and radicals, structure, synthesis, and reactivity. Rearrangements, including to electron deficient oxygen and nitrogen. General reactions of radicals.

Heteroatoms in Organic Synthesis

The chemistry of organic compounds containing boron, silicon, phosphorus and sulfur including their use in the construction of complex organic molecules and mechanistic and stereochemical aspects. Brief extension to other elements e.g. Se

Organic Synthesis II

Regioselectivity, chemoselectivity, and stereoselectivity. Oxidation, reduction, selective alkene oxidation and reduction. Site blocking and protecting groups and their utility; selective carbohydrate manipulations as exemplars. Principles of retrosynthetic analysis and worked examples.

Organic Chemistry of Biomolecules

Chemical synthesis of nucleic acids: solid-phase phosphoramidite DNA synthesis, synthesis of building blocks, synthesis of modifications that are commonly introduced into synthetic DNA for biological applications. Microarray DNA synthesis for the synthesis of entire genomes. Solid-phase RNA synthesis: protecting group strategies. Large scale oligonucleotide synthesis for diagnostic and therapeutic applications: backbone-modified DNA and DNA analogues. Applications: antisense oligonucleotides, exon skipping oligonucleotides, siRNA. Enzyme kinetics; Michaelis-Menten model to determine steady state parameters, the use of kinetic parameters to understand enzyme mechanisms, multi-substrate reactions, reaction intermediates, other tools to investigate enzyme mechanisms, e.g. isotopes. Enzyme inhibition; pharmaceutical motivation, classes of enzyme inhibitor and mechanism of action, effects of inhibitors on enzyme kinetics and use of kinetic data to identify potent inhibitors. Concepts will be illustrated throughout with a range of case studies, highlighting the contribution of enzyme structure to function.

PHYSICAL CHEMISTRY

The Examination will consist of questions relating to the lecture courses given in the second year, together with all the first year material:

Quantum Theory

Operators: basic notions and properties; linear operators, eigenvalue equations; degeneracy; expansion in a complete set. Postulates of QM and deductions there from; expectation values and the meaning of measurement in QM; the time-dependent Schrödinger equation; stationary states and the time-independent Schrödinger equation. Commutators: definition, evaluation, properties. Physical significance of commutators; complementary observables, simultaneous dispersion-free measurement and the uncertainty principle (weak and strong). Bra-ket notation; definition and properties of Hermitian operators. One-body problems: the free particle (wave-particle duality; commutation and measurement; peculiarities). The particle in a d -dimensional box (quantization via boundary conditions; zero-point energy; the correspondence principle; degeneracy). Rotational motion: angular momentum; angular momentum operators, commutation relations and their significance; particle on a ring; particle on a sphere and eigenfunctions of L^2 ; the rigid rotor. The H-atom. The simple harmonic oscillator: wavefunctions, energy levels and properties. The variational principle. The existence of electron spin. Spin functions for a single electron. Spin functions for two electrons; singlet and triplet states. The Pauli principle, antisymmetric wavefunctions, Slater determinants. Introduction to atomic spectra. He atom: variational calculation of ground state $1s^2$; orbital approximation. $1s^1 2s^1$ configuration; singlets and triplets. Atomic states: LS coupling; treatment of spin-orbit coupling. The Zeeman effect in atoms (magnetic fields), g -factors. The Stark effect (electric fields).

Liquids and Solutions

Ideal solutions: entropy of mixing, zero enthalpy of mixing, Raoult's law, ideal solubility, depression of freezing point, osmotic pressure. Regular solutions: the effects of non-zero interactions, non-zero enthalpy of mixing, Henry's law, vapour pressure, phase separation. Polymer solutions: polymer dimensions in solution (theta and good solvents, radius of gyration), Flory-Huggins model, entropy and enthalpy of mixing, osmotic pressure. Electrolyte solutions: activity coefficients of ions in solution, Debye-Hückel (D-H) theory, Debye-length, ionic strength, application of D-H to solubility and dissociation. Surface of liquids and solutions: surface tension, Laplace's law, the Kelvin equation, the Gibbs dividing surface and the Gibbs adsorption equation.

Statistical Mechanics.

Systems of independent particles. Aims of statistical mechanics. Distribution of molecules over molecular quantum states: microstates, configurations and the weight of a configuration. The most probable configuration and derivation of Boltzmann distribution for independent molecules. Definition and significance of molecular partition function, q . Factorization of q into translational, rotational etc. components; calculation of q_{trans} and q_{elec} . Determination of internal energy, E , and specific heat, C_v , from q ; application to monatomic gas.

Limitations of Maxwell-Boltzmann statistics.

Mean values of observables; applications to bulk magnetization, paramagnetic susceptibility and derivation of Curie Law. Interacting particles. Concept of an ensemble. The canonical ensemble and the canonical distribution. The canonical partition function, Q , its physical significance and determination of internal energy from Q . Entropy in statistical mechanics, and its relation to Q . Determination of enthalpy, Helmholtz free energy, Gibbs free energy and chemical potential from Q .

Independent particles II. Reduction of Q for special case of independent molecules: the relation of Q to q for (i) independent distinguishable and (ii) independent indistinguishable particles. Summary of thermodynamic functions for independent particles expressed in terms of q ; separability of thermodynamic functions into contributions from different modes.

Calculation of molecular partition function and selected applications. q_{trans} , q_{elec} and the statistical thermodynamics of a monatomic gas; molar entropies and the Sackur-Tetrode equation. Rotational contribution to q for heteronuclear molecules; the high temperature limit and characteristic rotational temperature, Θ_{rot} . Rotational contributions to S and C_V . The effects of nuclear spin: symmetry numbers and q_{rot} for homonuclear diatomics and other symmetrical molecules. Applications to rotational spectroscopy.

Vibrational partition functions, q_{vib} , for diatomic molecules and polyatomics. Chemical equilibrium. Statistical mechanical result for the equilibrium constant K of a general chemical reaction. Calculating the equilibrium constant and selected examples: dissociation reactions, isotope exchange reactions, thermal ionization equilibria.

Transition state theory – the derivations. Concept of the transition state and the reaction coordinate. Transition state theory in terms of separable motion. The quasi equilibrium hypothesis. Derivation of the explicit expression for $k(T)$ in terms of partition functions.

Atomic and Molecular Spectroscopy

General aspects of Spectroscopy: Energy levels of molecules; Born-Oppenheimer separation; the photon; interaction of radiation with matter; absorption; emission; transition moments; Einstein Coefficients, selection rules. Atomic Spectroscopy: Revision of H-atom; wavefunctions; atomic orbitals; selection rules; Grotrian diagrams; Many electron atoms; Alkali metal (and pseudo-1-electron) atoms; Penetration and shielding; The quantum defect; Selection rules and spectra; Determination of ionisation energies; Russell Saunders coupling; Atomic term symbols; The Helium atom; Singlet and triplet states; configurations, terms and levels; Hund's rules; electron correlation; Effects of external fields – Zeeman interactions; spin-orbit coupling; Molecular Spectroscopy (General) Molecular Rotational Spectroscopy; Rotors and their symmetry; revision of rigid rotor; moments of inertia; isotope effects; centrifugal distortion; selection rules; Stark effect; Complications of nuclear spin statistics. Molecular Vibrational Spectroscopy; Revision of harmonic oscillator and selection rules; Anharmonicity; normal vs local modes; symmetry considerations; vibration rotation spectroscopy. Molecular electronic spectroscopy; Potential energy curves/surfaces; Description of diatomic (linear) molecules; Classification of electronic states; Electronic selection rules; Franck-Condon Principle;

Band heads; Dissociation energies; Birge-Sponer extrapolation; Predissociation. Raman and Rayleigh Scattering; rotational and vibrational transitions; selection rules; mutual exclusion in centrosymmetric molecules; Raman vs. IR

Valence

Born-Oppenheimer Approximation. Bonding in H_2^+ (LCAO approximation). Many-electrons - the Orbital Approximation. Deficiencies of the orbital approximation. binding of He_2 , splitting of degenerate configurations, dissociation of H_2 . Application of Variation Principle to find LCAOs - the Secular Equations. Simplification due to symmetry and electronegativity differences. Examination of energy levels of diatomic molecules. Splitting into terms (O_2) and levels (NO). Electronic and Photoelectron Spectra of Molecules. Franck-Condon Effects. Selection Rules. Examination of vibrational and rotational structure. Band heads. Birge-Sponer extrapolation. Predissociation. Radiationless transitions. Polyatomics - Hückel simplifications of the secular equations. Use of symmetry. Properties from the wavefunction - bond-order, electron density, dipole moments, spectral properties, organic reactivity.

