The mass spectrum of an unknown compound has a molecular ion peak with a relative intensity of 46.60% and an M+1 peak of 2.57%. How many carbon atoms are in the compound? (Fill in an integer number)

$$\text{Number of carbon atoms} = \frac{\text{Intensity of M+1 peak}}{0.011 \times \text{Intensity of M peak}}$$

$$\text{Number of carbon atoms} = \frac{2.57\%}{0.011 \times 46.60\%}$$

2016-08-24 Q1 **Correct Answer = 5**

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**

Exam 1

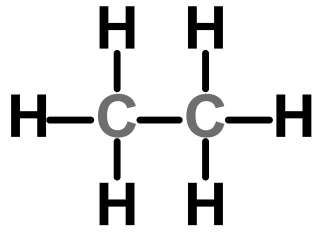
- **Time:**
  - **Tuesday, September 20: 7:00 – 9:00PM**
  - **Wednesday, September 21: 7:00 – 9:00PM OR**
  - **Thursday, September 22: 7:00 – 10:00PM**
- **Location – Soc/Anthro Testing Center**
  - Chapters will be covered in this order: Chapter 11, 14, 15, 19, 13
- **Practice Exams are Posted**
  - 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**

Chemically Equivalent Hydrogens

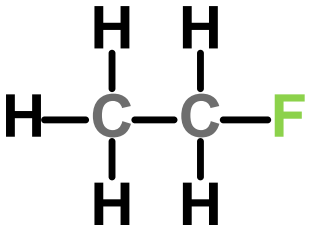
- Equivalent hydrogens are H-atoms that are completely interchangeable as to their role in the molecule.
  - One way is to determine whether H's are equivalent is to replace each H with a different group and see if you get a different compound.

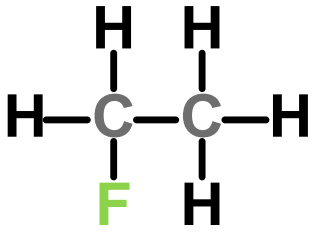
Chemically Equivalent Hydrogens

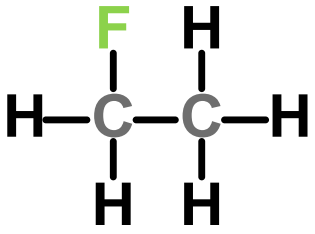
- One way is to determine whether H's are equivalent is to replace each H with a different group and see if you get a different compound.

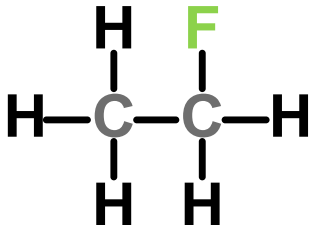


All H's in ethane are chemically equivalent!





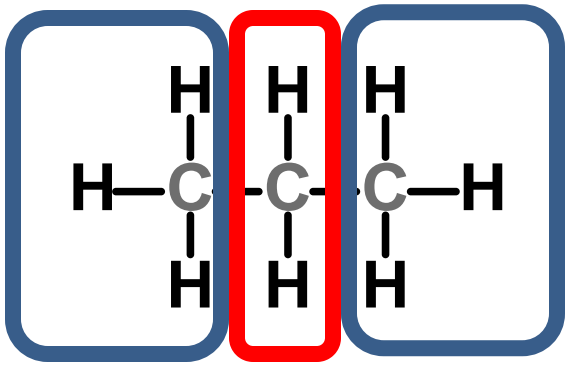




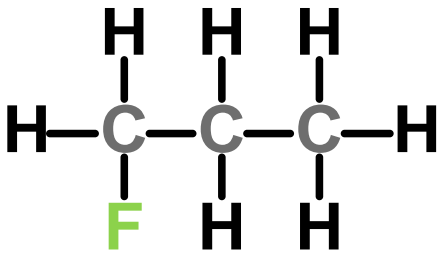
Replacement of any H with an F results in the same compound!

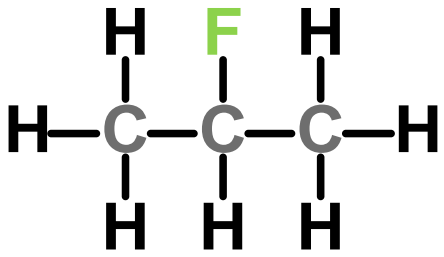
Chemically Equivalent Hydrogens

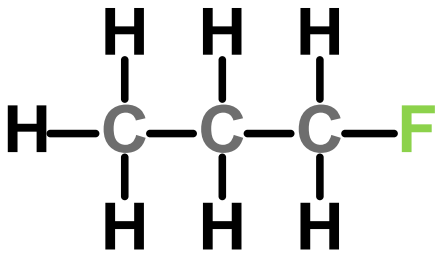
- Propane has two (2) groups of chemically equivalent hydrogens.



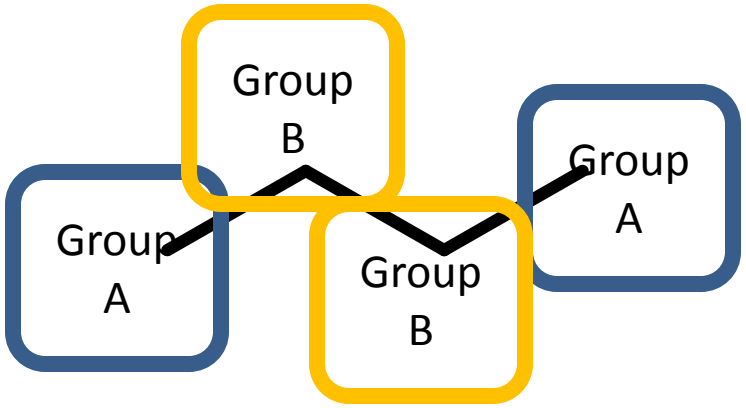
Substitution of any one of the blue H's results in 1-fluoropropane, while substitution of either of the red H's results in 2-fluoropropane







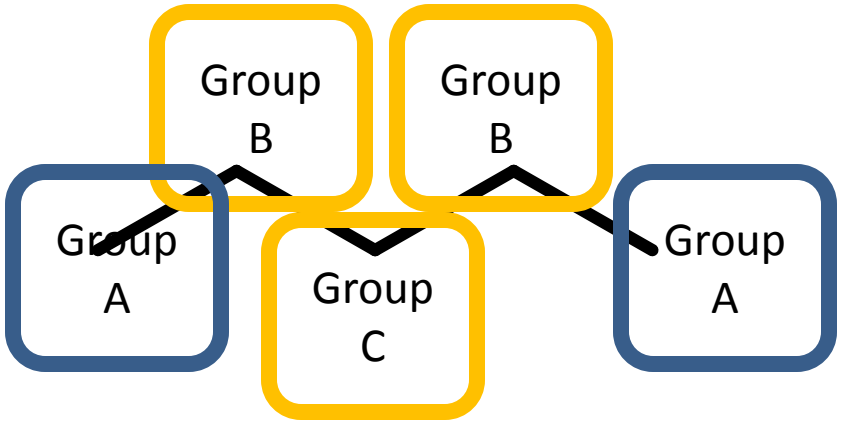
How many different groups of chemically equivalent hydrogen atoms are in the following compound? Give a number.



Answer = 2

2016-08-24 Q2

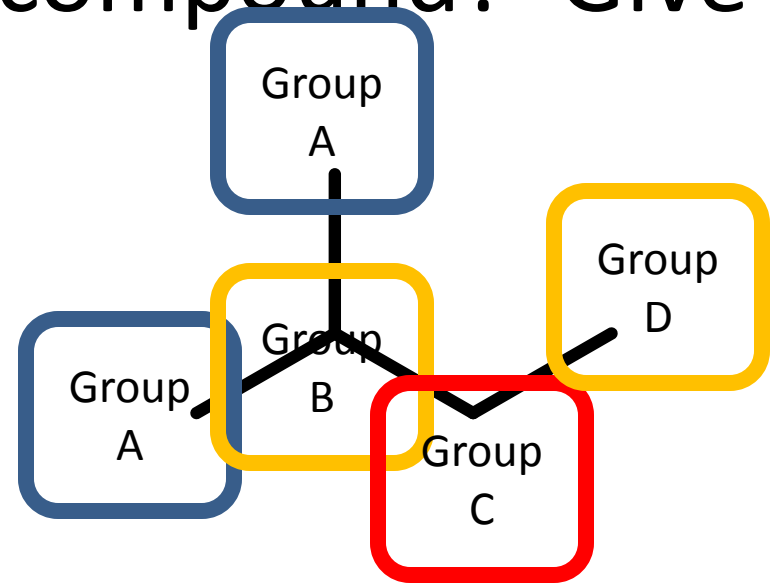
How many different groups of chemically equivalent hydrogen atoms are in the following compound? Give a number.



Answer = 3

2016-08-24 Q3

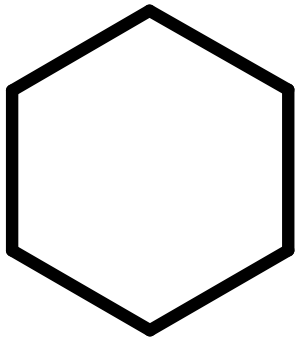
How many different groups of chemically equivalent hydrogen atoms are in the following compound? Give a number.



Answer = 4

2016-08-24 Q4

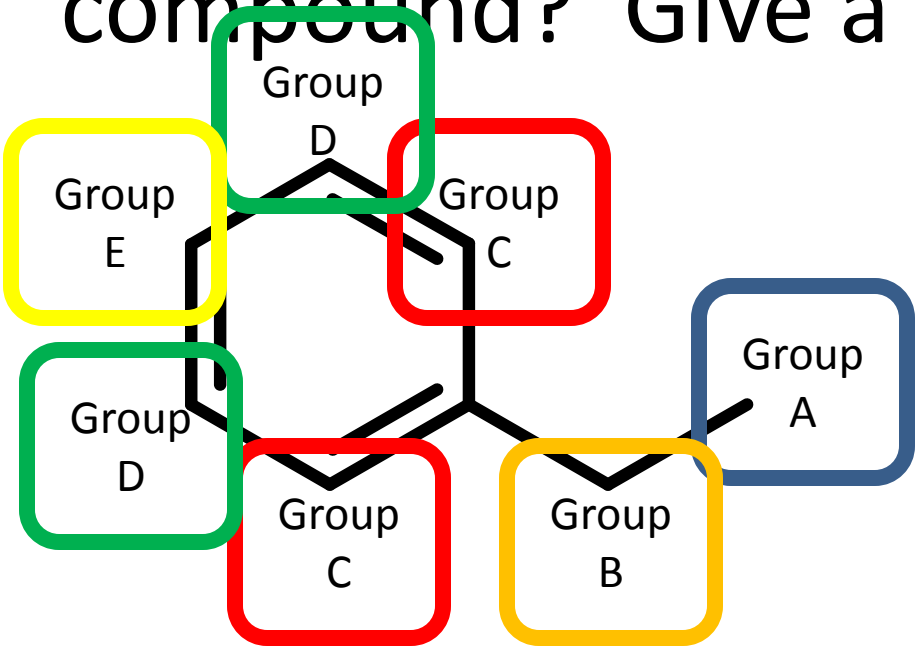
How many different groups of chemically equivalent hydrogen atoms are in the following compound? Give a number.



