GEO 391/371T: Geochemical Problem Solving with Ions & Atoms Spring 2016

Tuesdays 12-2 Lecture – EPS 4.104; Thursdays 11-2 Lab – various JGB labs UT Austin

"At first there were very few who believed in the existence of these bodies smaller than atoms. I was even told long afterwards by a distinguished physicist who had been present at my [1897] lecture at the Royal Institution that he thought I had been 'pulling their legs'."
— J.J. Thomson (1936)

"The real value of science is in the getting, and those who have tasted the pleasure of discovery alone know what science is. A problem solved is dead. A world without problems to be solved would be devoid of science." *— Frederick Soddy (1912)*

"I think there's a little bit of sizzling here. Honestly, I can feel it. The ions are flying back and forth." *— Regis Philbin (2013)*

Instructors (office hours by appointment):
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Course Overview: Mass spectrometers are analytical balances that operate at molecular and atomic levels. Compositional data (both isotopic and elemental) provided by mass spectrometry are invaluable to many lines of scientific inquiry. Many types of mass spectrometers have been developed to suit a wide range of applications (>10 in the Jackson School of Geosciences!), but all involve the conversion of sample molecules into charged particles (ions) that are then measured according to their mass-to-charge ratio. This course provides an introduction to inorganic mass spectrometry methods and their applications to the Earth sciences. Five key modalities are surveyed (TIMS, ICP-MS, LA-ICP-MS, MC-ICP-MS, and IRMS) in lecture and accompanying weekly labs. Knowledge and skills developed in this course are intended to provide an understanding of how mass spectrometers work, what can be analyzed, and what is necessary to generate and critically evaluate high-quality data.

Prerequisites: Graduate standing in geosciences, upper division undergraduate standing in geosciences and consent of instructor, or graduate standing in another field and consent of instructor.

Learning Goals: *The overarching goal of this course is for you to become a critical consumer and producer of data using inorganic mass spectrometry techniques.* Through understanding of key concepts and processes underlying operation of modern mass spectrometers introduced through lecture and lab, successful students completing this course should be able to:

- Explain basic principles of operation for each mass spectroscopic technique
- Articulate important sample preparation considerations for each technique
- Describe how instrumental parameters should be optimized for robust operating conditions
- Explain the strengths and limitations of each mass spectroscopic technique
- Explain how raw data generated by each technique should be processed to obtain high quality data (corrections for drift, mass fractionation, dilution)
- Calculate and evaluate important figures of merit to evaluate analytical quality (accuracy, precision, mass resolution, abundance sensitivity)
- Explain how the various techniques complement each other and can be used to evaluate geoscience problems (geologic applications of the techniques)

Evaluation:	Lab exercises and write-ups	30%
	Student synthesis final project	30%
	Discussion forum participation	10%
	Discussion forum summary presentation	5%
	Class synthesis (comparison matrix) project	10%
	Mini-quizzes (top 10 scores)	10%
	Class participation/engagement	5%

Overview of Course Requirements/Assignments

Class participation/engagement: It is important to be prepared for each lecture and lab. You should critically read assigned reading materials and be prepared for class discussions. Because there are only a few lectures and labs per mass spectrometry technique, it is vital that you regularly attend class. The Canvas activities, described below, are designed to help keep you engaged outside of class.

Weekly mini-quizzes (Due Thursdays before lab): Let's face it, lectures are short and there is a lot of time to forget between classes. To promote engagement and help reinforce lecture content, there will be weekly "mini-quizzes" based on reading assignments. The quizzes, worth 10 pts each, are hosted on Canvas, and must be taken at least 1 hour prior to class. There will be >10 mini quizzes during the semester, of which your top 10 scores will count toward this component of your grade.

Weekly discussion forum (Due Sundays): As we survey each MS technique, you are required to populate a discussion topic forum (Canvas) by responding to weekly threads that are synced to lecture and/or lab material. Your response should be concise and well written, and consist of two components: (1) your response to the discussion topic, and (2) a critique of a fellow student's posting. Critiques should be constructive, pointing out what may be missed or incorrect, or how your understanding of the topic may have been improved. Your first critique should be to a response that has not previously been critiqued by another student, however you may comment on as many responses as you wish. Thread responses must be submitted no later than 6pm on Sundays (Canvas time stamp) for full credit or they are considered late and worth half-credit. Grading criteria are:

- 3 pts Full thoughtful response to thread and at least one other classmate; responses are clear, concise and well written.
- 2 pts Response to original thread and at least one other classmate made, but responses are incomplete, vague, or poorly written.
- 1 pt Response to only original thread or only one classmate, regardless of content and quality
- 0 pts no submission (please don't do this!!!)