Rate Processes

Simple collision theory. Collision frequency and collision cross section. Reaction cross section and steric factor. Potential energy surfaces. Classical motion over PES's. Link between reaction cross sections and rate constants. Transition state theory. Comparison with simple collision theory. Calculation of rate constants. Estimation of pre-exponential factors. Temperature dependence of rate constants. Kinetic isotope effects. Quantum mechanical tunnelling. Non-Arrhenius behaviour. Thermodynamic formulation of TST. Liquid-phase kinetics. Comparison of liquid-phase and gas-phase reactions. Encounter pairs, cage effect, and geminate recombination. Wavelength and viscosity dependence of photodissociation, radical scavenging, kinetics of I_2 photodissociation, cluster reactions, spin effects. Diffusion controlled reactions. Smoluchowski theory. Stokes-Einstein relation. Effects of solvent viscosity and temperature, reactions between ions, spin effects. Activation controlled reactions. Gibbs energy of reaction, effect of electrostatic interactions, influence of solvent permittivity, entropy and volume of activation, electrostriction, influence of pressure and ionic strength. Electron transfer reactions. Marcus theory. Gibbs energy and reorganization energy. Marcus inverted region. Homogeneous and heterogeneous electron transfers. Interfacial kinetics. Electric potential and its effect on interfacial reaction rates. Butler-Volmer equation. Transfer coefficients. Overpotential. Tafel relations. Voltammetry.

GENERAL CHEMISTRY

Symmetry I - Molecular symmetry, group theory, and chemical bonding

Symmetry operations and symmetry elements. Symmetry classification of molecules – point groups. Symmetry and physical properties: Polarity, Chirality. Combining symmetry operations: 'group multiplication' Mathematical definition of a group. Review of Matrices. Definitions, matrix algebra, inverse matrices and determinants. Transformation matrices. Matrix representations of groups. Properties of matrix representations. Similarity transforms. Characters of representations. Reduction of representations. Irreducible representations and symmetry species. Character tables.

Orthogonality relationships in group theory. Using the LOT to determine the irreps spanned by a basis. Symmetry adapted linear combinations. Bonding in diatomics. Bonding in polyatomics - constructing molecular orbitals from SALCs. The variation principle. Solving the secular equations. Matrix formulation of a set of linear equations. Solving for the orbital energies and expansion coefficients. Summary of the steps involved in constructing molecular orbitals. Hückel molecular orbital theory

Symmetry II

Character tables and their meaning: C_{2v} , C_{3v} and T_d revisited. The reduction formula and its application to SALCs in CH_4 . Projection operators and the SALCs of NH_3 . p orbitals in C_6H_6 . Another look at the origins of degeneracy in molecular systems. Ligand field splitting of d levels. Tables of descent in symmetry. Jahn-Teller theorem. 2nd order Jahn Teller effect. Direct products - symmetry of many electron states. Selection rules in electronic spectroscopy: octahedral versus tetrahedral systems. IR and Raman selection rules. Overtones and combination bands. Vibronic transitions.

Vibrational spectroscopy: stretching vibrations of CF_4 , SF_4 and XeF_4 . The mutual exclusion rule. Complete 3N basis sets and the vibrations of NH_3 . The vibrations of C_{60} .

Maths for Chemists

Ordinary differential equations: Series solution, Frobenius method. Special functions: Bessel functions, Legendre, Laguerre, Hermite polynomials. Partial differential equations, separation of variables. The Schrödinger equation; particles in rectangular and circular boxes, the H atom. The diffusion equation. Numerical methods. Finite difference and finite element approaches. Explicit and implicit methods. COMSOL. Fourier series and Fourier transforms. FT infra-red spectroscopy and the Michelson interferometer. The Fellgett advantage.

Introduction to NMR

Introduction to magnetic resonance, including the background physics of magnetic resonance, the origin of shielding, multiplet structures, exchange phenomena and an overview of experimental methods.

APPENDIX E2

Syllabus for Part IB 2017-18

INORGANIC CHEMISTRY

General Papers

The examination papers in Part 1B will include all the topics considered in the core courses in Inorganic Chemistry delivered in the 1st, 2nd and 3rd years of the course. Candidates should also be familiar with the material covered in the practical course. The style of questions will be similar to questions used recently in Part 1B examination papers. For each paper, candidates will be required to answer 4 questions taken from a choice of 6.

Core Lecture Courses

Inorganic Spectroscopy and Magnetism

Electronic spectra of metal complexes

The different types of electronic transition. Characteristics of absorption bands: transition energy, intensity and band width. Selection rules: allowed and forbidden transitions. Ligand field (d-d) spectra: trends in the orbital splitting parameter (spectrochemical series); ligand field terms; Orgel diagrams and spectral assignment. The Racah parameter B and the nephelauxetic effect. Tanabe-Sugano diagrams. Charge-transfer (CT) spectra: (a) ligand-to-metal CT transitions in tetrahalide, tetroxo and hexahalide complexes; the redox connection; (b) metal-to-ligand CT transitions in octahedral ML_6 . Magnetic properties of metal complexes. Definition of magnetic quantities. Curie paramagnetism: the Curie law and the effective Magnetic moment; the spin-only formula. Lanthanide compounds: the Hund-Landé formula and its scope. Compounds of the transition elements: (a) quenching of the orbital magnetic moment; scope of the spin-only

formula; (b) residual orbital angular momentum and deviations from the spin-only magnetic moment.

Bioinorganic Chemistry

Introduction to bioinorganic chemistry: Cellular compartmentalisation. The roles of the Group 1 and Group 2 ions Na^+ , K^+ , Mg^{2+} , Ca^{2+} . Electrolytes, ion channels, signalling. Properties of complexes between metals and proteins – how one influences the chemistry of other. Haem proteins and enzymes. Cytochrome c and electron transfer. The biological chemistry of oxygen: haemoglobin, peroxidases, catalases, and monooxygenases. Oxygen binding. Reactive oxygen species and oxidative damage. Cobalt and radical chemistry. The cobalamin co-factor. Cobalt oxidation states and their stabilization and chemistry. Mutases and methyl transferases. The bioinorganic chemistry of proteins and enzymes containing M–S and M–O clusters. Iron-sulphur clusters in electron transfer, nitrogen fixation, and hydrogenases. Manganese-oxo chemistry and the oxygen-evolving centre.

Solids state chemistry

Overview of the material covered in the 2nd year: the basic electronic properties of stoichiometric solids and the effect of introducing defects. Defects and ion transport Defects in solids: thermodynamic and structural aspects. Non-stoichiometry and electronic consequences. Applications to metal oxides and other inorganic solids. Outline of experimental techniques used to study defects – diffraction, EXAFS, solid state NMR, electron microscopy (without detail on the techniques: focus is on information they provide) Ionic mobility in the solid state: factors affecting ionic

conductivity in various types of solid. Applications in technology. *Structures, Reactivity and Synthesis*
Chemical aspects of solid state chemistry: general synthetic methods. Low temperature reactivity of solids illustrated by intercalation chemistry (e.g. graphite, layered oxides and sulfides, C_{60}). Application of redox processes in solid state systems, for example in Li-ion secondary batteries).

Modern Main Group Chemistry

"Traditional" conceptions of chemical behaviour in main group and transition metal systems. Modern interpretations of electronic structure and bonding in main group compounds: Multiple bonding; Carbenes and their heavier analogues; Stable main group radicals. Novel modes of reactivity of main group systems: Frustrated Lewis Pairs; Small molecule activation using singlet carbenes and heavier group 14 carbene analogues; Reactivity of group 14 alkyne analogues. Catalysis using main group systems: Catalysis using Frustrated Lewis Pairs; "Redox" based catalysis using p-block elements - formal oxidative-additions, reductive eliminations; Catalysis using s-block complexes.

