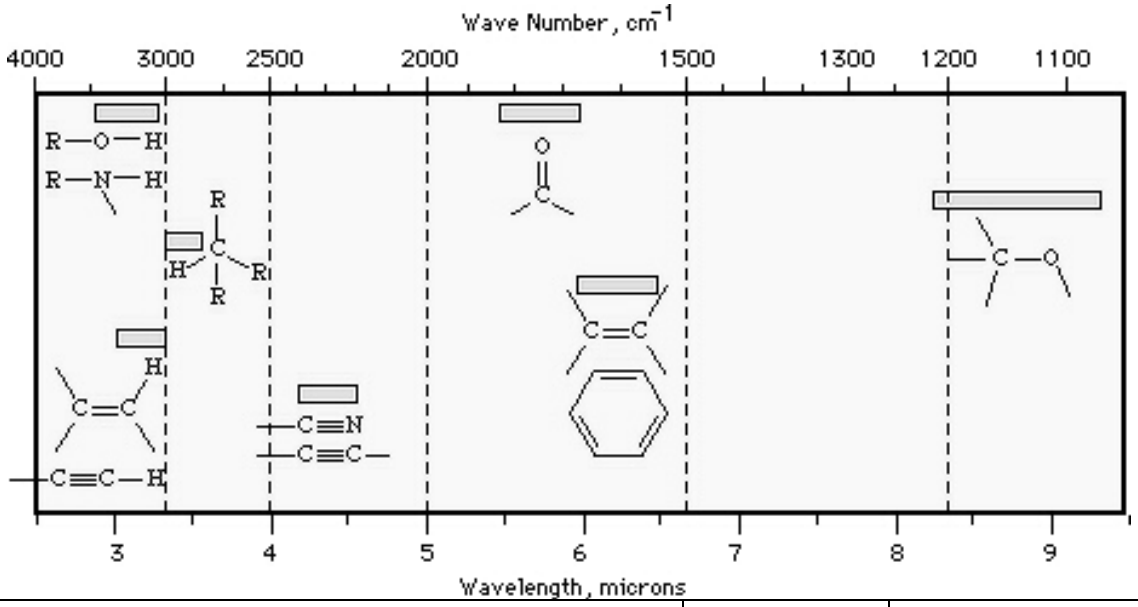
IR Absorbances



	Type of Vibration		Frequency (cm^{-1})	Intensity
C—H	Alkanes	(stretch)	3000–2850	s
	—CH_3	(bend)	1450 and 1375	m
	—CH_2—	(bend)	1465	m
	Alkenes	(stretch)	3100–3000	m
		(out-of-plane bend)	1000–650	s
	Aromatics	(stretch)	3150–3050	s
		(out-of-plane bend)	900–690	s
	Alkyne	(stretch)	ca. 3300	s
	Aldehyde		2900–2800	w
			2800–2700	w
C—C	Alkane		Not interpretatively useful	
C=C	Alkene		1680–1600	m–w
	Aromatic		1600 and 1475	m–w
C≡C	Alkyne		2250–2100	m–w
C=O	Aldehyde		1740–1720	s
	Ketone		1725–1705	s
	Carboxylic acid		1725–1700	s
	Ester		1750–1730	s
	Amide		1680–1630	s
	Anhydride		1810 and 1760	s
	Acid chloride		1800	s
C—O	Alcohols, ethers, esters, carboxylic acids, anhydrides		1300–1000	s
O—H	Alcohols, phenols			
	Free		3650–3600	m
	H-bonded		3400–3200	m
	Carboxylic acids		3400–2400	m
N—H	Primary and secondary amines and amides			
	(stretch)		3500–3100	m
	(bend)		1640–1550	m–s
C—N	Amines		1350–1000	m–s
C=N	Imines and oximes		1690–1640	w–s
C≡N	Nitriles		2260–2240	m
X=C=Y	Allenes, ketenes, isocyanates, isothiocyanates		2270–1940	m–s
N=O	Nitro (R—NO_2)		1550 and 1350	s
S—H	Mercaptans		2550	w
S=O	Sulfoxides		1050	s
	Sulfones, sulfonyl chlorides, sulfates, sulfonamides		1375–1300 and 1350–1140	s
C—X	Fluoride		1400–1000	s
	Chloride		785–540	s
	Bromide, iodide		< 667	s

