No (specifically) Required Textbook: Notes for this course will be provided online; Complete understanding of the activities will require external resources to be sourced by the individual. It is assumed that you have access to a typical Physical Chemistry textbook, such as the one used in CHM4411.

Contact Brucat if you have questions...

Instructor: PJ Brucat
- Office hours (subject to optimization):
  Wednesday 10:00 - 12:00; 15:30-16:30
  Friday 09:00 - 10:00
- or by appointment (message three choices)
- Contact method: Canvas Messaging only. No Email.

TA: Yiheng Yan

Course Website:
https://ufl.instructure.com/courses/471120

All communication and activities related to this course will be accessible from within UF’s campus-wide eLearning system (Canvas) at the URL above. Please become familiar with our course website as soon as possible. Much of the materials there are subject to revision, so pay careful attention to all announcements, updates, and revision dates. It is strongly advised that hardcopy or static downloads of course materials be avoided due to their continuous incremental improvement.

Etiquette

Your polite, courteous, and civilized behavior is expected in all aspects of our course. This holds especially true in these times of stress and uncertainty. Be Human. Be good to each other. Smile.
Goals and Objectives

Course Goals
Successful completion of this course will enable the learner to:
- Apply the Scientific Method to the Investigation of the Natural World
- Synthesize the Concepts of Thermodynamics, Transport, and Kinetics (Topics in CHM4411) into Testable Hypotheses
- Master the Basic Concepts of Experimental Design
- Apply Modern Computational Tools to Diverse Data Analyses
- Communicate Scientific Observations and Conclusions Concisely and Effectively

Course Objectives
Accomplishment in the course material will be assessed in the following:

Knowledge
- Statistical Methods in Extracting Model Parameters from Data
- Basic Elements of Scientific Programming
- Proper Conventions and Requirements for Rendering Scientific Observations

Skills
- Collection and Manipulation of Data
- Creation of Publication-Quality Figures
- Authoring High-Quality Short Reports/Executive Summaries

Course Operation

Course Meetings
There are two meeting types intrinsic to the learning experience of this course.

1. Lectures This course has regularly-scheduled meeting times designated for synchronous meetings of the entire class. These meetings are a one-on-many environment primarily for discussion and explanation of new material outlined in the course. Attendance at these meetings is strongly encouraged. If you fail to absorb information from these discussions, you will have difficulty completing the laboratory challenges.

2. Laboratory Sessions The actual experimentation will take place in the PChem Teaching Laboratory, LEI 248. It should go without saying that physical attendance in the lab session is required. If you are unable to attend the lab session, notify the instructor as soon as possible prior to that session. If the absence is allowable by University policy https://catalog.ufl.edu/UGRD/academic-regulations/attendance-policies/, a makeup session will be arranged. No grade points will be awarded for any assignment associated with a session you did not attend.
Communication with your Instructor

To guarantee rapid, reliable, and secure transmission, all course communications with your instructor(s) are to occur within the Canvas environment using the embedded tools. Configure your Canvas account profile for immediate automatic notification of course announcements and updates, and make sure that email forwarding, if desired, is set up correctly. It is expected that all replies to messages between instructor and student occur within 24 hours. Responsibility for receiving and responding to electronic course communication in a timely fashion is entirely that of the student.

Groups

Laboratory activities will be undertaken in groups of two. Your group designation will determine the laboratory activity schedule. Group assignments may be found in the course Canvas website.

You are expected to work professionally and efficiently with your group partner. Troublesome partnerships will suffer from poor subjective grades.

All graded assignments will be be worked and submitted as individuals. Clearly, data sharing and other collaboration is expected between the group members, but copying assignment submissions or other is not allowed. Assignment submission are to be your own original work. Plagiarism in any way is a violation of UF’s Honor Code.

Graded Assignments

Analysis Quizzes (AQ)

For each lab activity, short question sets will be delivered online through our course website. These are intended to be formative assessments, in that these activities focus on and cement concepts in the learners mind. These quizzes are entirely based on material relevant to the analysis and interpretation of your observations, and should be helpful in the crafting of your ES report, vide infra. Any resources may be used to solve these quiz problems, as long as they are worked entirely individually, without consultation with anyone except your instructors. You may discuss the quiz only with your instructors until after the due date has passed for everyone in the class.

