CHM3915 PHYSICAL CHEMISTRY LAB - GOALS AND STRUCTURE

Prerequisites:  Physical Chemistry CHM3910 (grade of C or better is recommended)

Instructors:  Dr. R.A. Peebles  Rm. PSB4037 ; 581-5906 ;  cfsp@eiu.edu
Dr. S.A. Peebles     Rm. PSB3420 ; 581-2679 ;  cfsp@eiu.edu


Additional lab materials:  You must have a 50 or 100 page duplicate copy lab notebook (“The Official Laboratory Notebook”, available from the bookstore) to record your pre-lab assignments, in-lab data, and any hand-calculated analysis.  These notebooks are from Jones and Bartless Publishers: 50 page ISBN 0-7637-0515-2; 100 page ISBN 0-7637-0516-0

Course Format:  The course consists of one hour of lecture and one four hour laboratory period per week.  Both are mandatory; you will not be allowed to perform the experiment if the pre-lab lecture is missed without a valid excuse.  Arriving more than 10 minutes late for an experiment will result in a 5% deduction on your grade for that experiment.

Goals:
1. To obtain hands-on experience with a number of instruments and techniques commonly used in physical chemistry.
2. To obtain measurements of physical phenomena and to develop an awareness of the influence of experimental errors on data.
3. To develop competence in technical report writing in the form of laboratory reports.
4. To develop a good working knowledge of Excel and to learn how to use it for efficient data analysis.
5. Last, but not least, to allow you to develop good time management and organizational skills.  In order to produce a good quality, detailed lab report on time, you must prepare well ahead of the deadline! Starting work on the lab report the night before it is due is not acceptable!  Start the writing as soon as you start the experiment.  If you are in any doubt as to whether this sort of approach is really necessary in a class at this level, talk to one of the graduating seniors and ask their advice!!

Structure and Grading:
  Eight experiments and laboratory reports carried out according to the attached schedule will constitute the core of the course.

  You are expected to perform all laboratory experiments in the time allotted.  Your overall grade depends very heavily on the quality of your lab reports.  Approximately 85% of the course grade will be determined from eight formal laboratory reports and 15% from pre-lab assignments/your notebook/your general lab preparation.  In this and other handouts you will find the objectives of the course, a list of the experiments, and style guidelines for writing the reports.  You are urged to consult The ACS Style Guide to help you with your writing.  Although it is possible to write a competent report with poor laboratory data, the task of writing the report will be considerably more difficult.  It is worth taking the time to carefully collect data; make sure you seek help in the analysis or writing if there is anything you don’t understand.

You must perform every experiment and hand in every laboratory report in order to pass this course.

Late reports increase the time taken to return graded reports and so inconvenience every student in the class.  Therefore, late reports will be penalized 5% for every day they are late, including weekends.  A second late lab report will be penalized 7% per day, a third late report will lose 9% per day and so on.  Please make every effort to turn in your labs ON TIME.

Lab reports not turned in by 7 days beyond the posted deadline will receive a grade of zero. Lab reports must be turned in by 3:00 pm on the due date to avoid late penalties.
Labs can be made up only for documented reasons. If you know ahead of time that you will miss a lab, you must notify the instructor before the lab, as soon as possible.

Grading will be on the following scale – subject to change by the instructors:

<table>
<thead>
<tr>
<th>Grade</th>
<th>Percentage</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>88 - 100%</td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>78 - 87</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>68 - 77</td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>58 - 67</td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>0 - 57</td>
<td></td>
</tr>
</tbody>
</table>

**General Comments:**
You must thoroughly familiarize yourself with the experiment before you enter the lab. Pre-lab assignments will be given for each lab to familiarize you with the material and the nature of the measurements you will be taking. Pre-lab assignments (which will be completed in your duplicate copy notebook) must be turned in by 9 am on the day of your lab (8 am for 8 o’clock sections) and form an essential part of your preparation for the lab. Failure to turn in a completed pre-lab assignment (or turning in a plagiarized pre-lab assignment) will mean you will be unable to carry out the experiment, and hence will receive a grade of zero for that lab.