Correlation Chart

Aromatic Strong Vibrations

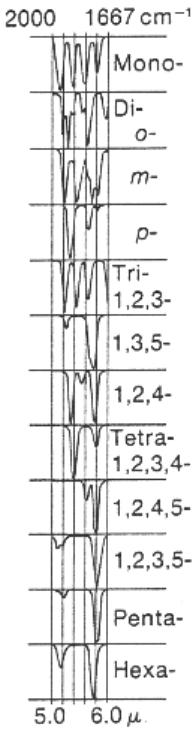
Monosubstituted : 730-770 and 690-710 cm-1

Ortho-disubstituted: 735-770 cm-1

Meta-disubstituted: 750-810 and 680-730 cm-1

Para-disubstituted: 790-840 cm-1

Aromatic Patterns



Mass Spectrometry: Common Mass Fragments

Commonly Lost Fragments

m-15 $\cdot CH_3$

m-17 $\cdot OH$

m-26 $\cdot CN$

m-28 $H_2C{=}CH_2$

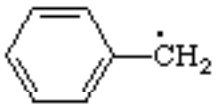
m-29 $\cdot CH_2CH_3$ $\cdot CHO$

m-31 $\cdot OCH_3$

m-35 $\cdot Cl$

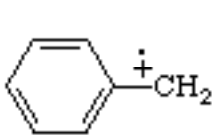
m-43 $CH_3\dot{C}{=}O$

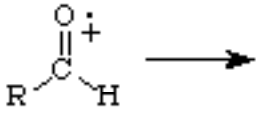
m-45 $\cdot OCH_2CH_3$

m-91 

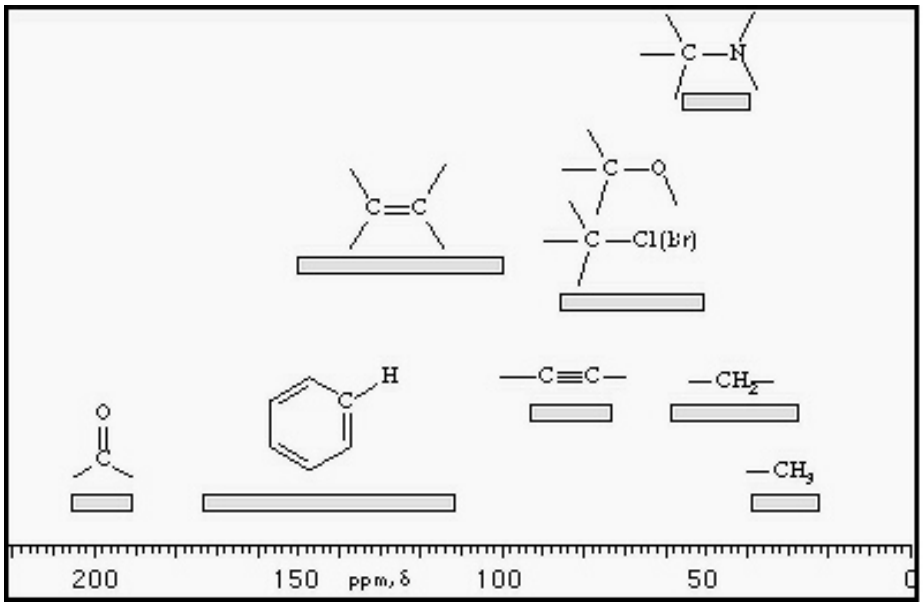
Common Stable Ions

m/e = 43 $CH_3{-}C{\equiv}O^+$

m/e = 91 

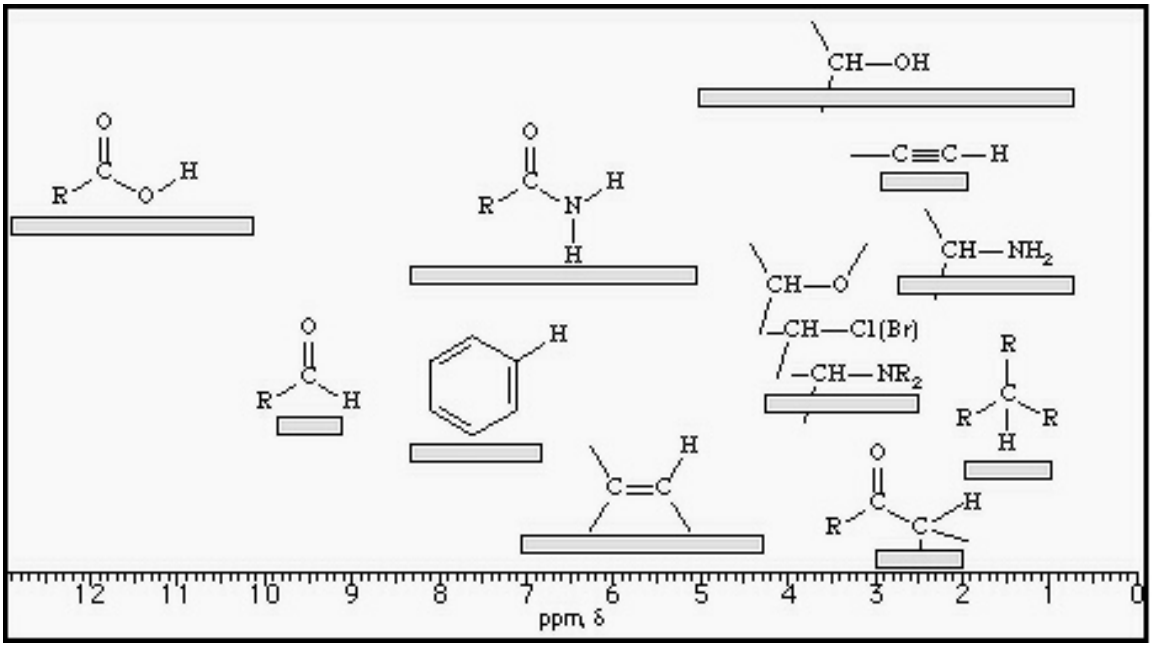
m/e = m-1 

^{13}C NMR Chemical Shifts



Refer to: *http://www.chem.wisc.edu/areas/reich/Handouts/nmr-c13/cdata.htm*

^{1}H NMR Chemical Shifts



Structure	Chemical Shift (ppm)
RCH_3	0.8 - 1.2
R_2CH_2	1.1 - 1.5
R_3CH	~1.5
$ArCH_3$	2.2 - 2.5
R_2NCH_3	2.2 - 2.6
R_2CHOR	3.2 - 4.3
R_2CHCl	3.5 - 3.7
$RC(=O)CHR_2$	2.0 - 2.7
$RCHCR=CR_2$	~1.7
RC=CH	4.9 - 5.9
ArH	6.0 - 8.0
RC(=O)H	9.4 - 10.4
RCCH	2.3 - 2.9
R_2NH	2 - 4
ROH	1 - 6
ArOH	6 - 8
RCO_2H	10 - 12

Chemical Shifts

^{1}H NMR Coupling Constants

