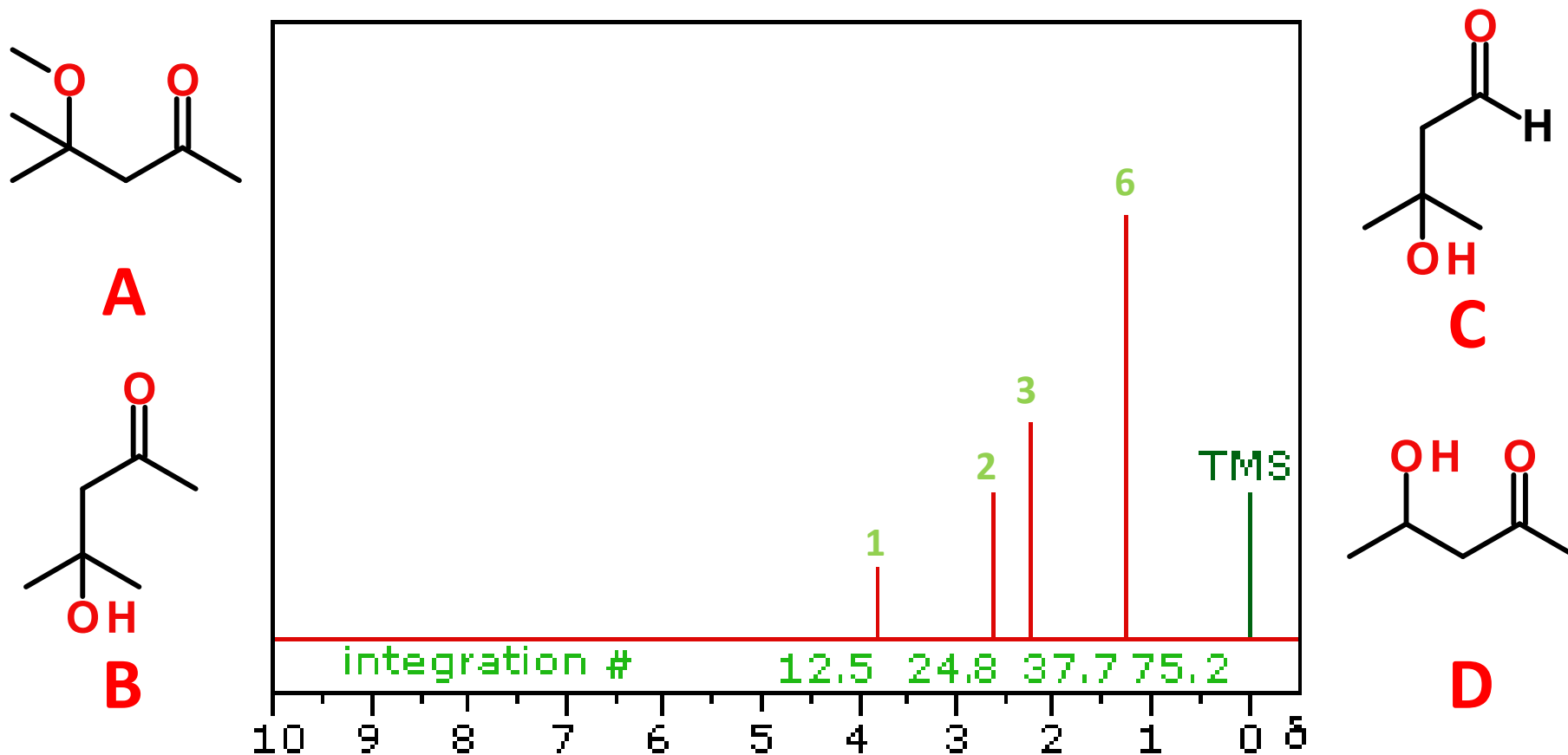
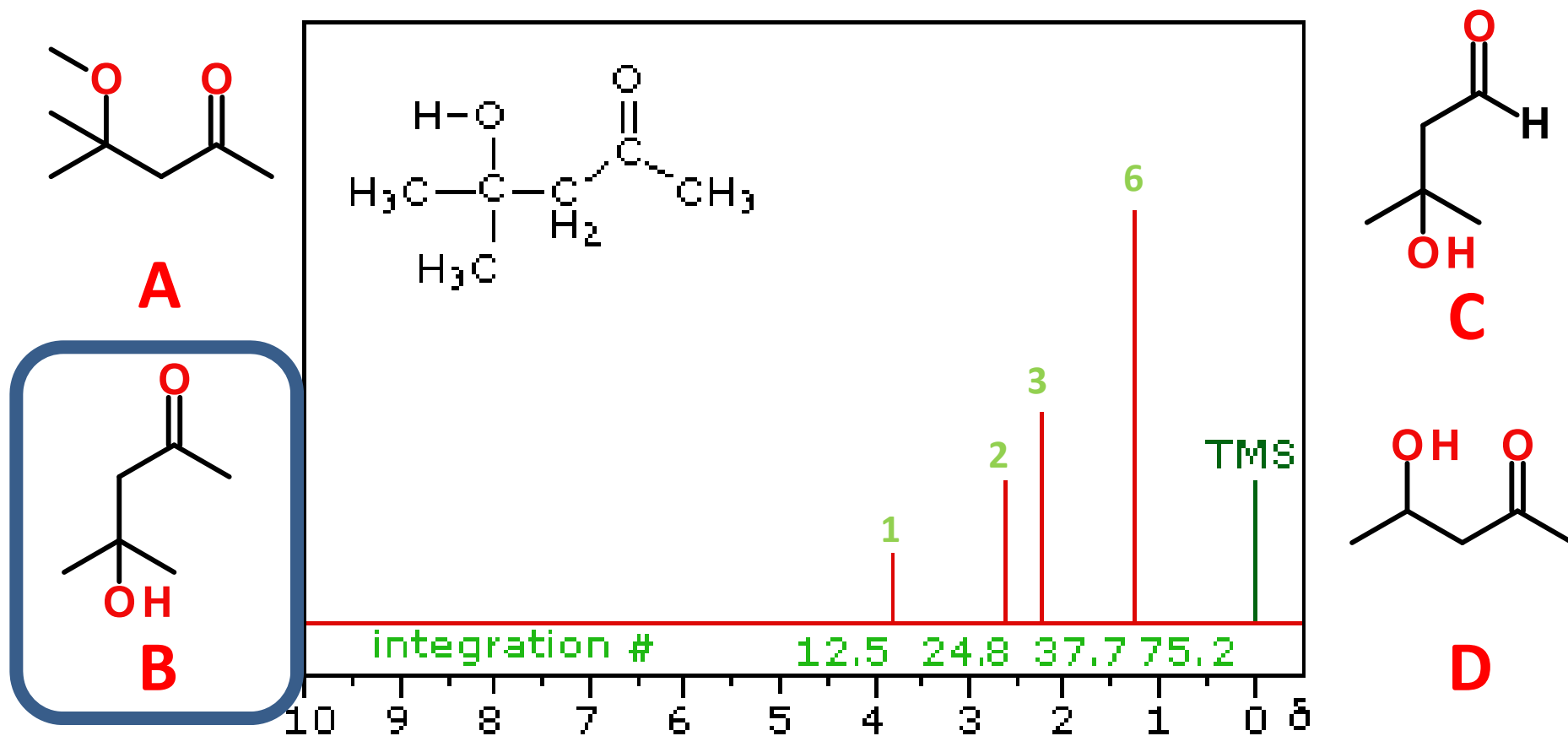


Chemical Shift and Integration Examples



2016-08-29 Q1

Chemical Shift and Integration Examples



2016-08-29 Q1

Exam 1

- **Time:**
 - Tuesday, September 20: 7:00 – 9:00PM
 - Wednesday, September 21: 7:00 – 9:00PM OR
 - Thursday, September 22: 7:00 – 10:00PM
- **Location – Soc/Anthro Testing Center**
 - Chapters will be covered in this order: Chapter 11, 14, 15, 19, 13
- **Practice Exams are Posted**
 - B7-19-98A Practice Exam 1A
 - B7-19-98B Practice Exam 1B
- **Deadline for alternate arrangements is Monday, 9/19/2016 at 4:30 PM (i.e., close of business)**
 - An oral make-up exam will be required for making up the exam for all students not taking the exam on the above dates or having already made prior arrangements

