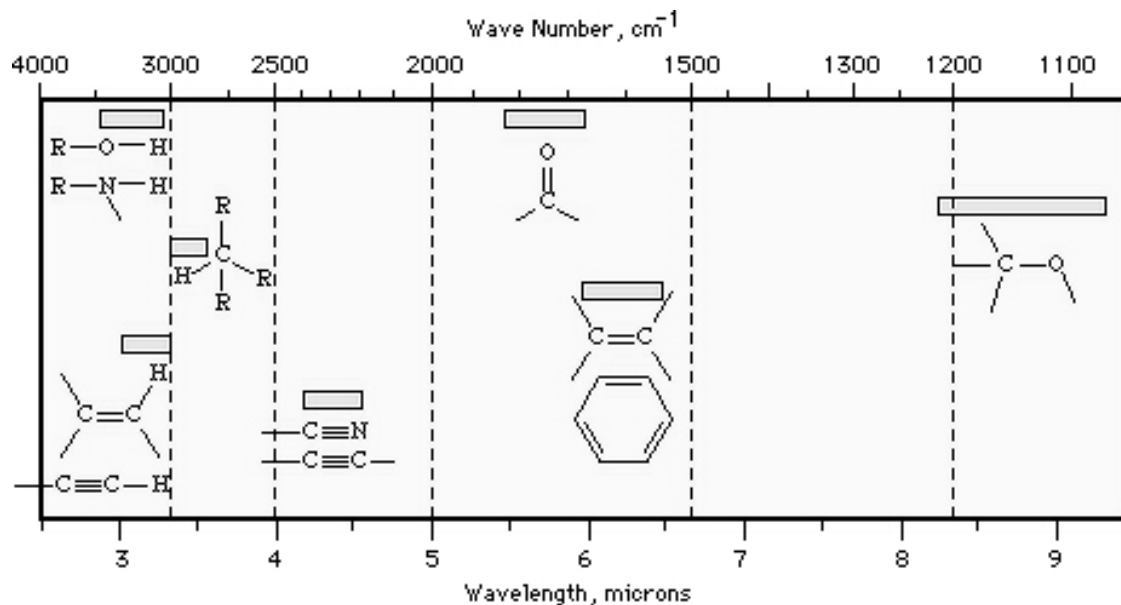


IR Absorbances



	Type of Vibration	Frequency (cm <sup>-1</sup> )	Intensity
C-H	Alkanes (stretch)	3000-2850	s
	-CH <sub>3</sub> (bend)	1450 and 1375	m
	-CH <sub>2</sub> - (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
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 <sub>2</sub> )	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

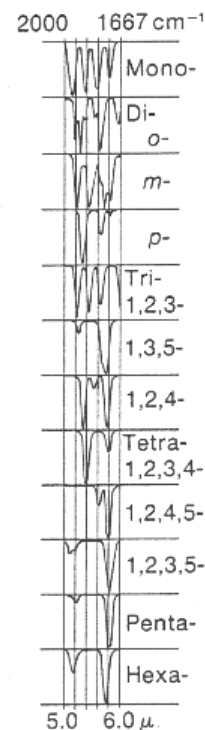
Monosubstituted:  
730-770 and 690-710 cm<sup>-1</sup>

Ortho-disubstituted:  
735-770 cm<sup>-1</sup>

Meta-disubstituted:  
750-810 and 680-730 cm<sup>-1</sup>

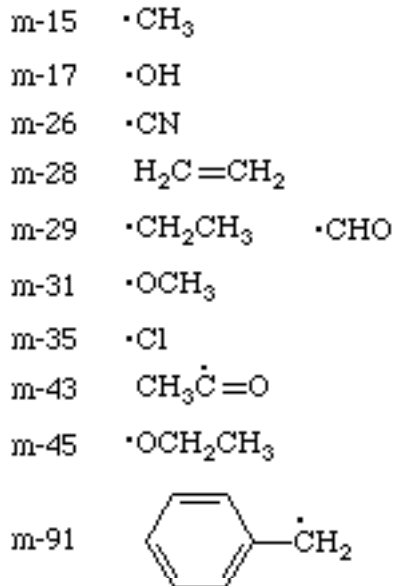
Para-disubstituted:  
790-840 cm<sup>-1</sup>

