**CHEM3117/3917**

**SPECTROSCOPY & QUANTUM CHEMISTRY**

**Course syllabus and learning objectives**

Spectroscopy and quantum chemistry are ubiquitous techniques, and in the past decade have moved beyond the realm of spectroscopists and theoretical chemists. Researchers are frequently required to provide computational support for structures and mechanisms. Optical spectroscopy is now used throughout biological and materials science via specifically-designed fluorophores, e.g. green fluorescence protein, and quantum dots with the consequence that knowledge of spectroscopy is now required throughout biological and materials science.

**Learning objectives:**

* To understand to role of symmetry in chemistry and how to use group tables;
* To learn how to compute molecular structure, molecular orbitals, energy levels and spectra;
* To understand vibrational and electronic spectra in terms of symmetry and to connect real spectra with the computations they have performed

**These learning objectives should prepare students to**

* Carry out their own computations of molecular structure in research or industry;
* Understand when the theory is inadequate for the task at hand;
* Understand the structure of an unfamiliar UV-vis or IR spectrum and interpret the spectrum with respect to symmetry and molecular structure.

**Course outline:**

**CHEM3117** will provide students with an introduction to the role of symmetry in chemistry. Symmetry will be illustrated through molecular symmetry, the symmetry of molecular orbitals and the connection between molecular motion (vibrations and rotations) and symmetry elements, which will be linked back to existing knowledge of IR and Raman spectroscopy (CHEM2401). They will use symmetry to determine quickly and simply which vibrational states (IR and Raman) and electronic states (UV-vis) are able to be excited in the interaction with light.

Students will be introduced to the principles and methods of computational chemistry. They will learn in detail about the approximations in Hartree-Fock theory and in the use of Gaussian basis sets. Theories beyond HF, including density functional theory, will be described. Students will run computational chemistry software to calculate molecular structures and predict spectra, interpreting all results in terms of nuclear and electronic symmetry. Students will understand the limitations in such calculations.

Students will learn how to interpret experimental IR and UV-vis spectra of molecules in terms of the symmetry of the molecule or orbitals, and to compare the spectrum with predictions of their calculations. Students will learn that there are different models of spectroscopy that are suited to different situations (e.g. Born-Oppenheimer, Franck-Condon, Herzberg-Teller approximations), and that these approximations are mirrored in the different levels of theory used in computational chemistry.

**CHEM3917** includes the outline above, but the advanced students are extended in three ways. i) advanced students will learn how to predict the number and symmetry of vibrations of an unknown molecule; ii) advanced students receive additional tuition in density functional approaches; and iii) advanced students learn about the quantum mechanical basis of Herzberg-Teller coupling in molecular spectra.

**Assessment:**

This Unit has learning objectives that are both conceptual and practical. Assessment of these learning objectives will be achieved by the following assessment tasks:

**CHEM3117:**

1. Conceptual objectives will be assessed by formal closed book examination (65%). This examination will be in the regular end-of-semester examination period.
2. Practical skills will be assessed via individual assignment (i.e. every student will receive a different assignment). This assignment focuses on the students’ ability to carry out a HF calculation of a specific molecule, to predict its structure and spectrum (30%, due beginning of week 10).
3. There will also be a mostly formative assignment on the basics of symmetry. This will be conducted early in the semester. Although there is a summative component to the assignment (5%), the assignment is mostly to provide feedback to the students on their understanding of symmetry, which is essential for later parts of the Unit (due in lecture 8).

**CHEM3917:**

The assessment for 3917 students will reflect the additional learning objectives for this class. The overall weight of the assessment elements is the same. Changes to the assessment are as follows:

1. The final exam will have two elective components at the end (meaning that the students must choose to do section A or B). This component will constitute 25% of the exam assessment. Section A will probe student learning against 3117 obectives, while Section B will be aligned with 3917 objectives. Grading in sections A & B will be normalized against the common (75%) section to ensure equity of grading for the harder 3917 section. Advanced students must complete Section B to complete 3917, else they will be graded with the 3117 cohort.
2. 3917 students will perform a DFT calculation rather than HF.
3. The formative assessment item will a question on predicting the symmetry of molecular vibrations.

**Support for learning:**

**Textbook**: The students’ learning is scaffolded by appropriate chapters in Engle and Reid, which they should already have from 2nd Year. In particular, Chapters 28 (Molecular Symmetry), 27 (Computational Chemistry) and 26 (Electronic Spectroscopy) underpin their learning against the three objectives above. Some material goes beyond E&R, and suitable materials will be provided.

**Lectures:** The unit has 22 lectures (lecture outline attached).

**Tutorials:** The Unit has 2 scheduled tutorials to support the conceptual objectives. Tutorials will be held at the normal lecture time, and held in triplicate (2 for 3117 and 1 for 3917) and conducted by all three teaching staff. The 3917 tutorial will include the additional material.

**Workshops:** Two workshops will be held in week 9. The 3rd floor computer rooms will be booked from 8-11 am on Wed & Thurs of week 9. This includes the regular lecture time of 10-11am on these days, so all students should be able to attend for at least these hours. In these workshops students will be taught the practical elements of running their own calculations. Advanced students will be taught about DFT (perhaps in the 3rd year computer room). All three teaching staff will be available at different times during these 3 hour blocks.

**Website:** All course materials will be provided on the Unit website. Support materials beyond E&R will be provided.