Read through the lab handout and know what data you will be collecting so you can utilize your time in lab efficiently. Preparing a rough table for data collection before coming to lab will help to ensure that you are well organized and that you don’t waste time in lab trying to figure out what to do. Writing up the Introduction section before the lab period will assist you in understanding the requirements for the experiment and will reduce the amount of effort spent on writing up the lab after you complete the experiment. You will need a bound duplicate notebook to record the data (available from the bookstore – see start of this handout). The duplicate pages for each experiment will be turned in with the completed report and will be checked for clarity, completeness and accuracy. Note that poorly kept and incomplete lab notebooks will negatively impact your final grade in this class.

**Laboratory Reports (including an important note on plagiarism):**
Your report must be prepared by a word processor. Graphs and regression calculations should be prepared with Excel or other graphics/spreadsheet software. Equations and unusual symbols may be neatly handwritten or prepared using the Equation Editor function in Microsoft Word. Occasionally an experiment may not function as expected. The fault may lie with the experimenter or with the apparatus. On these occasions when the problems are beyond your control (e.g., the apparatus breaks down) you can still write a satisfactory report. Your write-up should describe the experiment, analyze the difficulty and describe the data. In cases such as these, you should describe where the experiment failed and propose what may have been the cause of the problems. Experiments that do not work according to plan provide considerably more material for discussion than those that function as expected.

All laboratory reports should follow the prescribed format (attached). Be sure to give a reference for any data or material that you cite in your lab reports but do not copy large portions of the handout or text books or any other source – this is plagiarism and will be dealt with according to university policy on cheating. Likewise, copying of text, graphs, spreadsheets, diagrams etc. from other students’ lab reports will be regarded as plagiarism and you risk failing this course if you are caught doing this. **ANY cases of plagiarism or cheating of any form will be referred to the Office of Judicial Affairs.** Remember that this is a writing intensive course and one of the aims of this laboratory is to give you experience in writing good quality, informative lab reports of the same format as a manuscript that would be submitted to a peer reviewed journal. You should therefore make an effort to improve the quality of your reports with each experiment. Read the comments on your graded lab reports and make sure you address these problems in future reports; there’s nothing more depressing and frustrating than seeing points being lost for the same mistakes you made on previous lab reports.

Carefully proofread the final report, check the spelling and grammar, and make sure the report is clear and concise. Spelling, grammar and overall clarity will make up a portion of the grade for each experiment. The report should be written at a level designed to be understood by a chemist who is reasonably experienced, but not familiar with your particular experiment.
To give you an opportunity to adjust to the different report writing styles in this course from the lab courses you have had previously, you have the option of rewriting the first lab from each instructor – be sure to pay close attention to the comments on the returned lab and you will be guaranteed to improve your grade (more details in the next section)!

Finally, note that there is a minimum required standard of lab report that must be met for you to pass this course. Repeated poor grades (<70%) in lab reports are an indication that your data analysis/report writing skills are poor; such grades will seriously affect your overall grade – do not rely on a curve in this class to pass you (it won’t happen).

Report rewrite
Since this is a writing intensive class, to improve your skills in editing a manuscript, the first lab report from each instructor can be rewritten. We will give you back your original draft, with comments, and you will make the corrections and additions and turn back in the edited copy. Remember to turn in the original report as well! Note that any late penalties that applied to the original will also apply to the rewrite and any additional late penalties will also be assessed on the rewrite. You will only be able to regain up to 50% of the points you lost on the original draft so it is important that you do the best job possible on the original version. For instance, if you get a 90% on the original, you can get a maximum of 95% on the rewrite. If, however, you decide to do a very poor job on the original since you know that you can rewrite it, and end up with a 40% (highly likely if you give the original less than your best effort) the best you could do is 70% on the rewrite.

Short form reports
For students who maintain a B average (78% or better) on four consecutive lab reports, a short form report may be submitted. This short form report omits the Abstract and Introduction sections (so any equations that you use must be included in the Results section). As long as your average over 4 consecutive labs remains above a B you may continue to submit short form reports.

A complete report format and checklist is provided below. Points will be lost for each section that is missing or incomplete. See separate handout for additional details on each section.

General format (also see separate handout)
Double spaced, 10 or 12 point, 1-1.25 inch margins, numbered pages

Cover Sheet
1. Course and section number.
2. Title and number of experiment as given in handouts.
3. Your name.
4. Your partner's name(s).
5. Date submitted.

Abstract
A short paragraph summary of:
1. Experimental purpose.
2. Experimental technique.
3. Principal experimental results including numbers with uncertainties.
4. Major conclusions.

