THOMPSON RIVERS UNIVERSITY

Department of Physical Sciences (Chemistry)

CHEM 4430 – 1 Credit
Advanced Physical Chemistry Laboratory (0,1,3)
Fall 2016

Instructor:	Dr. Nelaine Mora-Diez
Office:	S-254, Science Building
Phone/Voice Mail:	828-5442
E-mail:	nmora@tru.ca
Office Hours:	Mon, Wed 1:30 – 2:30 pm Additional office hours are available by appointment.

Description

This is a half semester (6 weeks) course is a practical course on computational chemistry that builds on the knowledge students have acquired in CHEM 3060, 3070 and 3080. Students will become familiar with the use and operation of the Linux (UNIX) operating system, the Gaussian series of programs for electronic structure calculations, and a visualization software (GaussView). Students will engage in a short research project.

Prerequisites

CHEM 3070 and CHEM 3080 (C- minimum).

Laboratory Classes

4 hours/week Tue 2:30 – 6:30 pm S 266 (October 25 – November 29, 2016)

Moodle

Any electronic course-related materials will be available through Moodle. You have to enroll in the Moodle course "CHEM 4430 – Advanced Physical Chemistry Laboratory" by using the enrolment key: *4430-2016*. To access Moodle on the Internet, use the Moodle quick link from the TRU homepage (www.tru.ca).

Academic Policy

It is the responsibility of all students to be aware of TRU Student Academic Policies, Regulations and Procedures found in the TRU Calendar (www.tru.ca/calendar/current/). These include: Academic Honesty Policy ED-5-0 (p. 24), Appeals Policy ED-4-0 (p. 25), Students Attendance ED-3-1 (p. 24), and Exams Policy ED-3-9 (p. 24). Forms of Academic Dishonesty are summarized and described on the TRU Calendar, and include cheating, misconduct, fabrication and plagiarism.

Assessment

Students will perform two labs during the first three weeks of the course. Work on a short research project on a topic of choice, to be discussed with your instructor, will take place during the last three weeks.

Grades will be assigned on the following basis:

Oral Pre-Lab Quizzes (Weeks 1 and 3)	10%
UNIX quiz (Week 3)	10%
Lab reports (Due on weeks 3 and 4)	30%
Draft of project proposal (Due on week 3)	5%
Lab work on project (Weeks 4, 5 and 6)	15%
Project class presentation (End of week 6)	10%
Final Report (Due the last day of classes)	20%

A letter grade will be awarded using the TRU Grading System (Policy ED-3-5) on page 24 of the TRU Calendar. This one-semester course is worth 1 credit.

Schedule

Week 1: Oral Pre-Lab Quiz; Lab 1

Week 2: Lab 1 (Cont.)

Week 3: Report for Lab 1 due at the beginning of the lab
UNIX quiz
Oral Pre-Lab Quiz; Lab 2
Provide in writing your ideas for the class project

Week 4: Report for Lab 2 due at the beginning of the lab
Work on class project

Week 5: Work on class project, the report and presentation
Meet with your instructor to discuss progress before the end of the lab

Week 6: Work on class project, the report and presentation
Project class presentation (15 minutes followed by 5 minutes of questions)

The final class project report is due the last day of classes.

Lab 1: Introduction to Linux and some computational chemistry software (Weeks 1 and 2)

Lab 2: Thermodynamic and kinetic calculations in the gas phase (Week 3)