

Chemistry 5000/7000

Statistical Mechanics

Spring 2009

Instructor: Marc R. Roussel
Offices: E862 and A534
Phone: 403-329-2326
Email: roussel@uleth.ca
Course web site: <http://people.uleth.ca/~roussel/C4000>

Textbook

Thermodynamics, Statistical Thermodynamics, & Kinetics by Engel and Reid

Email

Important information will frequently be communicated to the class via email. It is *your responsibility* to keep an eye on your email during the term. This includes making sure that you do not exceed your email quota. You can check your email account status at https://www.uleth.ca/webtools/account_tools/acctstatus.

Office hours

I operate on an open-door basis: If I'm in, you are welcome to stop in to ask questions. Some parts of the term are busier than others, and I have offices at both ends of the building, so it's probably a good idea to phone ahead if you're making a special trip to see me.

Grading scheme

Evaluation type	Number	Formula 1	Formula 2	Dates
Participation	—	8%	8%	
In-class tests	2	12% each	0%	Feb. 13, March. 20
Assignments	8	16%	16%	see syllabus
Final exam	1	32%	56%	April 27, 9:00 a.m.
Lecture	1	20%	20%	April

I will compute your course mark using each of the two formulas given above. Your grade will be based on the better of the two scores.

If you miss one of the in-class tests, you will receive a grade of zero unless you have a medical or other equally serious, documentable reason. **It is your responsibility to notify me.** You should be prepared to present appropriate documents on request to support any

claims you make with respect to a missed test. If you do miss an in-class test with a valid reason, the weight of the final exam will be increased accordingly in Formula 1.

If you miss the final exam, the provisions of the University Calendar (2008–09 edition, Part 4 (Academic Regulations), section 4, subsection f) take effect.

Conduct of exams

In each exam, you will be permitted to bring one $8\frac{1}{2} \times 11$ -inch piece of paper containing any information you want (formulas, instructions for using your calculator, etc.). Any numeric data you need (universal constants, etc.) will be given on the exams, so you don't have to put those on your formula sheet. You can also bring a calculator if you wish.

The exams will be held in the computer lab. You will have access to the full range of scientific software available at the University. Any use of communications software or devices of any kind, including browsers, is strictly forbidden.

Conduct of the lectures

As a means of instruction, they [lectures] ought to have become obsolete when the printing press was invented. We had a second chance when the Xerox machine was invented, but we seem to have muffed it.

— R. P. Boas

In this course, I do not lecture. Rather, you will be assigned readings from the book which you must work through *before* you come to class. In each class, we will engage in the following three activities:

1. We will draw out the key ideas from our readings.
2. I will answer any questions you have about the readings.
3. We will work on some problems together to consolidate your learning.

Note the careful use of the word “we” in two of the above three points. This is intended to be a participatory exercise since, as noted above, learning is an active process. Note also that 10% of the evaluation will be based on your participation in class.

Class participation

Class participation will be evaluated on the basis of both the frequency and continuity of your contributions. I set the threshold at a reasonable level so that everybody who makes a consistent effort to participate will get 10/10, but I do insist on hearing your voice regularly over the term.

Participation can take many forms. Here are just a few:

- Helping to put together the key ideas from the readings

- Asking a question
- Helping to solve a problem

Don't worry if you miss one or two classes over the term. That won't make any difference to your participation mark. However, if you miss several classes for good reason, please let me know and I will take this into account when setting your participation mark.

Assignments

Assignments will generally be released on Fridays and due the following Friday. The detailed schedule of assignment due dates is included in the syllabus. There will not be an assignment due the week of a test, nor the following week.

While I expect that you will talk to each other and to me about the assignments, each assignment must be the product of your own work. My advice, in order to avoid misunderstandings and charges of plagiarism, is not to take written notes of any kind when talking to fellow students about the assignment.

