CHEM 6371 – Spectroscopic Identification of Organic Compounds CHEM 4341 – Applied Spectroscopy

M 17-Aug	-						Topic	Reading (4e)
No. P. P. P. Votur undergraduate Intro-2 L.G. Elemental analysis, sites of unsaturation 1:1-1.5	M	17-Aug	Introduction	Intro-1		LG	*	8 ()
F 21-Aug Pavia Chap Aug Intro-5 Box Aug Aug								1:1-1.5
M 24-Aug		_						
W 26-Aug Intro-5 DC H NMR 3:10-17 M 31-Aug Intro-6 DC H NMR 3:10-17 M 31-Aug Intro-7 DC H NMR 3:10-17 M 31-Aug Intro-8 HW 2 DC Problems 3:q1-12 M 5-8ep Infrared IR-1 DC CH, CC bonds 2:8-11 F 11-Sep Spectroscopy IR-2 DC OH, NH bonds 2:12, 14F, 15 M 14-Sep Pavia Chap 2 IR-3 DC CO bonds 2:24, 16, 17-21 F 18-Sep IR-5 IR-5 DC CO bonds 2:24, 16, 17-21 F 18-Sep IR-5 IR-5 DC CO bonds 2:24, 116, 17-21 F 18-Sep IR-5 IR-5 DC CO bonds 2:24, 116, 17-21 F 18-Sep IR-5 IR-5 DC CO bonds 2:24, 116, 17-21 F 18-Sep IR-5 IR-5 DC CO bonds 2:24, 116, 17-21 F 18-Sep IR-5 IR-5 DC CO and CN bonds, reporting IR data 2:14, 16, 17-21 F 18-Sep Pavia Chap 8 MS-2 DC MS techniques R salve untrures F 2-3-Sep Pavia Chap 8 MS-2 DC Fragmentation, Hydrocarbons 8:8A-C, I-M M 28-Sep IR-5 IR-5 IR-5 DC MS-5 DC Hal-containing compounds, reporting MS data 8:8V M 5-0ct MS-6 IR-5 IR-5 DC H-5 M 5-0ct MS-5 DC H-7 Cellosing crisciples of IR and NMR to solve structures F 9-Oct MS-5 DC H-7 Cellosing crisciples of IR and NMR to solve structures F 9-Oct MS-5 DC H-7 Cellosing crisciples of IR and NMR to solve structures F 9-Oct MS-6 IR-5 IR-5 IR-5 IR-5 IR-5 M 19-Oct MS-6 IR-5 IR-5 IR-5 IR-5 IR-5 M 19-Oct MS-6 IR-5 IR-5 IR-5 IR-5 M 19-Oct		_			HW 1			
F 28-Aug		_	_F -,-					
M 31-Aug Intro-7 DC IH NMR and 13C NMR 3:19 + 4:14.2A F 4-Sep F 4-Se		_						
W 2-Sep		_						
F 4-Sep W 7-Sep 1.5ep 1.5ep 1.5ep 1.6ep 1.7ep 1.7e		_			HW 2			
M 7-Sep						20		
W 9-Sep		-			DAY			
F 1-Sep M 14-Sep M 18-Sep M			Infrared			DC	CH, CC bonds	2:8-11
M 14-Sep	F							
W 16-Sep R-4 R-5 HW 3 DC C=O and CN bonds, reporting IR data 2:14,16,17-21	M	-						
F R-Sep R-S R-S	W		1					
M 21-Sep Mass Spectrometry MS-1 DC Ms techniques 8:intro-6 F 25-Sep Pavia Chap 8 MS-2 DC Ms techniques 8:8A-C,I-M M 28-Sep MS-3 DC Alcohols, ethers and amines: α-cleavage 8:8N-O,T W 30-Sep MS-4 HW 4 DC C=O compounds 8:8P-U F 2-Oct MS-5 DC Hal-containing compounds, reporting MS data 8:8V M 5-Oct MS-6 HW 5 DC Problems 8:q1-15 W 7-Oct MS-6 HW 5 DC Problems 8:q1-15 W 7-Oct MS-6 HW 5 DC Problems 8:q1-15 W 12-Oct					HW 3			
W 23-Sep	M							
F 25-Sep	W		Mass Spectrometry			DC		
M 28-Sep MS-3 DC Alcohols, ethers and amines: α-cleavage 8:8N-Q,T W 30-Sep MS-4 HW 4 DC C=O compounds 8:8P-U F 2-Oct MS-5 DC Hal-containing compounds, reporting MS data 8:8V M 5-Oct MS-6 HW 5 DC Problems 8:q1-15 W 7-Oct EXAM 3 MS. plus use of basic principles of IR and NMR to solve structures F 9-Oct Indicate Indicat		-						8:8A-C,I-M
W 30-Sep MS-4 HW 4 DC C=O compounds 8:8P-U	M		•					
F 2-Oct MS-5 MS-6 HW 5 DC Hal-containing compounds, reporting MS data 8:8V M5-6 HW 5 DC Problems 8:q1-15	W	-		MS-4	HW 4	\mathbf{DC}		8:8P-U
M 5-Oct MS-6 HW 5 DC Problems 8:q1-15	F	-		MS-5		\mathbf{DC}		8:8V
F 9-Oct	M	5-Oct		MS-6	HW 5	\mathbf{DC}		8:q1-15
M 12-Oct	W	7-Oct		EXAM 3			MS, plus use of basic principles of IR and NMR to solve str	uctures
Note	F	9-Oct		no lecti	ıre			
F 16-Oct Spectroscopy NMR-2 DC H Chemical Shift 6:1-5	M	12-Oct		MID-SEN	<i>IESTER</i>	BREA	K	