Python/Jupyter Notebook (NB)

Data visualization and quantitative analysis is key to any experiment, and the Scientific Method in general. The Jupyter notebook environment, running a Python3 kernel, will be used for processing the numerical results of the guided inquiries of the lab. No, Excel or other spreadsheet programs will not be suffient. Students will submit Python notebooks to our class Jupyter server as part of their reporting. Fear not. No prior programming experience is necessary to master the creation and use of these notebooks. Extensive hints and templates will be provided.

Executive Summary (ES)

After each lab session you will be asked to report your observations. This will be in the form of an executive summary of the hypotheses, procedures, findings, and conclusions. Some form of data analysis and graphical representation, usually in the form of publication-quality captioned figures will be required. The ES is a shorter, more focused, and less formal than a typical journal publication.

Each ES will be submitted to the appropriate Canvas assignment page the format requested for grading. Some materials may be need to be authored on or uploaded to the class Jupyter server. Submissions not in the format requested will be ignored.
### Laboratory Activity Schedule

(Tentative; see course website)

<table>
<thead>
<tr>
<th>Week</th>
<th>Date</th>
<th>Lecture</th>
<th>Group ID</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>MG1</td>
</tr>
<tr>
<td>1</td>
<td>01/09</td>
<td>01</td>
<td>PD</td>
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<tr>
<td>2</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>01/23</td>
<td>02</td>
<td>HPA</td>
</tr>
<tr>
<td>4</td>
<td>01/30</td>
<td>03</td>
<td>HPB</td>
</tr>
<tr>
<td>5</td>
<td>02/06</td>
<td>04</td>
<td>AE</td>
</tr>
<tr>
<td>6</td>
<td>02/13</td>
<td>05</td>
<td>ARA</td>
</tr>
<tr>
<td>7</td>
<td>02/20</td>
<td>06</td>
<td>ARB</td>
</tr>
<tr>
<td>8</td>
<td>02/27</td>
<td>07</td>
<td>CEA</td>
</tr>
<tr>
<td>9</td>
<td>03/06</td>
<td>08</td>
<td>CEB</td>
</tr>
<tr>
<td>10</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>11</td>
<td>03/20</td>
<td>09</td>
<td>PKA</td>
</tr>
<tr>
<td>12</td>
<td>03/27</td>
<td>10</td>
<td>PKB</td>
</tr>
<tr>
<td>13</td>
<td>04/03</td>
<td>11</td>
<td>PT</td>
</tr>
<tr>
<td>14</td>
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<td>MUW</td>
</tr>
<tr>
<td>15</td>
<td>04/17</td>
<td>12</td>
<td>XX</td>
</tr>
</tbody>
</table>

**PD** is ‘Plotting Data’, an introduction to Jupyter/Python and data visualization and regression.

**AE** is ‘Adiabatic Expansion’, a quantitative study of expansion and compression processes in gases and the extraction of heat capacity information.

**HP** is ‘Heat Pump’, the analysis of the performance of a thermoelectric heat pump and its evaluation with respect to maximum thermodynamic efficiency. This is a two session activity (A and B) which will include a draft and final report, as well as a quiz.

**AR** is ‘Acoustic Resonator’, the thermodynamic study of sound in various gases. Several types of types of acoustic spectroscopy will be explored, revealing common features of all spectroscopic methods. Heat capacity information will be extracted and compared with the AE activity. This is a two session activity (A and B) which will include two reports, as well as a quiz.

**CE** is ‘Chemical Equilibrium’, the analysis of aqueous equilibrium by simultaneous colorimetry, conductometry and pH. This is a two session activity (A and B) which will include two reports, as well as a quiz.

**PK** is ‘Photolysis Kinetics’, a study of the reversible photophysics of azobenzene. This is a two session activity (A and B) which will include a draft and final report, as well as a quiz.

**PT** is ‘Passive Transport’, a study of the migration of ions through a membrane as a result of a concentration gradient.