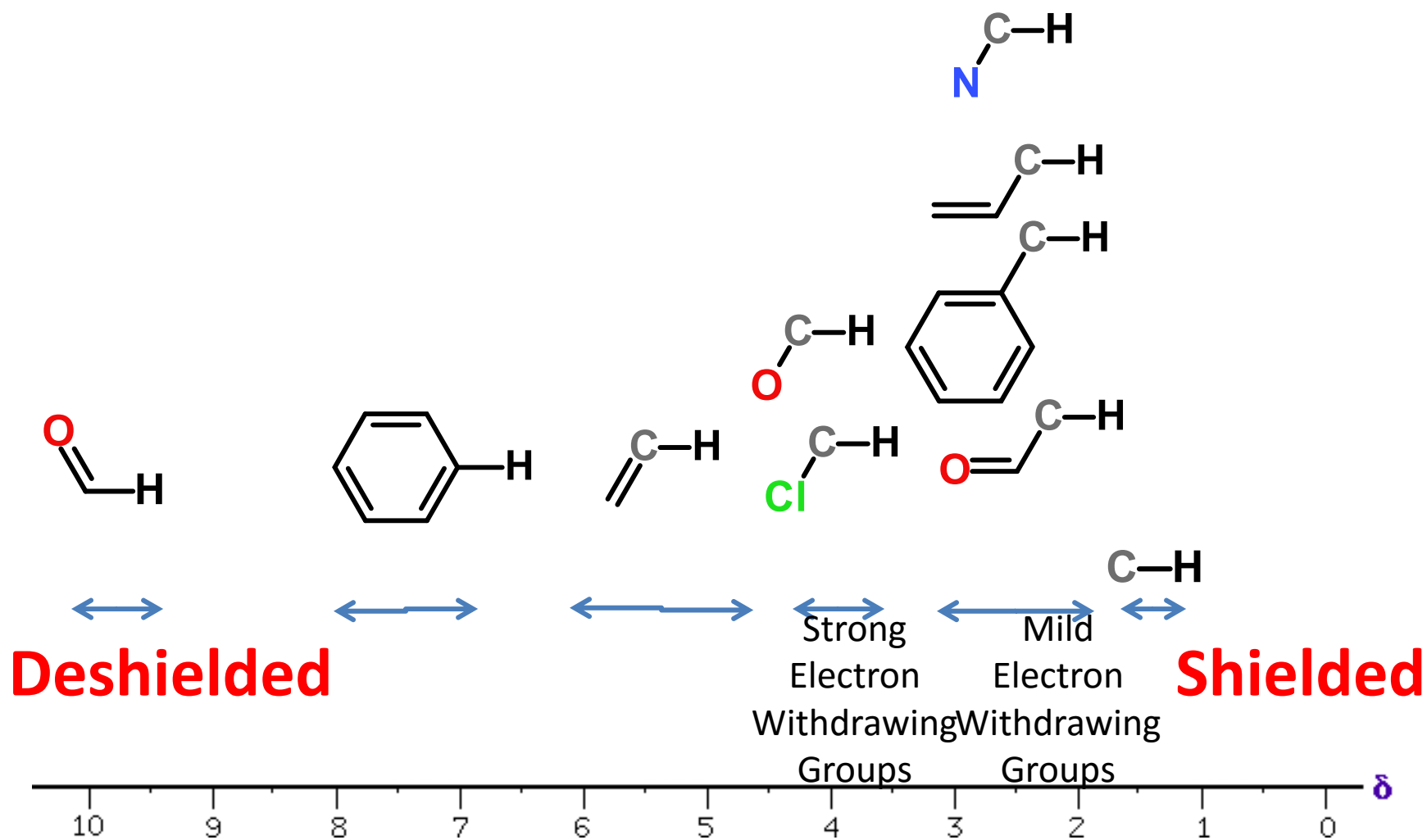
Order of Coverage (Exam 1)

	Homework Assignment	Due Date
1	B4-11-01 IR Functional Groups (wDeadline)	Tuesday, August 23
2	B7-14-02 Mass Spec - Molecular Ion (wDeadline)	Wednesday, August 24
3	B7-14-03 Mass Spec - Isotope Effects (wDeadline)	Thursday, August 25
4	B7-15-01 Number of Peaks 1H NMR Spectra (wDeadline)	Friday, August 26
5	B7-15-06 Number of Peaks 13C NMR (wDeadline)	Saturday, August 27
6	B7-15-02 Theoretical NMR Chemical Shift (wDeadline)	Sunday, August 28
7	B7-15-03 Theoretical NMR Integration (wDeadline)	Monday, August 29
8	B7-15-04 Theor. NMR Spin-Spin Splitting (wDeadline)	Tuesday, August 30
9	B7-15-05 NMR Spectroscopy Problems (wDeadline)	Wednesday, August 31
10	B7-15-07 13C NMR Structure ID (wDeadline)	Thursday, September 1
11	B7-13-01A Nomenclature Alkyl Halides (wDeadline)	Friday, September 2
12	B7-13-01B Alkyl Halide Nomenclature (wDeadline)	Saturday, September 3
13	B7-13-02A Halogenation of Alkanes (wDeadline)	Sunday, September 4
14	B7-13-02B Halogenation of Alkanes (wDeadline)	Monday, September 5

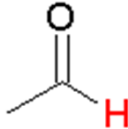
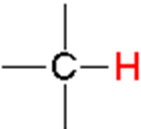
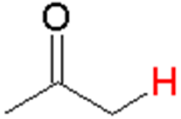
Order of Coverage (Exam 1)

	Homework Assignment	Due Date
15	B7-13-03A Oxidation and Anti-oxidants (wDeadline)	Tuesday, September 6
16	B7-19-01 Aromaticity (wDeadline)	Wednesday, September 7
17	B7-19-02B Arene Nomenclature (wDeadline)	Thursday, September 8
18	B7-19-03A Halogenation of Arenes (wDeadline)	Friday, September 9
19	B7-19-03B Halogenation of Arenes (wDeadline)	Friday, September 9
20	B7-19-04A Arene Rxns Inorganic Acids (wDeadline)	Saturday, September 10
21	B7-19-04B Arene Rxns Inorganic Acids (wDeadline)	Saturday, September 10
22	B7-19-05A Friedel-Crafts (wDeadline)	Sunday, September 11
23	B7-19-05B Friedel-Crafts (wDeadline)	Sunday, September 11
24	B7-19-06 Arene Mechanistic Issues (wDeadline)	Wednesday, September 12
25	B7-19-06B Arene Mechanisms (wDeadline)	Wednesday, September 12
26	B7-19-07A Nucleophilic Aromatic Subs (wDeadline)	Thursday, September 13
27	B7-19-07B Nucleophilic Aromatic Subs (wDeadline)	Friday, September 14
	Exam 1	September 18, 19, 20

