References

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E. Breitmaier, W. Voelter, *Carbon 13 NMR Spectroscopy*, 3rd. ed., VCH, New York, NY, 1987.
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Computer Programs for Help in Spectral Interpretation

Name	Type of Program	Host Application	Spectroscopy covered
ChemDraw: NMR spectrum simulation, Rule based spectrum prediction, first order multiplets			
ChemDraw	CAI	PC, Mac	H,^{13}C-NMR
^{1}H Chemical Shift Prediction: Rule based spectrum prediction			
H1pred.html	Simulation	Web	H-NMR
Upsol Assemble: Automatically generates all possible molecular structures (www.upstream.ch)			
Assemble2	Structure generator	PC	Any
IRHelper: Spectral Interpretation guidance			
IRHelper.html	CAI	Web	IR
MS Interpreter: NBS Mass Spectral Interpretation, fragment prediction			
MS Interpreter	Simulation, Helper	Varian Saturn PC	MS
First Order Multiplet Maker: First Order Multiplet prediction			
jmmset.html	Simulation	Web	H-NMR
Sweet J: J coupling calculator, Karplus relations			
altona.html	Helper	Web	H-NMR
garbisch.html	Helper	Web	H-NMR
Sweet J ppc	Helper	Mac	H-NMR
http://www.inmr.net/sweetj.html			
MestReJ	Helper	PC	H-NMR
http://www.mestrelab.com/ mestrej.html			
Spin-Spin Splitting Simulation: Second order multiplets			
jdplot.html	Simulation	Web	NMR
Fragment Finder: Formulas from molar mass			
Fragment.html	Helper	Web	MS
Formula Finder: Formulas from molar mass			
Formula.html	Helper	Web	MS
Molecular Modeling Programs			
MM3	Molecular Modeling	Web	H-NMR J_{AB}
MOE	Molecular Modeling	Schupf Lab	H-NMR J_{AB}

Key: CAI= computer aided instruction
Mac= Macs in Keyes 203 and filerserver1: /academics/chem/CH255J
Web= NMR course Web page

Grading

900-1000 A 800-899 B 700-799 C 600-699 D

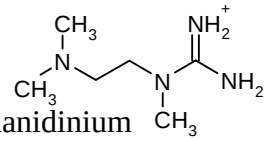
unknown 1	40	
unknown 2	60	
unknown 3	100	
drivers license (See below)	300	^{1}H, ^{13}C, probe tuning, 90° pulse determination, SW set, DEPT
water suppression	50	Watergate on glucose
molecular modeling	40	WF pp. 96-101 pulmericin, Fig. 3.29
MO chemical shift calculation	40	Spartan on camphor or β-ionone using GIAO approach
analysis of a complex spin-spin pattern	60	jdset.html or nmrsim
matched filter and sine-bell apodization	40	data work up

(try different BF's on a noisy spectrum. Find the BF for a "matched filter" and try sine-bell apodization.)

T_1 determination and partially relaxed spectra	90	
HMQC	40	
HMBC	50	
phase sensitive COSY	80	(double quantum filtered)
1D-gradient NOE	70	(camphor, beta-ionone or one of your unknowns)
1D-gradient TOCSY	70	
NOESY	120	camphor
TOCSY	120	camphor, limonene, or betulin
HMQC-TOCSY	120	limonene or betulin
GC/MS	40	
Chromatoprobe MS	60	on solid unknown or candy
direct infusion MS and MS/MS	100	unknown or transition metal complex
LC/MS	100	on unknown or tea infusion
Mirror rate optimization in FT-IR	60	choose 4 cm^{-1} and 8 cm^{-1} resolution and optimize mirror rate
KBr pellet IR sample prep	30	
CHN analysis	50	

• some of the above techniques are combined in the projects below:

unknown monosacharride	200
purity of 4-amidino-N -methylpiperizinium ion samples	200
unknown dipeptide	300
assign resonances in N-[2-(dimethylamino)ethyl]-N-methylguanidinium	100
+ guest-host complex NOESY	250
^{31}P of phosphate complex with N-[2-(dimethylamino)ethyl]-N-methylguanidinium	250
assign resonances in cimetidine	250
assign resonances in dextromethorphan	300
assign resonances in α or β-pinene or lemonene	300
assign resonances in dipeptide from NutraSweet	300
assign resonances in catechin, ^{1}H and ^{13}C	400
assign resonances in betulin (from birch bark)	500



Quizzes and homework also add to the point total

Varian VNMR 500 MHz NMR
License Activities

Take a 1D Proton, adjust the phasing on the spectrum
Find Z0, adjust lock gain, power, and phase
Manual shim
Tune the proton probe
Narrow SW
Retake 1D Proton
Find proton high-power 90° pulse
Do a DEPT135 (CH & CH_3 up/CH_2 down, suppress quaternaries)

You can work on an unknown or just the ethylbenzene or other standard sample