

Final Preparation Guide (Chem 111, Spring 2008)

The final will test your knowledge and understanding of all the topics and techniques that we have covered in this class. Your three recommended study sources are the textbook(s), the posted tutorials, and the notes that you took in the class. Some of the posted tutorials were used as my lecture notes and I expect that you know all the background material presented there. Others demonstrated how to solve kinetics problems with *Mathematica*; you do not need to know the mathematical details of these solutions by heart. Below is a list of important topics that we have covered since the second midterm. Please consult Midterm Guides for other important topics that you should know.

NMR: principles and applications

- a. Basic principles of NMR, spin and the resonance phenomenon
- b. Shielding and NMR chemical shifts
- c. NMR as a tool to study kinetics of slow reactions
- d. Vector model to describe NMR
- e. Longitudinal and transverse relaxation, Bloch equations
- f. Determination of T₂ relaxation time from the NMR line width
- g. Spin saturation transfer experiment (Forsen–Hoffman double resonance)
- h. Line-shape analysis: simulation of spectra for two-site exchange
- i. Practical aspects of performing kinetics by NMR

The Final has two parts. The first in-class part is similar to the in-class part of your midterm exams. The main difference is that your answers to questions are worth a lot more on the final than they were on the midterms. Also, the final has a larger fraction of multiple-choice and true-false type questions. The second take-home part has two questions:

- 1) Calculate the rate constant for the unimolecular process that consists of internal rotation around the amide bond in of N,N-dimethylacetamide based on the Forsen–Hoffman double-resonance experiment that we performed in the class. The relative areas of the two N-methyl peaks were 1.000 and 0.338 in this year's experiment. If you were not able to attend the NMR experiment, you'll receive the relevant spectra at the final. (10 points)
- 2) Perform the analysis for a system under chemical exchange by line shape analysis as outline in the handout that you were given Friday. You could use either the Lineshape Analysis tutorial or the Lineshape Generation File to simulate these spectra. If you missed class on Friday, you'll get the assignment at the final. (30 pts)

Extra credit: 5 pts if you can figure out how to perform nonlinear least-squares fitting to the McConnell equations to refine HIDDEN parameters. I have not quite done this but it seems doable. I suspect that the best route is to use the solution to McConnell equation from that was derived in the Lineshape Analysis tutorial as a model. The values for relevant fixed parameters, such as relaxation times are given in the Lineshape Generation File. For things to work, initial guesses for HIDDEN parameters must be close to the true values.