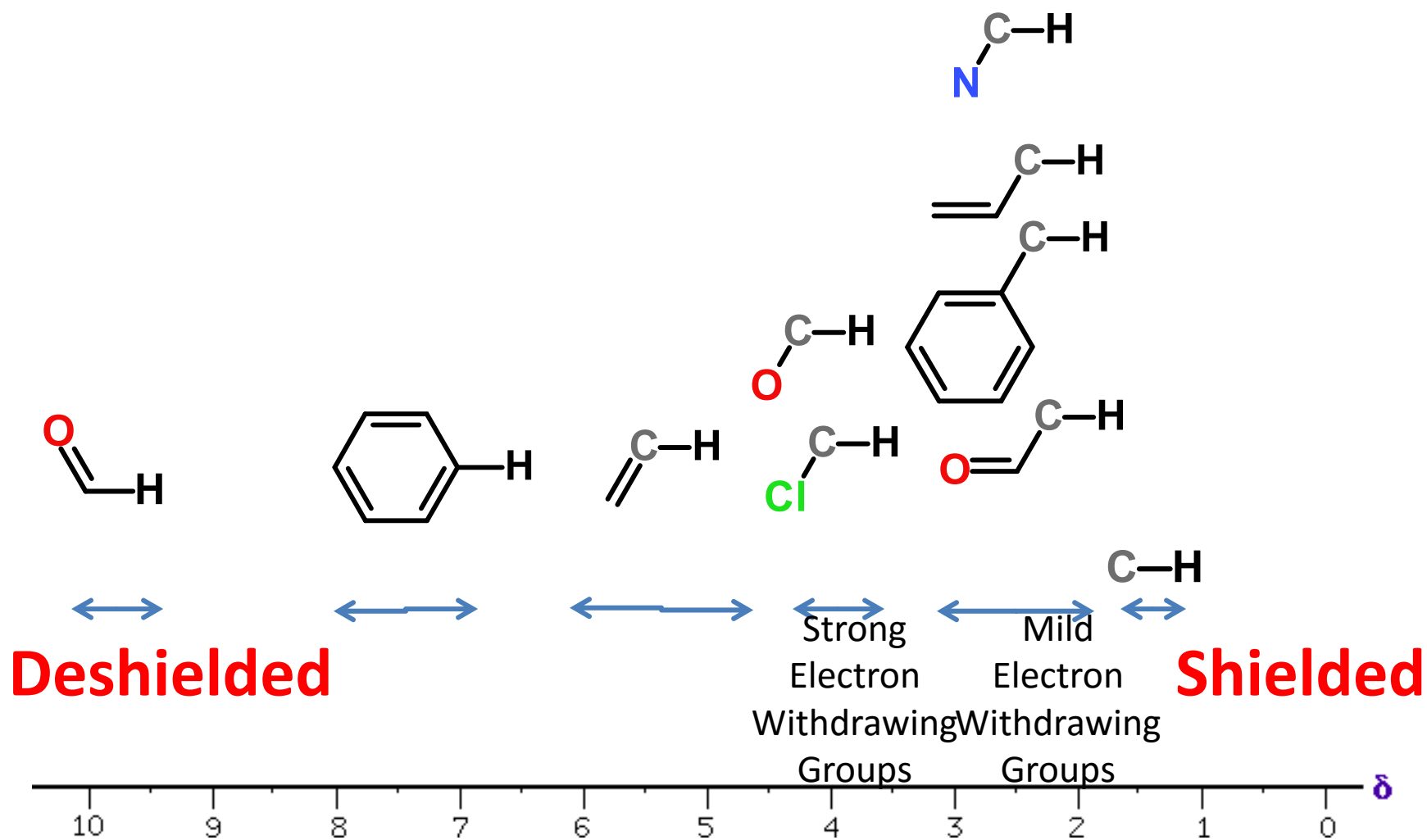
Penn's View of ^1H Chemical Shifts



Approximate Values of Chemical Shifts for ^1H NMR

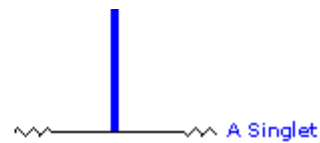
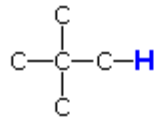
Type of Proton	Approximate Chemical Shift (δ)	Type of Proton	Approximate Chemical Shift (δ)
$-\text{CH}_3$	0.9	Ar-H	6.8-8.0
$-\text{CH}_2-$	1.2-1.3		9.7-10.5
	1.4	I-C-H	3.1-3.3
$\text{C}=\text{C}-\text{CH}_3$	1.5-2.5	Br-C-H	3.4-3.6
	2.1-2.6	Cl-C-H	3.6-3.8
Ar- CH_3	2.3-2.6	RNH_2	Variable
$-\text{C}\equiv\text{C}-\text{H}$	2.5-3.0	R-O-H	Variable
R-O-CH	3.3-4.0	ArOH	Variable
$\text{R}_2\text{C}=\text{CHR}$	4.5-6.5	RCO_2H	Variable

Penn's View of ^1H Chemical Shifts

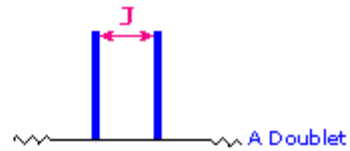
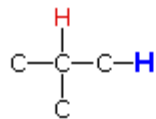


Splitting Patterns

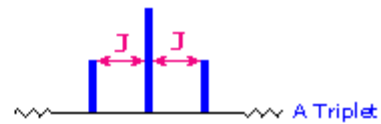
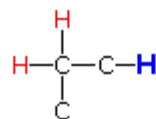
No Coupled
Hydrogens



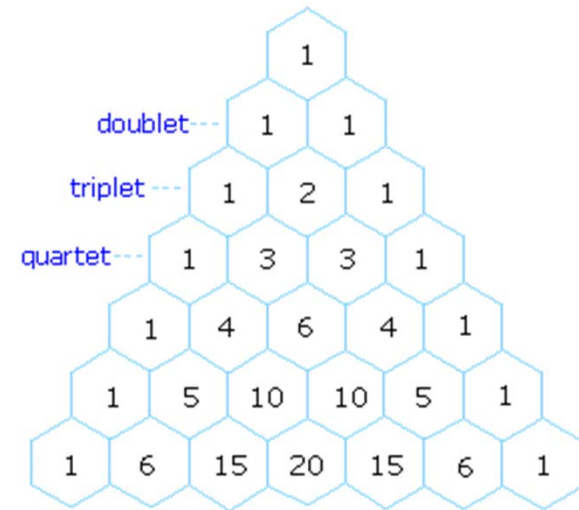
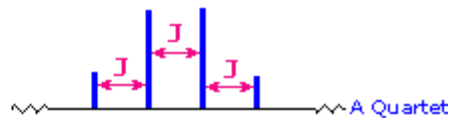
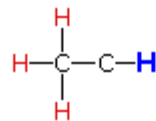
One Coupled
Hydrogen



Two Coupled
Hydrogens



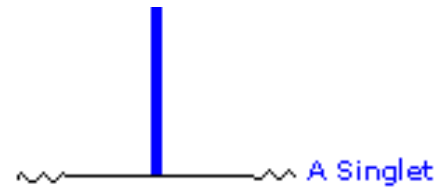
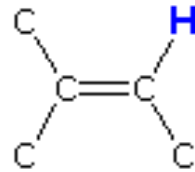
Three Coupled
Hydrogens



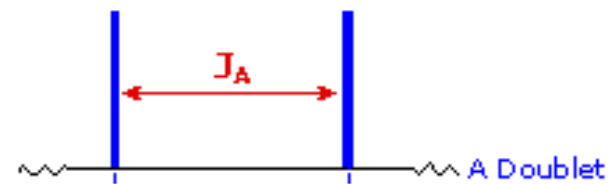
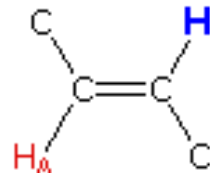
Pascal's Triangle

Splitting Patterns

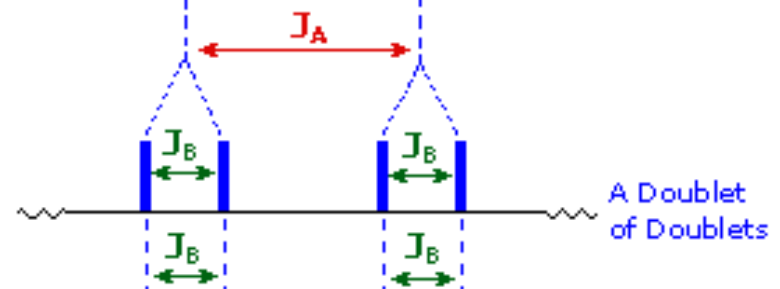
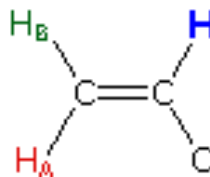
No Coupled
Hydrogens