Inorganic Reaction Mechanisms

Ligand substitution reactions in square planar metal complexes (including the *trans* effect) and in octahedral metal complexes: *D*, *A*, σ , π mechanisms, anation and solvolysis reactions. Electron transfer reactions: inner sphere and outer sphere electron transfer. Introduction to Marcus theory: interplay between donor-acceptor overlap, thermodynamic driving force and reorganisation energy. Two-electron transfer and non-complementary reactions.

Organometallic Reaction Mechanisms and Catalysis

Oxidative addition and reductive elimination. Mechanistic evidence including: dihydrogen compounds, agostic bonding. Brief mention of C-H bond activation. α - and β -hydrogen transfer; migratory insertion reactions. Introduction to homogeneous catalysis and a consideration of various important and representative systems. Including the isomerisation and hydrogenation of olefins; hydroformylation; Monsanto acetic acid process; Wacker process. Brief introduction to olefin polymerization by metallocene or similar systems.

ORGANIC CHEMISTRY

The course is designed to develop the concepts of organic chemistry introduced in the first and second years; to show some of the key experimental evidence which supports these concepts; to apply these data and concepts to chemical problem solving. The core course will provide a comprehensive treatment of more elaborate aspects organic chemistry, with an emphasis on synthesis and biological chemistry.

General Papers

The examination papers will be based upon topics covered by the third year organic chemistry core lecture courses below, and will also include topics covered in the first and second year organic chemistry lecture courses and possibly from the practical laboratory course. For each paper, candidates will be required to answer 4 questions taken from a choice of 6.

Advanced Organic Spectroscopy

NMR Spectroscopy: Assigning proton NMR spectra: spin decoupling and 2D NMR, 1H COSY; Assigning carbon NMR spectra: using carbon-proton spin coupling; spectrum editing (DEPT), 2D NMR- one-bond (HSQC) and multiple-bond (HMBC) 1H - ^{13}C correlations. Defining molecular stereochemistry using the nuclear Overhauser effect (NOE).

Mass Spectrometry: Principles of hard and soft ionisation methods. Qualitative mass spectrometry analysis: Chemical formulae calculation; nitrogen rule; high resolution analysis of isotopes signatures. Tandem mass spectrometry: Post-source fragmentation processes; molecular and structural identification. Selected applications and examples.

Organic Synthesis III

This course will cover the strategies and tactics adopted for the controlled and efficient synthesis of organic molecules. It will address aspects of the what, the why and the how of complex molecule synthesis in both academic and industrial settings. A large focus will be on stereocontrol and in particular we will look at the approaches to synthesising compounds as single enantiomers through, for example, classical resolution methods, chiral auxiliary approaches and enantioselective catalytic transformations. The course will cover the discovery and development of various methodologies for effecting stereoselective carbon-carbon, and carbon-heteroatom bond formation, as well as their strategic incorporation as key steps in applied total synthesis. Aspects of retrosynthesis, protecting group chemistry and mechanism will also be covered.

Pericyclic Reactions

Hückel molecular orbitals; conservation of orbital symmetry; frontier molecular orbital theory; Woodward-Hoffmann rules. Cycloaddition Reactions. Diels-Alder reaction: endo-preference, Lewis acid catalysis; [2+2] cycloaddition of ketenes, dipolar cycloaddition, cheletropic reactions; photochemical reactions. Electrocyclic Reactions. ring opening of cyclobutenes, ring closure of hexatrienes, cyclopropyl halide solvolysis; charged systems. Sigmatropic Rearrangements. Dewar method compared to FMO approach, [1,n] H-atom shifts, Cope and Claisen variants; ene reactions. Applications of pericyclic reactions in synthesis.

Transition Metal Catalysis

Introduction to organometallic chemistry of transition metals. Organopalladium chemistry: Suzuki coupling, Heck coupling and related cross couplings. Copper-catalysed cross-coupling reactions. Alkene metathesis.

Curly Arrows of Biology

An Introduction to the Chemistry of Metabolism / Bioenergy. Primary and secondary metabolisms. Glycolysis and the citric acid cycle, Amino acid metabolism and the nitrogen cycle.

Radical Reactions

Occurrence and structure of free radicals; definitions; characteristic reactions. Free radical substitution reactions; reactivity and regioselectivity. Kinetics and mechanism: addition to multiple bonds; selectivity and chain reactions. Kinetics and mechanism: rearrangement chemistry; kinetic and thermodynamic control. Radicals in synthesis: functional group chemistry; tandem, cascade processes in complexity generation and application for natural product synthesis.

Revision – Molecular Structure and Reactivity

This course provides revision for essential knowledge of the organic chemistry course taken over the three years of the undergraduate course, considered under two broad headings, molecular structure and molecular reactivity. Each of the reaction types will be illustrated with examples showing their application to synthetic organic chemistry.

PHYSICAL CHEMISTRY

General Papers

Candidates will be required to answer 4 questions out of 6. The style of questions on the two papers will be similar to that of the 2012 - 2017 papers and of Part IB papers in the years up to 2011. Students will be informed about the distribution of topics between the two papers when this has been decided by the examiners

Magnetic Resonance

A revision of the principles of Nuclear Magnetic Resonance (NMR): magnetic moment, space quantization, the resonance condition, the vector model, populations and bulk magnetization, selection rules, the origin of shielding, diamagnetic and paramagnetic shielding, neighbouring group anisotropy, ring current effects, electronic effects, intermolecular interactions. *J*-coupling, multiplet splitting, coupling to spins with *I* greater than ½, discussion of Fermi contact interaction, an introduction to dipolar coupling. Magnetic resonance spectroscopy of two coupled spin-½ particles: a quantum mechanical treatment. The rotating frame, linear and circularly polarized fields, NMR as a coherence phenomenon; experimental methods: continuous wave and pulsed NMR, Free Induction Decay (FID) and Fourier Transformation for simple FIDs. Spin relaxation: spin-lattice and spin-spin relaxation, the rotational correlation time and the spectral density function, spin relaxation and the vector model, measurement of relaxation times, the inversion recovery experiment, the spin-echo experiment.

Soft Condensed Matter

Interaction between surfaces: dispersion forces; Van der Waals attraction; Hamaker constant; double layer repulsion; measurements of forces. Surfactants: Gibbs adsorption equation; thermodynamics of micelle formation; geometric model for micelle shapes; interface curvature, wetting, capillarity. Colloidal phase behaviour; hard sphere crystallization; fluid-fluid phase separation; entropy driven phase transitions; polymers; elastic properties of polymers; depletion interaction; polymer brushes; Brownian motion; Langevin equation; Einstein-Smoluchowski equation; velocity autocorrelation function; diffusion; mean square displacement; Timescales.

Photophysics and photochemistry

Electronic transitions of polyatomic molecules. Beer-Lambert law, selection rules and absorption strength, vibronic transitions, radiative lifetime, Franck-Condon Principle. Fates of excited states: Jablonski diagram, fluorescence and phosphorescence, vibrational relaxation, intersystem crossing and internal conversion, intramolecular vibrational redistribution, dissociation / predissociation.

Lifetimes of excited states: quantum yield, photochemical kinetics, fluorescence / phosphorescence quenching, Stern-Volmer plot. Intramolecular energy transfer: application of Fermi's Golden Rule, rates of intersystem crossing (El-Sayed rule), and internal conversion, energy-gap law, isotope effects, conical intersections. Delayed fluorescence. Intermolecular energy transfer, Electronic energy transfer, long-range (dipolar, FRET) and short-range (exchange) mechanisms, spin correlation rules. Triplet annihilation. Triplet sensitization and delayed fluorescence. Exciplex formation. Chemical reactivity of electronically excited molecules; isomerisation, acidity, redox, orbital character etc. The role of intersections in returning to the ground state. Geminate recombination, escape probability and recombination timescale. Photoionisation and photoelectron spectroscopy. Ion chemistry, ZEKE. Photodissociation, and predissociation, ozone destruction. Ultrafast photochemistry and photophysics. Pulsed lasers. Pump-probe spectroscopy. Generation and fate of nuclear wavepackets. Chemistry in real time.