Each week, a different student will be responsible for summarizing the results of the discussion thread and preparing a short (<5 minute) presentation for the class (to be presented at the start of lecture on Tuesdays). You will be assigned a date on the first day of class. Write it down here: ________________

Lab exercises (Due Tuesdays before next class): Lab exercises are intended to be experiential, and to allow time for observation and hands-on participation. Out-of-class time will be required for evaluations of data sets, and participation may also be through Canvas. We urge you to begin the lab write-ups as soon as possible while the lab content is fresh in your minds, and you have time to ask any questions prior to the next class. Where practical, some of the data sets generated in labs will be used for student synthesis projects.

Class synthesis project: To promote understanding and comparison of the mass spectrometry techniques and how they compare in terms of generation of high quality MS data, we will construct a comparison matrix via Canvas. You are required to provide input for each cell of the matrix as the various MS modules are covered, but will also be assigned a subset for which you are responsible for compiling and editing all student responses toward construction of a final integrated class matrix.

Student synthesis project: Each student will be assigned a mass spectrometry technique dataset for which you will be responsible for documenting methodology and data quality. You will demonstrate that you have become a critical consumer of mass spectrometric data by (1) presenting your individual project methodology and results on Synthesis Day (May 5 or May 10) and by (2) documenting your knowledge of course content in a final report.

1) Presentation (15 pts) – Each student will make a brief GSA-type presentation (10-12min + questions) based on their assigned MS topic and data set.
2) Final Report
   a) Methods sections (12 pts per module) - During each mass spectrometer module, you will be given a representative data set. You are responsible for documenting, in the form of a mock methods section, the means by which the data were acquired and the resulting quality of the data. It is important to include all necessary measures of data quality, including how the instrument was optimized and performed during data collection. Components of good (and bad) methods sections will be discussed in class and also shown from literature examples. We strongly recommend that you complete each methods section as you complete each module. This component of the final report will thus consist of five (5) methods sections.
   b) Comparison (15 pts) - You will prepare a short essay comparing and contrasting the 5 modalities presented in this class, based on the class matrix questions provided during the first week of class.
   c) Personal impact (10 pts) - Describe how what you have learned in this class impacts your ongoing or future research. This question is intentionally open-ended, as we want you to reflect on how you might apply what you have learned in this class.

Grading Policy: Your attendance, participation and preparation for class are expected. Assignments are due by class meeting time on the dates indicated in the course syllabus. For schedule conflicts, contact us well in advance to see if alternative arrangements can be made.

Required and recommended materials: Rather than refer to a single text, we will instead examine relevant foundational and application-based papers documenting aspects of each technique. Course readings will be made available in pdf form on the course Canvas site.

Class Websites: We will use Canvas throughout the semester: http://canvas.utexas.edu
We will try to adhere to the course schedule as much as possible, but some modifications are possible for logistical reasons. Any such changes will be communicated weekly and/or updated.

- The SERC Geochemical Instrumentation and Analysis website provides information on mass spectrometry as well as other geochemical techniques. http://serc.carleton.edu/research_education/geochemsheets/index.html
- The website for the JSG ICP-MS lab will also be useful: http://www.jsg.utexas.edu/icp-ms/

Notice: Students with disabilities may request appropriate academic accommodations from the Division of Diversity and Community Engagement, Services for Students with Disabilities, 471-6259: http://ddce.utexas.edu/disability/

Academic Dishonesty: Academic dishonesty and plagiarism will not be tolerated. You are expected to do your own work in accordance with the UT Honor Code: http://deanofstudents.utexas.edu/sjs/spot_honorcode.php