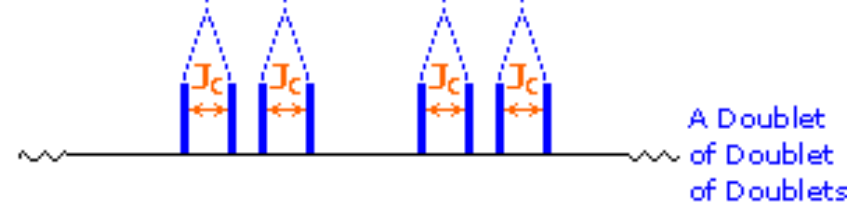
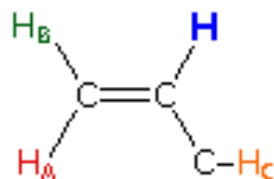
One Coupled
Hydrogen



Two Coupled
Hydrogens

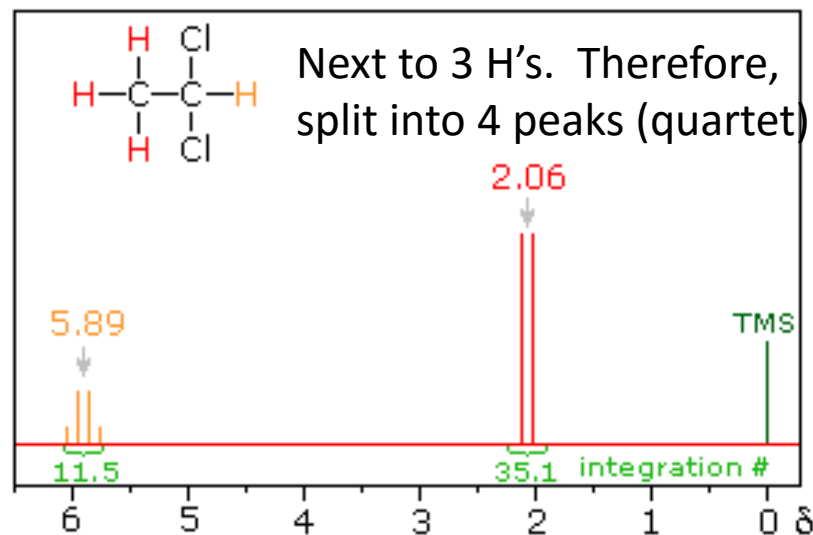
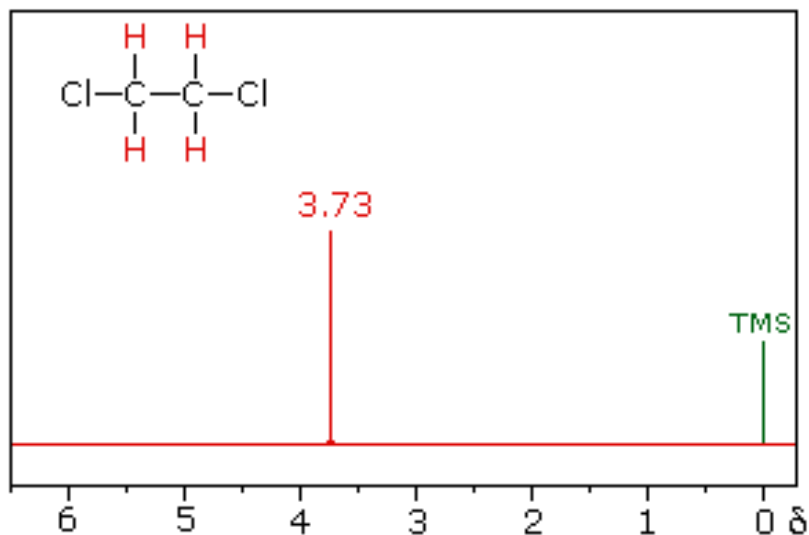


Three Coupled
Hydrogens



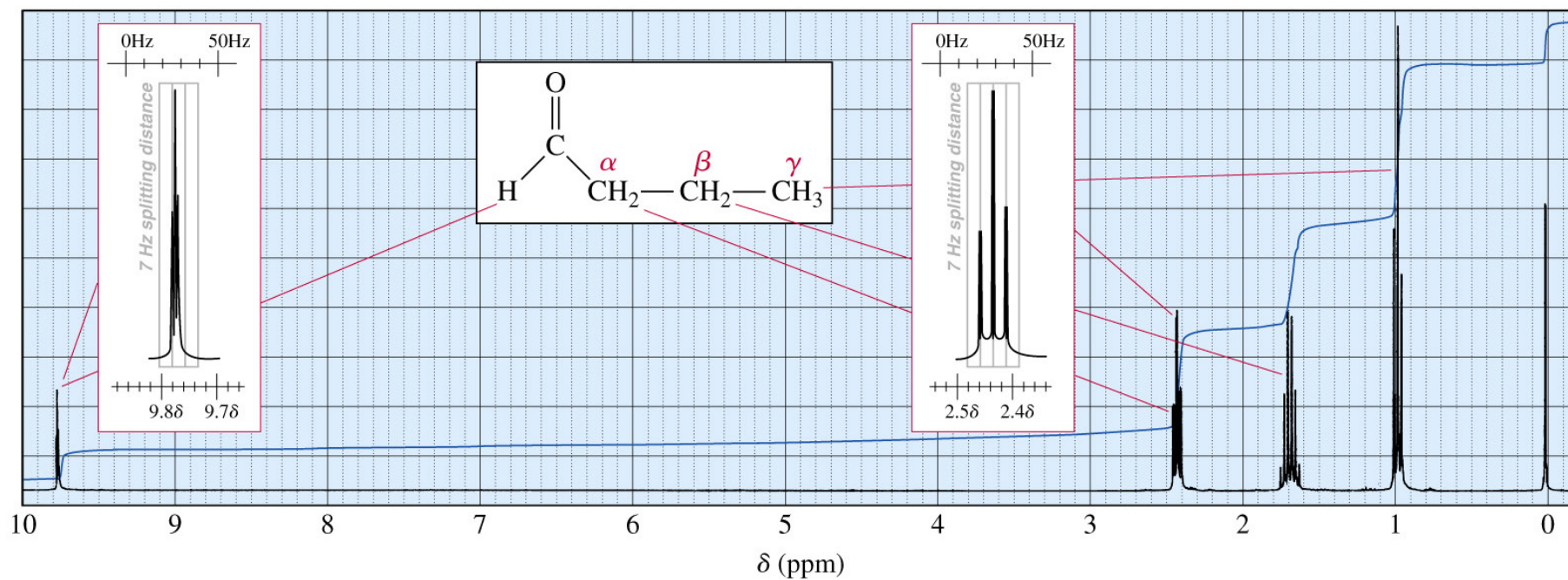
Spin-Spin Splitting

Next to 1 H. Therefore,
split into 2 peaks (doublet)