Physical Principles of Solids

Electrons in solids: free electron gas in differing dimensionality, DOS and Fermi energy, electronic heat capacity, Pauli paramagnetism, electrical conductivity, Wiedemann-Franz law, deficiencies in free electron model. Phonons in solids: Einstein theory of heat capacity, deficiencies, Debye model, optical and acoustic phonons, thermal conductivity in insulators. Defects and disorder in solids: Classification of defects, thermal population of point defects, Schottky heat capacity, theory of the order-disorder transition in alloys. Surfaces: structure of surfaces, types of adsorption, Langmuir and BET isotherms, dissociative and competitive adsorption, heterogeneous catalysis, heat of adsorption.

Options Paper

The option courses are designed to develop advanced concepts and methods in chemistry to cover some areas of contemporary interest, for example in technology and in the environment. The options are dynamic, and will be updated annually to reflect modern developments. The courses are at M (Masters level), assume knowledge of the core material in the first three years of the course and build on it. The options examination will be three hours and students will be expected to answer three questions. Each of the 14 options offered will have one 1-hour question on the paper. Each option course comprises 8 lectures in Hilary Term and 1 problem class in Trinity term.

Advanced Chemical Biology

Peptide Chemistry. Peptide synthesis: Methods, strategy, factors compromising yields, including loss of stereochemistry, and analysis. Use of different types of protecting groups, coupling reagents (including use of protein-splicing and, in outline, enzymes) for solid and solution phase peptide synthesis. Comparison with nucleic acid synthesis, and, in outline, with biological peptide biosynthesis. Roles (in brief) and extent of post-translational modifications including enzyme catalysed peptide hydrolysis; importance of hydrolytic enzymes as pharmaceutical targets.

Preparation and applications of chemically modified biopolymers. Functional groups in proteins and nucleic acids. Synthesis of modified nucleic acids. Phosphoramidite reagents and post synthetic modifications. Phosphorothioates, dithioates, PNA and other DNA analogues. Applications of modified oligonucleotides, fluorescent probes – Taqman, Molecular Beacons, Forensic analysis of DNA.

Advanced Synthesis and Total Synthesis

This course builds from the core 3rd year lecture course Organic Synthesis III and will draw together many core synthesis topics. The course will illustrate advances in the total synthesis of major classes of natural products, selected pharmaceuticals, and other challenging molecules, with asides to cover important reactions, reagents, reactivity and strategy principles.

Contemporary Methods in Catalysis for Organic Synthesis

The lecture course will focus on new methods of catalysis, both organometallic and organocatalytic, applied to organic synthesis. Sustainability (Green), industrially relevant chemistry, enantioselective syntheses, mechanistic studies, and applications of key reactions will all be considered.

Functional Organic Polymers and Materials Chemistry

Dyes- Mauveine, chromophores, commercial dyes, synthesis of azo dyes and cyanines, direct dyes, reactive dyes for cellulose, fluorescence, chemiluminescence, photochromics, photoinduced electron-transfer. *Polymers and polymer synthesis*- Polymerisation reactions: condensation vs. addition, step-growth vs. chain-growth, DP, Mn, Mw, polydispersity index, Carothers equation, epoxy-resins, ring opening, stereochemistry, Ziegler Natta, metallocene catalysts, living polymerisation (anionic, cationic, ring opening metathesis) architecture, dendrimers.

Living Polymerisation and Conjugated Polymers

Living polymerisation will be considered in more detail, including living free-radical polymerisation (nitroxide-mediated polymerization, ATRP and RAFT). Approaches to the synthesis of conjugated polymers will also be discussed: using polyacetylene, polyphenylene vinylene, poly-para-phenylene and polythiophene as examples. *Liquid Crystals*- Classification: hermotropic / lyotropic, calamitic/isotropic, nematic / smectic/columnar; examples; molecular structural requirements; synthesis; techniques: polarised optical microscopy, differential scanning calorimetry; orientation: by electric fields, by rubbed surfaces, by surfactants; twisted nematic LCD; LC thermometers; LC polymers: main-chain e.g. Kevlar, side-chain *Organic Surface Chemistry*- Comparison of different techniques for preparing and analysing organic surface functions. *Organic Surface Chemistry*-Grafting to and grafting from approaches, polymer brushes, applications of organic surface chemistry. *Organic Semiconductors* Types of organic metals and semiconductors: charge-transfer salts, conjugated polymers, molecular crystals; polyacetylene and poly-para-phenylene: band structure, solitons and bipolarons, synthesis, precursor routes, substituted derivatives, conformation. *Organic Electronic Materials* Types of organic metals and semiconductors: charge-transfer salts, conjugated polymers, molecular crystals; band structure, solitons and bipolarons; electroluminescence: how an LED works; photovoltaic devices: the basic principles, dye-sensitised cells, polymer blend devices; controlling energy transfer and electron transfer.

Inorganic Molecular Spectroscopy

How various spectroscopic techniques are used to characterise inorganic systems. The complementary nature of all the techniques will be illustrated.

1. Electronic spectroscopy – The use of spectroscopic techniques to probe transition metal and lanthanide systems.
2. Vibrational spectroscopy – underpinned by the course “Symmetry II”, but going further and demonstrating the value of matrix isolation, the use of polarised light and time resolved studies to probe various systems.
3. Applications of NMR spectroscopy quantitative dynamics, 2D spectra.

An Introduction to the Liquid State

Classical statistical mechanics: classical partition function, phase space; pairwise additivity, second virial coefficient. Statistical mechanics of the liquid state: pair distribution function, osmotic compressibility, Ornstein-Zernike equation, structure factor. Light scattering: Rayleigh scattering (point scatterer), Rayleigh-Gans-Debye theory (larger particles), form factor, Guinier and Porod's laws, structure factor and link to statistical mechanics of liquids, partial structure factors, contrast variation, computer simulation of liquids.

Magnetic Resonance

Overview of how modern NMR experiments work. Conceptual and theoretical tools needed to understand something of the inner workings of some of the more important multi-pulse, multi-nuclear, multidimensional techniques used to probe the structures and dynamics of molecules.

Brief review of spin interactions in NMR. Zeeman interaction, chemical shift. *J*-coupling. Energy levels. Appearance of spectra.

Vector model. Magnetization. Rotating frame. Radiofrequency pulses. Free precession. T_1 and T_2 relaxation. Free induction decay. Spin echoes, echo modulation. Fourier transformation, lineshapes. Product operators for one spin. Product operators for two coupled spins. Spin echoes, homonuclear and heteronuclear. INEPT. Polarization transfer. Multiple quantum coherence. Double quantum filter, INADEQUATE. Two-dimensional NMR. COSY. NOESY. HSQC Review of quantum mechanics of spin angular momentum. Spin Hamiltonian. Density matrix. Time-dependent Schrödinger equation. Liouville-von Neumann equation. Pulses and delays. Density matrix description of two-spin systems. Product operator and density matrix calculations in *Mathematica*.

Molecular Reaction Dynamics

Thermally averaged collision properties: state resolved properties. Individual collision events: conservation of energy and angular momentum. Concept of a cross-section, and the relationship with opacity functions and impact parameter. Elastic and inelastic scattering. Total and differential cross sections: molecular beam scattering experiments. Types of energy transfer and their relationship to intermolecular forces. Potential energy surfaces. Origin of the PES, and examples. Inelastic and reactive scattering in terms of classical trajectories on surfaces. Reactive scattering: determining the angular distribution. Crossed molecular beam methods. Reaction mechanisms: stripping mechanism and the harpoon model; rebound reactions; complex formation. Stereochemistry and cones of acceptance. Reactive scattering: controlling reagents and characterizing products. Selection of reagent states and control molecular orientation. Laser based methods for reagent state selection. Spectroscopic based methods for detecting products. Infrared emission. Laser based methods. Reactive scattering: interpretation. Potential energy surfaces and attractive and repulsive energy release. Mass effects. Microscopic reversibility: use of reagent energies. Non-adiabatic processes. Probing the transition state. Half collisions and photodissociation dynamics. Femtochemistry. Photoelectron detachment spectroscopy. Applications of molecular reaction dynamics. Atomic and molecular lasers. Excimer lasers. Energy transfer and the CO₂ laser. Chemical lasers: CO laser. Chemistry in extreme environments: low and high energy collisions.