Aromatic Patterns

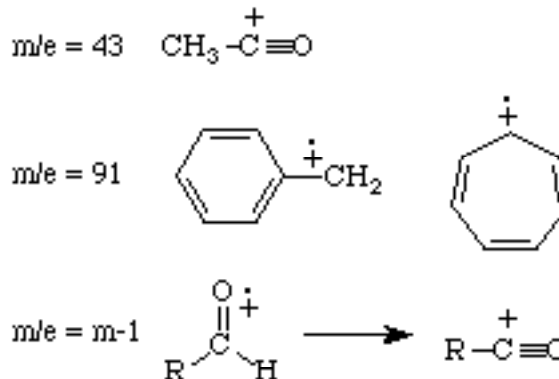


Mass Spectrometry: Common Mass Fragments

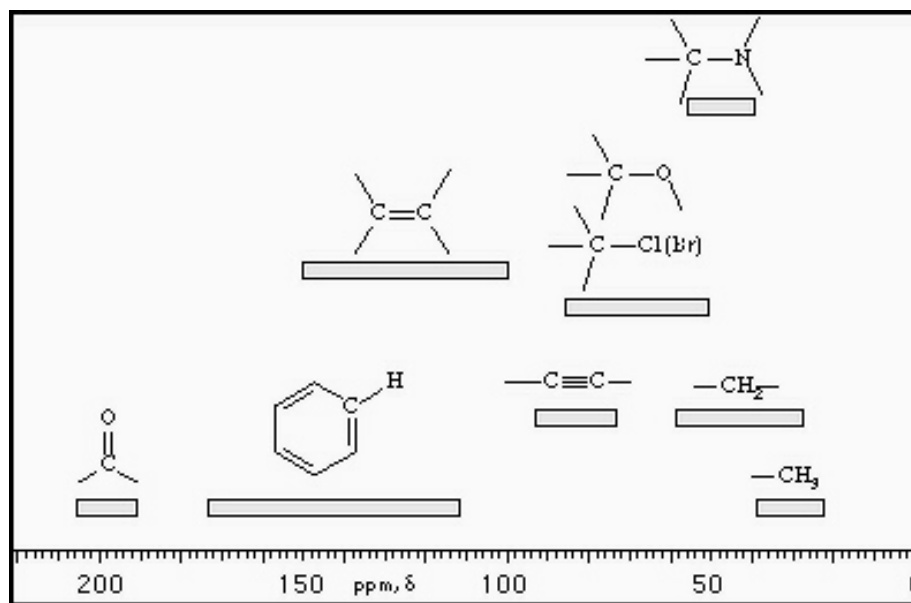
**Commonly Lost Fragments**



**Common Stable Ions**

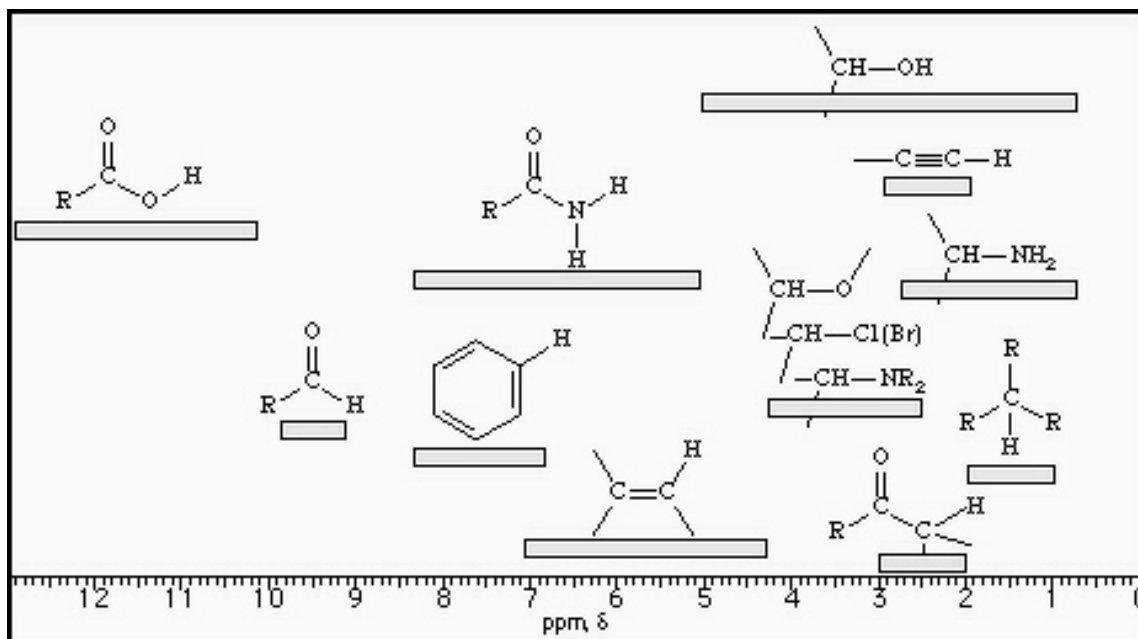


<sup>13</sup>C NMR Chemical Shifts



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

# <sup>1</sup>H NMR Chemical Shifts



Structure	Chemical Shift (ppm)
RCH <sub>3</sub>	0.8 - 1.2
R <sub>2</sub> CH <sub>2</sub>	1.1 - 1.5
R <sub>3</sub> CH	~1.5
ArCH <sub>3</sub>	2.2 - 2.5
R <sub>2</sub> NCH <sub>3</sub>	2.2 - 2.6
R <sub>2</sub> CHOR	3.2 - 4.3
R <sub>2</sub> CHCl	3.5 - 3.7
RC(=O)CHR <sub>2</sub>	2.0 - 2.7
RCHCR=CR <sub>2</sub>	~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 <sub>2</sub> NH	2 - 4
ROH	1 - 6
ArOH	6 - 8
RCO <sub>2</sub> H	10 - 12

*Chemical Shifts*

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