Answer = 1

2016-08-24 Q5

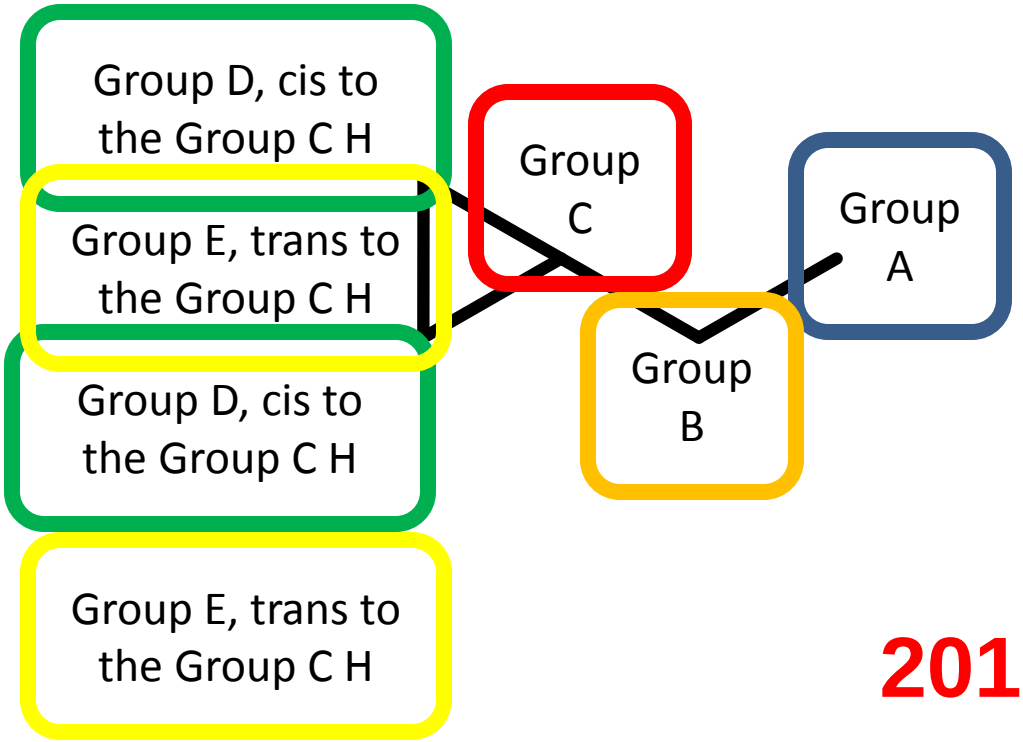
How many different groups of chemically equivalent hydrogen atoms are in the following compound? Give a number.



Answer = 5

2016-08-24 Q6

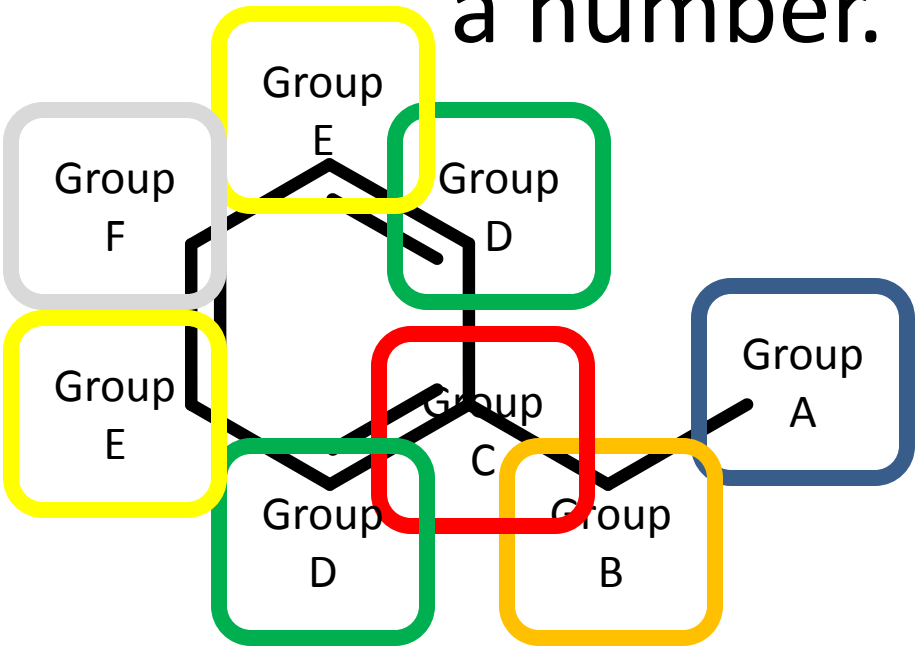
How many different groups of chemically equivalent hydrogen atoms are in the following compound? Give a number.



Answer = 5, due to *cis*, *trans*- issues

2016-08-24 Q7

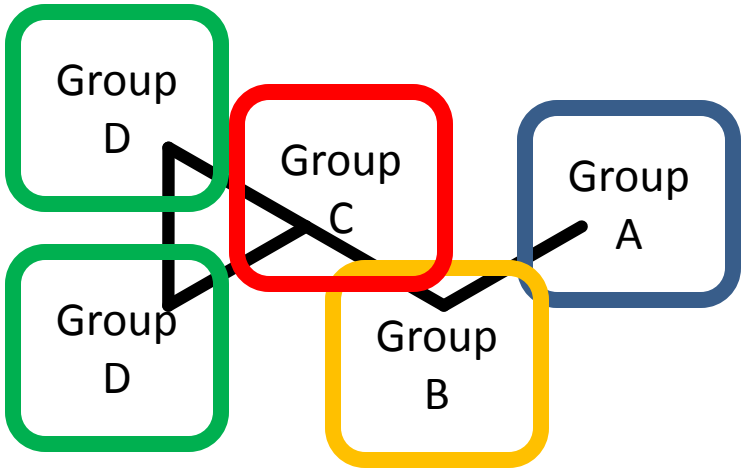
How many different groups of chemically equivalent **carbon** atoms are in the following compound? Give a number.



Answer = 6

2016-08-24 Q8

How many different groups of chemically equivalent **carbon** atoms are in the following compound? Give a number.



Answer = 4

2016-08-24 Q9

Background Material

- http://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/Spectrpy/nmr/nmr1.htm
  - (Last accessed August 23, 2016)
- OR Google “NMR Tutorial”

What can I learn from ^{1}H NMR?

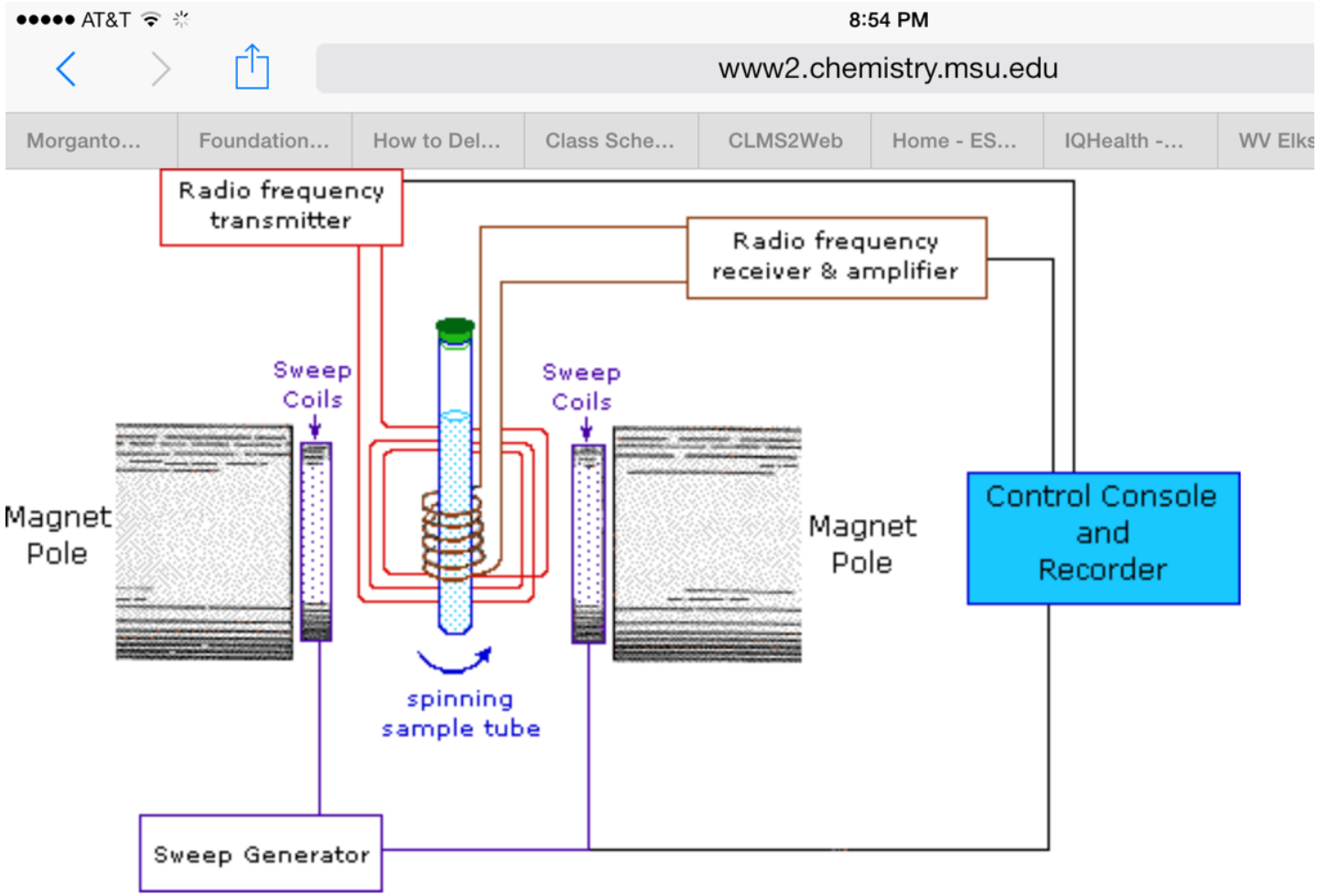
- **Each group of chemically equivalent hydrogens gives a signal!**
- Three pieces of information from each signal
  - Chemical Shift
    - Deshielding from Nearest Neighbors
      - Electronegativity (e.g., O, N, C=O, Ar)
      - Pi system effects
  - Integration
    - Number of H's on that carbon atom
  - Spin-spin splitting
    - Number of H's on next carbon atom