Natural Product Chemistry

This course builds upon previous courses on primary metabolism and synthesis and covers secondary metabolism and biosynthesis of polyketides, fatty acids, terpenes, and alkaloids. The total synthesis of members of these classes of natural product using a biomimetic approach will be discussed. The course will include: the link between primary and secondary metabolism; enzymes, cofactors and common metabolic pathways; the acetate hypothesis, fatty acid, prostaglandin and polyketide biosynthesis; mevalonic acid formation, terpene, squalene and steroid biosynthesis; amino acid biosynthesis; biosynthesis of alkaloids derived from lysine/ornithine and phenylalanine/tyrosine leading to the biosynthesis of complex polycyclic alkaloids such as morphine.

Organometallic Catalysts: From fundamentals to application

An advanced-level options course that will highlight contemporary organometallic chemistry ranging from fundamental aspects of synthesis, bonding and stoichiometric reactivity to the application of organometallic compounds in catalytic transformations. **Homogeneous olefin polymerisation.** Homogeneous vs. heterogeneous olefin polymerisation catalysts; examples of homogeneous transition metal catalysts focussing initially on metallocene-types; co-catalysts: types and mode of operation; polymerisation mechanism: initiation, propagation, termination; α -olefins and control of tacticity. Extension to constrained geometry and post-metallocene systems; brief examination of the use of isoelectronic and isolobal relationships in catalyst design.

Ring Opening Polymerizations to oxygenated polymers Homogeneous catalysts. Ring opening polymerization of lactones: thermodynamic factors and monomer scope; homogeneous catalysts; proposed mechanism for coordination-insertion polymerizations: initiation, propagation, termination, chain exchange reactions, rates of polymerizations, living polymerizations, control of tacticity (stereocontrol) in lactide ring-opening polymerizations – enantiomorphic site control vs. chain end control mechanisms.

Copolymerizations of Oxiranes: alternating copolymerizations: thermodynamics and monomer scope; metal catalysts for CO₂/epoxide copolymerizations – homogeneous and heterogeneous; catalyst nuclearity – mono- vs. dinuclear complexes; polymerization rates and mechanisms; exemplification of other alternating copolymerizations and block copolymerizations.

Sigma complexes, C-H activation and functionalization, Transition metal sigma complexes: structure and bonding. Fundamental issues of electronic structure and bonding in sigma complexes featuring H-H, C-H, Si-H and B-H bonds, relevance to oxidative addition chemistry, spectroscopic probes of the nature of the interaction with the metal.

C-H activation: Fundamentals and catalysis. C-H...M bonds in organometallic chemistry, a brief survey. C-H activation processes and their mechanisms. Use of C-H activation in synthesis. A discussion of representative catalytic processes using C-H activation, concentrating on mechanism.

Catalytic functionalisation of organic molecules by borane reagents. Direct borylation of C-H bonds in arenes and alkanes – mechanism, selectivity and synthetic utility.

Solid State Compounds in Technology

This builds on the core topics of solid state chemistry. The focus is on properties which confer technological value on solid state compounds (e.g. telecommunications, ICT, energy generation and storage).

For example:

1. Materials for Energy applications. Photovoltaics, Battery Materials, Transparent Conductors, Fuel Cell materials, Thermoelectric materials. How do we use our knowledge of Inorganic Chemistry to devise new compounds with particular properties?
2. Superconductivity. Classical and non-BCS superconductors. Factors affecting T_c . Recent developments; superconductors in action.

3. Magnetism. The collective magnetism in solids. The uses of magnetic materials in technology – magnetoresistance, multiferroic materials.

Structural Methods

The focus is on using various structural methods to probe materials in the solid state.

The complementarity of the various techniques will be emphasised and modern instrumentation will be described. 1. Diffraction techniques – X-ray, neutron and electron diffraction techniques for characterising long range order in extended and molecular solids. 2. Local Probes – EXAFS and X-ray absorption techniques for elucidating local structure. Pair distribution function analysis. X-ray photoelectron spectroscopy for probing electronic structure. NMR spectroscopy

Supramolecular and Medicinal Inorganic Chemistry

This course focuses on specific examples of uses of coordination compounds. 1. Supramolecular Chemistry: nature of the non-covalent interactions involved, illustrated with biological and synthetic examples of cation, anion and neutral guest recognition. Importance of preorganisation in host design. Extension of Template Effect to self-assembly, in particular metal-directed self-assembly of polymetallic architectures dictated by polydentate ligand design and stereochemical preference of metal. Catalysis within polymetallic cage frameworks. Anion coordination chemistry: biological importance; exploiting electrostatics, hydrogen bonding and Lewis acidity in anion receptor design illustrated with synthetic examples. Simultaneous cation and anion (ion-pair) binding by heteroditopic host systems for extraction, salt solubilisation and membrane transport applications. Case studies will be discussed which highlight the principles of transition metal optical and redox selective sensing of cation and anion analytes of biological and environmental importance.

2. Inorganic Medicinal Chemistry: how inorganic compounds and complexes can be used to treat and diagnose disease. For example: *Therapy*: platinum complexes in cancer chemotherapy, lithium carbonate, photodynamic therapy using porphyrin complexes), radiotherapy (choice of

radioisotopes. Ligand design), targeted radiotherapy (bifunctional chelating agents, antibody and peptide targeting, antibody directed prodrug therapies). *Diagnosis: Magnetic Resonance Imaging*: principles of contrast imaging, development of paramagnetic contrast agents; factors influencing contrast agent design; targeted and responsive MRI imaging agents. *Radioisotope Tomography* (Positron Emission Tomography and Single Photon Computer Tomography): blood pool and organ targeted imaging agents, application of bifunctional chelating agents to targeted imaging of receptors. *Luminescent imaging* (responsive probes for endogenous metal ions and anions): time-resolved imaging using lanthanide complexes, lanthanide based bioassay in drug discovery and diagnosis. *Multi-modal imaging* (MRI-PET, optical-PET and optical-MRI).

Theoretical Chemistry

Time-Dependent Quantum Mechanics

Review of time dependence in quantum mechanics; stationary and non-stationary states. Two level system in a rotating field (*e.g.*, ESR/NMR), Rabi oscillations. Perturbation theory: derivation of 1st order amplitudes, application to two-level systems and a continuous final spectrum (Fermi Golden rule rates). Applications of Fermi Golden rule rates to non-radiative processes in molecules, *e.g.* inter-system crossing and interconversion.

The interaction of light and matter 1: dipole approximation, derivation of the Einstein *A* and *B* coefficients. Derivation of the Einstein *A* and *B* coefficients. The interaction of light and matter 2: electric susceptibilities, oscillator strengths, and sum rules. Applications to radiative processes in molecules. Molecular electric susceptibilities, oscillator strengths, sum rules. *Statistical Mechanics – Mean-field theory*

Recap of statistical mechanics of non-interacting systems; consequences of interactions; role of theory, models and simulation. Introduction to mean-field theory and concept of molecular field. Ferromagnetic to paramagnetic transition; Ising model and its mean-field description.

Liquid-gas phase transition; classical partition functions; mean-field derivation of van der Waals equation of state.

Syllabus for Supplementary Subjects 2017-18

CHEMICAL CRYSTALLOGRAPHY

A supplementary course exploring the way in which crystallography is used to determine the atomic scale structure of chemical compounds covering crystal structure, symmetry, diffraction, reciprocal space, experiments, structure solutions, modelling and refinement.