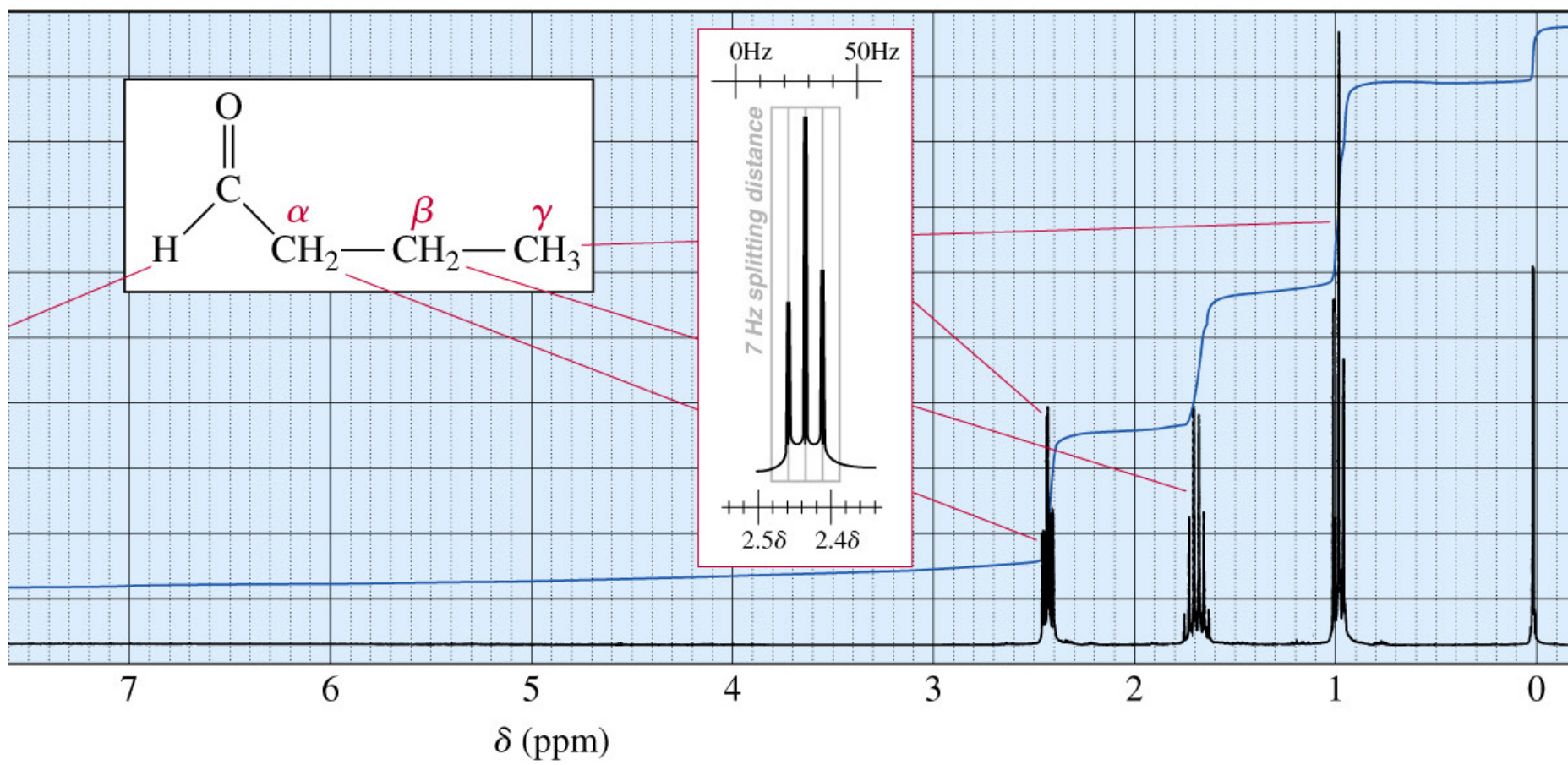


All hydrogens are chemically equivalent. Therefore, no splitting!

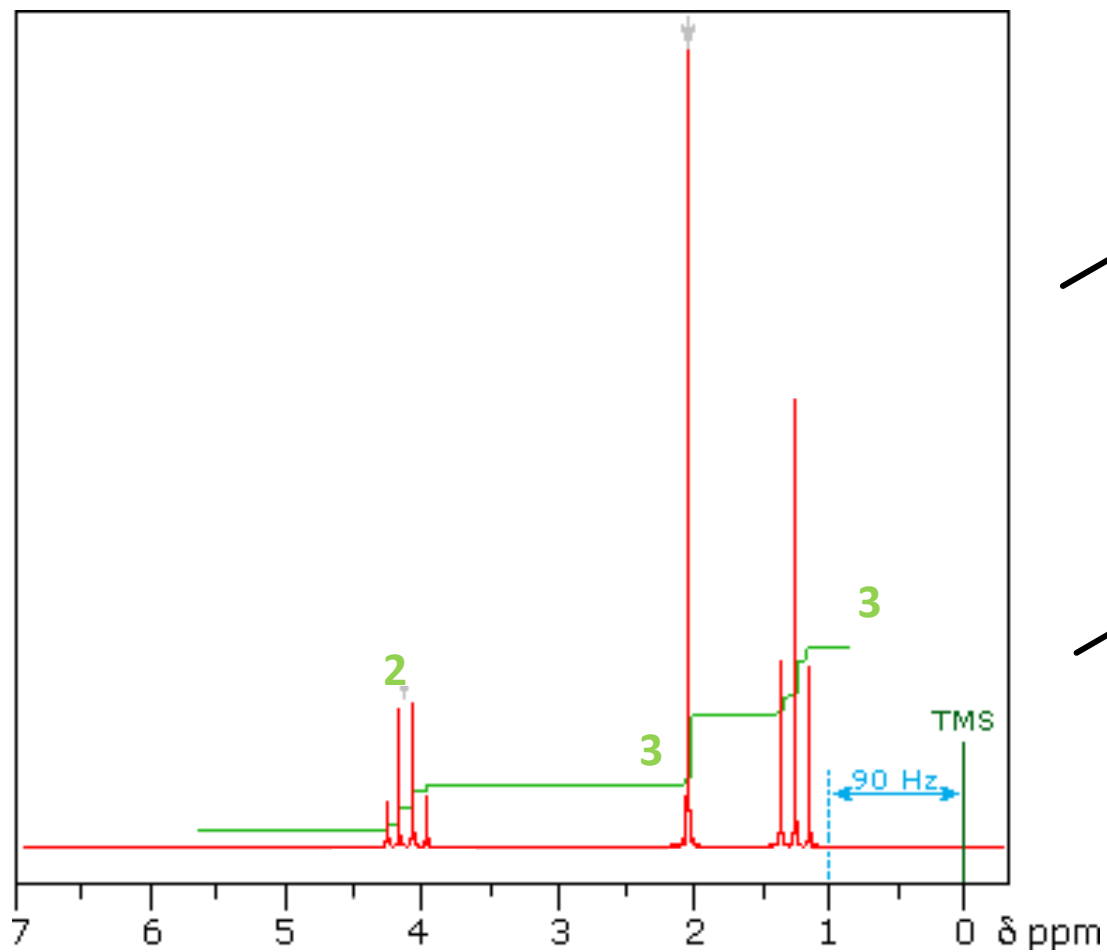
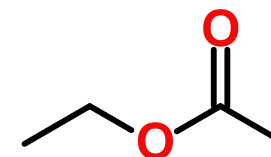
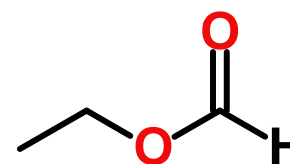
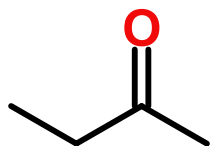
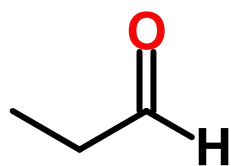
9.78 (1H, t), 2.45 (2H, dt), 1.7 (2H, tt),
0.9 (3H, t)



