13-140
LSC: App-3/13/14
UWUCC: App-4/1/14
Senate: App-4/29/14

REVISION APPROVAL COVER SHEET FOR CONTINUATION OF W-DESIGNATION

TYPE II DEPARTMENT COMMITMENT

Professor Anne Kondo

Department Chemistry

Email akondo@iup.edu

Course Problems in Chemistry

Please provide answers to these questions on the next page:

1. Include the most recent syllabus for the Type II course.
2. Include a new "Statement Concerning Departmental Responsibility". The statement of departmental responsibility" explains how the department will ensure that the writing component is present regardless of who is teaching the course. It needs to identify the specific department group or individual who is responsible for ensuring this.

Approvals:	**Signature**	**Date**
Professor (s)	Anne Kondo	2/4/14
Department Chair		11/31/14
College Dean		2/5/14
Director of Liberal Studies		3/14/14
UWUCC Co-chair(s)	Gail Sechrist	4/1/14

Received
FEB 10 2014
Liberal Studies

TYPE II DEPARTMENT COMMITMENT

Professor Anne Kondo Department Chemistry

1. Include the most recent syllabus for the Type II course: Sample from chemistry student [redacted] with Dr. Justin Fair is attached

2. Include a new "Statement Concerning Departmental Responsibility". The statement of departmental responsibility" explains how the department will ensure that the writing component is present regardless of who is teaching the course. It needs to identify the specific department group or individual who is responsible for ensuring this.

Chemistry Department/Biochemistry Program Statement of Responsibility for All Writing-Intensive Courses:

The chair/coordinator shall provide a copy of this agreement to each faculty member assigned to teach a Writing-Intensive course.
Each faculty member assigned to teaching a Departmental/Program Writing Intensive Course agrees to the following criteria:

- Writing assignments are an integral part of the course, which promise to enhance student learning (not 'exercises in writing for writing's sake').
- Writing assignments will include various forms of writing such as case studies, laboratory reports, journals, letters, memos, formal essays, research articles, project or grant proposals, etc.
- The improvement of student writing is a clear objective of the course.
- Students will be provided with written instructions that cover major criteria for the evaluation of the assignment(s).
- Students will receive guidance in conceiving, organizing, and presenting written material in ways appropriate to the field of Chemistry/Biochemistry.
- Students will produce at least 5000 words (15-20 typed pages) of writing that will be critically evaluated.
- Each writing assignment will have specified length in terms of minimum number of pages required.
- Writing assignments include at least one major assignment and several shorter different assignments.
- Students will be required to submit drafts of at least one major writing assignment that will be returned with instructor comments/suggestions for improvement before the final copy of the assignment is due, so that students have an opportunity to revise their written work.
- Students will submit final copies of writing assignments for critical evaluation.
- Instructor evaluation of written work will comprise at least 50% of the course grade.
- At the end of the semester, faculty teaching W courses will submit copies of their syllabi to the curriculum committee for review and discussion, if needed.
- At the end of the semester, faculty teaching CHEM 498 W courses will submit copies of completed final writing assignments to the department chair, which is a standard part of the review for re-certification of the American Chemical Society certified degree.

Problems in Chemistry
SYLLABUS – FALL, 2013

Instructor: Dr. Justin Fair
138 Weyandt Hall
Or by Appointment
Campus Phone: (724)-357-4477
Email: jfair@iup.edu

Office Hours:
M: 8:30-11:30 am
T: 9:15-10:15 am
R: 9:15-10:15 am
or by appointment

CHEM 498 **0c-0l-1cr**
Prerequisites: CHEM 112 or 114, CHEM 231 and permission of the department chairperson.

Catalog Description: A course of supervised undergraduate research in conjunction with a faculty member in the chemistry department.

1) **Rationale for Conducting an Independent Study**
[redacted] is requesting to take one credit of CHEM 498 in Fall 2013 to complete the research requirement necessary for graduation with a B.S degree in chemistry.
2) **The Purpose of the Study**
[redacted] plans to computationally study the kinetics of the Finkelstein reaction and, using the results, develop an undergraduate computational kinetics exercise to complement an exercise developed based on experimental data obtained by another student. The addition of the computational chemistry will be able to add a stronger understanding of the different states (ground, transition, and product) involved in the reaction.
Throughout the computational study, multiple reaction schemes will be studied as well: a Finkelstein reaction with different alkyl bromides as the reactants. The experiment will be used to study the effects of adding carbons to the beta carbon on different kinetic factors of the reaction.
3) **Objectives**
    1. The transition state for the reaction of butyl bromide with iodide will first be determined using transition-state optimization, verified with vibrational frequency calculations. These geometries will be determined and evaluated using quantum mechanical means with CCSD, MP2, HF. Within each of these QM methods each available basis set for the necessary atoms will be run (3-21G, 6-311G, 6-311G* 6-311G**).
    2. Ground state geometries for the starting materials, products, and their complexes will be found and evaluated using the methods in objective 1 above.
    3. The effects of solvation in acetone will be determined using the dielectric constant and solvent radius as the solvation parameters in the COSMO solvation model.
    4. Compare the experimental kinetics in acetone to those calculated in acetone and determine best QM method and basis set.
    5. After determining the optimal QM method and basis set, the following substrates will be evaluated and compared to literature kinetic data: methyl bromide, ethyl bromide,

propyl bromide, isopropyl bromide, isobutyl bromide, neopentyl bromide, and tert-butyl bromide.

6. The final write up will include a thorough background of literature and include discussion on the kinetics of a Sn2 reaction on 1) substituents at the alpha carbon and 2) substituents at the beta carbon.
7. My research will be concluded with a presentation of my findings at an ACS regional conference.