M 19-Oct Pavia Chap 4,5,6 NMR-3 DC 1H Chemical Shift 6:6-10	W	14-Oct	¹ H and ¹³ C NMR	NMR-1		LG	Nuclear magnetic resonance theory	
NMR-4	F	16-Oct	Spectroscopy	NMR-2		\mathbf{DC}	¹ H Chemical Shift	
F 23-Oct NMR-5 LG	M	19-Oct	Pavia Chap 4,5,6	NMR-3		\mathbf{DC}	¹ H Chemical Shift	6:6-10
M 26-Oct W NMR-6 NMR-6 NMR-7 LG Decoupling, noe, etc 4:1-4,11-16 W 28-Oct Solve NMR-9 LG Edited spectra, APT, DEPT 4:5-9 and 6.11 F 30-Nov MR-9 LG Edited spectra, APT, DEPT 4:10 and 10.4-5 M 2-Nov NMR-9 LG Problems 9:intro-q21 W 4-Nov Follows NMR-10 HW 7 LG Problems 9:q22-43 F 6-Nov Problems 9:q22-43 M 9-Nov Problems NMR-9 W 11-Nov NMR Adv-1 LG COSY 10:1,6 W 11-Nov Pavia Chap 10 Adv-2 LG COSY 10:7 F 13-Nov Pavia Chap 10 Adv-3 LG NOESY 10:10 M 16-Nov W 18-Nov Pavia Chap 10 Adv-4 HW 8 LG HETCOR, HSQC 10:8-9 W 18-Nov F 20-Nov Adv-5 LG HMBC Adv-6 HW 9 LG Problems 10:12,q1-11 W 25-Nov - Pavia Chap 10 Adv-6 HW 9 LG Problems Basic and Adv NMR, and use of MS and IR to solve structures W 25-Nov - Problems Problems LG Problems LG W 25-Nov Problems Problems Problems LG Problems LG	W	21-Oct		NMR-4		\mathbf{DC}	¹ H Multiplicity	5:1-6
W 28-Oct NMR-7 LG Decoupling, noe, etc 4:5-9 and 6.11 F 30-Nov NMR-8 LG Edited spectra, APT, DEPT 4:10 and 10.4-5 M 2-Nov NMR-9 LG Problems 9:intro-q21 W 4-Nov NMR-10 HW 7 LG Problems 9:q22-43 F 6-Nov EXAM 4 NMR, plus use of MS and IR to solve structures M 9-Nov NMR Adv-1 LG 2D NMR Theory 10:1,6 W 11-Nov NMR Adv-2 LG COSY 10:7 F 13-Nov Pavia Chap 10 Adv-3 LG NOESY 10.10 M 16-Nov NAR-Nov Adv-4 HW 8 LG HETCOR, HSQC 10.8-9 W 18-Nov Adv-5 LG HMBC 10:12,q1-11 F 20-Nov Adv-6 HW 9 LG Problems 10:12,q1-11 W 25-Nov Adv-6 HW 9 LG Problems 10:12,q1-11 W 25-Nov Adv-6 HW 9 LG Problems Basic and Adv NMR, and use of MS and IR to solve structures W 25-Nov Adv-6 HW 9 LG Problems LG Problems W 25-Nov Adv-6 HW 9 LG Problems LG Problems W 25-Nov Adv-6 HW 9 LG Problems LG Problems	F	23-Oct		NMR-5		LG	¹ H Multiplicity, reporting NMR data	5:7-11
F 30-Nov NMR-8 LG Edited spectra, APT, DEPT 4:10 and 10.4-5 M 2-Nov NMR-9 LG Problems 9:intro-q21 W 4-Nov NMR-10 HW 7 LG Problems 9:q22-43 F 6-Nov EXAM 4 NMR, plus use of MS and IR to solve structures West of the problems 10:1,6 M 9-Nov 2D, Advanced and Adv-1 LG 2D NMR Theory 10:1,6 W 11-Nov NMR Adv-2 LG COSY 10:7 F 13-Nov Pavia Chap 10 Adv-3 LG NOESY 10:10 M 16-Nov Adv-4 HW 8 LG HETCOR, HSQC 10:8-9 W 18-Nov Adv-5 LG HMBC 10:12,q1-11 EXAM 5 Basic and Adv NMR, and use of MS and IR to solve structures 10:12,q1-11 W 25-Nov no lecture THANKSGIVING BREAK W 2-Dec Problems LG HANG LG HA	M	26-Oct		NMR-6	HW 6	LG	¹³ C Chemical shift, shift calculations	4:1-4,11-16
M 2-Nov NMR-9 LG Problems 9:intro-q21 W 4-Nov NMR-10 HW 7 LG Problems 9:q22-43 F 6-Nov EXAM 4 NMR, plus use of MS and IR to solve structures M 9-Nov 2D, Advanced and Adv-1 LG 2D NMR Theory 10:1,6 W 11-Nov NMR Adv-2 LG COSY 10:7 F 13-Nov Pavia Chap 10 Adv-3 LG NOESY 10:10 M 16-Nov Adv-4 HW 8 LG HETCOR, HSQC 10.8-9 W 18-Nov Adv-5 LG HMBC 10:12,q1-11 M 23-Nov Adv-6 HW 9 LG Problems 10:12,q1-11 W 25-Nov no lecture THANKSGIVING BREAK M 30-Nov More problems Problems LG W 2-Dec Problems LG	W	28-Oct		NMR-7		LG	Decoupling, noe, etc	4:5-9 and 6.11