A Modern Spectrometer

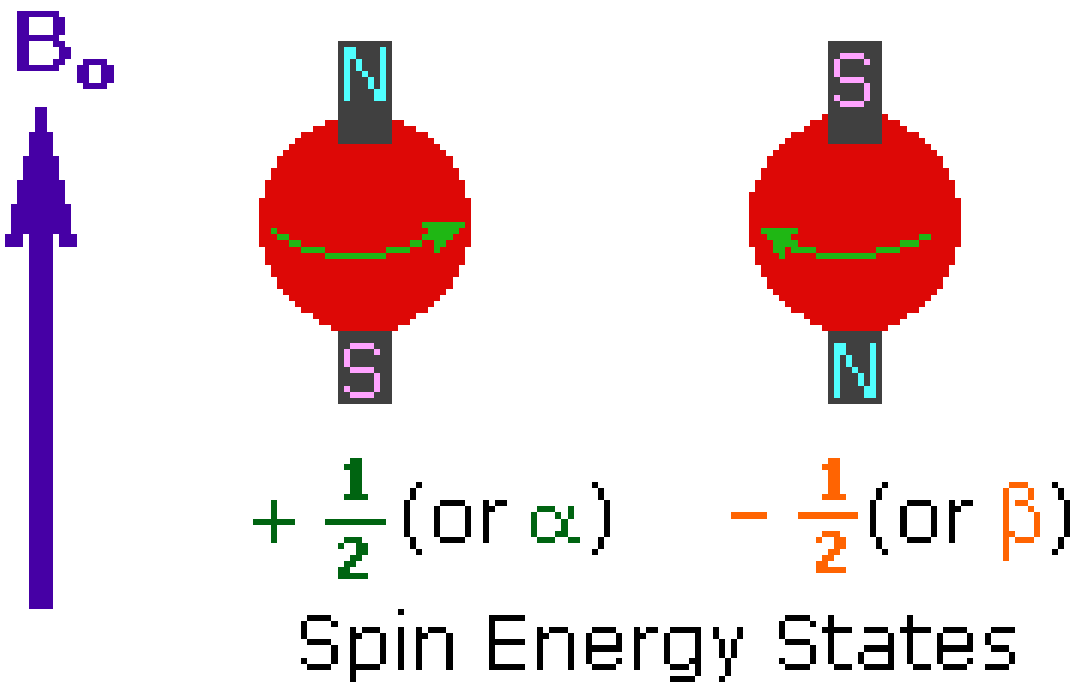
Cost:
$600,000

Room 110
Clark Hall

Schematic view of an NMR Spectrometer

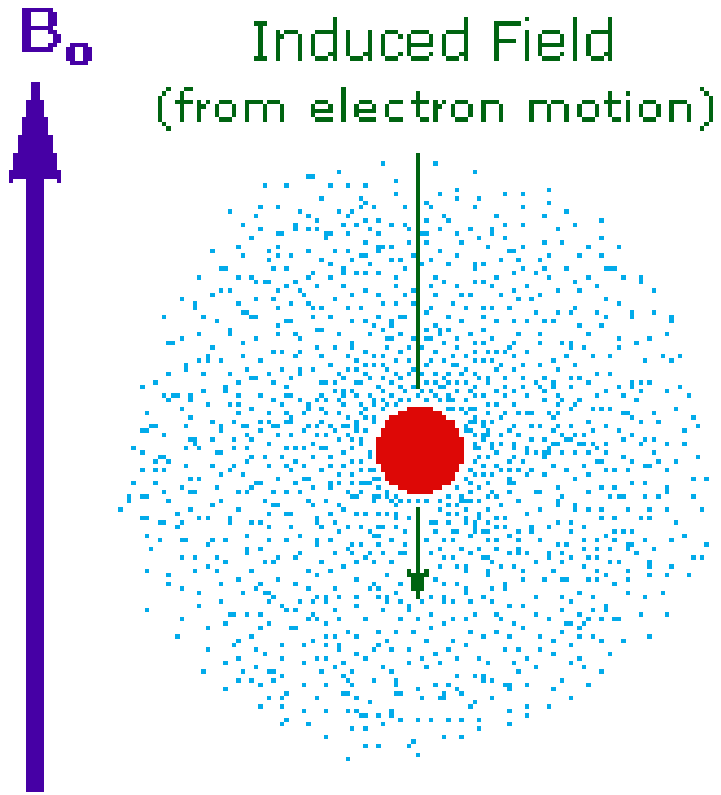


Introduction to Chemical Shift



H nucleus (among others) has a magnetic moment, due to spinning of the charged nucleus. In a magnetic field, there are two possible energetic states where the nuclei are stable. The energy range for changing from one allowed state is in the radio frequency range and is measured in Nuclear Magnetic Resonance.

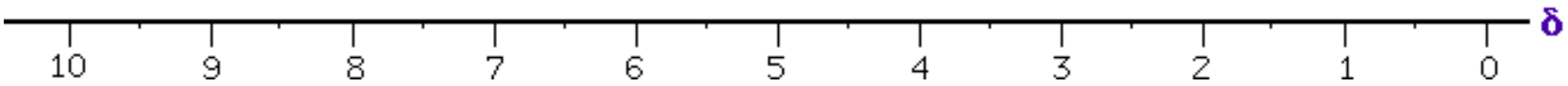
Chemical Shift Depends Primarily on the Electron Cloud Surrounding the Nucleus



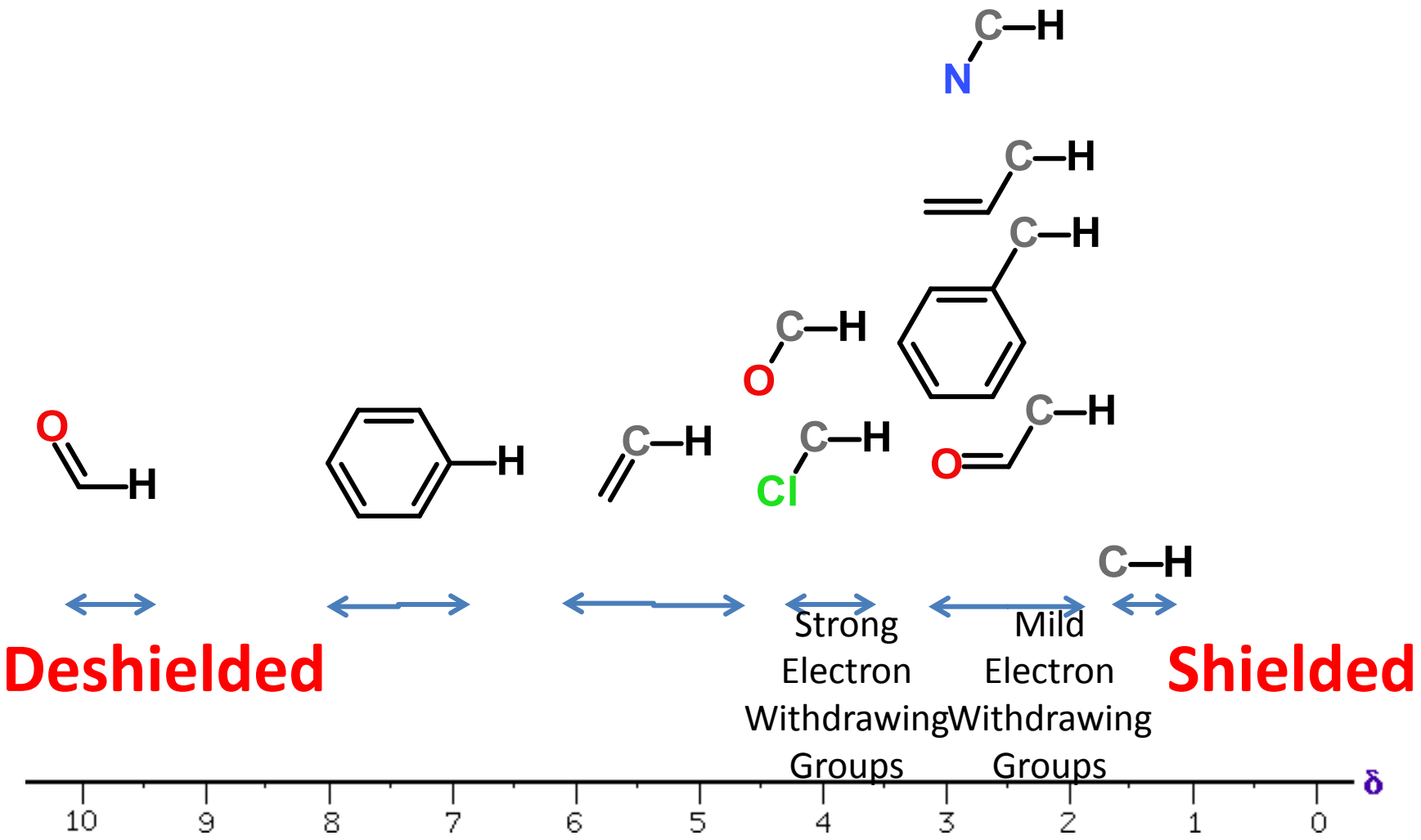
- An electronegative group will remove electrons from the cloud and “deshield” the nucleus
- More electron density results in a more “shielded” nucleus

