CHE 344: Applications of Nuclear Magnetic Resonance
Course syllabus and policies

Spring 2009

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See our course page at moodle.gac.edu	

Introduction: This course will survey the application, hardware, and theory of a diverse range of nuclear magnetic resonance (NMR) spectroscopic techniques across the scientific disciplines. The course will focus on non-routine applications of NMR such as methods to probe structure and dynamics of large molecules or samples in the solid state, hyphenated methods (UV-NMR, LC-NMR, etc.), multidimensional spectroscopy (2-D, 3-D, 4-D), and heteronuclear methods. A vast majority of the course will involve student-led presentations and discussions of NMR use in the major chemistry subdisciplines as well as geochemistry, food science, medicine, materials science, and emerging sciences. Course work will involve discussions, literature research and short professional presentations.

Course Format: The course objectives are three fold: (i) to provide greater insight into the theory behind NMR, (ii) to break down traditional barriers by introducing the diverse research applications of NMR within the undergraduate curriculum, and (iii) provide an opportunity for you to practice preparing, delivering, and critically analyzing professional presentations, a life skill of exceptional importance post-graduation. To meet these goals, Dr. Russell and Dr. Bowers will present a few lectures of background information delving more deeply into NMR theory, relaxation behavior of nuclei, and instrument hardware over the first three weeks. After the third week, we will switch to a predominantly peer learning environment where each class period will involve student presentations and student-moderated discussions of the presentation topics. We have established broad categories to help guide your choices of topic, but exactly what we discuss is up to you!

Attendance: Because of the course objectives and format, attendance each week is mandatory. If you have a conflict you believe to be of legitimate academic merit or a family emergency, please contact Dr. Russell or Dr. Bowers as soon as possible and PRIOR TO YOUR ABSENCE. Some sort of make-up assignment will be arranged, likely a short paper related to the major topic of discussion for that particular week.

Participation: While everyone will be making an equal number of presentations over the duration of the course, not everyone will be presenting or moderating a discussion each week. However, you are expected to submit an article for every deadline (see below), read the articles that will be presented each week, and participate frequently in class discussions. Discussion

participation includes asking the presenters intelligent questions or providing insightful comments to questions posed by others.

Grade: Grading in this course is on the ABCDF scale. Grades will be based on in-class participation, quality of your oral presentations, and thoughtful critical evaluations of presented research topics.

Participation:	25%
Presentations:	50%
Research Critiques:	25%

Presentations:

Part I - The Literature Search

To help spread the workload, you will each be paired with another student to form a team. Each week, **both** student team members will be required to find and submit one research article that interests both of you and is related to the following week's topic. There is no need to read the entire article, but you should at least read the abstracts before you make your choice. A digital copy of your paper should be submitted via email to Dr. Russell or Dr. Bowers by the deadlines listed on the class schedule below (also see the schedule to determine which professor should receive your submission). Dr. Russell and Dr. Bowers will review the submissions and select articles we feel are most appropriate for presenting to the entire class while ensuring that each student makes an equal number of presentations. You will be informed via email and the course Moodle site if one of your articles is selected for presentation to the class.

A brief list of appropriate journals include American Chemical Society publications (JACS, Journal of Physical Chemistry A/B/C, Langmuir, Biochemistry), American Physical Society publications (Chemical Physics Letters, Physical Review A/B/C/etc.), Proceedings of the National Academy of Sciences, the Journal of Magnetic Resonance, Journal of Biomolecular NMR, and the Journal of Magnetic Resonance Imaging. If you find an interesting article and are unsure about the quality of the publication, see Dr. Bowers or Dr. Russell in person and we will approve or reject your request.

NOTE: Interlibrary loan is often very fast (1-3 days)! Do not ignore interesting articles because we do not have access to their content online—just submit an ILL request.