Lecture

You will be expected to deliver one lecture on statistical mechanics, and to provide a range of support materials to go with your lecture. You can choose any topic in statistical mechanics not covered in the syllabus. The topic covered in your lecture will be examinable material, although you will be excluded from answering questions on your own topic in the exam.

Here are the deadlines you must meet, along with the breakdown of the 20% of the grade assigned to the lecture:

Date		Marks
Feb. 27	Lecture proposal	2
March 13	Lecture outline	2
March 27	Lecture notes	4
April 3	Problem set	4
	Lecture	8

The **lecture proposal** should clearly identify the topic chosen and the *print* resources you plan to use to prepare your lecture. (No web resources, please.) I will comment on your proposal and return it. If there are problems with your topic (e.g. too close to another student's topic), I will talk to you about possible alternative topics at this point. Grading of this assignment will be based on making a reasonable effort to identify an interesting topic and relevant sources.

The **lecture outline** should list the key ideas you intend to cover, along with some estimate of the time you think you will spend on each. When marking this assignment, I will be looking for a clear and reasonable plan.

The **lecture notes** should be a complete set of notes for your lectures. You will be given an opportunity to revise them after I have commented on them. Only the final version will be graded. Clarity and completeness of exposition will be the main criteria of evaluation.

You will also be responsible for distributing the final version to your classmates at least three days before your lecture. You can decide on the best distribution method (email, your web site, print).

You are also required to generate a short **problem set** with solutions which your classmates can use to prepare for the final exam. The problem set will be graded for clarity and appropriateness of the questions, as well as for the quality of the solutions. Again, you will be given an opportunity to revise your problem set after I have commented on it and before I grade it. You will also be responsible for distributing the problem set to your classmates no later than the day of the lecture.

Failing to distribute either the lecture notes or problem set on time will result in a penalty of 5 marks (out of the 20 total marks).

The **lecture** will be graded for clarity of exposition, quality of the presentation, and completeness.

Syllabus

Note that the syllabus is subject to change. Any changes will be announced by email and posted to the course web site.

Date	Readings	Assignment due
Jan. 7	Orientation	
Jan. 9	Sections 12.1–12.3	
Jan. 12	Sections 12.4–12.6	
Jan. 14	Section 13.1	
Jan. 16	Sections 13.2–13.5	X
Jan. 19	Molecular energy levels (handout)	
Jan. 21	Sections 14.1–14.4	
Jan. 23	no class today	
Jan. 26	Section 14.5	X
Jan. 28	Sections 14.6, 14.7	
Jan. 30	Section 14.8 and handout	X
Feb. 2	Section 14.9	
Feb. 4	Sections 15.1, 15.2	
Feb. 6	Section 15.3	X
Feb. 9	Sections 5.12, 6.2	
Feb. 11	Sections 15.4, 15.5 and handout	
Feb. 13	Test 1	
Feb. 23	Section 15.6	
Feb. 25	Section 15.7	
Feb. 27	Lattice models of polymers (handout)	
Mar. 2	Lattice models of proteins (handout)	
Mar. 4	Sections 6.4, 6.5, 6.7	
Mar. 6	Other ensembles (handout)	X
Mar. 9	Entropy, again (handout)	

Date	Readings	Assignment due
Mar. 11	Sections 16.1–16.4	
Mar. 13	Sections 16.1–16.4 (continued)	X
Mar. 16	Sections 16.5–16.7	
Mar. 18	Sections 16.5–16.7 (continued)	
Mar. 20	Test 2	
Mar. 23	Sections 17.1–17.3	
Mar. 25	Section 17.4	
Mar. 27	Discrete random walks (handout)	
Mar. 30	Continuous random walks (handout)	
Apr. 1	Sections 18.13, 18.14	
Apr. 3	Section 19.3 and RRK(M) theory (handout)	X
Apr. 6	Catch up/sum up	
Apr. 8	Graduate student lecture	
Apr. 15	Graduate student lecture	
Apr. 17	Graduate student lecture	X