Schedule of Class Activities

Wk		Day	Method Topic (Instructor)	Class/ Graded Labs	JGB Lab Location	Class Topic
1	19-Jan	T	Intro (Miller/Loewy)	Lecture	EPS 4.104	Course outline, grading, deliverables; History & basics of mass spectrometry
1	21-Jan	Th		Lecture	EPS 4.104	Mass spectrometers & metrology - the science of measurement
2	26-Jan	T		Lecture	EPS 4.104	Ions, Tigers & Bears: Elements, Atoms, Isotopes, Ions, Interferences
2	28-Jan	Th		Lecture	EPS 4.104	Generating & documenting defensible MS data: Sample collection & prep, MS optimization & measurement, data processing & quality control metrics
3	2-Feb	T	ICP-MS (Miller)	Lecture	EPS 4.104	What is ICP-MS & how does it work? Applications, strengths, weaknesses
3	4-Feb	Th		Lab	6.310b	ICP-MS Lab introduction - Demo: solution mode instrument optimization
4	9-Feb	T		Lecture	EPS 4.104	ICP-MS components; Sample preparation, quality control planning
4	11-Feb	Th		**Lab 1**	6.310b	What's in my sample? Semi quant analysis 72 full spectral scans
5	16-Feb	T		Lecture	EPS 4.104	Dealing with interferences; Data reduction - assessing quality control
5	18-Feb	Th		**Lab 2**	6.310b	Designing a method; Cal/QC stds/unknown analysis/data processing
6	23-Feb	T	Laser Ablation ICP-MS (Miller)	Lecture	EPS 4.104	What is LA-ICP-MS & how does it work? Applications, strengths, weaknesses
6	25-Feb	Th		Lab	6.310b	LA-ICP-MS lab demo - designing a laser experiment & ICP-MS method
7	1-Mar	T		Lecture	EPS 4.104	What are lasers? Types of lasers & geologic applications
7	3-Mar	Th		**Lab 3**	6.310b	LA-ICP-MS data reduction & assessment of data quality
8	8-Mar	T	Intro to MC - MS (Loewy/ Koleszar)	Lecture	EPS 4.104	What is MC MS? Isotope ratios, isotope dilution, mass fractionation
8	10-Mar	Th		Lab	6.310ab/ 1.126	MC MS Lab tours - Isoprobe and Triton, Parts of the Machines (must wear socks!)
8		F	**Final Project Road Check - drafts of TIMS and ICP-MS methods portions due**			
			March 14-18 Spring Break			
9	22-Mar	T	MC-ICP-MS (Koleszar)	Lecture	EPS 4.104	How does MC-ICP-MS work? Applications, strengths, weaknesses
9	24-Mar	Th	Clean lab (Loewy)	Lab	1.126	Clean chemistry sample prep:- general technique, dissolution, chemical separation, Clean Lab tour and Demos (must wear socks!)
10	29-Mar	T	MC-ICP-MS (Koleszar)	Lecture	EPS 4.104	MC-ICP-MS method design (interferences, data acq, cup configuration); Data processing & QC
10	31-Mar	Th		**Lab 4**	3.216B	The Isoprobe MC-ICP-MS - Analyzing samples & processing data for isotope ratios & concentrations
11	5-Apr	T	TIMS (Loewy)	Lecture	EPS 4.104	TIMS - Applications, strengths, weaknesses
11	7-Apr	Th		**Lab 5**	EPS 4.104	The TIMS - Analyzing samples & processing data for isotope ratios & concentrations
12	12-Apr	T	Noble Gas MS	Lecture	EPS 4.104	Noble Gas mass spectrometry (D. Stockli)
12	14-Apr	Th	LA-HR-ICP-MS	Lab	3.104	LA-HR-ICP-MS for U-Pb zircon geochronology (L. Stockli)
13	19-Apr	T	Gas Source MS (Larson)	Lecture	EPS 4.104	IRMS principles & operation; Applications, strengths, weaknesses
13	21-Apr	Th		Lab	5.140	IRMS lab tour - Sample & run log preparation
14	26-Apr	T		Lecture	EPS 4.104	Sampling strategies; IRMS optimization (calibration) & data reduction
14	28-Apr	Th		**Lab 6**	5.140	IRMS data measurement & data reduction
15	3-May	T	Final Synthesis	Lecture	EPS 4.104	***Synthesis, "wrap up" and Pizza***
15	5-May	Th	Final Synthesis	Lecture	EPS 4.104	***Student presentations***
16	10-May	Tu	Final Synthesis	Lecture	EPS 4.104	***Student presentations***
16	13-May	Fri	Write-up due			***submitted by email***