**MUW** is a makeup week. Activities scheduled *ad hoc*

**XX** is ‘Experimental Design’, a trail run of an untested experimental activity.
**Assignment Schedule**  (Tentative; see course website)

<table>
<thead>
<tr>
<th>Week</th>
<th>AQ</th>
<th>Due</th>
<th>NB</th>
<th>Due</th>
<th>ES</th>
<th>Due</th>
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<tbody>
<tr>
<td>1</td>
<td>SYLQ</td>
<td>01/11</td>
<td>NB-PD</td>
<td>01/13</td>
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<tr>
<td>2</td>
<td>SAFQ</td>
<td>01/20</td>
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<td></td>
<td></td>
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<tr>
<td>3</td>
<td>AQHP</td>
<td>01/25</td>
<td>NB-HP</td>
<td>01/27</td>
<td></td>
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</tr>
<tr>
<td>4</td>
<td>AQAE</td>
<td>02/08</td>
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<td></td>
<td>ES-HP</td>
<td>02/03</td>
</tr>
<tr>
<td>5</td>
<td>AQAR</td>
<td>02/15</td>
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<td>ES-AE</td>
<td>02/10</td>
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<td></td>
<td>ES-ARA</td>
<td>02/17</td>
</tr>
<tr>
<td>7</td>
<td>AQCE</td>
<td>03/01</td>
<td>NB-ARB</td>
<td>02/22</td>
<td>ES-ARB</td>
<td>02/24</td>
</tr>
<tr>
<td>8</td>
<td></td>
<td></td>
<td>NB-CE</td>
<td>03/03</td>
<td>ES-CE</td>
<td>03/10</td>
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<tr>
<td>9</td>
<td></td>
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<tr>
<td>11</td>
<td>AQP K</td>
<td>03/22</td>
<td>NB-PK</td>
<td>03/24</td>
<td></td>
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</tr>
<tr>
<td>12</td>
<td>AQPT</td>
<td>04/05</td>
<td></td>
<td></td>
<td>ES-PK</td>
<td>03/31</td>
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<tr>
<td>13</td>
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<td></td>
<td></td>
<td>ES-PT</td>
<td>04/07</td>
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</tbody>
</table>

**SYLQ** is the Syllabus Quiz.

**NB-*** are a Jupyter/Python notebooks submitted via our class Jupyter server. They are the backbone of the data analysis and visualization for all the activities in the course. In most cases hints and templates will be provided. No previous Python or programming experience is required.

**SAFQ** is the Safety Quiz. It is based on the materials found on the Resources page under Safety and Waste Management. Stay safe, my friends.

**AQ-*** are Analysis Quizzes. They preceed every experiment with a review of concepts and computations.

**ES-HP** is the Executive Summary report for the entire Heat Pump activity.

**ES-AE** is the Executive Summary report for the entire Adiabatic Expansion activity.

**ES-ARA** is the Executive Summary report for Session A of the Acoustic Resonance activity.

**ES-ARB** is the Executive Summary report for Session B of the Acoustic Resonance activity.

**ES-CE** is the Executive Summary report for the entire Heat Pump activity.

**ES-PT** is the Executive Summary report for the entire Passive Transport activity.

**ES-PK** is the Executive Summary report for the entire Photolysis Kinetics activity.

All ‘official’ activity dates and grades are posted on the secure course website. Assignments are to be submitted in full by the assignment deadline in the requested format for credit.
Course Resources

... Activity Descriptions
Notes guiding and describing course activities are posted on the course website. The expectation is that these notes guide your preparation prior to attending the lab meetings. It is not expected that these notes will be sufficient on their own — This laboratory relies heavily on all the Chemistry that you have learned in all the courses you have taken thus far, and in particular CHM4411 Thermodynamics and Kinetics. The lab notes are subject to constant revision, so make sure you are using the latest copy. For that reason, static downloads of the material are discouraged.

... The Course Jupyter Server
The majority of scientific data processing, data mining, and AI research relies on the computing ‘language’ Python. It is ubiquitous in Chemistry and has lots of community support around the globe. There are libraries (packages) for almost everything a Chemist wants to do already written in Python, so it is an obvious choice for a student of Chemistry. Moreover, Python is easy to learn. The internet provides multiple tutorials and helpful hints for almost any imaginable task in Python. Python can be used in an interactive development environment, Jupyter, which breaks up the commands into ‘cells’ which are executed in a flexible order. Jupyter has many of the features and behavior of other powerful apps like Mathematica or MATLAB, but is free, has huge support among Chemists, and has a shallower learning curve. Familiarity with Python in some form may just be what it takes to get you a job.

Graded data analysis and visualization assignments in this course will use a server spun up specifically for us. This Chemistry Department jupyter server can be found here: https://jupyter.chem.ufl.edu:8000/. Login there with your Gatorlink username (the part of your @ufl.edu email address before the @ symbol) and the initial password ‘mechanicup’. Instructions for changing your password to protect your work will be provided in our first meeting. You must change your password to protect your work. You may choose any password, but it is advised not to reuse a password from any other system. Note: If you are off campus, you must VPN into the UF network before hitting the server login page. Instructions for using VPN are on UF’s website.