^{1}H Chemical Shifts

Deshielded **Shielded**



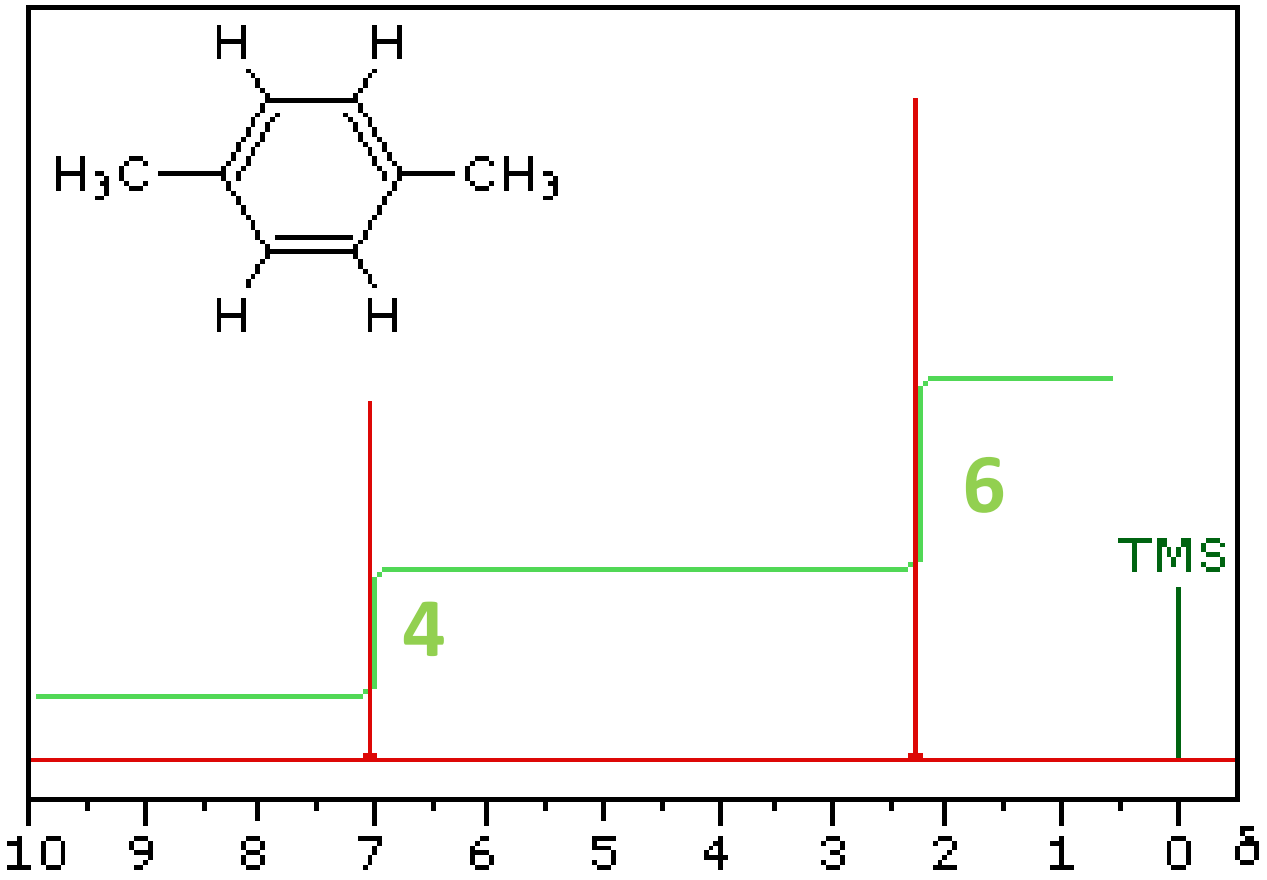
Penn's View of ^{1}H Chemical Shifts



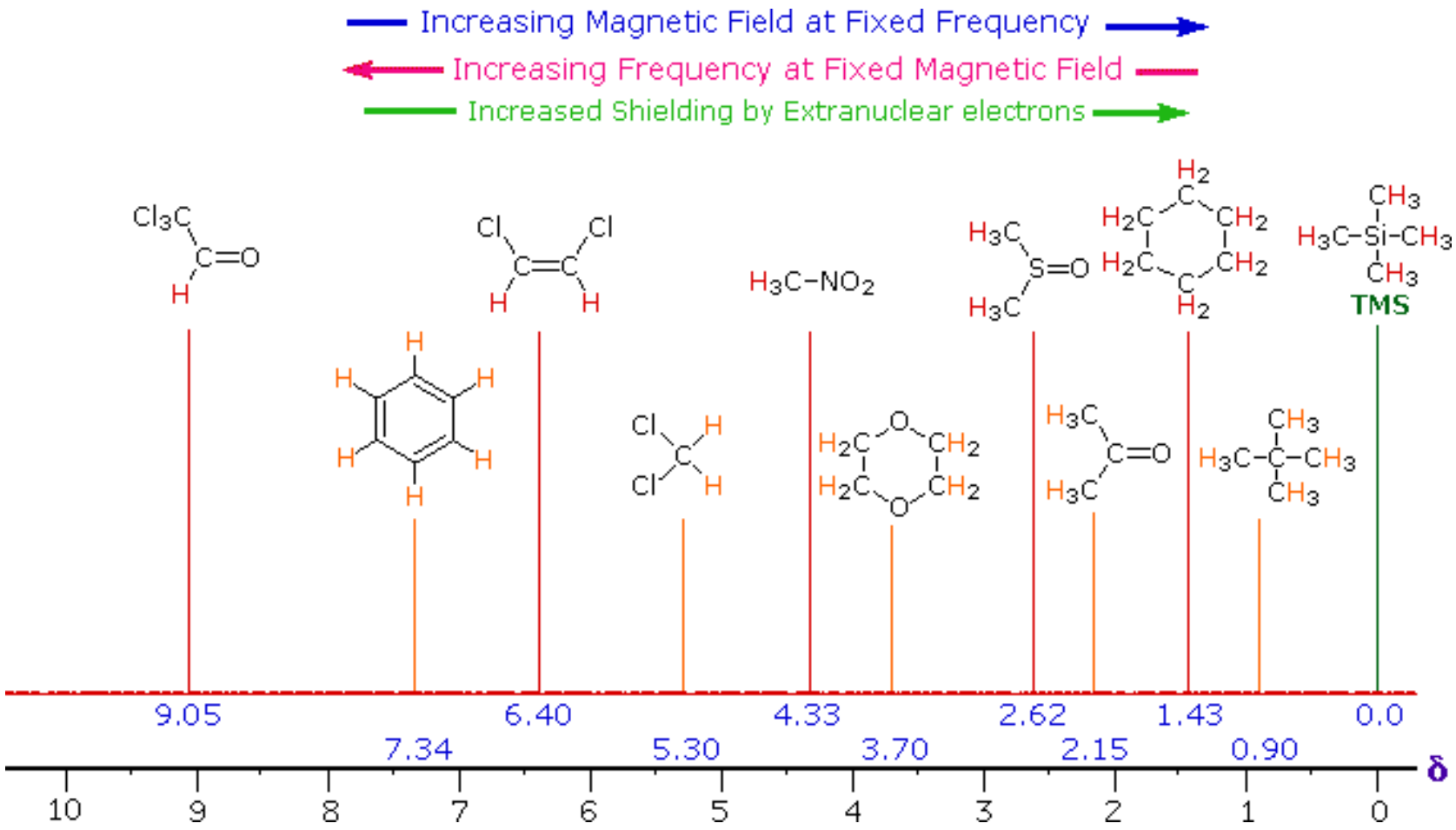
Integration

- Area under the peak is proportional to the number of hydrogen atoms

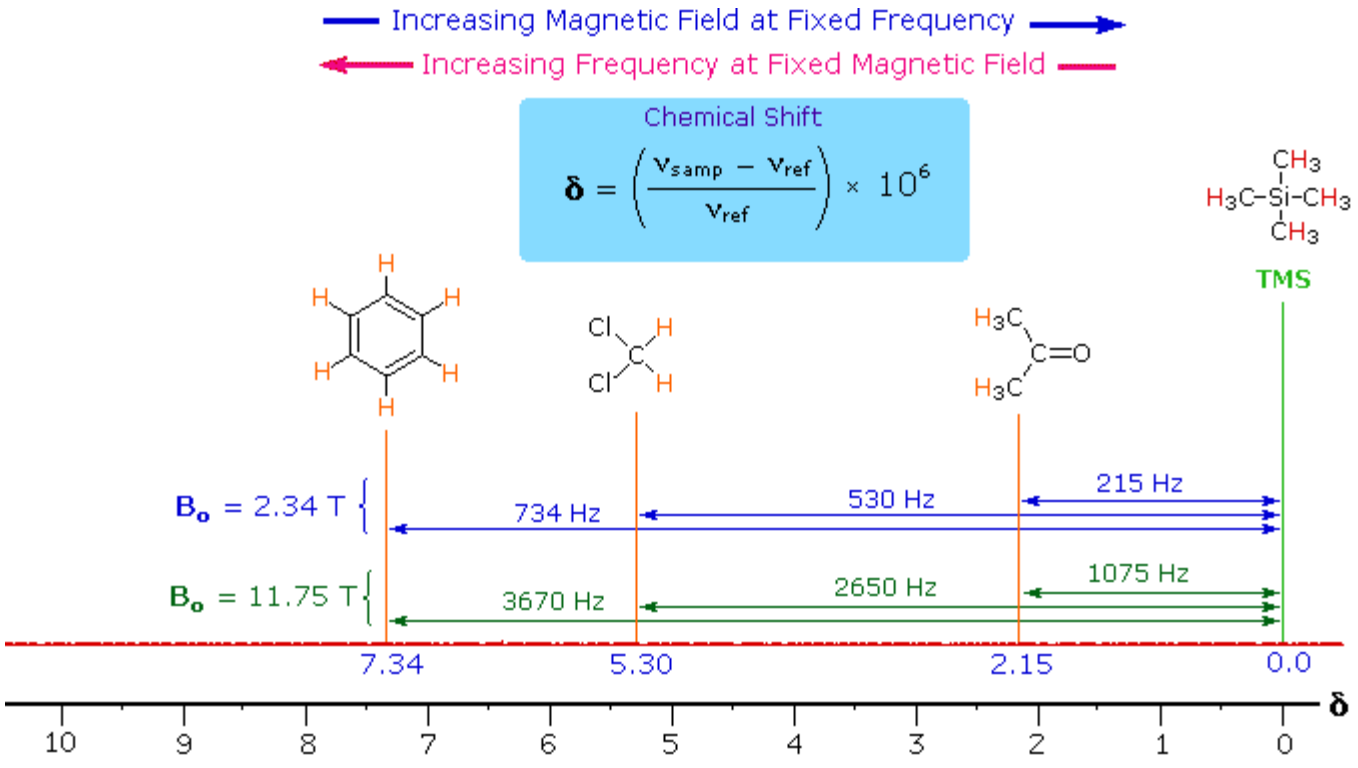
Chemical Shift and Integration Examples

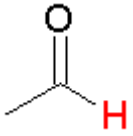
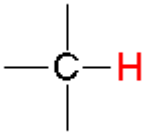
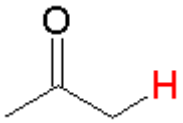
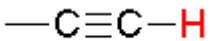