W 4-Nov NMR-10 HW 7 LG Problems 9:q22-43 F 6-Nov EXAM 4 NMR, plus use of MS and IR to solve structures M 9-Nov 2D, Advanced and Adv-1 LG 2D NMR Theory 10:1,6 W 11-Nov NMR Adv-2 LG COSY 10:7 F 13-Nov Pavia Chap 10 Adv-3 LG NOESY 10.10 M 16-Nov Adv-4 HW 8 LG HETCOR, HSQC 10.8-9 W 18-Nov Adv-5 LG HMBC 10:12,q1-11 M 23-Nov Adv-6 HW 9 LG Problems 10:12,q1-11 W 25-Nov no lecture THANKSGIVING BREAK W 2-Dec Problems LG	F	30-Nov		NMR-8		LG	Edited spectra, APT, DEPT	4:10 and 10.4-5
F 6-Nov EXAM 4 NMR, plus use of MS and IR to solve structures M 9-Nov 2D, Advanced and Adv-1 LG 2D NMR Theory 10:1,6 W 11-Nov NMR Adv-2 LG COSY 10:7 F 13-Nov Pavia Chap 10 Adv-3 LG NOESY 10.10 M 16-Nov Adv-4 HW 8 LG HETCOR, HSQC 10.8-9 W 18-Nov Adv-5 LG HMBC 10:12,q1-11 F 20-Nov Adv-6 HW 9 LG Problems 10:12,q1-11 M 23-Nov no lecture no lecture F 27 Nov THANKSGIVING BREAK M 30-Nov More problems LG W 2-Dec Problems LG	M	2-Nov				LG		9:intro-q21
M 9-Nov 2D, Advanced and William Adv-1 LG 2D NMR Theory 10:1,6 W 11-Nov NMR Adv-2 LG COSY 10:7 F 13-Nov Pavia Chap 10 Adv-3 LG NOESY 10.10 M 16-Nov Adv-4 HW 8 LG HETCOR, HSQC 10.8-9 W 18-Nov Adv-5 LG HMBC 10:12,q1-11 M 23-Nov EXAM 5 Basic and Adv NMR, and use of MS and IR to solve structures W 25-Nov no lecture F 27 Nov THANKSGIVING BREAK M 30-Nov More problems LG Problems LG Problems LG	W				HW 7	LG		9:q22-43
W 11-Nov NMR Adv-2 LG COSY 10:7 F 13-Nov Pavia Chap 10 Adv-3 LG NOESY 10.10 M 16-Nov W 18-Nov F 20-Nov F 23-Nov F 27 Nov S 27 Nov S 2-Dec Adv-4 HW 8 LG HETCOR, HSQC 10.8-9 W 25-Nov F 27 Nov S 2-Dec Adv-6 HW 9 LG Problems F 27 Nov F								
F 13-Nov Pavia Chap 10 Adv-3 LG NOESY 10.10 M 16-Nov Adv-4 HW 8 LG HETCOR, HSQC 10.8-9 W 18-Nov Adv-5 LG HMBC F 20-Nov Adv-6 HW 9 LG Problems 10:12,q1-11 M 23-Nov no lecture Basic and Adv NMR, and use of MS and IR to solve structures W 25-Nov no lecture F 27 Nov THANKSGIVING BREAK M 30-Nov More problems LG Problems LG Problems LG								
M 16-Nov Adv-4 HW 8 LG HETCOR, HSQC 10.8-9 W 18-Nov Adv-5 LG HMBC 10:12,q1-11 F 20-Nov EXAM 5 Basic and Adv NMR, and use of MS and IR to solve structures W 25-Nov no lecture F 27 Nov THANKSGIVING BREAK M 30-Nov More problems Problems LG W 2-Dec Problems LG	W							
W 18-Nov F 20-Nov Adv-5 LG Problems HMBC M 23-Nov EXAM 5 Basic and Adv NMR, and use of MS and IR to solve structures W 25-Nov no lecture no lecture F 27 Nov THANKSGIVING BREAK M 30-Nov More problems Problems W 2-Dec Problems	F		Pavia Chap 10					
F 20-Nov Adv-6 HW 9 LG Problems 10:12,q1-11 M 23-Nov EXAM 5 Basic and Adv NMR, and use of MS and IR to solve structures W 25-Nov no lecture F 27 Nov THANKSGIVING BREAK M 30-Nov More problems LG W 2-Dec Problems LG	M				HW 8			10.8-9
M 23-Nov W 25-Nov no lecture F 27 Nov THANKSGIVING BREAK M 30-Nov More problems W 2-Dec Basic and Adv NMR, and use of MS and IR to solve structures Hand III to solve structures No lecture LG Problems LG Problems LG	W							
W 25-Nov no lecture F 27 Nov THANKSGIVING BREAK M 30-Nov More problems Problems LG W 2-Dec Problems LG	F					LG		
F 27 Nov THANKSGIVING BREAK M 30-Nov More problems Problems LG W 2-Dec Problems LG							Basic and Adv NMR, and use of MS and IR to solve structure	res
M 30-Nov More problems Problems LG W 2-Dec Problems LG	W							
W 2-Dec Problems LG					GIVING		K	
			More problems					
F 4-Dec Problems I C								
	F	4-Dec		Problems		LG		
W 9-Dec (8:00 am – 10:50 am) FINAL Comprehensive	W	9-Dec (8	3:00 am – 10:50 am)	FIN	AL		Comprehensive	

