Chem 115

Instrumental Analysis and Bioanalytical Chemistry

http://faculty.ucmerced.edu/emenke/Chem115_f09/index.html

Chem 115

Instrumental Analysis and Bioanalytical Chemistry

This is the course syllabus for Chemistry 115, the instrumental analysis and bioanalytical chemistry class at UC Merced.

A note about printing this page: Please don't. This page will be at this URL long enough to share with your children and grandchildren. You don't need a paper copy of it.

Instructor: Professor Erik Menke

Class Room and Hours: COB 209, MWF 9-9:50 am

Office: Science and Engineering, Room 358

Office Hours: Drop by my office any time if you have questions or concerns. If I don't have time to talk, we can schedule a time. In addition, I will be available for the half-hour immediately following class at the Lantern Café in the library.

Contacting me: In addition to visiting my office, you can reach me by e-mail or leaving a message on the UCMCrops website for the class.

Course description and objectives: Analytical chemistry is one of the broadest disciplines of chemistry, with the primary goal of developing the tools and experiments to either qualitatively or quantitatively measure chemical composition. Historically, analytical chemistry was primarily perfomed by wet methods, most notably titrations, but over the last decade instrumental tools and techniques have come to dominate the field. This course focuses on how these instruments work, and what samples they are best suited for. The instruments and experiments we will look at are FTIR, FT-NMR, UV-Vis, GC, HPLC, AAS and AES, and electrophoresis.

Expected Student Learning Outcomes: By the end of the semester you should be able to:
-Identify the most useful technique and instrument for a given analytical problem.
-Identify the different parts of analytical instruments and explain how they work.
-Calculate relative and absolute amounts of an unknown substance from instrumental data, as well as the error in the measurements.

Required Text: Undergraduate Instrumental Analysis by James W. Robinson, Eileen M. Skelly Frame, and George M. Frame II (Sixth Edition)

Prerequisites: Chem 112, which may be taken concurrently.

Class Policies: The number one rule is to respect the time of everybody in the class, including the instructor. Ultimately, I believe that this is the only rule we should need, but it is rather vague. To help overcome the vagueness of said rule, here are some examples of what this covers:
-Refrain from using cell phones in class (this includes texting or having the ring volume above vibrate).
-Refrain from talking out of turn.
-Do not tease, taunt, or belittle others.
-Anything that someone else reads (e-mails, homework, message posts) should be legible, with (mostly) proper grammatical structure and spelling.

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Academic Integrity: This is a topic that I take very seriously. While I understand that shortcuts are attractive, they very rarely end up helping in the long run. Dishonest practices, like cheating and plagarism, typically prevent you from understanding the material, which is ultimately why you are here in school. A full description of the University policy, as well as the judicial process and potential penalties, can be found on the student life website. Students should be familiar with the University policy as anyone caught violating the policy will be dealt with harshly.

Disability Services: A disability should not impede learning. To this end, UC Merced provides a number of options to help people with disabilities suceed in their academic career. If you have a disibility, I encourage you to contact the University Disability Services Office to find out how they can help. You can find out more information on their website, e-mailing them at disabilityservices@ucmerced.edu, or calling them at 209.228.6996. In addition, please let me know so that we can take measures to ensure that it has a minimal effect on your ability to understand the material.

Exams: There will be three in-class exams, worth 50 points each. The final will consist of a 15 minute presentation on an instrumental topic or technique of your choice, and will be worth 50 points. There will be no make-up's allowed for missed exams. If you miss an exam and have a legitimate excuse (i.e. doctor's note or equivalent) the other exams will be renormalized to make up the point difference (i.e. the other two exams will be worth 75 points each).

Exam Schedule:

Exam 1: Friday, October 2.

Exam 2: Friday, November 6.

Exam 3: Wednesday, December 9.

Presentation: Friday, December 11 from 8-11 am.

Homework: There will be two kinds of homework problems:

"Practice" problems will be assigned for you to practice the material. We will attempt to go over them in class, but they will not be graded. Exam problems are typically of this difficulty.