I. Introduction
1. Purpose of the experiment.
2. Brief description of the theoretical model(s) including equations which relate the data to the results.
3. How information is obtained.
4. How and why the information is useful.
II. Experimental
1. Apparatus.
2. Reagents.
4. Block diagram.

III. Data
1. Instrumental readout/spectra (with descriptive captions and figure numbers).
2. Data tables (again with captions and table numbers).
3. Text describing/introducing the tables, spectra, etc. and referring to these by number.

IV. Calculations, Precision Limits, and Results
1. Sample calculations.
2. Precision limits based on propagation of error or appropriate statistics.
3. Tabulated summaries of redundant calculations.
4. Table of final results with:
   a. precision limits.
   b. correct number of significant figures.
   c. appropriate units.
   d. literature values.
   e. accuracy (as measured by percent deviation from literature values).

V. Discussion
1. Interpretation and comparison of results.
2. Logical implications of results.
3. Results versus goals of the experiment.
4. Comparison of results with literature or expected values.
5. Suggested improvements for the experiment and alternate methods for meeting the goals of the experiment, if appropriate.

VI. References
1. ACS format for journal articles, books, etc.
2. ACS format for private communications and handouts.

"THE ACS STYLE GUIDE—2nd Edition"
SELECTED SECTIONS OF PARTICULAR IMPORTANCE

Grammar, Style and Usage (Chapter 2)
1. Grammar p. 49
2. Punctuation p. 56
3. Spelling p. 67
4. Hyphenation p. 75
5. Capitalization p. 83
6. References* p. 176
   Periodicals
   Books p.186
   Internet sources p. 211
Illustrations and Tables (Chapter 3)
1. Illustrations* pp. 295
2. Tables* pp. 300
3. Lists pp. 135

* Make special note.

SAMPLE TABLE
One of the many skills you will be improving this semester is the ability to present data and results in a table. A sample table layout is shown below and illustrates many of the important aspects of setting up a table.

Note that the table title and column headings should be informative. A well thought-out table should stand alone, without the need for reference to the text of the report. If necessary, define any relevant terms in a footnote to the table. An example is shown below.

Table III. Comparison of calculated and experimental methyl cation affinities (MCAs). a)

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Basis set</th>
<th>HF b)</th>
<th>Level of calculation</th>
<th>MP2 c)</th>
<th>MP3 c)</th>
<th>MP4 c)</th>
<th>Expt. d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H2O</td>
<td>6-31G*</td>
<td>56.2</td>
<td>72.3</td>
<td>69.5</td>
<td>71.1</td>
<td>68.5</td>
<td></td>
</tr>
<tr>
<td></td>
<td>6-31G**</td>
<td>56.2</td>
<td>72.1</td>
<td>69.4</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>6-31+G*</td>
<td>52.7</td>
<td>66.7</td>
<td>64.8</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>6-31+G**</td>
<td>52.0</td>
<td>65.8</td>
<td>64.1</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td></td>
<td>6-311+G**</td>
<td>51.2</td>
<td>66.2</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>6-311++G(2d,2p)</td>
<td>50.3</td>
<td>64.9</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH3OH</td>
<td>6-31G*</td>
<td>68.3</td>
<td>85.0</td>
<td>82.2</td>
<td>81.2</td>
<td>84.0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>6-31G**</td>
<td>68.0</td>
<td>84.8</td>
<td>81.9</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>6-31+G*</td>
<td>63.6</td>
<td>78.5</td>
<td>76.3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>6-31+G**</td>
<td>65.1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(CH3)2O</td>
<td>6-31G*</td>
<td>74.2</td>
<td>92.1</td>
<td>89.2</td>
<td>91.0</td>
<td>93.0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>6-31G**</td>
<td>74.1</td>
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<td></td>
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<td></td>
</tr>
<tr>
<td></td>
<td>6-31+G*</td>
<td>72.1</td>
<td>89.2</td>
<td>86.9</td>
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<td></td>
</tr>
</tbody>
</table>

a) MCA values are in kcal/mol, and are calculated utilizing total electronic energies from this work and references 4, 7 and 25. See text for details.
b) Hartree Fock level calculation
c) Møller-Plesset perturbation calculations to second order (MP2), third order (MP3) or fourth order (MP4)
d) Experimental values - this work or reference 2.