INSTRUCTORS

 David M. Collard
 Leslie Gelbaum

 MS&E 2100J
 MS&E 113A

 404-894-4026
 404-894-4079

david.collard@chemistry.gatech.edu lg2@prism.gatech.edu

LECTURES

Come prepared to ask <u>and answer</u> questions! MWF, 11:05-11:55 Molecular Science & Engineering Building (MSE) 1201A

OFFICE HOURS

Collard – first half of course
Friday noon-1 p.m.

Gelbaum – second half of course
Tuesday 1:00 - 2:00 p.m.

or by appointment!

WORK PROBLEMS

Work as many problems as possible, from the notes, from the book, from other sources.

REQUIRED TEXTBOOK

Introduction to Spectroscopy, *4e or 5e*, Donald L. Pavia, Gary M. Lampman, George S. Kriz, and James A. Vyvyan; *Brooks Cole*; ISBN-10 / ASIN: 0495114782; ISBN-13 / EAN: 9780495114789. Note: Section numbers and problems vary for different editions (U.S.)

GRADES

Exam 1

Exam 2

Exam 3

Exam 4

Graded Assignments Tonic

Topic	
Fundamental principles and using basic information to solve structures	100 points†
IR, plus use basic principles of MS and NMR to solve structures	100 points†
MS, plus use of basic principles of IR and NMR to solve structures	100 points†
NMR, plus use of MS and IR to solve structures	100 points†

Exam 5 Basic and Advanced NMR techn., plus use of MS and IR to solve structures

Homework Nine HW assignments (score normalized to 100 points)

Final 8:00 am-10:50 am: Comprehensive

100 points

100 points

200 points

The lowest score of the five mid-term exams (†) will be dropped. If you miss an exam that score (0) will be dropped. The course grade will be determined based on your score out of 700 points.