"Real" problems will be tougher, and will be graded. There will be, on average, one problem set assigned each week, and it will be due one week later. Each set of "real" problems will be worth 10 points, although the overall homework grade will be renormalized to 100 total points. If you work with, or receive help from, someone, please put their name under yours. There is no policy against outside help, and collaboration is an important skill to learn, but it is also important to credit others when help is received.

Grading: Overall, there will be a total of 300 points, 50 points for each exam, 50 points for the presentation, and 100 points for homework. The grading will follow a standard 10 point scale (100 - 90 = A, 89 - 80 = B, 79 - 70 = C...), with any +/- to be left for the instructors discretion.

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This is a tentative schedule for the class. However, as this class has never been taught before, deviations from this schedule are likely.

Week	Lecture #	Week of...	Topic(s)	Chapter(s)
1	Lecture 1 Lecture 2	August 26th	Concepts, data analysis	1
2	Lecture 3 Lecture 4 Lecture 5	August 31st	Sample prep, solution chemistry	1
3	Lecture 6 Lecture 7	September 9th	Light-matter interaction, optics	2
4	Lecture 8 Lecture 9 Lecture 10	September 14th	NMR	3
5	Lecture 11 Lecture 12	September 21st	2-D NMR, solid state NMR	3
6	Lecture 13 Lecture 14 Exam 1	September 28th	IR spectroscopy	4
7	Lecture 15 Lecture 16 Lecture 17	October 5th	IR spectroscopy	4
8	Lecture 18 Lecture 19 Lecture 20	October 12th	UV-Vis, Fluorescence	5
9	Lecture 21 Lecture 22 Lecture 23	October 19th	Atomic absorption	6

10	Lecture 24 Lecture 25 Lecture 26	October 26th	Atomic emission	7
11	Lecture 27 Lecture 28 Exam 2	November 2nd	Mass Spectrometry	9, 10
12	Lecture 29 Lecture 30	November 9th	Gas Chromatography	12
13	Lecture 31 Lecture 32 Lecture 33	November 16th	Liquid Chromatography	13
14	Lecture 34 Lecture 35	November 23rd	Electrophoresis	13
15	Lecture 36 Lecture 37 Lecture 38	November 30th	X-ray techniques	8
16	Lecture 29 Exam 3	December 7th	X-ray techniques	8

- I will post these lectures as a pdf on the website after each class.

- So, when taking notes, make sure to write down what I'm saying that DOESN'T appear on the slides.

- Each slide has a unique serial number, so if you have a question about a slide, refer to that number.

- For example, this slide is number 1-7

Lecture number

- For example, this slide is number 1-8

Slide number

Chem 115

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Part 1: Concepts and analysis

What's in this lecture?

- What is analytical chemistry?
- How do analytical chemists approach problems?

What is analytical chemistry?

The qualitative and quantitative characterization of matter.

- Qualitative - What is this?
- Quantitative - How much is there?

Analytical chemistry is broad...

- Pharmaceuticals
- Manufacturing
- Law enforcement
- Museums

Why instrumental analysis?

- Faster than wet methods
- More sensitive
- Less operator error
- Typically non-destructive

What goes into instrumental analysis?

- Chemistry
- Physics
- Electronics
- Biology
- Materials science
- Food science
- ...

It is the analytical chemist's job to communicate with other scientists.

The analytical approach:

1. Define the problem.
2. Design the method.
3. Sampling and sample storage.
4. Sample preparation.
5. Perform the measurement.
6. Assess the data.
7. Validate the method.
8. Document.

Define the problem...

- How precise and accurate?
- Organic, inorganic, or both?
- Possible interferences?
- Qualitative or quantitative?

Qualitative analysis...

- **What** is this?
- Distinguish between molecular analysis and elemental analysis:
  - Molecular - Sucrose vs. Fructose.
  - Elemental - Carbon vs. Oxygen.