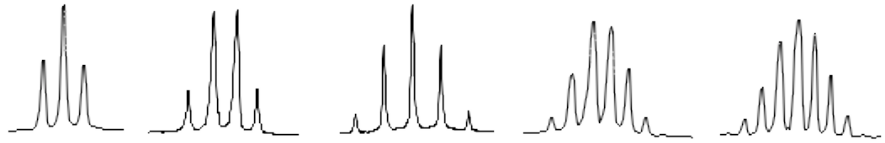
A signal that is split by three identical protons takes a shape known as a **quartet**, each peak having relative intensities of 1:3:3:1.

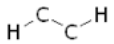
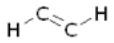
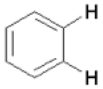
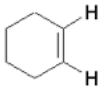
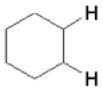
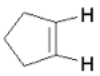
A peak is split by *n* identical protons into components whose sizes are in the ratio of the *n*th row of Pascal's triangle:

n		
0	singlet	1
1	doublet	1 1
2	triplet	1 2 1
3	quartet	1 3 3 1
4	quintet	1 4 6 4 1
5	sextet	1 5 10 10 5 1
6	septet	1 6 15 20 15 6 1
7	octet	1 7 21 35 35 21 7 1
8	nonet	1 8 28 56 70 56 28 8 1

Because the *n* th row has *n*+1 components, this type of splitting is said to follow the "*n*+1 rule": a proton with *n* chemically equivalent neighbors appears as a cluster of *n*+1 peaks.

Peaks for protons that split each other will always have the same coupling constant. Multiplets are often skewed in the direction of the peak to which they are coupled.



Functional Group	*J* (Hz)
	6 - 8
	11 - 18
	6 - 15
	4 - 10
	6 - 10
	8 - 11
	a,a: 8 - 14 a,e: 0 - 7 e,e: 0 - 5
	*cis*: 6 - 12 *trans*: 4 - 8
	5 - 7

Refer to: *http://www.chem.wisc.edu/areas/reich/Handouts/nmr-h/hdata.htm*