Typical Grade Cut-offs

A: 85%+ B: 70-84.99 C: 60-69.99 D: 50-59.99

RETURNED WORK AND REGRADES

All graded assignments will be returned as soon as possible, usually within a week. If you want any work regraded you must make a written request and return the assignment within one week. Work will not be regraded after this deadline.

LECTURE ATTENDANCE

It is strongly recommended that you attend all lectures.

MATERIAL COVERED, KEEPING UP, WORKING PROBLEMS, STUDENT RESPONSIBILITIES

You are responsible for all material presented in lectures and in assigned readings. You are also responsible for announcements made in class or by email. You must check your *gatech.edu* email account on a regular basis. Note: there are potential problems associated with automatic forwarding of messages from your *gatech* mail to other email addresses; check your *gatech* account even if you have it set up to forward email elsewhere.

By the end of each section you should have completed all reading associated with that section, and worked <u>all of the end-of-chapter problems</u> and any additional problems which have been distributed. These questions should form the basis for discussion with your peers, and serve as a guide for the types of questions to appear on examinations (some of these questions might even appear on the exams!) Do not submit answers to these problems, they will not be graded.

EXAMS: SCHEDULE, MAKE-UPS AND DROPS

You must take the exam at the assigned time. All exams are closed to textbooks, class-notes and electronic devices (unless otherwise stated prior to the exam). *Tables of NMR*, *IR*, *MS data*, *along with a periodic table*, *will be provided*.

The only valid reasons for missing an exam are illness and official GA Tech business. Make-up exams can only be given if advance notification is given or upon presentation of a doctor's note. All make-up exams must be administered before the exams are returned to the class (typically before the next class). Exams not made-up by this time for any reason will receive a score of zero and will be the drop grade for the class (i.e., it will be the lowest score).

WORK PROBLEMS

Work as many problems as possible, from the notes, from the book, from other sources.

WORKING IN GROUPS

Most learning takes place *outside* of the classroom. Although lectures should provide a framework for learning and put things in perspective, working through the textbook and solving the problems is when you will come to terms with the material. We encourage you to work together on these reading and problem assignments. For most students, it is actually unwise to try to work alone. Although you might study in groups, remember that you are ultimately responsible for your learning. Everybody can benefit from team work. If you are struggling with the material you stand to learn a lot; if you are a "spectroscopy wizard" you also stand to learn from the challenge of presenting your understanding to others - you will learn through teaching.

Office hours are available for individual instruction. No *new* information will be introduced during office hours. Come prepared to ask *and answer* problems.

COMPETITION AND GRADING

Formal education often puts students in competition with each other for good grades. We do not believe that competition for grades, and the exclusion of everything else, is the most effective way to foster student development. Although grades will be assigned based on a numerical score, which judges attainment on exams/homework, we hope that the course is structured such that if you show a desire to learn, put *the effort in*, and have the intellectual ability, you can get the grade you want.

CANCELLATION OF CLASSES

If class is cancelled by Georgia Institute of Technology owing to campus closing, the entire schedule for the course will be delayed by one lecture. This will move all exams and the homework due dates back by one lecture.

TIME COMMITMENTS

We all have extensive demands on our time. For each hour of lecture you should aim to put in *at least* another two hours of your own time. You will need to spend more time preparing for exams. Some students will require more, some less.

WORK PROBLEMS

Work as many problems as possible, from the notes, from the book, from other sources.

SOME STUDY TIPS

Work Problems. Understand and Rationalize. Read the text, prepare your own summaries. Study in groups. **Keep up to date!** Ask Questions!! Work more problems.

STUDENT CLASS ACCOMMODATIONS

Students with disabilities who require reasonable accommodations to fully participate in course activities or meet course requirements are encouraged to register with ADAPTS-Disability Services Program at (404)894-2564 or www.adapts.gatech.edu

Contact the instructors within the first two weeks if you expect to take exams with ADAPTS. Please send reminders one week before each exam.

GEORGIA TECH ACADEMIC HONOR CODE

Please visit www.honor.gatech.edu

For Graded Homework Assignments: You may work with others in developing approaches to solve problems, but submitted work must be in your own handwriting.

For Tests: Cheating from another person's exam and use of unauthorized materials are direct violations of the GT Academic Honor Code, and will be dealt with accordingly.

For any questions involving these policies, please discuss them with the instructors or consult www.honor.gatech.edu.

LASTLY

Work as many problems as possible, from the notes, from the book, from other sources; work hard; enjoy.