**CHEM3117/CHEM3917
Spectroscopy and Quantum Chemistry**

**Lecture 1:** Course Administration; Introduction and Overview; Review of Assumed Knowledge; Revision: the Electromagnetic Spectrum, Classical Absorption of Light, Molecular Vibrations.

**Lecture 2:** Introduction to Symmetry, Symmetry Operations: identity, inversion, rotation, reflection, improper rotation; Symmetry Elements, Molecular Point Groups (E&R 28.1)

**Lecture 3:** Common Molecular Point Groups; Flow Chart for determining Molecular Point Groups; Examples of Molecular Point Groups (E&R 28.2)

**Lecture 4:** Representations; Characters; Character Tables; Irreducible Representations; Application to Molecular Orbitals of Diatomic Molecules. (E&R 28.4, 28.5)

**Lecture 5:** Reduction in Symmetry; Subgroups of the Molecular Point Group; Application to the 3 and 4 orbital problems. (E&R 28.6)

**Lecture 6:** The Interaction of Light with a Molecule; the Transition Moment Integral for Vibrational Transitions; The Symmetry of the Transition Moment Integral. (E&R 19.4, 28.7)

**Lecture 7:** Vibrational Selection Rules; Electronic Selection Rules.

**Tutorial 1:** CHEM3117: Symmetry Tutorial/ CHEM3917: Extension Material Determining the Symmetry of Molecular Vibrations.

**Lecture 8:** The Schrodinger Equation; Matrix Representation of the Schrodinger Equation; The Secular Determinant; Dirac Notation. (E&R 24.2)

**Lecture 9:** Solution of the 2 orbital problem for H2+/H2; The Resonance Integral; The Variation Principle. (E&R 24.2, 24.3, 21.4)

**Lecture 10:** Matrix Representation of 3 and 4 orbital problems; Atomic Orbital Basis Sets. (E&R 27.3, 27.7)

**Lecture 11:** Hartree-Fock Self-Consistent Field Theory (E&R 21.5, 27.3)

**Lecture 12:** Beyond Hartree-Fock Theory: Electron Correlation, Density Functional Theory. (E&R 27.6)

**Lecture 13:** The Adiabatic Born-Oppenheimer Approximation; Molecular Potential Energy Surfaces. (E&R 27.2)

**Lecture 14:** Applications of Computational Chemistry: Selecting a Computational Method, Predicting Molecular Structure and Thermochemistry. (E&R 27.8)

**Lecture 15:** Applications of Computational Chemistry: Predicting Molecular Spectra. (E&R 27.9)

**Workshop 1:** Computational Chemistry Workshop. H2O as an example

**Workshop 2:** Computational Chemistry Workshop: Setting up the problem for a new (assignment) molecule.

Mid-Semester Break

**Lecture 16:** Introduction to Experimental Spectroscopy; The Transition Moment Integral; Revision of Electronic Selection Rules. (E&R 26.2, 26.3)

**Lecture 17:** Vibrational Fine Structure; The Franck-Condon Principle for Absorption (E&R 26.4, 26.5)

**Lecture 18:** The Franck-Condon Principle for Emission (E&R 26.6)

**Lecture 19:** Vibronic Spectroscopy; Vibronic Selection Rules.

**Lecture 20:** Vibronic Spectroscopy; Vibronic Selection Rules.

**Lecture 21:** Rotational Fine Structure in Electronic and Vibrational Spectroscopy. (E&R 19.6)

**Tutorial 2:** CHEM3117 Spectroscopy Tutorial/ CHEM3917: Tutorial plus extension material.

**Lecture 26:** Summary / catch-up / public holiday provision