1. Describing structure in real and reciprocal space. Understanding symmetry in diffraction patterns. Relationship between space group symmetry and diffraction patterns.
2. Space group symmetry notation and conventions. Lattices, symmetry operations and space groups.
3. Experimental considerations. Structure solutions methods. Parameterisation of structure. Obtaining the best fit of a model to data. Analysis and comparison of crystal structures.

QUANTUM CHEMISTRY

Time independent quantum mechanics

Operators and Commutators. Postulates of quantum mechanics; Linear operators; Hermitian operators; The unit operator; Commutators; The uncertainty principle; Constants of the motion.

The Harmonic Oscillator. Hamiltonian. Creation and annihilation operators; Eigenvalues and eigenstates; Matrix elements.

Angular Momentum. Angular momentum operators; Commutation relations; Raising and lowering operators; Eigenvalues and eigenstates; Coupling of angular momenta.

Matrix Formulation. Matrix representations; Hermitian matrices; Hamiltonian matrices; The variational method; Secular equations; Examples.

Group Theory

Group Theory in the abstract: definition of a group, examples, multiplication tables, abelian groups, conjugacy classes. Symmetry and Quantum Mechanics: 'true' symmetries of the molecular Hamiltonian. Molecular point groups, Matrix representations and similarity transformation, Reducible and Irreducible representations. Great and Little Orthogonality theorems, including results arising from them. Reduction of representations. Projection formula and SALCs. Direct Product representations, Full Rotation Groups and Russell-Saunders coupling. Symmetry Properties of integrals and application to selection rules. Application of group theory to electronic transitions and molecular vibrations.

Perturbation Theory and Time Dependent Quantum Mechanics

Stationary State Perturbation Theory, Non-degenerate and degenerate cases Applications, e.g. helium atom, Stark Effect, Time Dependence in Quantum Mechanics Equations of Motion, Time-independent Hamiltonians, Stationary and Non-stationary States; Time-dependent Hamiltonians

Molecular Electronic Structure

Introduction: Schrödinger equation, Born-

Oppenheimer, wavefunctions; The linear combination of atomic orbitals (LCAO) approach to molecular orbitals; Pauli principle, Slater determinants Formulation of the Hamiltonian for H_2^+ , H_2 . Matrix formulation and the secular determinants for a 1-electron system (H_2^+); Formulation of H_2 in the LCAO approach; Formulation of Hamiltonian for H_2 . ; Coulomb integrals, Triplet state of H_2 and the exchange integral, Expansion of the Coulomb and exchange integrals in an atomic basis, Self-consistent fields and Hartree-Fock theory, Hartree-Fock and Roothaan equations, Basis sets, Slaters vs Gaussians, Hierachy of basis sets, Beyond the HF approximation, Configuration interaction, Density functional theory, Semi-empirical methods, Hückel and Extended Hückel theory.

HETEROCYCLIC, AROMATIC AND PHARMACEUTICAL CHEMISTRY

Aromatic and heterocyclic chemistry is a very large and important branch of chemistry with which those students who enter the chemical industry are almost certainly going to intimately involved. Mechanistic rationales for the synthetic basis of aromatic chemistry that is practised today will be presented; more descriptive organic chemistry than would be reasonable in a main lecture course will be given. The relationship of reactions in aromatic chemistry to those of aliphatic chemistry will be emphasised. This is an area that provides a substantial part of the profits of the pharmaceutical industry, the syntheses of some of the past and potential blockbusters will be exemplified. The course will consist of 5 modules each having 5 lectures and 1 problems class. **Heterocyclic Synthesis I** - Objectives of the course. Range of 5 ring heterocycles: synthesis of 1,4-dicarbonyls in many different guises. Cheap natural sources. Fused systems and in particular indole. **Benzenoid Chemistry** - Comparison with heterocyclic reactions. Reactions of benzenoid systems: electrophilic aromatic substitution; early and late transition states; reactivity-selectivity in electrophilic and oxidative attack; electrophilic reactivity; ipso attack; kinetics versus thermodynamics; nucleophilic substitution; SNAr, SRN1, benzyne mechanisms; applications in synthesis. Aromatic rearrangements. Arene metallations and cross couplings.

Heterocyclic Synthesis II - Range of 6 ring heterocycles: 1,5-dicarbonyls by aldol, base-catalysed dehydration and Michael reactions. Synthesis of frameworks with more than one heteroelement towards purines and pyrimidines.

Reactions of Heterocycles - C=C versus C=O frameworks. Electrophilic attack easy on pyrroles and pyridines (at nitrogen). Dichotomies of electrophilic substitution mechanisms. Mannich and Vilsmeier in aromatic and aliphatic systems. Decarboxylation and other ipso substitutions. Easy attack by nucleophiles - sometimes by electrophilic catalysis. Ring opening reactions. Difference from benzene.

Pharmaceutical Chemistry

Key topics of medicinal chemistry will be covered and exemplified with the story of the discovery of ground-breaking medicines: introduction to drug discovery and medicinal chemistry; physicochemical properties of drugs; case study – *sildenafil* introduction to pharmacology; drug targets; receptors; transporters; case studies – *cimetidine* and *omeprazole* introduction to small molecule drug design; drug-protein interactions; structure-based drug discovery; case study – *crizotinib* introduction to

pharmacokinetics; half life, dose, volume of distribution and clearance; case studies – *amlodipine* and *azithromycin*, Introduction to drug safety; the central nervous system; drug-drug interactions; case studies – *ketoconazole*, *terfenadine*, *fexofenadine* and *maraviroc*

Problem Session – designing better drugs

APPENDIX F1

PRELIMS (First Year)	Term	Department / Faculty			College	Comments
		Lectures	Classes	Practicals	Tutorials	<i>Figures in this table are in hours unless otherwise stated.</i>
INORGANIC CHEMISTRY						Tutorials - 1 or 2 of c.90 minutes each <u>per week</u> - See NOTES
Atomic Structure and Periodic Trends	M	6				
Ionic Model and Structures of Solids	M	10				
Molecular Shapes, Symmetry and Molecular Orbital Theory	H	6				
Acids, Bases and Solution Equilibria	H	4				
Non-metal Chemistry	H	6				
Transition Metal Chemistry	T	4				
Revision topics	T	4				
Practical Course (Inorganic)	Total of 60 credit hours (10 days)					See NOTES
ORGANIC CHEMISTRY						
Introduction to Organic Chemistry	M	7				
Organic Spectroscopy I	M	2				
Orbitals and Mechanisms	M	7				
Substitution and Elimination at Saturated Carbons	H	8				
Chemistry of C–C σ Bonds	H	8				
Core Carbonyl Chemistry	H	8				
Introduction to Biological Chemistry	T	12				
Revision Course	T	4				
Practical Course (Organic)	Total of 60 credit hours (10 days)					See NOTES
PHYSICAL CHEMISTRY						
Foundations of Physical Chemistry: Chemical Thermodynamics	M	13				
The Physical Basis of Chemistry: Classical Mechanics	M	4	1			All physics classes are 90 minutes
The Physical Basis of Chemistry: Properties of gases	M	4	1			All physics classes are 90 minutes
The Physical Basis of Chemistry: The role of charge I	M	4	1			All physics classes are 90 minutes
The Physical Basis of Chemistry: The role of charge II	H	4	1			All physics classes are 90 minutes
Quantum Theory of Atoms and Molecules	H	10				
Reaction Kinetics	H	6				
Electrochemistry	H	4				
States of Matter	T	4				
Practical Course (Physical)	Total of 60 credit hours (10 days)					See NOTES
MATHEMATICS FOR CHEMISTRY						
The Calculus of One and Two Variables	M	20	6			
The Calculus of One and Two Variables	H		1			
Introduction to Vectors	M	2	1			
Vector Algebra and Determinants	H	6	3			

Continues overleaf

Complex Numbers, Multiple Integrals and Ordinary Differential Equations	H	10	4			
Complex Numbers, Multiple Integrals and Ordinary Differential Equations	T		1			
Matrix Algebra	T	8	4			
Revision	T		1			
Practical Course - IT*	A total of c. 12 hours with workshops and directed private study *					

NOTES

Tutorials are the college teaching system whereby undergraduates are taught in very small groups by a tutor (usually a Fellow of the college). Undergraduates attend, on average, one or two tutorials every week, either on a one-to-one basis or with one or two other students. Students must undertake a considerable number of hours' preparatory work for each tutorial, including background reading, essay-writing and problem-solving. Colleges may, at their discretion and as appropriate, provide teaching in different quantities or formats than those indicated above.