Quantitative analysis...

- **How much** is there?
- Generally expressed as a concentration.
- Sensitivity is important!

Concentration...

- Molarity - moles per liter
- Percent
  - Atomic percent
  - Weight percent
  - Volume percent
- Parts per _____
  - Hundred (same as %)
  - Thousand
  - Million
  - Billion
  - Trillion

Concentration, cont...

- Molality - moles per gram
- Mole fraction
- Normality

Molarity vs. molality

- Molarity
- Depends on mass and volume
- Temperature dependent

- Molality
- Depends on mass only
- Temperature independent

Common instrumental methods...

Method	Qualitative?		Quantitative?	
	Elemental	Molecular	Elemental	Molecular
Atomic absorption	No	No	Yes	No
Atomic emission	Yes	No	Yes	No
Capillary electrophoresis	Yes	Yes	Yes	Yes
Electrochemistry	Yes	Yes	Yes	Yes
Gas chromatography	No	Yes	No	Yes
ICP-Mass spectrometry	Yes	No	Yes	No
IR spectroscopy	No	Yes	No	Yes
Ion chromatography	Yes	Yes	Yes	Yes
Liquid chromatography	No	Yes	No	Yes
Mass spectrometry	Yes	Yes	Yes	Yes
Nuclear magnetic resonance	No	Yes	No	Yes
Raman spectroscopy	No	Yes	No	Yes
Thermal analysis	Yes	Yes	Yes	Yes
UV/Vis spectroscopy	Yes	Yes	Yes	Yes
UV absorption	No	Yes	No	Yes
UV fluorescence	No	Yes	No	Yes
X-ray absorption	Yes	No	Yes	No
X-ray diffraction	No	Yes	No	Yes
X-ray fluorescence	Yes	No	Yes	No

Concentration ranges...

Method	Destructive	Ultratrace <1 ppm	Trace 1 ppm - 0.1%	Minor 0.1 - 10%	Major >10%
X-ray diffraction	No	No	No	Yes	Yes
NMR	No	No	Yes	Yes	Yes
X-ray fluorescence	No	No	Yes	Yes	Yes
IR spectroscopy	No	No	Yes	Yes	Yes
Raman spectroscopy	No	No	Yes	Yes	Yes
UV/VIS	No	No	Yes	Yes	Yes
Colorimetry	No	Yes	Yes	Yes	No
Molecular fluorescence	No	Yes	Yes	Yes	Yes
Atomic absorption	Yes	Yes	Yes	Yes	No
Atomic emission	Yes	Yes	Yes	Yes	Yes
ICP-MS	Yes	Yes	Yes	Yes	No
GC-MS	Yes	Yes	Yes	Yes	Yes
LC-MS	Yes	Yes	Yes	Yes	Yes
Potentiometry	No	Yes	Yes	Yes	Yes
Voltammetry	No	Yes	Yes	Yes	Yes
HPLC	Maybe	Yes	Yes	Yes	Yes
Ion chromatography	Maybe	Yes	Yes	Yes	Yes
Capillary electrophoresis	No	Yes	Yes	Yes	Yes
Thermal analysis	Yes	No	No	Yes	Yes

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Defining the problem

1. What accuracy is required?
2. How much sample is available?
3. What is the concentration range?
4. What are likely interferences?
5. What are the matrix properties?
6. How many samples?

Designing the analytical method

- Limits
  - Time
  - Sample
  - EH&S
- Blank
  - Matrix
  - Reagent
- Standard
- Literature
  - Journals
  - Books
  - Associations

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Sampling...