Reusch's View of ^{1}H Chemical Shifts

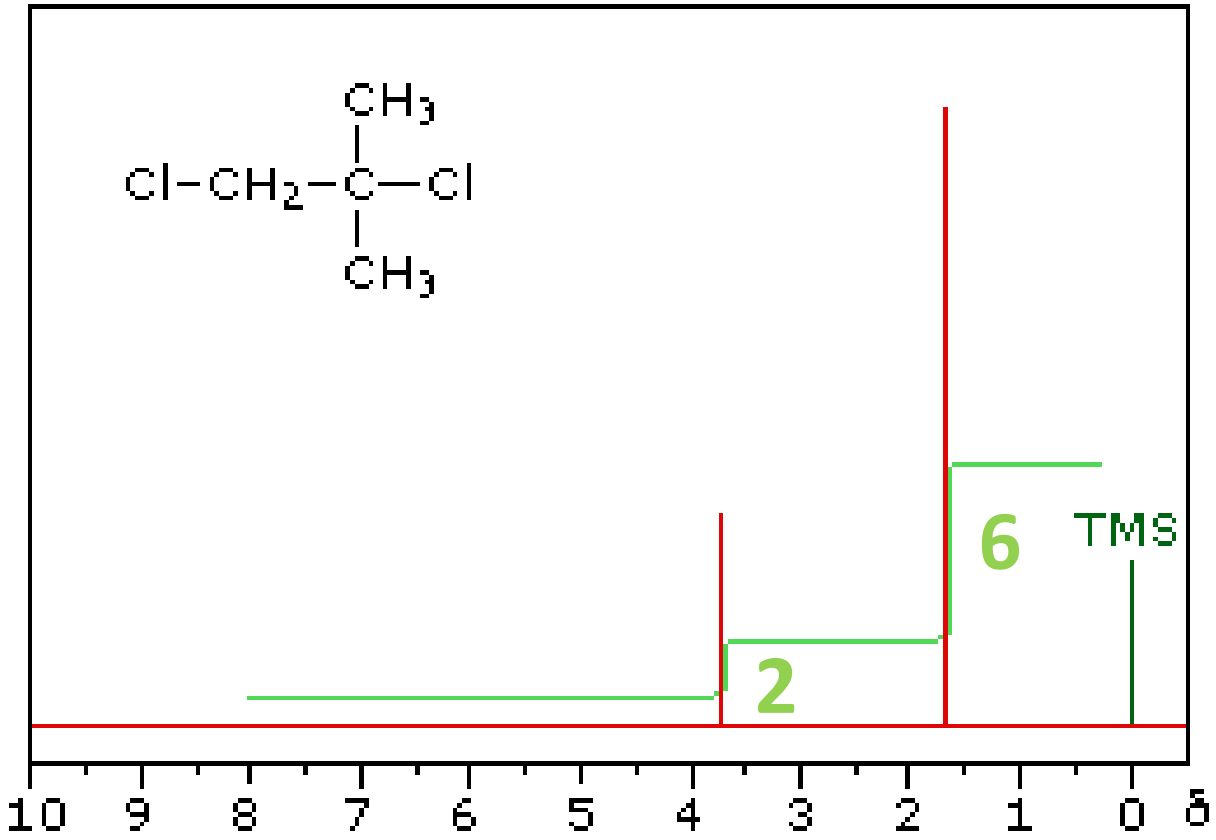


Chemical Shift

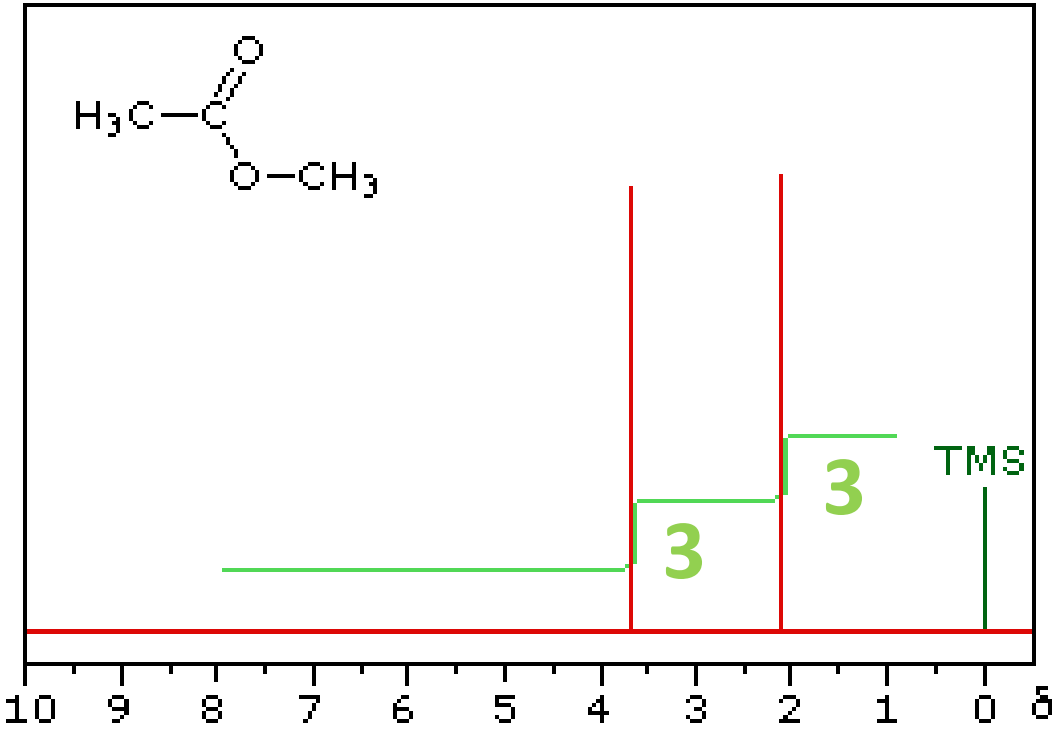


Approximate Values of Chemical Shifts for ^{1}H NMR			
Type of Proton	Approximate Chemical Shift (δ)	Type of Proton	Approximate Chemical Shift (δ)
-C**H**$_3$	0.9	Ar-**H**	6.8-8.0
-C**H**$_2$-	1.2-1.3		9.7-10.5
	1.4	I-C-**H**	3.1-3.3
C=C-C**H**$_3$	1.5-2.5	Br-C-**H**	3.4-3.6
	2.1-2.6	Cl-C-**H**	3.6-3.8
Ar-C**H**$_3$	2.3-2.6	RN**H**$_2$	Variable
	2.5-3.0	R-O-**H**	Variable
R-O-C**H**	3.3-4.0	Ar**O**H	Variable
R$_2$C=C**H**R	4.5-6.5	RC**O**$_2$H	Variable