It is also strongly encouraged that you install Python on your own devices, if it is not already. ‘Anaconda’ is a free code suite that allows one to easily setup Jupyter/iPython/R on your personal devices. Free download and instructions can be found on the website: https://www.anaconda.com/distribution/. Anaconda is also available through UF apps for all UF students. My experience with UFapps is mixed, and I cannot recommend it except for casual use.

... Notebook Hints
To assist mastery of data processing and manipulation, detailed Python notebook ‘hints’ will be provided for each activity. These are not meant to represent the unique solution to the posed problem, but provide example code for scrutiny and modification. These ‘hints’ will be placed in your workspace on the course jupyter server or on the course website.
Grades

Course Grade Computation

Course grades will be computed from the weighted-average of the earned percentages of each graded items described under Course Activities, submitted by the individual student. The weighting factors of the activity categories are as follows:

<table>
<thead>
<tr>
<th>Grade Category</th>
<th>weight %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Analysis Quiz (AQ)</td>
<td>20</td>
</tr>
<tr>
<td>Jupyter/Python Notebook (NB)</td>
<td>20</td>
</tr>
<tr>
<td>Executive Summary (ES)</td>
<td>40</td>
</tr>
<tr>
<td>Instructor Subjective (IS)</td>
<td>20</td>
</tr>
</tbody>
</table>

The grading scheme will generate a aggregate assignment percentage, which will be converted into a letter grade as follows:

<table>
<thead>
<tr>
<th>Grade</th>
<th>A</th>
<th>A−</th>
<th>B+</th>
<th>B</th>
<th>B−</th>
<th>C+</th>
<th>C</th>
<th>D</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>Minimum percentage</td>
<td>87.5</td>
<td>80.0</td>
<td>77.5</td>
<td>72.5</td>
<td>70.0</td>
<td>67.5</td>
<td>60.0</td>
<td>50.0</td>
<td>&lt; 50.0</td>
</tr>
</tbody>
</table>

Regrade Requests

Grade accuracy is a high priority for this course. Assignments will be regraded if a grading error is suspected. Regrade requests from students must be submitted through Canvas Messaging to Brucat within 48 hours of the grade post. Regrades will be performed on the entire assignment following the standard assignment rubric. Grade adjustments may be positive or negative.

UF’s Grading Policy

See https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx
**Honesty and Truthfulness**

Ethical, moral, and professional behavior is expected and required of all participants in this course. Moreover, all participants in UF’s Academic activities are bound by Rules of Conduct, from which can be found the following excerpt:

> “UF students are bound by The Honor Pledge which states, ‘We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honor and integrity by abiding by the Honor Code.’

On all work submitted for credit by students at the University of Florida, the following pledge is either required or implied:

> ‘On my honor, I have neither given nor received unauthorized aid in doing this assignment’

The Honor Code (http://www.dso.ufl.edu/scmr/process/student-conduct-honor-code/) specifies a number of behaviors that are in violation of this code and the possible sanctions. Furthermore, you are obligated to report any condition that facilitates academic misconduct to appropriate personnel. If you have any questions or concerns, please consult with the instructor or TAs in this class.”

**Accommodations**

The Disability Resource Center at UF offers this advice:

> “Students with disabilities who experience learning barriers and would like to request academic accommodations should connect with the Disability Resource Center by visiting our Get Started page. It is important for students to share their accommodation letter with their instructor and discuss their access needs, as early as possible in the semester.”

**Counseling**

Useful non-academic services are available in many forms at UF.

- **U Matter, We Care**: If you or a friend is in distress, please contact unmatter@ufl.edu or 352 392-1575 so that a team member can reach out to the student.
- **The Counseling and Wellness Center**: http://www.counseling.ufl.edu/cwc/

**GatorEvals**

The UF course evaluation policy includes the following statement:

> “Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. Guidance on how to give feedback in a professional and respectful manner is available at https://gatorevals.aa.ufl.edu/students/. Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals, in their Canvas course menu under GatorEvals, or via https://ufl.bluera.com/ufl/. Summaries of course evaluation results are available to students at https://gatorevals.aa.ufl.edu/public-results/.”

All course policies and procedures are subject to change at any time at the sole discretion of Brucat

*We, the members of the University of Florida Community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity*

--- Revision: January 10, 2023 ---