The **practical course** requirement consists of a single introductory day, **plus** ten days (60 credit hours) in each of the three laboratories, **plus** a c. 8 hour IT course.

As part of a national **survey investigating the practical skills** of incoming undergraduates, the department is participating in the OFQAU study. There will be an introduction session on the 2nd day of your group's allocation in week 1. This will be followed by a practical test. It is hoped that all students will take part in this as it will influence our new course as well as add to the overall picture.

If you have any **issues with teaching or supervision** please raise these as soon as possible so that they can be addressed promptly. Details of who to contact are provided in 'Complaints Procedures' (Page 7)

APPENDIX F2

PART 1A (Second Year)	Term	Department / Faculty			College	Comments
		Lectures	Classes	Practicals		
INORGANIC CHEMISTRY						<i>Figures in this table are in hours unless otherwise stated.</i>
						Tutorials - 1 or 2 of c.90 minutes each <u>per week</u> - See NOTES
Diffraction	M	4				
Bonding in Molecules	M	8				
Transition Metal Chemistry	M	6				
Coordination Chemistry	H	4				
Chemistry of the Lanthanides and Actinides	H	4				
Organometallic Chemistry	H	8				
Electronic properties of solids	H	8				
Periodic trends in main-group Chemistry	T	5				
NMR in Inorganic Chemistry	T	4				
Course overview	T	8				
Revision Topics	T	2				
Practical Course (Inorganic)	Total of 60 credit hours (10 days)					See NOTES
ORGANIC CHEMISTRY						
Organic Synthesis I	M	4				
Aromatic and Heterocyclic Chemistry	M	4				
Organic Spectroscopy I	M	6				
Conformational Analysis and Ring Chemistry	M	10				
Physical Organic Chemistry	H	8				
Heteroatoms in Organic Synthesis	H	8				
Rearrangements and Reactive Intermediates	H	8				
Organic Synthesis II	T	8				
Organic Chemistry of Biomolecules	T	8				
Problem Solving	T	2				
Practical Course (Organic)	Total of 60 credit hours (10 days)					See NOTES
PHYSICAL CHEMISTRY						
Quantum Mechanics: Principles and Applications	M	12				
Liquids and Solutions	M	8				
Statistical Mechanics	H	12				
Atomic & Molecular Spectroscopy	H	10				
Valence	H	8				
Rate Processes	T	8				
Revision Lectures	T	3				
Practical Course (Physical)	Total of 60 credit hours (10 days)					See NOTES
GENERAL CHEMISTRY						
Symmetry I	M	5				
Introduction to NMR	M	4				
Maths for Chemists	M	5	2			All Maths classes are 90 minutes

Continues overleaf

Symmetry II	M	4				
SUPPLEMENTARY SUBJECTS (Optional)						<i>See NOTES</i>
Aromatic & Heterocyclic Pharmaceutical Chemistry	M	16				
Aromatic & Heterocyclic Pharmaceutical Chemistry	H	14				
Quantum Chemistry	M	16				
Quantum Chemistry	H	14				
Quantum Chemistry - Operators and Commutators	M		4			All Quantum classes are 1 hour
Quantum Chemistry - Group Theory	M		3			All Quantum classes are 1 hour
Quantum Chemistry - Group Theory	H		1			All Quantum classes are 1 hour
Quantum Chemistry - Perturbation Theory	H		4			All Quantum classes are 1 hour
Quantum Chemistry - Electronic Structure Theory	H		3			All Quantum classes are 1 hour
Chemical Crystallography	M	12				
Chemical Crystallography	H	9				
History and Philosophy of Science	M	8				
History and Philosophy of Science	H	8				
Chemical Pharmacology	M	4		3		
Chemical Pharmacology	H	14				
Modern Language	T	32				

NOTES

Tutorials are the college teaching system whereby undergraduates are taught in very small groups by a tutor (usually a Fellow of the college). Undergraduates attend, on average, one or two tutorials every week, either on a one-to-one basis or with one or two other students. Students must undertake a considerable number of hours' preparatory work for each tutorial, including background reading, essay-writing and problem-solving. Colleges may, at their discretion and as appropriate, provide teaching in different quantities or formats than those indicated above.

The **practical course** requirement consists of a single introductory day, **plus** ten days (60 credit hours) in each of the three laboratories.

Supplementary Subjects are available each year, on an optional basis. Normally, they are taken in the Second Year but they may be taken in any of years 2, 3 or 4, with a maximum of three in total. See - <http://course.chem.ox.ac.uk/supplementary-sub.aspx>.

If you have any **issues with teaching or supervision** please raise these as soon as possible so that they can be addressed promptly. Details of who to contact are provided in 'Complaints Procedures' (Page 7).

APPENDIX F3

PART 1B (Third Year)	Term	Department / Faculty			College	Comments
		Lectures	Classes	Practicals		
INORGANIC CHEMISTRY						<i>Figures in this table are in hours unless otherwise stated.</i>
						Tutorials - 1 or 2 of c.90 minutes each per week - See NOTES
Inorganic Reaction Mechanisms	M	4				
Modern main group chemistry	M	5				
Organometallic Chemistry	M	5				
Solid State Chemistry	M	5				
Spectroscopy and Magnetism in Inorganic Chemistry	M	5				
Bioinorganic Chemistry	M	4				
Revision of Topics Inorganic Chemistry	T	6				
Review of Periodic Table	T	3				
ORGANIC CHEMISTRY						
Advanced Organic Spectroscopy	M	6				
Curly Arrows of Biology	M	4				
Organic Synthesis III	M	8				
Transition Metal Catalysis	M	4				
Pericyclic Reactions	M	6				
Radical Reactions	M	4				
Revision Lectures	T	4				
PHYSICAL CHEMISTRY						
Physical Principles of Solids	M	8				
Soft Condensed Matter	M	8				
Photophysics and Photochemistry	M	8				
Magnetic Resonance	M	8				
Revision Lectures	T	4				
Practical Course (Physical)	Total of 72 or 36 credit hours (12 or 6 days)					See NOTES
Practical Course (IT) *	Total of c.6 hours directed private study					See NOTES
OPTION COURSES						
Molecular Spectroscopy	H	8 + 1				plus 1 lecture in Trinity Term
Structural Methods	H	8 + 1				plus 1 lecture in Trinity Term
Organometallic Chemistry: Structures, Bonding and Catalysis	H	8 + 1				plus 1 lecture in Trinity Term
Solid State Compounds in Technology	H	8 + 1				plus 1 lecture in Trinity Term
Supramolecular Nano and Medicinal Inorganic Chemistry	H	8 + 1				plus 1 lecture in Trinity Term
Natural Product Chemistry	H	8 + 1				plus 1 lecture in Trinity Term

Continues overleaf

Advanced Synthesis and Total Synthesis	H	8 + 1				plus 1 lecture in Trinity Term
Contemporary Methods in Catalysis for Organic Synthesis	H	8 + 1				plus 1 lecture in Trinity Term
Advanced Chemical Biology	H	8 + 1				plus 1 lecture in Trinity Term
Functional Organic Polymers and Materials Chemistry	H	8 + 1				plus 1 lecture in Trinity Term
Molecular Reaction Dynamics	H	8 + 1				plus 1 lecture in Trinity Term
Theoretical Chemistry	H	8 + 1				plus 1 lecture in Trinity Term
An Introduction to the Liquid State	H	8 + 1				plus 1 lecture in Trinity Term
Magnetic Resonance	H	8 + 1				plus 1 lecture in Trinity Term

NOTES

Tutorials are the college teaching system whereby undergraduates are taught in very small groups by a tutor (usually a Fellow of the college). Undergraduates attend, on average, one or two tutorials every week, either on a one-to-one basis or with one or two other students. Students must undertake a considerable number of hours' preparatory work for each tutorial, including background reading, essay-writing and problem-solving. Colleges may, at their discretion and as appropriate, provide teaching in different quantities or formats than those indicated above.