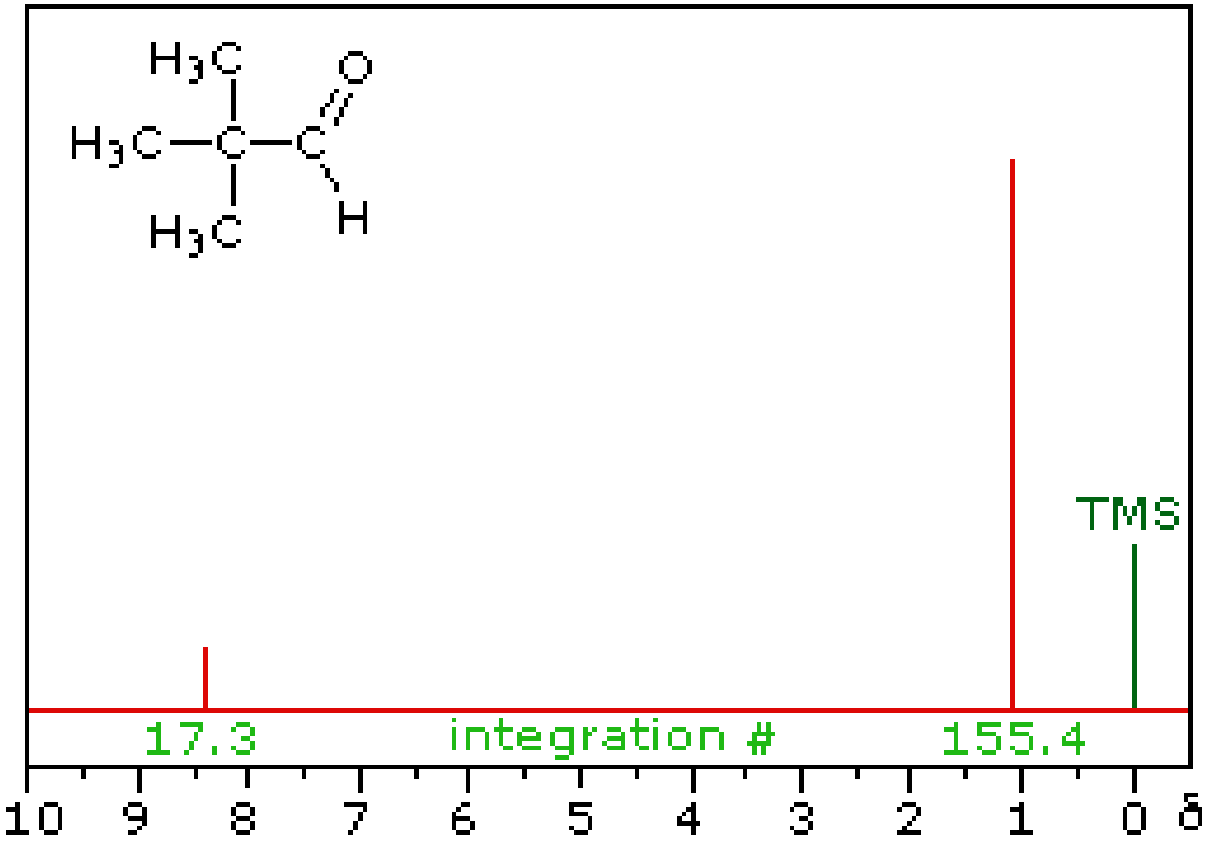
Chemical Shift and Integration Examples



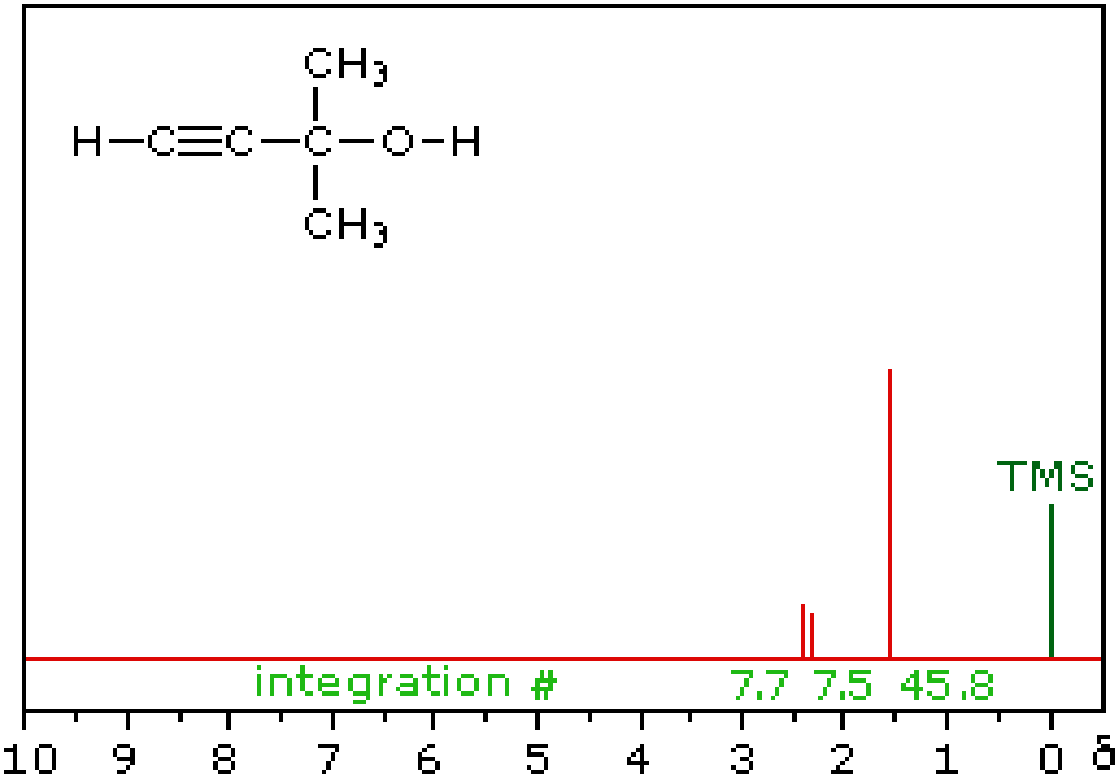
Chemical Shift and Integration Examples



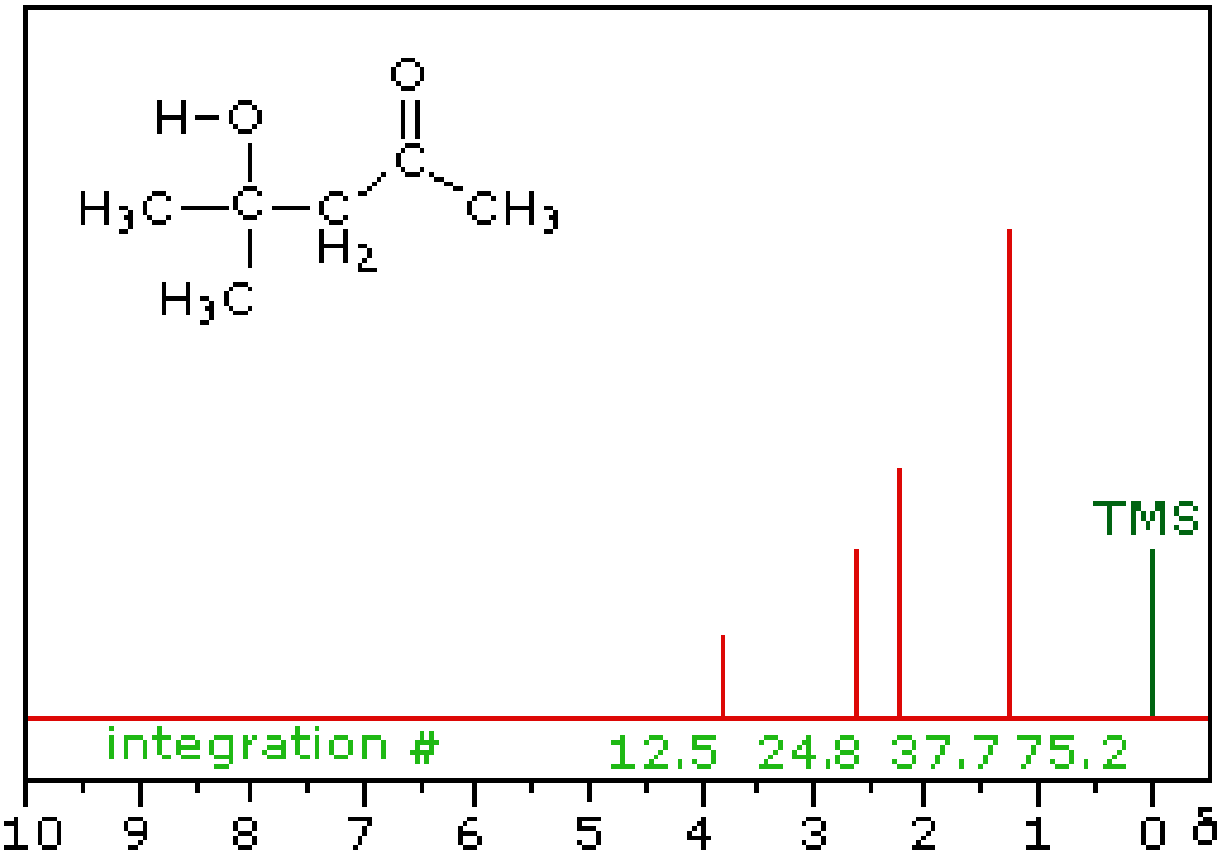
Chemical Shift and Integration Examples



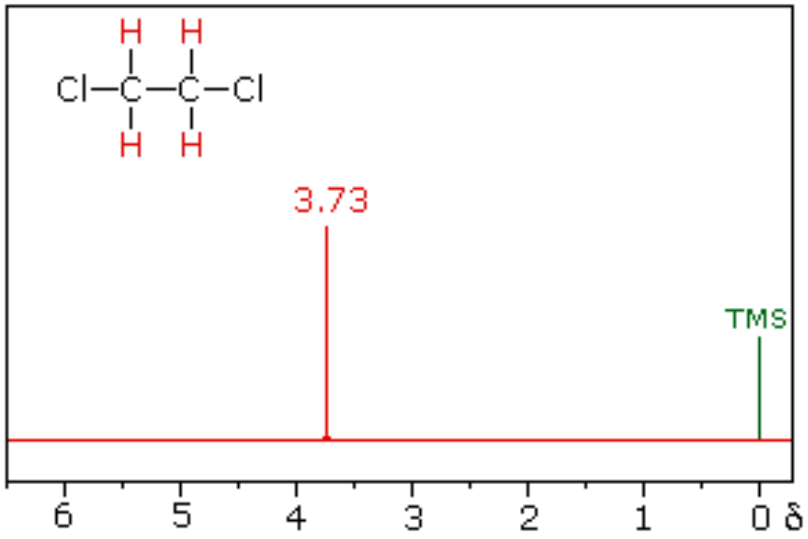
Chemical Shift and Integration Examples

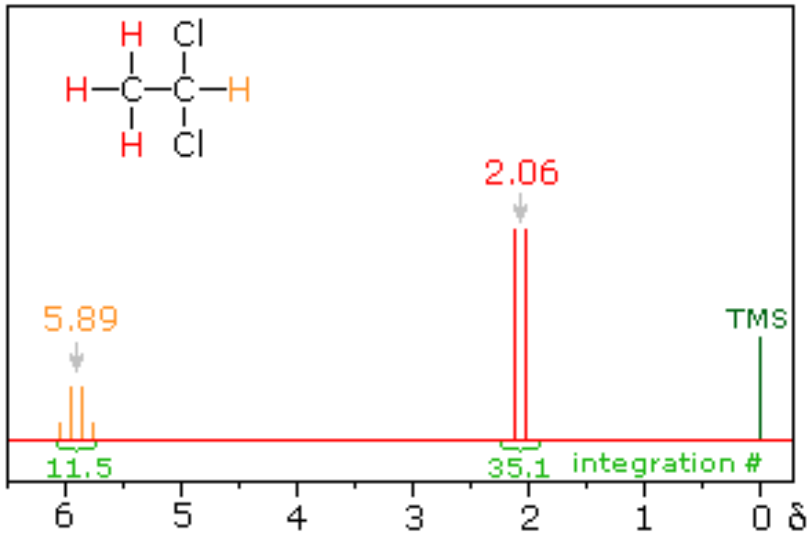


Chemical Shift and Integration Examples



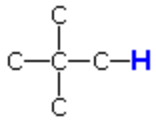
Spin-Spin Splitting

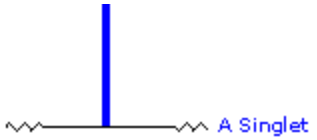




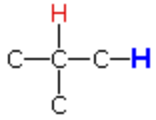