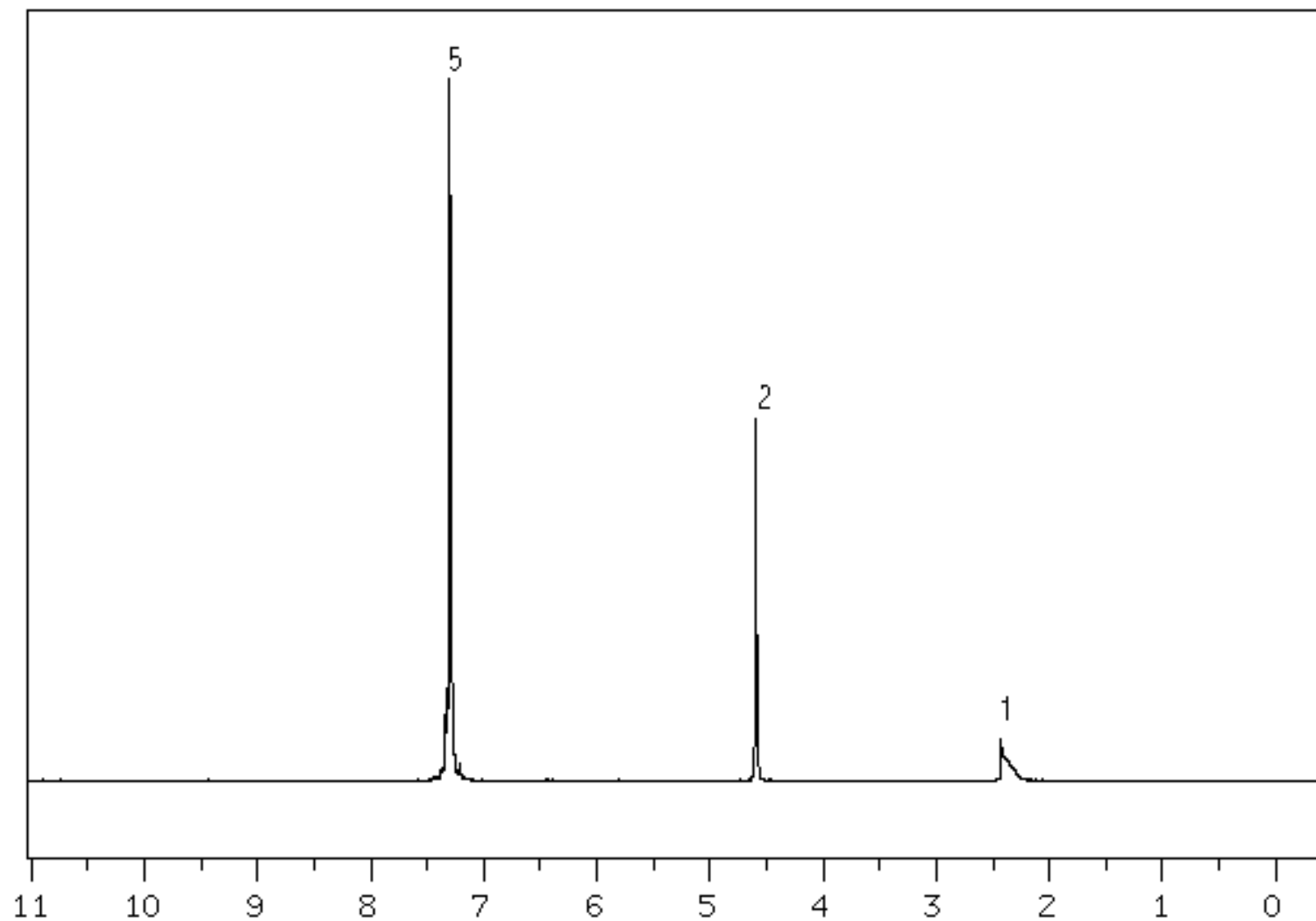
9.78 (1H, t), 2.45 (2H, dt), 1.7 (2H, tt),
0.9 (3H, t)



