

Course: CHMC20H3F, Intermediate Physical Chemistry

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Please use only UofT email accounts. When composing your email, please use professional language. Be sure to include the course code as part of the subject line and sign the email with your first and last name, as well as your student ID. Your email will be answered as soon as possible.

Web: CHMC20 maintains a Blackboard web space which archives a variety of course-related information including: grades, class announcements, lecture and lab materials, contact information and links to outside resources. In addition, class emails will periodically be sent via Blackboard. To receive these emails, you must have a valid “utoronto.ca” email account registered with ROSI.

Office: SW504D; office hours: Monday & Wednesday 14:00–15:30

Lectures: Room IC 320, Wednesday 12:00–14:00

Recommended Texts: 1) F. C. Andrews, Equilibrium Statistical Mechanics; 2) D. A. McQuarrie, Statistical Mechanics; 3) A. Szabo and N.S. Ostlund, Modern quantum chemistry: Introduction to advanced electronic structure theory

Marking Scheme: midterm test 35%, final exam 45%, homeworks 20%: will appear on Wednesdays (starting Sept 10, check BB), will be due noon of the next Wednesday, -50% late penalty.

Note: To pass this course you need to pass either the midterm test or the final exam, visit me during the office hours at least once before the midterm test, and receive a final grade of 50+.

Course Description: This course gives an introduction to statistical mechanics and electronic structure. These subjects will be applied to thermochemistry, kinetics, and spectroscopy. The list of topics is as follows.

- Motivation for statistical mechanics, elements of probability theory
- Ensembles in statistical mechanics: micro-canonical, canonical, and grand-canonical ensembles
- Relation between statistical mechanics and thermodynamics
- Partition function for molecular systems (translational, rotational, vibrational, and electronic components), chemical equilibrium
- Electronic structure, Hartree-Fock method, molecular geometry, harmonic frequencies