Course: CHMB21H3S, Chemical Structure and Spectroscopy

**Instructor:** Simon J. Fraser

e-mail UTSC: fraser@utsc.utoronto.ca; St. George: sfraser@chem.utoronto.ca

phone UTSC: (416) 287-7214; St. George: (416) 987-4650

OFFICES:

UTSC: Room SW 506A St. George: Room 420C

Office Hours at UTSC: Mondays 12:00–14:30, Wednesday 12:00–14:30

Lectures: Room SW 128 Monday 15:00-17:00 Room SW 128 Wednesday 15:00-16:00

**Required Text:** P.W. Atkins and J. de Paula (A&P), Physical Chemistry Ninth Edition (Freeman).

Marking Scheme for CHMB21H3S, 2012

 $\begin{array}{ccc} \text{Problem Sets} & 30\% \\ 1 \text{ Term Test} & 30\% \\ \text{Final Exam} & 40\% \\ \text{TOTAL} & 100\% \end{array}$ 

It is desirable that you take MATB41H3. Note that you must take MATB41H3 if you are going to take a 3rd year physical chemistry course.

Calendar Course Description: Atomic structure and spectra; term symbols and their meaning; valence bond theory: LCAO-MO; molecular spectroscopies.

**Course Description:** This course uses *Quantum Mechanics* extensively to describe atomic and molecular structure and bonding, including valence bond and molecular orbital theory. The theory of these systems will be treated first and their spectroscopy afterwards.

- Blackbody Radiation, Wave-Particle Duality, etc.
- The Time-Dependent (TDSE) and Time-Independent (TISE) Schrödinger Equations. Stationary states; operators and observables; eigenvalues and eigenfunctions.
- Quantum mechanics of two-body systems, e.g., diatomic molecules. Reduction to a one-body problem with internal potential and center-of-mass motion.
- Quantum mechanics of simple systems, especially hydrogen-like atoms.
- Many electron atoms.
- Theories of chemical bonding: valence bond theory and molecular orbital theory (LCAO-MO description). This is done in relation the the hydrogen molecule ion  $H_2^+$ , the hydrogen molecule,  $H_2$ , and more complex molecules.
- Quantum mechanics of the internal motion of molecules.

 $\bullet$  Spectroscopy of the above atomic and molecular systems.