Part II - The Presentation

If an article your team submitted is selected for presentation, you will be required to prepare and deliver a ~ 15 minute presentation to the class consisting of a ~ 10 minute Powerpoint slideshow summarizing the paper and a 5 - 7 minute student-lead discussion. Both team members should work together to prepare the Powerpoint slides and a list of questions to stimulate class discussion. The slide show should clearly explain the paper's topic, motivation, experimental methods, results, and conclusions to the class. You should also provide one slide where you critically evaluate the results of the study and its broader implications for the scientific community. Your list of questions should consist of three to

four questions about the paper that you feel will stimulate an interesting class discussion. One member of the team will be designated by Dr. Russell or Dr. Bowers to present the powerpoint slides and the other will be responsible for moderating the class discussion (introduce speaker, ask the audience questions, keep things moving, stop on time, etc.). Both of you should be prepared to field questions from the audience, including Dr. Russell and Dr. Bowers.

Your presentation will be evaluated according to the following criteria by both instructors. We will then average our evaluations to determine your presentation grade.

- Quality (20%) - Is the layout and design of the slides appealing? Were the slides too crowded or was space well utilized? Did you incorporate animations that were useful rather than distracting to the audience? Were there spelling errors on the slides? Was the formatting uniform on all slides? Did you incorporate too many words or not enough pictures? Did you include a bibliography slide? Was the slide background you chose distracting?
- Delivery (30%) - Did you dwell on the slides too long? Did you maintain eye contact with the audience? Did you look at the screen too often? Was the presentation well organized? Did the presentation flow smoothly from start to finish? Did you pause or stutter during delivery? How well did you handle the questions at the end of your presentation?
- Technical Merit (40%) - How informative was your presentation? Was the information accurate and supported with proper citations? Did you present the chemical concepts clearly to the audience? Did you use proper chemistry vocabulary during your presentation?
- Time Management (10%) - Was the presentation within a 10 ± 1 minute window? If it went over or under the goal, by how much did it miss the mark?

Research Critiques: Every student must critically evaluate the scientific content (not the actual presentation) of three papers presented by other teams over the course of the semester. From the notes you take in class, prepare a double-spaced summary and critique typed in 12 pt Times font and with 1" margins all around. This document should be no more than two pages with a target length of 1.5 pages. The first paragraph should summarize the presented research, focusing on the methods, key findings, and conclusions made by the authors of the source paper. Be sure to note the names of the authors and the title of the paper somewhere in this paragraph. The second paragraph should include your critique of their methods and conclusions and is also a venue for you to propose potential new hypotheses and methods of testing them. The critiques should be submitted via email to Dr. Bowers on the due dates listed in the schedule below. Grading will be based on timely submission, content (presence of a detailed summary and critique paragraphs), quality of the writing, and evidence of good critical thinking. The due dates for your critiques are listed in the course schedule below. A sample critique has also been included at the end of this document.

Honor code: As members of the Gustavus Adolphus College community of scholars, we have all agreed to abide by an excellent honor code, which you signed upon admission to the college. If you have forgotten the details of this code, please refer to the Academic Bulletin.

"On my honor, I pledge that I have not given, received, nor tolerated others' use of unauthorized aid in completing this work."

An integral part of the honor code is non-tolerance of violations. Under our code, students are not expected to police others' actions. Rather, you agree to report violations of which you become aware. Failure to do so will constitute an honor code violation in this class. Any student found in violation of the academic honesty policy and honor code will receive a grade of 0 for that assignment. A second offense will result in an F for the course and the Dean will be notified. If you have any questions about these policies, please come see us.

Accommodations: If you have specific physical, psychiatric, attentional, or learning disabilities and require accommodations to help you fulfill course expectations, please let us know during the first week of class so that your learning needs may be appropriately met. You will need to provide documentation of your disability to Laurie Bickett in the Academic Advising Center. Discussions will remain confidential.

Class schedule: Below is a rough/tentative outline of the course topics. The most updated version of the schedule will always be posted at our Moodle page (moodle.gac.edu).

Week	Course Topic	Homework Due
February 9-13	Planning & class overview	
February 16-20	NMR Review and New	
February 23-27	Relaxation: not quite as fun as it sounds	
March 2-6	NMR hardware	☐ Solution Structure Articles due 3/5 to Dr. Russell
March 9-13	Solution structure	
March 16-20	""	☐ Critique 1 due 3/20 ☐ Solid State Structure Articles due 3/19 to Dr. Bowers
March 23-27	NO CLASS - SPRING BREAK	
March 30-April 3	Solid state structure	
April 6-10	""	☐ Dynamics Articles due 4/9 to Dr. Russell
April 13-17	Dynamics	
April 20-24	""	☐ Critique 2 due 4/24
April 27-May 1	Unpaired electrons & the NMR spectrum	☐ Unpaired Electron Articles due 4/30 to Dr. Russell
May 4-8	Imaging	☐ Imaging Articles due 5/7 to Dr. Bowers
May 11-15	Hyphenated methods	☐ Hyphenated Articles due 5/14 to Dr. Bowers
May 18-20	TBD	☐ Critique 3 due 5/20