3rd Year Option Courses - The courses are at Masters level and assume knowledge of the core material in the first three years of the course and build on it. They are designed to develop advanced concepts and methods in chemistry to cover areas of contemporary interest, and will be updated annually to reflect developments.

The **practical course** requirement consists of a single introductory day, **plus** either 12 or 6 days (72 or 36 credit hours) with a free choice of experiments in **any** of the three laboratories, **plus** an IT course*. A pass or distinction in a Supplementary Subject may be offered as an alternative to half of the 3rd year practical requirement. Refer to section 'Examination Conventions'.

If you have any **issues with teaching or supervision** please raise these as soon as possible so that they can be addressed promptly. Details of who to contact are provided in 'Complaints Procedures' (Page 7)

APPENDIX G

Academic Staff

All Staff in the Department can be contacted by e-mail which is generally the best method.

Add chem.ox.ac.uk to the e-mail addresses listed below.

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Anderson Prof HL	OC	CRL	Keble	harry.anderson@
Armstrong Prof FA, FRS	IC	ICL	St. John's	fraser.armstrong@
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Beer Prof PD	IC	CRL	Wadham	paul.beer@
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Clary Prof DC, FRS	PTC	PTC	Magdalen	david.clary@
Compton Prof RG	PTC	PTCL	St John's	richard.compton@
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Cooper Prof RI	IC	CRL	Pembroke	richard.cooper@
David Prof W	IC	CRL		bill.david@
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Commonly used abbreviations:

OC = Organic Chemistry
 IC = Inorganic Chemistry
 PTC = Physical and Theoretical Chemistry
 CB = Chemical Biology
 CRL = Chemistry Research Laboratory
 ICL = Inorganic Chemistry Laboratory
 PTCL = Physical and Theoretical Chemistry Laboratory
 DP = Dyson Perrins Building
 T.Lab = Teaching Laboratory
 MPLS = Mathematical, Physical and Life Sciences Division

APPENDIX H**University Policies**

The University has a wide range of policies and regulations that apply to students. These are easily accessible through the A-Z of University regulations, codes of conduct and policies available on the Oxford Students website www.ox.ac.uk/students/academic/regulations/a-z. To ensure that these are up to date, please consult the relevant University web pages.

Intellectual property: <http://www.admin.ox.ac.uk/researchsupport/ip/>

Plagiarism: <http://www.ox.ac.uk/students/academic/guidance/skills/plagiarism>

Equal opportunities: <http://www.admin.ox.ac.uk/eop/>

Disability: www.ox.ac.uk/students/welfare/disability

Harassment: <http://www.admin.ox.ac.uk/eop/harassmentadvice/>

Health and safety: <http://www.admin.ox.ac.uk/safety/hs-mgement-policy/>

Chemistry Department safety: <http://safety.chem.ox.ac.uk/>

Computer usage: <http://www.it.ox.ac.uk/do>

Policy on recording lectures by students: <http://www.admin.ox.ac.uk/edc/policiesandguidance>

Examination regulations: <http://www.admin.ox.ac.uk/examregs/>

The Proctors' Memorandum: <http://www.proctors.ox.ac.uk/handbook/handbook/>

Data Protection Act 1998: <http://www.admin.ox.ac.uk/councilsec/dp/>

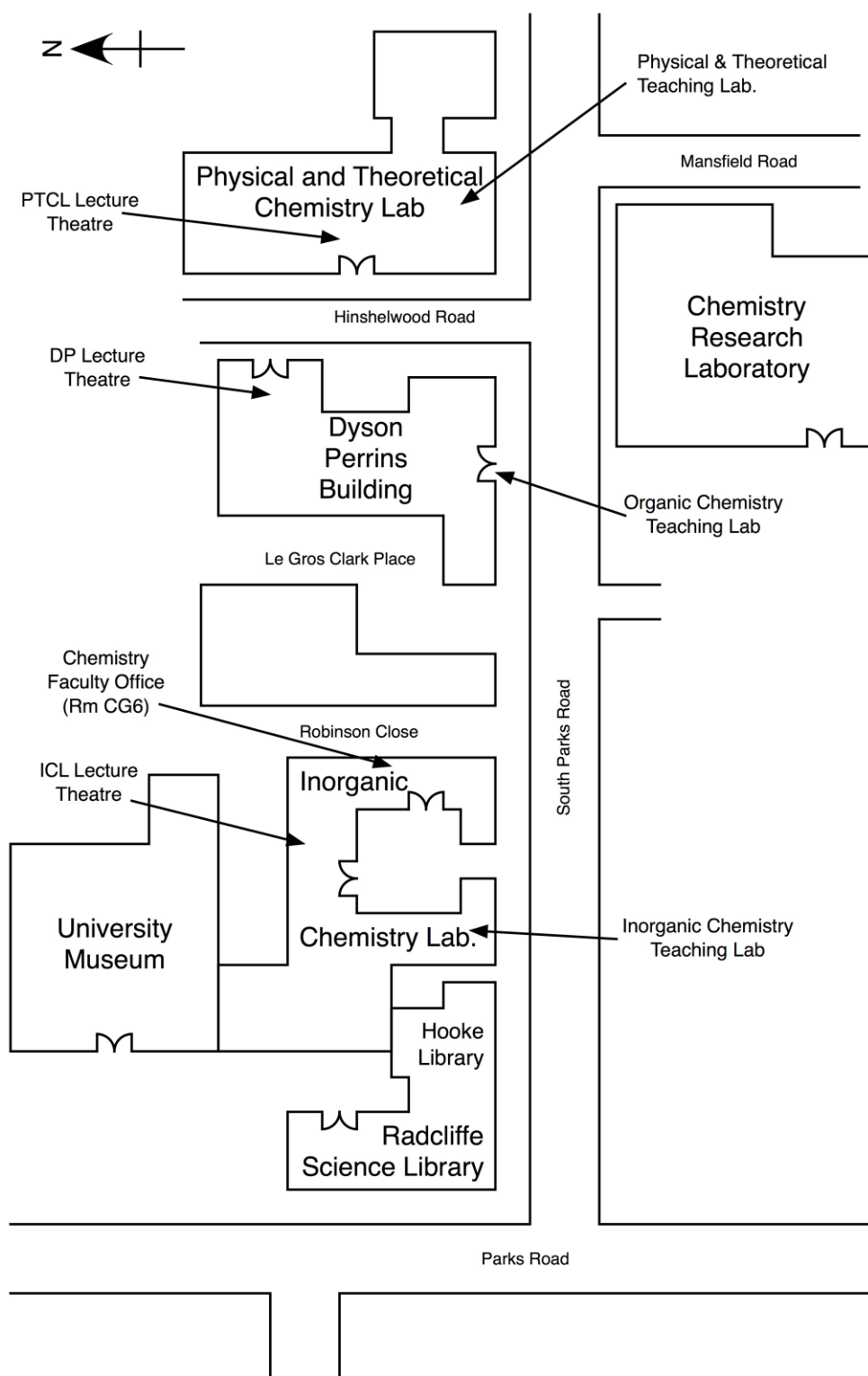
Resources

University Careers Service: www.careers.ox.ac.uk

Guidance on Paid Work: www.ox.ac.uk/students/life/experience

Skills and Work Experience: www.ox.ac.uk/students/life/experience

Enterprising Oxford: <http://eship.ox.ac.uk/> An online map and guide to innovation and entrepreneurship in Oxfordshire, developed here at the University of Oxford.



Commonly used abbreviations:

PTCL = Physical and Theoretical Chemistry Lab.
 DP = Dyson Perrins Building
 ICL = Inorganic Chemistry Laboratory
 CRL = Chemistry Research Laboratory
 UM = University Museum
 RSL = Radcliffe Science Library