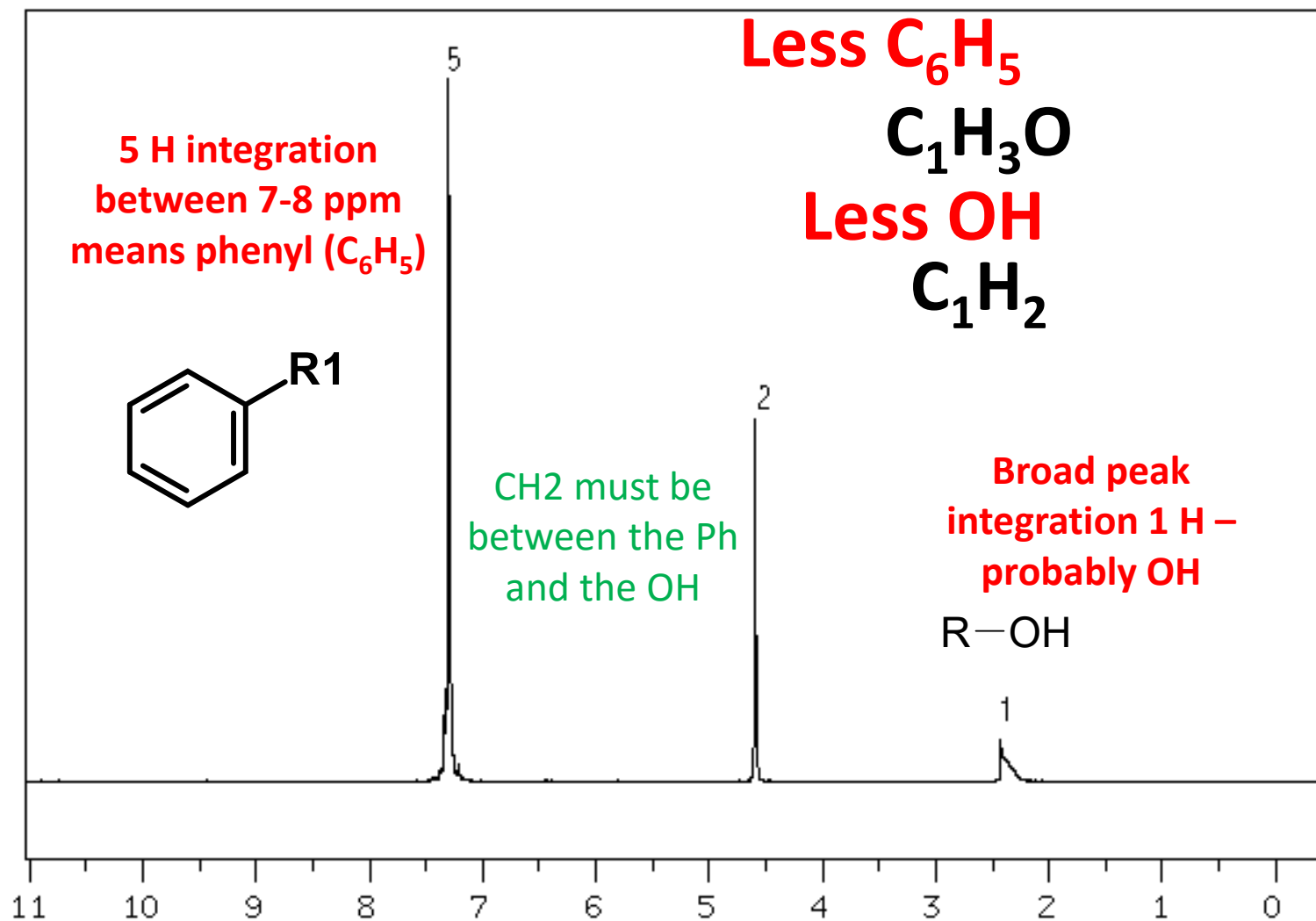
2016-08-29 Q2



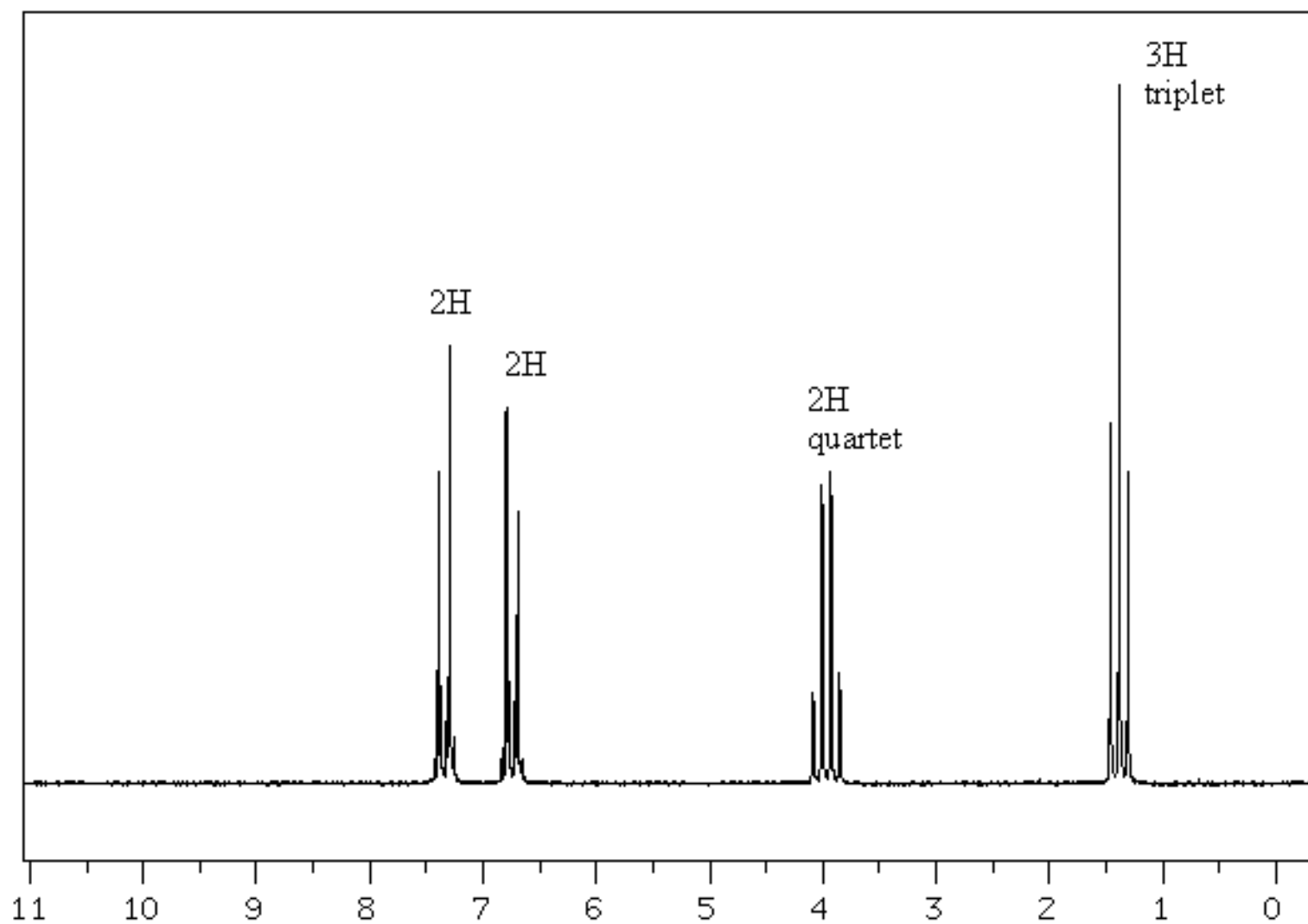
Worked Example C₇H₈O



Worked Example C₇H₈O

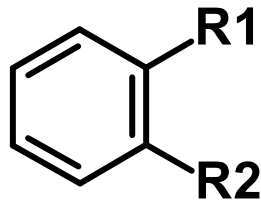


Worked Example (C_8H_9BrO)

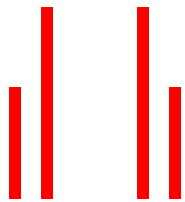


Di-substituted Aryl Groups

1,2-disubstituted

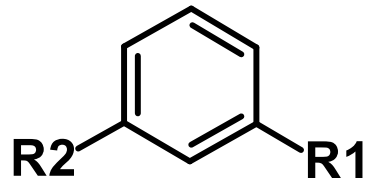


4 different H's,
"simpler" splitting
pattern



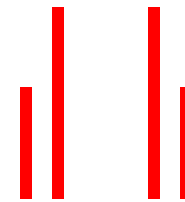
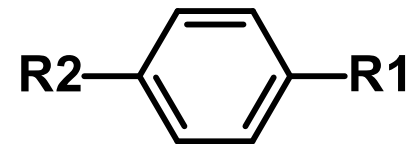
If R1 is chemically
similar to R2, then
doublet of doublet