Splitting Patterns

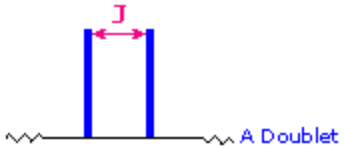
No Coupled Hydrogens



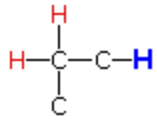


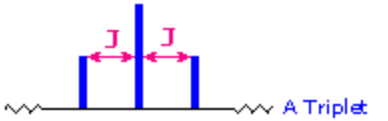
One Coupled Hydrogen



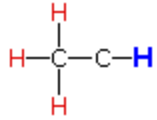


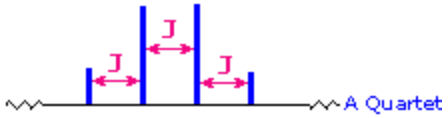
Two Coupled Hydrogens

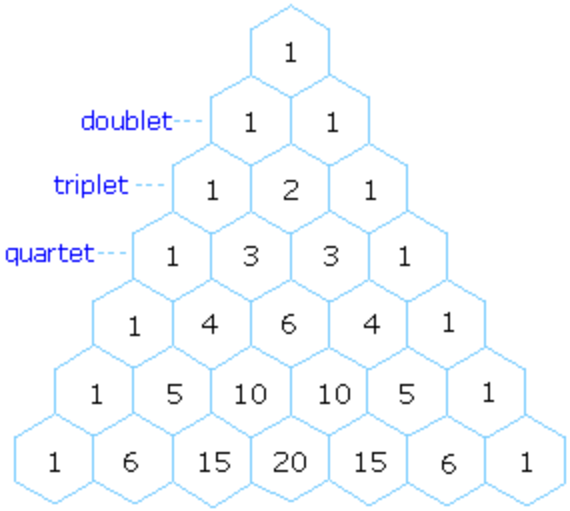




Three Coupled Hydrogens







Pascal's Triangle

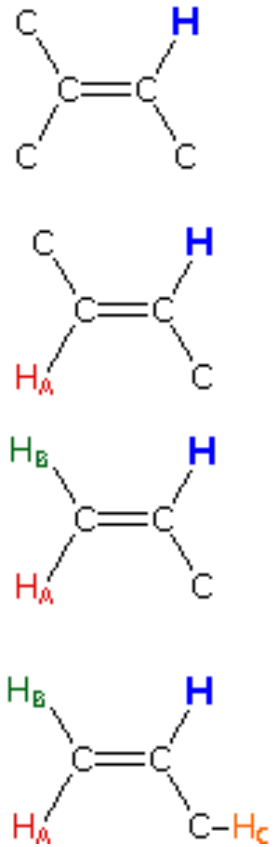
Splitting Patterns

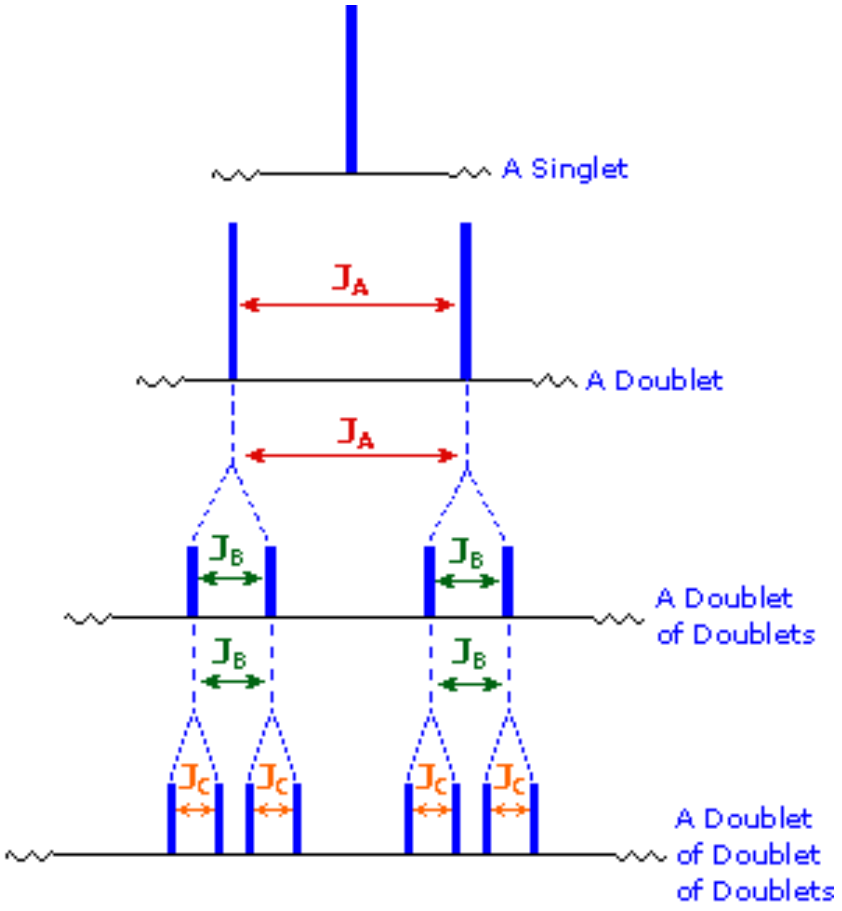
No Coupled Hydrogens

One Coupled Hydrogen

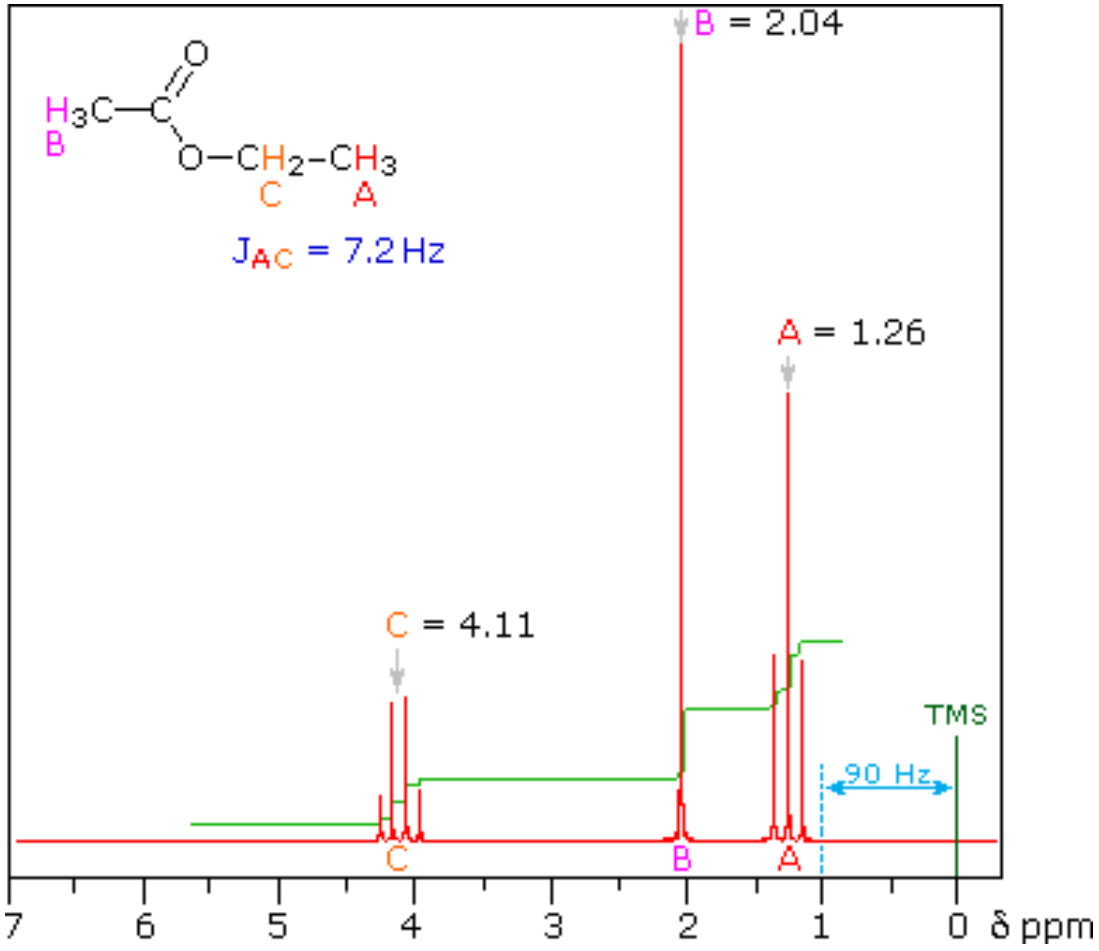