Sample Critique - Molecular Modeling in Environmental Chemistry

Scientific and public interest in environmental chemistry is rapidly on the rise. One motivating factor for this increased global awareness is the realization that pollution affects all members of our society. Because new chemicals and products are constantly being introduced into the environment, it would be beneficial if we had some method to predict the toxic effects of chemicals without lengthy biochemical or biomedical trials. On Friday, April 4, 2003, Dr. James Kubicki of the Penn State Department of Geoscience presented his work on modeling the toxicity of poly-aromatic hydrocarbons (PAH) in the environment, specifically the relationship between PAH's, mineral adsorption, and phototoxicity. Kubicki *et al.* set out to determine weather HOMO-LUMO energy gaps calculated by simulation would be capable of predicting the environmental partitioning and toxicity/phototoxicity of PAH's quickly and accurately. To this end, initial minimum energy structures were calculated with HyperChem 4.5 (a semi-empirical program) followed by further minimization with Gaussian 94 (G94) in the HF/3-21G** and B3LYP/6-31G* basis sets. Once the minimum energy structures were obtained, the HOMO-LUMO gap energies were calculated with Keith and Frisch's self consistent isodensity polarized continuum model (SCIPCM) predictions for the gas-phase PAH's[1]. A minimum energy solvation model was then constructed for the PAH's with G94 in the HF/3-21G** basis. The solvated PAH's were placed within a polarized continuum to model other solvents and the SCIPCM model was applied to calculate new minimum energy structures with HF/3-21G** and B3LYP/6-31G* basis sets. Adsorption of these solvated PAH's on various mineral surfaces were then modeled with varying levels of theory in G94, and the HOMO-LUMO gaps recalculated. It was found that the level of theory played an important role in both the accuracy of the gap calculations and the speed of the simulations. It appears that density functional theory provided good accuracy in combination with efficient computation.[2] They also conclude that HOMO-LUMO gaps do not explain/predict the

phototoxicity of adsorbed PAH's,[2] suggesting that the scientific community needs better ways of modeling these behaviors if we are to use computational chemistry to predict the behavior of other potentially toxic compounds.

It is apparent that the environmental systems that Dr. Kubicki and his colleagues try to model are extremely complex. The lack of modeling in environmental chemistry is likely a consequence of this complexity. It would be difficult to represent all of the factors in an environmental process to create a good simulation engine applicable to many real systems. It was unclear from the presentation how all of these complex interactions were taken into account, which makes the utility of simulations for environmental systems seem questionable. However, the complimentary nature of computational and experimental chemistry was quite evident in this work. More detailed research should continue if we are to use such models in a predictive fashion.

References

1. Keith TA, Frisch MJ. *Inclusion of Explicit Solvent Molecules in a Self-Consistent Reaction Field Model of Solvation.* In Smith, DA (ed), *Modeling the Hydrogen Bond*, ACS Symposium Series 56. American Chemical Society, Washington, DC. 1994, Pg. 22-35.
2. Kubicki J. D., Blake G. A., and Apitz S. E. **Molecular models of benzene and selected PAHs in the gas, aqueous, and adsorbed states**. *Environmental Toxicology and Chemistry*, 1999, *18*, 1656-1662.
3. Kubicki J. D., Sykes D., and Apitz S. E. **Ab initio calculation of aqueous aluminum and aluminum-carboxylate NMR chemical shifts**. *Journal of Physical Chemistry A*, 1999, *103*, 903-915.
4. Kubicki J.D., Itoh M.J., Schroeter L.M., Apitz, S.E. **Bonding Mechanisms of Salicylic Acid Adsorbed onto Illite Clay: An ATR-FTIR and Molecular Orbital Study.** *Env. Sci. and Tech.*, 1997, *31*, 1151-1156.