1,3-disubstituted

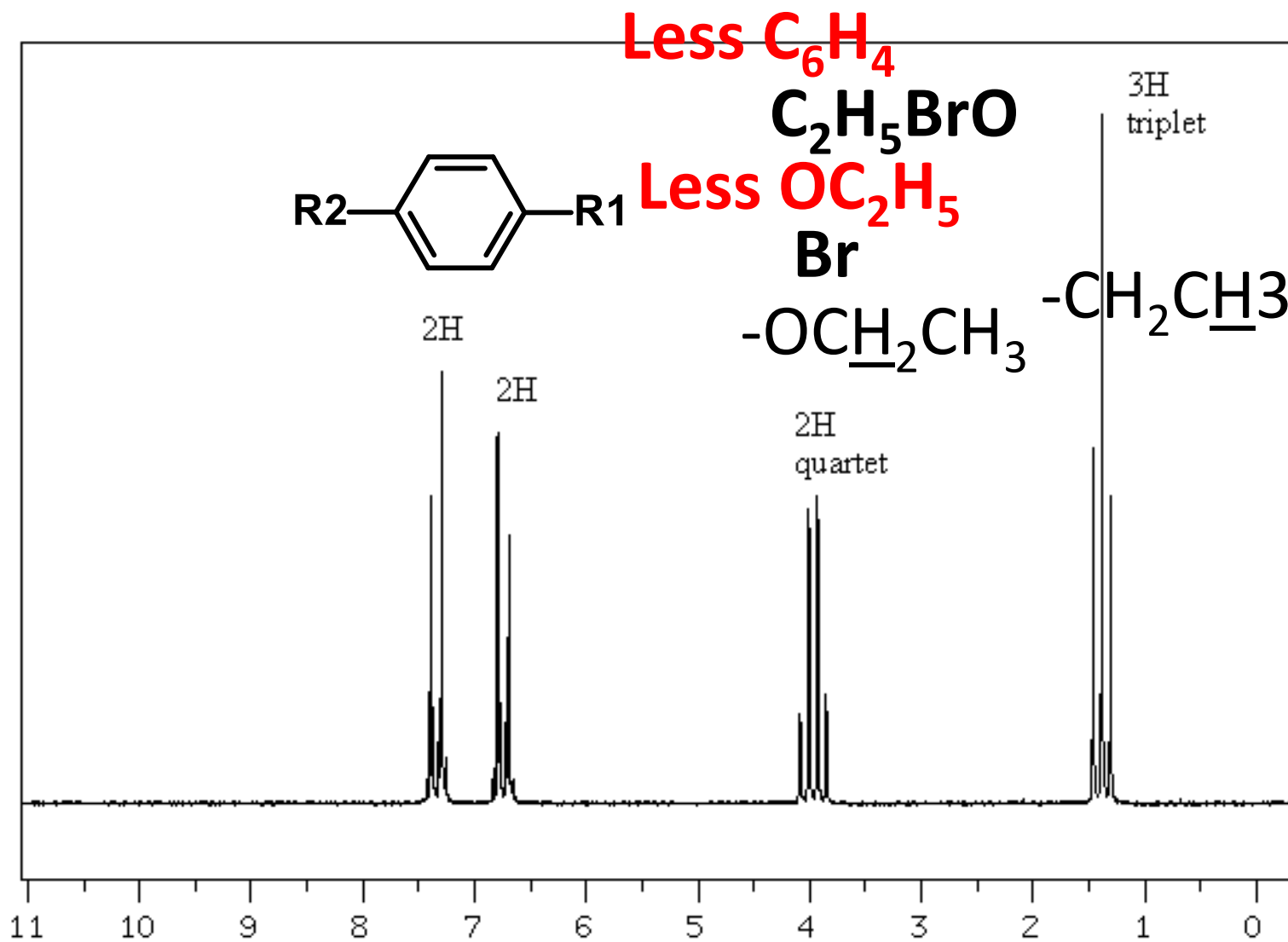


4 different H's, complex
splitting pattern

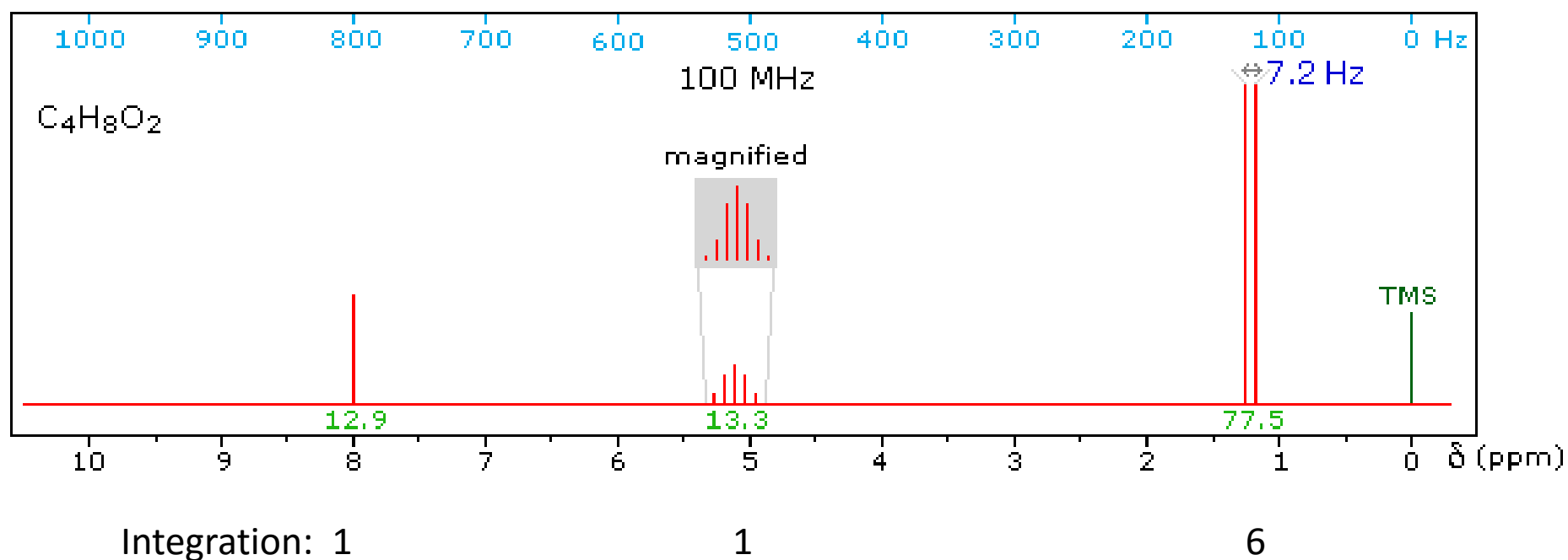
1,4-disubstituted



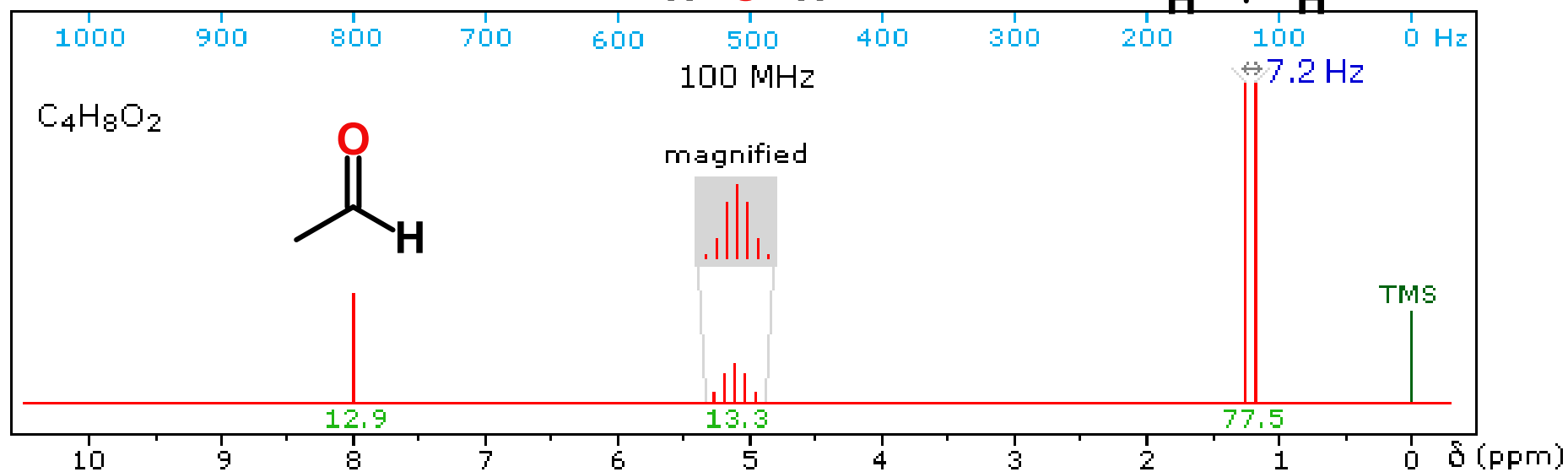
Worked Example (C_8H_9BrO)



Worked Example ($C_4H_8O_2$)



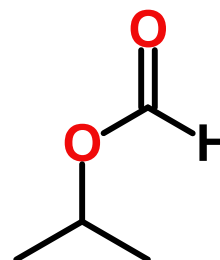
Worked Example (C₄H₈O₂)



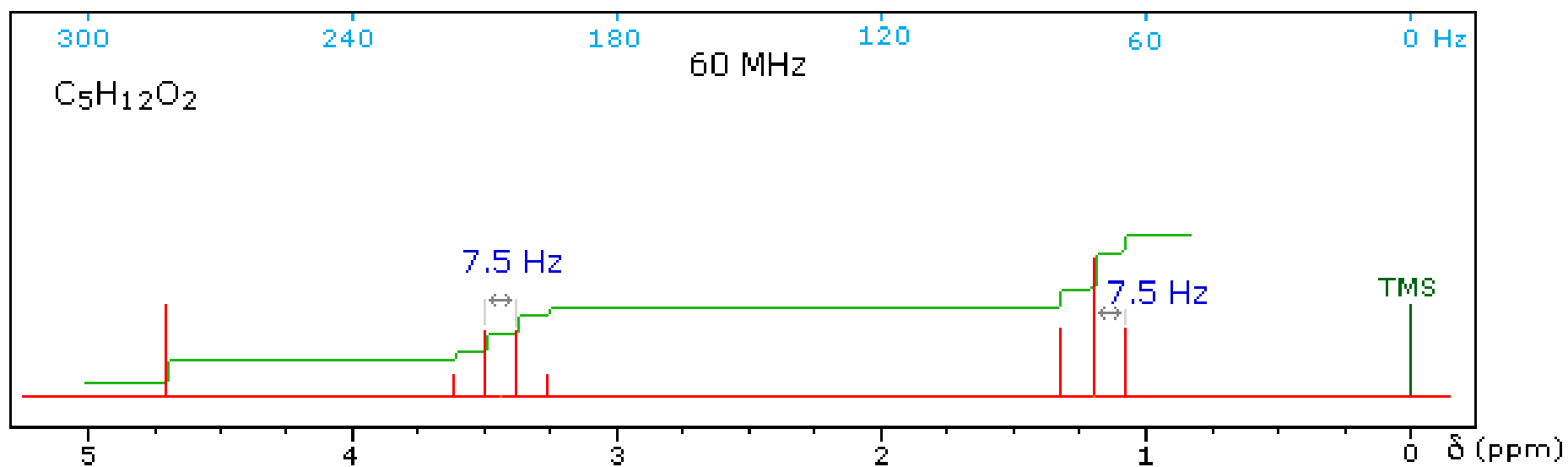
Integration: 1

1

6



Worked Example ($C_5H_{12}O_2$)



Worked Example ($C_5H_{12}O_2$)