4) Activities to Accomplish Objectives

1. *August 26 – September 30*
    - Determine transition state of methyl, ethyl, propyl, isopropyl, butyl, isobutyl, tert-butyl, and neopentyl bromide with iodide by transition state optimization, verified by vibrational frequency calculations with HF and MP2 using 3-21G initially. These two computational methods are used initially due requiring less calculation power.
    - Repeat calculations with HF and MP2, each with the following larger basis sets: 6-31G, 6-31G*, 6-311G, 6-311G**, 6-311+G**
    - Determine starting and product complexes with IRC Forward and IRC backward from each transition state. Optimize each complex with geometry optimization using 3-21G
    - Repeat calculations with HF and MP2, each with the following larger basis sets: 6-31G, 6-31G*, 6-311G, 6-311G**, 6-311+G**
    - Calculations will be repeated with higher cost computational methods (i.e.: CCSD), and the methods used will be determined based on the results of the HF and MP2 calculations.
2. *September 31 – October 14*
    - Research experimental kinetics for the reaction of butyl bromide with iodide in acetone and compare results to calculated energies
        i. Use comparison to determine best QM model and basis set for kinetic computations in acetone
3. *Week of November 4*
    - First draft of thesis paper will be turned in at weekly meeting
4. *Week of December 9*
    - Final draft of thesis will be submitted at weekly meeting along with a rough draft poster for a presentation at an ACS regional conference
5. *Week TBD*
    - Professional meeting to disseminate results via a poster

5) Required Reading/Bibliography

1. Pace, D.R; Regmi, Y. "The Finkelstein Reaction: Quantitative Reaction Kinetics of an S_N2 Reaction using Nonaqueous Conductivity." *J. Chem. Educ.* **2006**. 1344-1348

2. Carrion, F.; Dewar M.J.S. MNDO Study of S_N2 Reactions and Related Processes. *J. Am.Chem. Soc.*,**1984**, *106* (12), pp 3531–3539
3. Clauss, A; Nelson, S. Integrating Computational Molecular Modeling into the Undergraduate Organic Chemistry Curriculum. *J. Chem. Educ.* **2009,** *86 (8)*, 955-957
4. Wright, S.W. "A Demonstration of the S_N2 Reaction and the Effects of Structure, Leaving Group, and Solvent." *J. Chem. Educ.* **1992**, *69* (3), 235-236.
5. Ditchfield, R.; Hehre, W. J.; Pople, J. A., "Self-Consistent Molecular-Orbital Methods. IX. An Extended Gaussian-Type Basis for Molecular-Orbital Studies of Organic Molecules," *J. Chem. Phys.*, **1971**, *54*, 724-728.
6. Dunning, T. H., Jr., "Gaussian Basis Sets for Use in Correlated Molecular Calculations. I. The Atoms Boron Through Neon and Hydrogen," *J. Chem. Phys.*, **1989**, *90*, 1007-1023.
7. Finkelstein, Hans. "Preparation of Organic Iodides from the Corresponding Bromides and Chlorides *Berichte der Deutschen Chemischen Gesellschaft.* **1910**, 43, 1528
8. Hehre, W.J. *A Guide to Molecular Mechanics and Quantum Chemical Calculations.* Wavefunction Inc: Irvine, CA, 2003.
9. Cramer, C.J. *Essentials of Computational Chemistry: Theories and Models.* 2nd Ed. John Wiley and Sons: West Sussex, England, 2004.

6) Evaluation Process

1. 10% - Attendance at weekly meetings
    i. A letter grade will be dropped for each missed meeting
    ii. A power point will be presented at each meeting
2. 5% - Work on project 5 to 6 hours a week
    i. Time on project will be recorded in the back of the lab notebook as a log
    ii. Calculations will be kept organized to follow the different phases in which the reaction is analyzed in (gas versus solvent)
3. 5% - Keep a well-structured notebook with extensive data recording
    i. First couple pages will contain a table of contents
    ii. Data will be organized by day, and labeled by appropriate reaction schemes
    iii. The particulars of the structure will follow guidelines set by the research advisor
    iv. When project is complete, the notebook will be turned in, along with any other record of data. There will be no grade given if this is not done.
4. 10% - Progress power points
    i. It will be at least approximately 10 slides each week
    ii. It must cover progress gained over the past week's work
    iii. The end must explore plans for the current week
    iv. Include any new introduction material that would be necessary in a formal report for the progress and/or plans presented

5. 15% - Rough Draft Thesis Paper
    i. Includes rough draft of at least introduction, results, and conclusion
    ii. Introduction
        1. will include background on kinetics of Sn2 reaction
            a. At the alpha carbon
            b. At the beta carbon
        2. Will include a brief background of the quantum mechanics behind computational chemistry to afford the reader an understanding of the increasing basis sets and the difference between the models used
6. 35% - Final Thesis Paper
    i. Should include above mentioned information in introduction
    ii. Method should include discussion of overcoming errors in input files and specifications of parameters used to describe solvent in each solvent model
    iii. Conclusion will compare literature data to calculated results from Gaussian computational analysis and discuss the accuracy of each basis set/computational model.
    iv. Conclusion will discuss patterns apparent in the results as the alkyl bromide structure increases in number of carbons and with constitutional isomers
7. 20% - Regional meeting poster presentation
    i. Disseminate findings at a regional ACS meeting (this presentation can be done during the spring 2014 semester).

7) Use for Special Purpose

This semester of research will be used to fulfill one of the writing intensive requirements.

8) Number of Credits

This course is being taken for one credit.