Module Specification

Module Title	Physical and Quantum Chemistry	Module Code	CHE204a

Credit Value	15	Level	5	Mode of Delivery	On Campus	Semester A

Pre-requisite modules	Co-requisite modules	Overlapping modules

1) Content Description

Provide a description of the module, as it will appear in the Module Directory and on the Student Information System (approx. 70-80 words).

This module introduces key concepts of quantum mechanics in a chemical context, explaining how the theories of quantum mechanics can be applied to atoms and molecules so as to rationalise the structure, properties and chemical reactivity of such entities.

2) Module Aims

Specify the aims of the module, i.e. the broad educational purposes for offering this module.

This module aims to provide students with an understanding of the principles of quantum mechanics, and how the theories of quantum mechanics can be applied to atoms and molecules, including molecular orbitals and bondin. Objective is for the student to be able to rationalise the structure, properties and chemical reactivity of such entities. Such knowledge and understanding will underpin studies of molecular structure and reactivity in other chemistry modules.

3) Learning Outcomes

Identify the learning outcomes for this module, i.e. knowledge, skills and attributes to be developed through completion of this module. Outcomes should be referenced to the relevant QAA benchmark statements and the Framework for Higher Education Qualifications in England, Wales and Northern Ireland (2008). The SEEC Credit Level Descriptors for Further and Higher Education 2003 and Queen Mary Statement of Graduate Attributes should also be used as a guiding framework for curriculum design.

Academic Content:	
A 1	Introduction to Quantum Mechanics & Atomic Structure (6 hours) 1. Wave-particle duality & wavefunctions 2. Particle in a box & uncertainty relationships 3. Hydrogen atom: atomic orbitals and energies 4. Many electron atoms
A 2	Molecular Structure and Bonding (6 hours) 1. Molecular energy, potential energy curves 2. Harmonic and anharmonic potentials 3. Vibrational spectroscopy of diatomics & triatomics 4. Electronic states & atomic terms
A 3	Molecular Orbital Theory (6 hours) 1. Applying the Schrödinger equation to molecules. 2. Molecular orbitals as LCAOs. 3. Hückel theory, charge distributions and bond orders.

A4	Kinetics and Potential Energy Surfaces, (4 hours) 1. Potential energy surfaces (PESs) and hypersurfaces (PEHSs). 2. Reaction barriers and kinetics. 3. ZPE and entropy contributions to reaction dynamics.
A 5	Statistical Thermodynamics (2 hours) 1. Introduction to Statistical Mechanics. 2. Thermodynamic ensembles and partition functions. 3. Applications of statistical mechanics.

Disciplinary skills - able to:	
B1	Solve problems relating to the application of basic theorems of quantum mechanics (including those pertaining to diffraction, uncertainty relationships and spatial-confinement of particles)
B2	Rationalise and quantify aspects of bonding in molecules, by application of molecular orbital (MO) theory.
B3	Predict basic properties of molecules by application of appropriate models, including properties such as charge distributions, bond-orders and relative chemical reactivity.
B4	Understand the topological treatment of reaction surfaces and the implications that this has for predicting the outcome and likelihood of a reaction.
B5	Apply a Boltzmann distribution to independent distinguishable/indistinguishable systems and the consequences of such a treatment to a variety of systems.

Attributes:	
C1	Acquire and apply knowledge relating to the principles and practices of physical and quantum chemistry
C2	Produce analyses which are grounded in experimental evidence (e.g. structural, spectroscopic and computational)
C3	Apply existing knowledge and skills to investigate unfamiliar problems.
C4	Able to conduct calculations of intermediate complexity, in a confident and reliable manner.

4) Reading List

Provide an indicative reading list for the module. This should include key texts and/or journals but should not be an exhaustive list of materials.

Introduction to Quantum Theory and Atomic Structure, by P.A. Cox (Oxford Chemistry Primer 37)
Quantum Mechanics for Chemists, by D.O. Hayward (RSC Tutorial Chemistry Text 14)
Atkins' Physical Chemistry, 9th ed, P. Atkins & J. de Paula, Oxford Univ Press#

5) Teaching and Learning Profile

Provide details of the method of delivery (lectures, seminars, fieldwork, practical classes, etc.) used to enable the achievement of learning outcomes and an indicative number of hours for each activity to give an overall picture of the workload a student taking the module would be expected to undertake. This information will form the Key Information Set for each undergraduate programme and will be used to populate the KIS widget found on the QMUL programme information pages. More information can be found online about KIS. You may also wish to refer to the QAA guidance on contact hours when completing this section.

Activity Type	KIS Category	Time Spent (in hours)
Lecture	Scheduled	22
Practical Classes and Workshops	Scheduled	8
Guided Independent Study	Independent	120

Total	150

Specify the total module notional study hours. This should be a total of the hours given for each activity. The notional study hours for each academic credit point is 10. A 15 credit point module therefore represents 150 notional study hours.

Activity Type	Total Time Spent (in hours)	Percentage of Time Spent
Scheduled learning and teaching	30	20
Placement	0	0
Independent Study	120	80
Total	150	100

Use the information provided in the box above to specify the total time spent and the percentage time spent in each category of teaching and learning activity.

6) Assessment Profile

Provide details of the assessment methods used to assess the achievement of learning outcomes.

Description of Assessment	Assessment Type	KIS Category	Duration/Length	Percentage Weighting	Final element of assessment	Qualifying Mark
Coursework	Written Assignment including essay	Coursework		20%	No	
Examination	Written Exam	Written	2 Hours	80%	Yes	

Final element of assessment: The assessment that takes place last. There should normally be only one element of assessment marked as final unless two assessment or submission dates occur on the same day.
Qualifying mark: A specified minimum mark that must be obtained in one or more elements of assessment in order to pass a module. This is in addition to, and distinct from, the requirement to achieve a pass in the module mark to pass the module.

Reassessment

Provide details of the reassessment methods used, specifying whether reassessment is either standard reassessment or synoptic reassessment.

○ Standard Reassessment ◉ Synoptic Reassessment

Synoptic reassessment details (if you have indicated synoptic reassessment above, please give details)		
Brief Description of Assessment	Assessment Type	Duration/Length of Examination/ Coursework
Resit Examination	Written Exam	2 Hours