- Need a sample that is representative
- Worry about contamination
- Many standard methods

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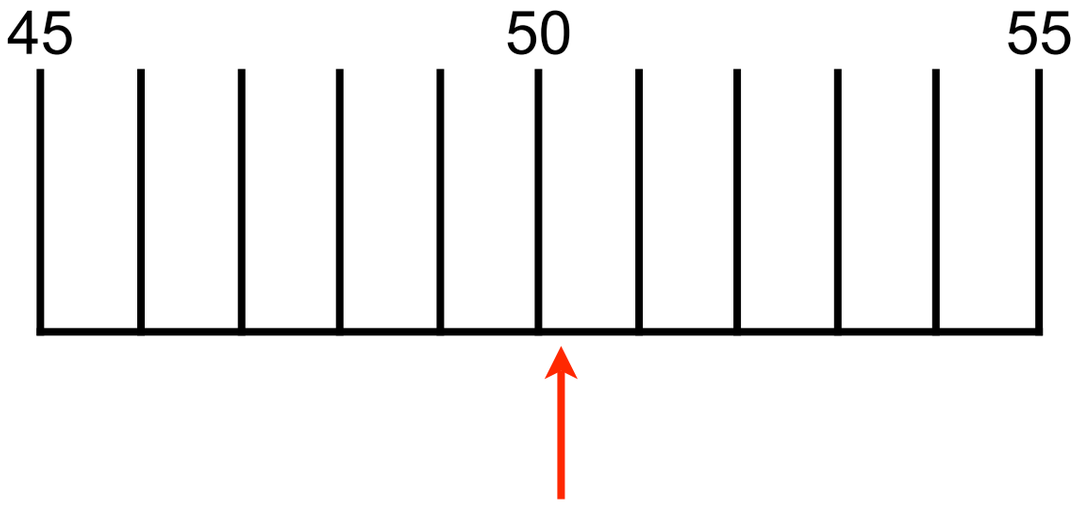
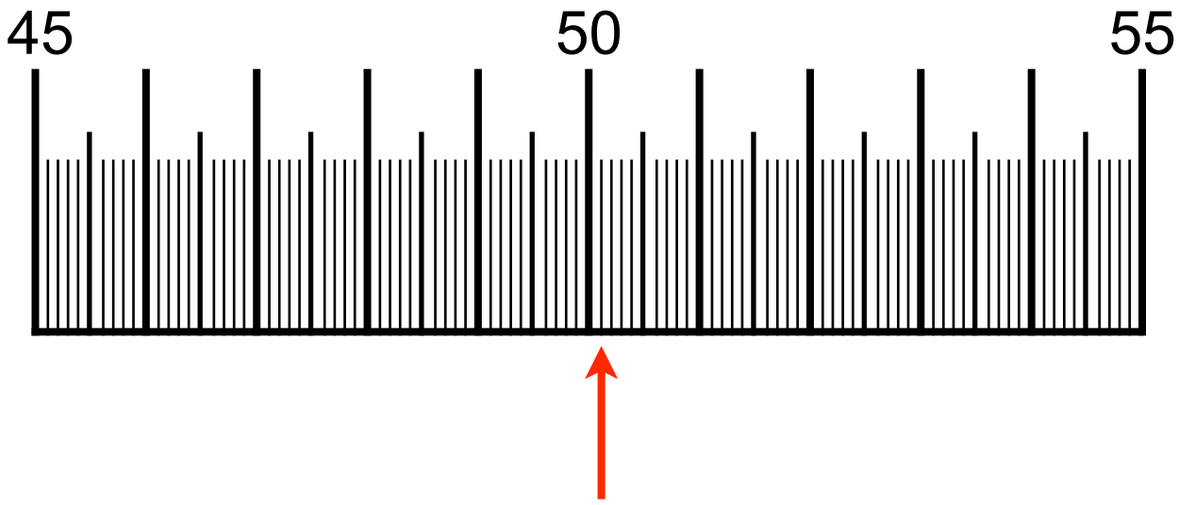
4. Sample preparation.
5. Perform the measurement.
6. Assess the data.
7. ~~Validate the method.~~
8. ~~Document.~~

Significant figures





50.1 ≠ 50.09

Uncertain digit Uncertain digit

When reporting numbers, report <u>all</u> certain digits, and <u>1</u> uncertain digit