Confirmation that this version of the module specification has been approved by the School Learning and Teaching Committee:

19th June 2015………………………………………

**MODULE SPECIFICATIONS**

1. Title of the module

CH532 Spectroscopy and Bonding

1. School or partner institution which will be responsible for management of the module

School of Physical Sciences

1. Start date of the module

Autumn Term 2015

1. The number of students expected to take the module

25

1. Modules to be withdrawn on the introduction of this proposed module and consultation with other relevant Schools and Faculties regarding the withdrawal

None, existing module.

1. The level of the module (e.g. Level 4, Level 5, Level 6 or Postgraduate Level 7)

Level 5

1. The number of credits and the ECTS value which the module represents

15 (ECTS value 7.5)

1. Which term(s) the module is to be taught in (or other teaching pattern)

Terms 1 and 2

1. Prerequisite and co-requisite modules

Students must have taken CH308, CH320 and CH382 before taking this module

1. The programmes of study to which the module contributes

Chemistry programme (MChem and BSc), stage 2

This is not available as a wild module.

1. The intended subject specific learning outcomes

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| Knowledge and critical understanding of: |
| 11.1 Basic quantum mechanical concepts.  11.2 Basic concepts of molecular symmetry and group theory.  11.3 How to obtain and interpret spectra to calculate molecular parameters from spectroscopic data. |
| . Intellectual skills: |
| 11.4 An ability to link quantum mechanical theories to experimental observables.  11.5 An ability to interpret spectroscopic data.  11.6 The skill to perform practical experiments to gain spectroscopic information. |
| 11.7 The skill to operate standard chemical instrumentation, record data and evaluate observations and errors. |
| . Subject-specific skills: |
| 11.8 A knowledge of basic spectroscopy; microwave, infra-red, UV-VIS, Raman.  11.9 An ability to perform calculations on molecular parameters from spectroscopic data. |
| 11.10 An ability to understand quantum mechanical concepts underlying bonding and energy transitions experimentally observed in spectroscopy. |
| 11.11 An ability to understand symmetry of molecules to determine spectroscopic data. |
| 11.12 An ability to make use of appropriate texts, or other learning resources as part of managing their own learning. |

1. The intended generic learning outcomes

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| 12.1 Problem-solving skills, an ability to formulate problems in precise terms and to identify key issues, and the confidence to try different approaches in order to make progress on challenging problems. |
| 12.2 Analytical skills – associated with the need to pay attention to detail and to develop an ability to manipulate precise and intricate ideas, to construct logical arguments and to use technical language correctly. |
| 12.3 Personal skills – the ability to work independently, to use initiative, to organise oneself to meet deadlines and to interact constructively with other people. |

1. A synopsis of the curriculum

Lectures (24 lectures);

1. Quantum theory (10 lectures)
2. Introduction: origins of quantum mechanics, wave-particle duality, Shrodinger equation, wave function, uncertainty principle.
3. Techniques and applications: translational motion – particle in a box, vibrational motion – harmonic approximation, rotational motion, spin – spin orbit coupling.
4. Atomic structure and spectra: structure of hydrogenic atoms, atomic orbitals and their energies, spectroscopy and selection rules, orbital approximation, spectra of complex atoms.
5. Molecular structure: valence-bond theory, homonuclear diatomic molecules, heteronuclear diatomic molecules and polyatomic molecules.
6. Molecular symmetry and group theory (6 lectures)
7. Symmetry elements: Operation and symmetry elements, symmetry classification of molecules, polarity and chirality
8. Molecular orbital theory: character tables and symmetry labels, overlap and symmetry, representations.
9. Applications of character tables to spectroscopy
10. Spectroscopy (8 lectures)
11. Rotation of molecules: energy levels, transitions, microwave spectroscopy, calculation of moments of inertia and bond lengths.
12. Vibration in molecules: molecular vibrations for a diatomic molecule, vibration–rotation spectra, vibrations of polyatomic molecules, infra-red spectroscopy, Raman spectroscopy, calculation of bond energies.
13. Electronic transition in molecules: electronic spectra of diatomic molecules, UV-VIS, fluorescence and phosphorescence.
14. Other spectroscopies: basic concepts on photoelectron and X-racademic year fluorescence spectroscopies, nuclear magnetic resonance (NMR) and Mössbauer spectroscopy.
15. Indicative Reading List
16. P.W Atkins, Physical Chemistry (2014)
17. C. N. Banwell and E. M. McCash , Fundamentals of molecular spectroscopy (1994)
18. Y. Jean, F. Volatron and J. Burdett, An introduction to molecular orbitals (1993)
19. Learning and Teaching Methods, including the nature and number of contact hours and the total study hours which will be expected of students, and how these relate to achievement of the intended module learning outcomes

- Lectures: 24 (24 hours). This will address learning outcomes 11.1, 11.2, 11.4, 11.5, 11.8, 11.9, 11.10, 11.11, 12.1 and 12.2.

- Laboratory work: 3 sessions (18 hours). This will address learning outcomes 11.3, 11.4, 11.5, 11.6, 11.7, 11.8, 11.9, 11.10, 11.11, 11.12, 12.1, 12.2 and 12.3.

- Assignments: 2 class tests (2 hours). This will address learning outcomes 11.1, 11.2, 11.4, 11.5, 11.8, 11.9, 11.10, 11.11, 11.12, 12.1 and 12.3.

- 11.111.211.411.511.811.911.1011.1111.1212.112.212.3- Private study hours (106 hours). This will address learning outcomes 11.1, 11.2, 11.3, 11.4, 11.5, 11.8, 11.9, 11.10, 11.11, 11.12, 12.1, 12.2 and 12.3

1. Assessment methods and how these relate to testing achievement of the intended module learning outcomes

Course work: 2 class tests (15%) This will address learning outcomes 11.1, 11.2, 11.4, 11.5, 11.8, 11.9, 11.10, 11.11, 11.12, 12.1, 12.3.

Course work: 3 practicals (25%). This will address learning outcomes 11.3, 11.4, 11.5, 11.6, 11.7, 11.8, 11.9, 11.10, 11.11, 11.12, 12.1, 12.2, 12.3.

Final written exam 2hrs (60%). This will address learning outcomes 11.1, 11.2, 11.4, 11.5, 11.8, 11.9, 11.10, 11.11, 11.12, 12.1, 12.2 and 12.3.

1. Implications for learning resources, including staff, library, IT and space

None, existing module.

1. The School recognises and has embedded the expectations of current disability equality legislation, and supports students with a declared disability or special educational need in its teaching. Within this module we will make reasonable adjustments wherever necessary, including additional or substitute materials, teaching modes or assessment methods for students who have declared and discussed their learning support needs. Arrangements for students with declared disabilities will be made on an individual basis, in consultation with the University’s disability/dyslexia support service, and specialist support will be provided where needed.
2. Campus(es) where module will be delivered:

Canterbury Campus