Two Coupled Hydrogens

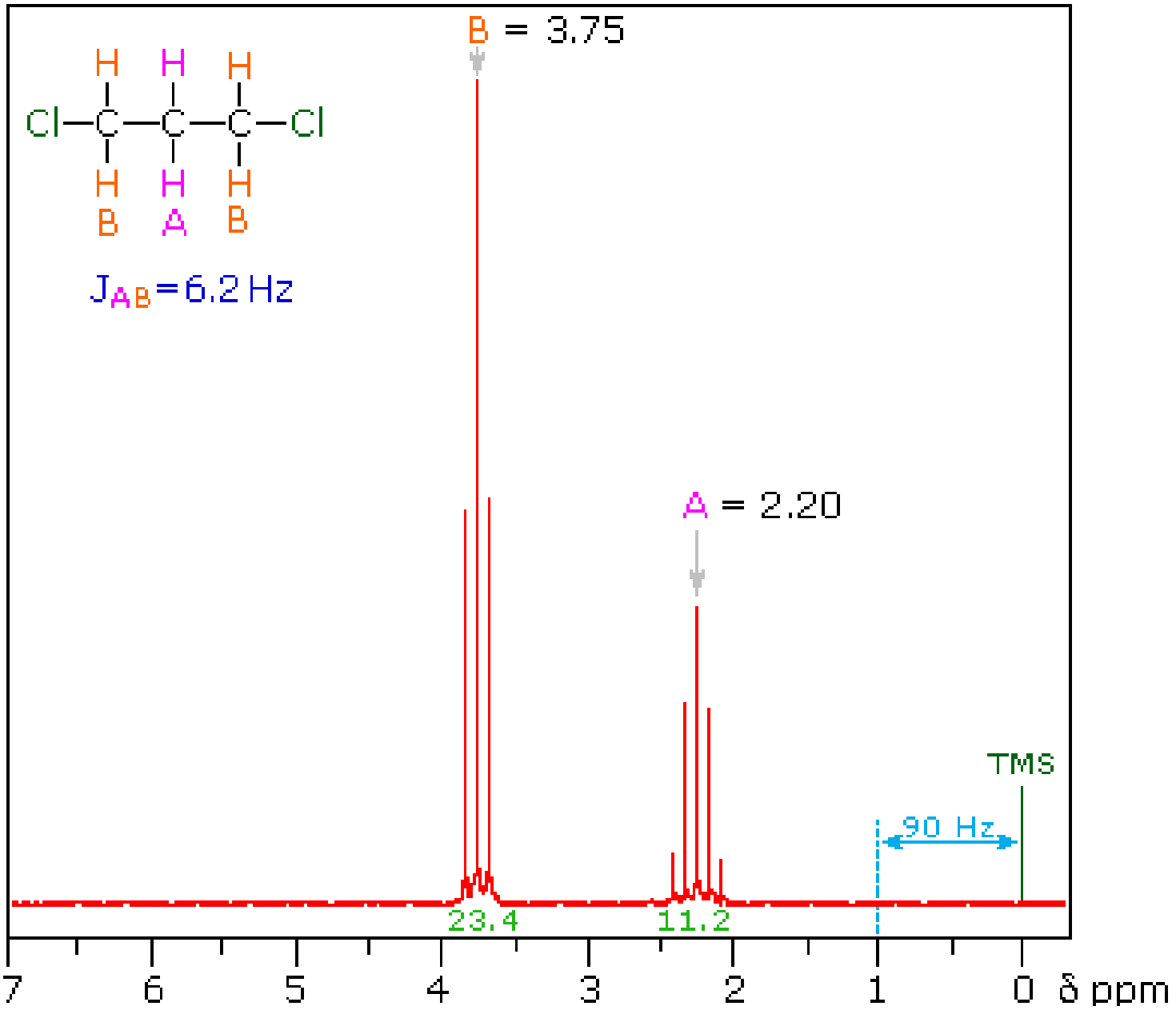
Three Coupled Hydrogens



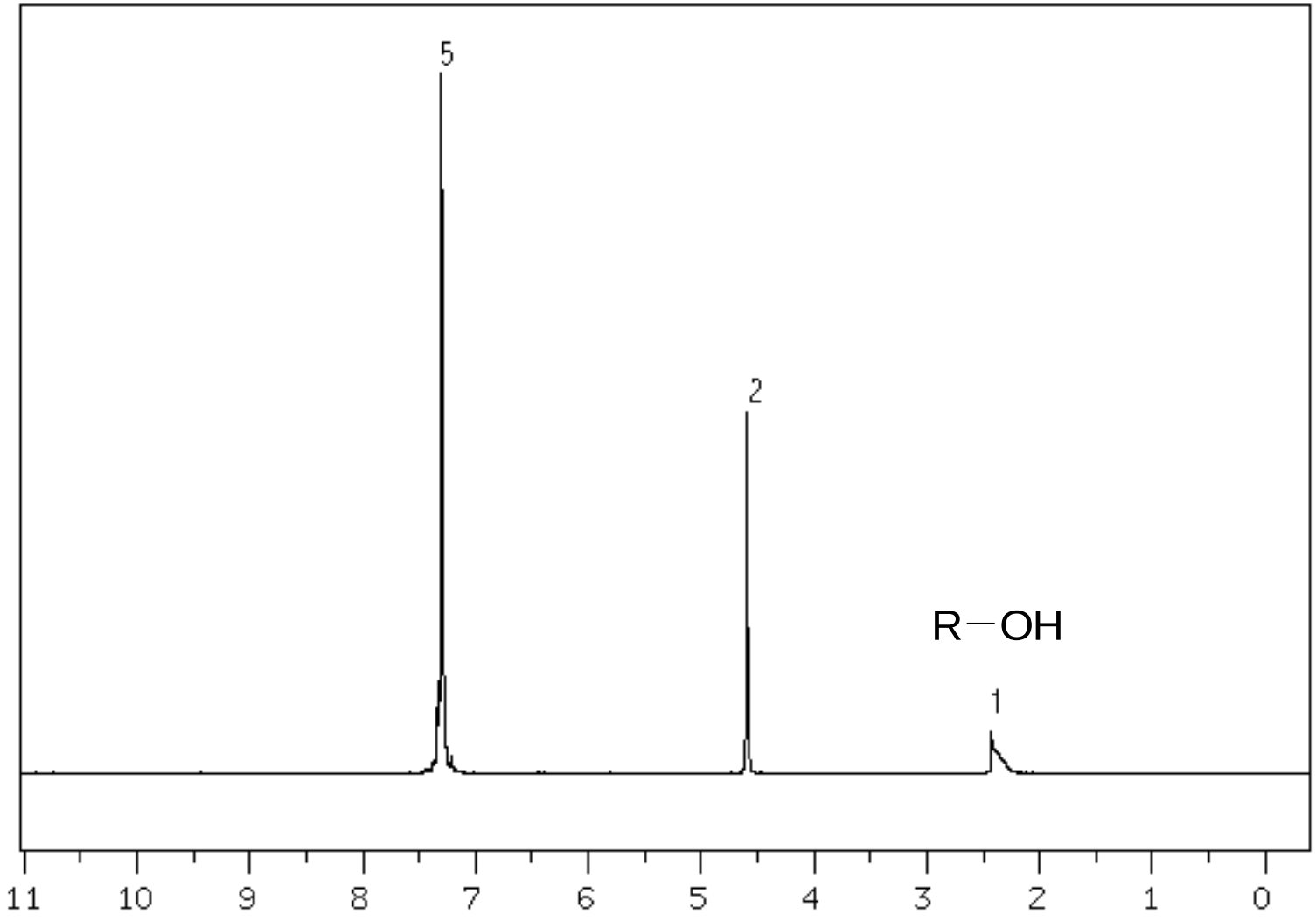


Spin-Spin Splitting of $C_4H_8O_2$

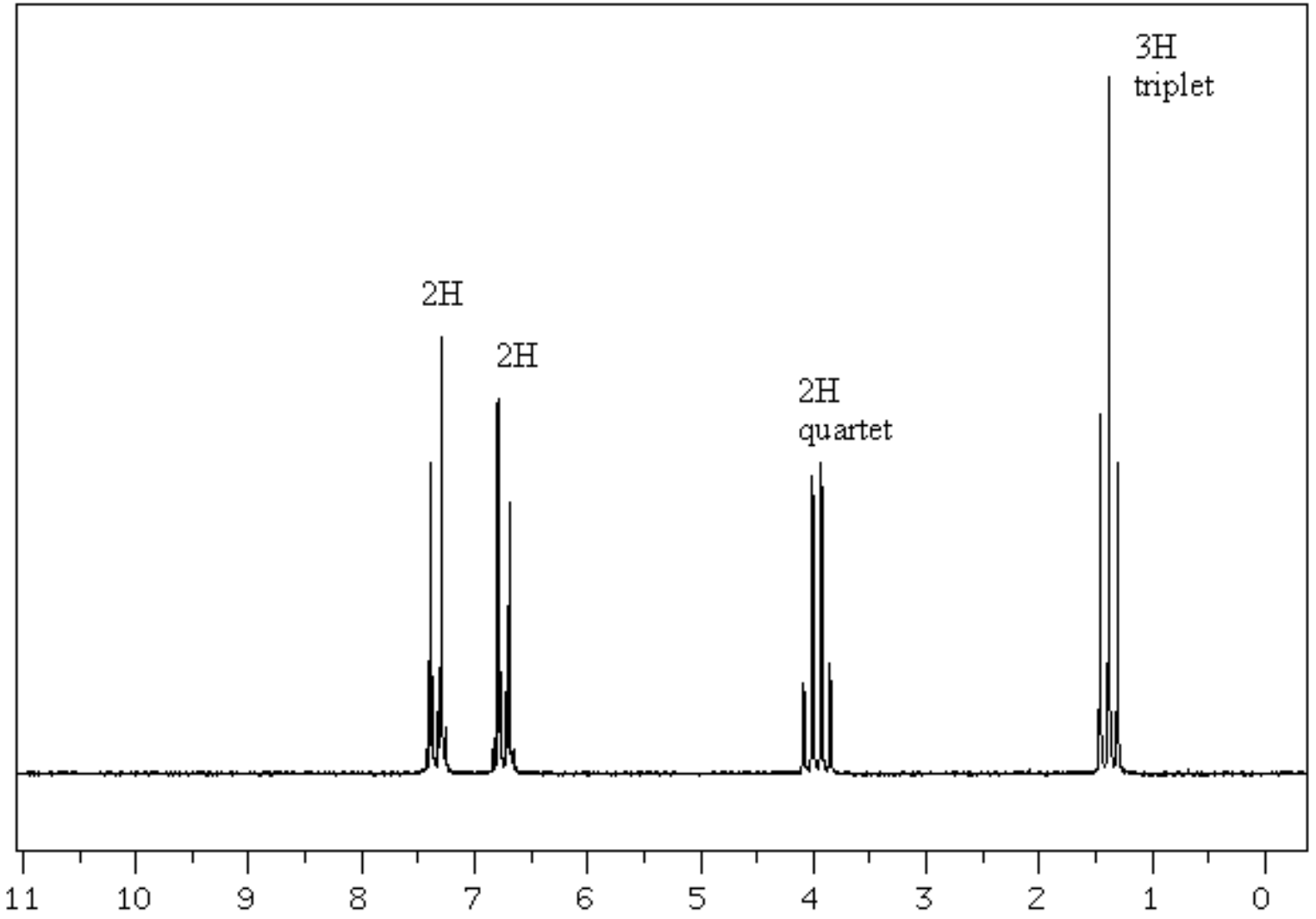



B = 3.75
A = 2.20
TMS
90 Hz
23.4
11.2
7
6
5
4
3
2
1
0 δ ppm
H H H
Cl C C C Cl
H H H
B A B
JAB = 6.2 Hz

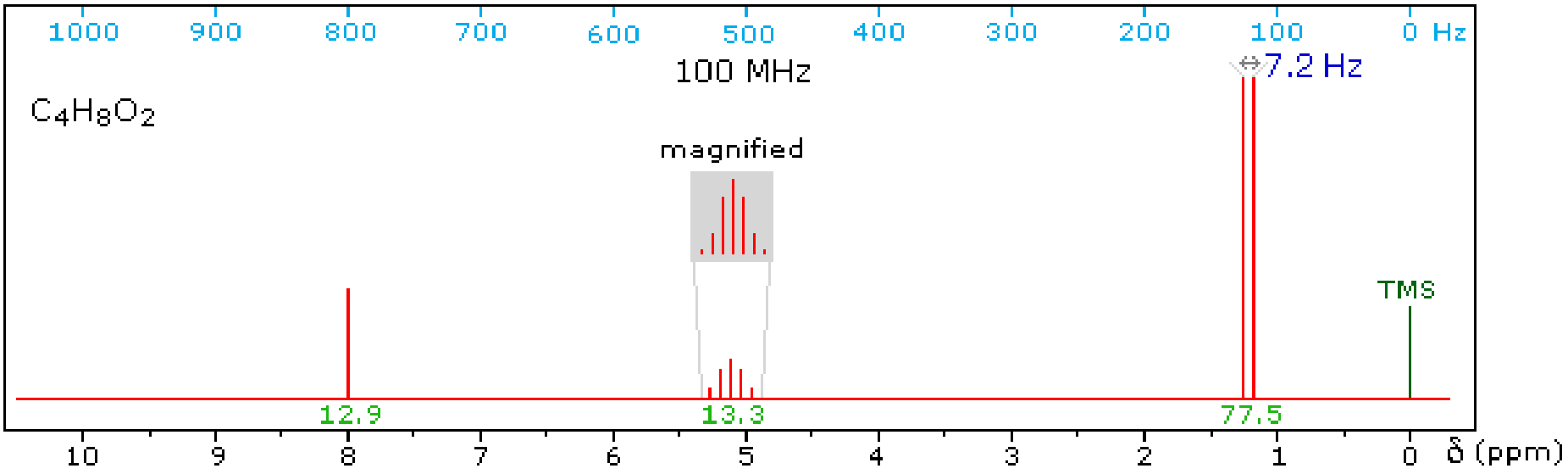
Worked Example C_7H_8O



Worked Example (C_8H_9BrO)

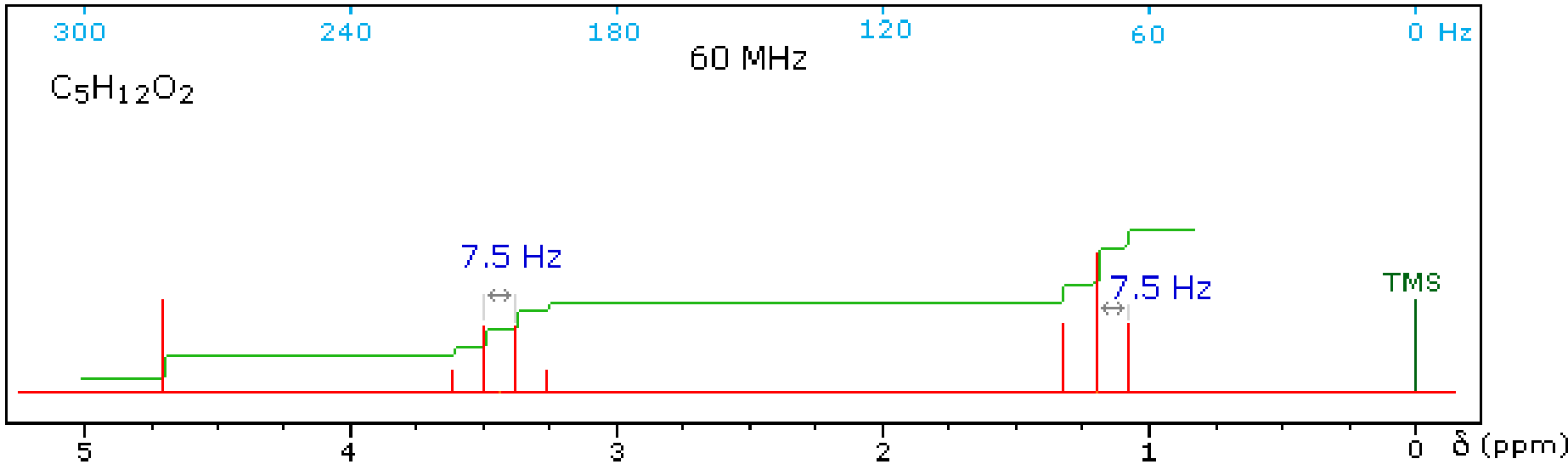


Worked Example ($C_4H_8O_2$)



Integration: 1 1 6

Worked Example ($C_5H_{12}O_2$)



Worked Example (C_5H_6O)