13C-NMR Spectroscopy

Unsaturated **C** atom next to O atom (**C**=O)	Unsaturated **C** atom (**C**=**C** & Aromatic **C**)	Saturated **C** atom next to O atom (**C**H_3O, **C**H_2O, etc...)	Saturated **C** atom (**C**H_3, **C**H_2, **C**H, etc...)

200 **150** **100** **50** **ppm** **0**

1H-NMR Spectroscopy

H atom on unsaturated C atom next to O atom (Aldehyde **H**)	**H** atom on unsaturated C atom (Aromatic **H**)	**H** atom on unsaturated C atom (Alkene **H**)	Saturated (**C**H_3, **C**H_2, **C**H, etc...) next to O atom	Saturated (**C**H_3, **C**H_2, **C**H, etc...)

10.5 **8.5** **6.5** **4.5** **3.0** **ppm** **0**

SOME PROTONS ATTACHED TO N and O (quite variable)

R–O**H** (alcohols)	1–6 ppm
R_2N**H** (amines)	1–6 ppm
Ar–O**H** (phenols)	4–8 ppm
RCO_2**H** (carboxylic acid)	9–13 ppm

IR Spectroscopy

Bonds to H	**Triple Bonds**	**Double Bonds**	**Single Bonds**
N—H O—H C—H	C≡N C≡C	C=O C=N C=C	Fingerprint Region

4000 **2500** **2000** **1500** **cm^{-1}** **500**

Mass Spectrometry

Significant **M+1** Isotopes (12C = 100%, 13C = 1.1%)

Significant **M+2** Isotopes (79Br = 100%, 81Br = 98%)

Significant **M+2** Isotopes (35Cl = 100%, 37Cl = 33%)

Significant **M+2** Isotopes (32S = 100%, 34S = 5%)

IR

Overtones of strong carbonyl absorptions can also appear 3600cm⁻¹ – 3200cm⁻¹

aryl overtones (rolling hills)

C – Hal (SINGLE BONDS)

FINGER PRINT REGION

Adapted from:
MOUSER, 130AL
FALL 2000
version 10/26/200

4000 cm⁻¹ | 2200 cm⁻¹ | 1680 1600 | 1400 cm⁻¹ | 500 cm⁻¹

3600-3200 (very broad) O–H

3500-3350 (broad) N–H

C≡C (weak)

C≡N ~2250 (strong)

alkene stretch (weak)

aromatic stretch (weak)

C=C stretch zone

NO_2 stretch 1550 cm⁻¹ and 1350 cm⁻¹ (STRONG)

Sp C–H ~3300, strong

=C–H stretch (unsaturated)

C–H stretch (saturated)

aryl or alkenyl

sp^2 sp^3

3000 line C-H

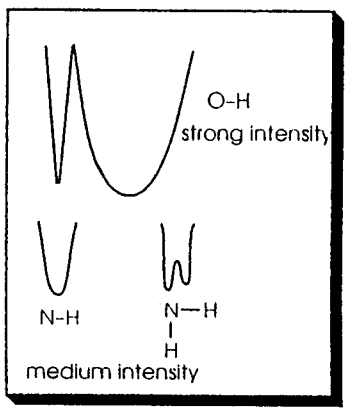
C=O stretch zone 1800-1560, strong

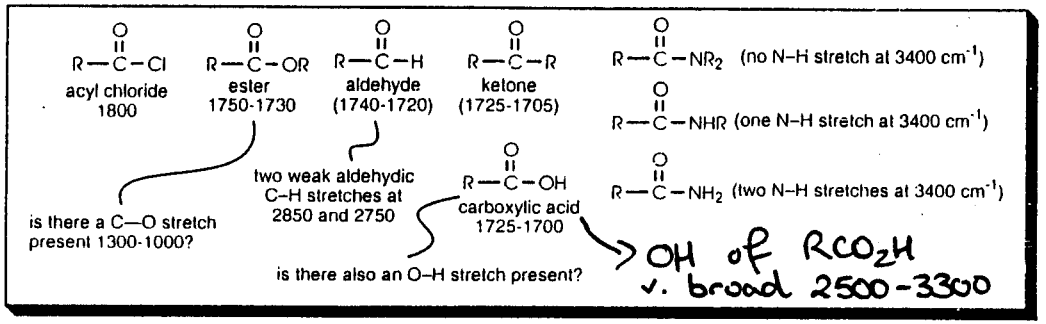
C-O-C Stretch 1250-1050 several, strong

AROMATIC RINGS

- monosubsituted
  - 2 peaks
  - 690-710 (s)
  - 730-770 (s)
- disubstituted
  - ortho
    - 735-770 (s)
  - meta
    - 750-810 (s)
    - 800-900 (w)
  - para
    - 800-860 (s)

OH vs. NH

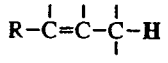
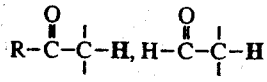
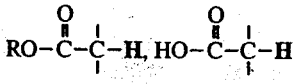
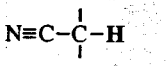
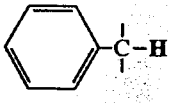
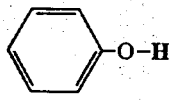
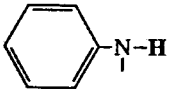
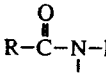
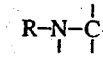
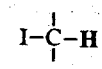
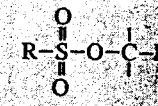
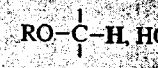
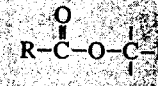
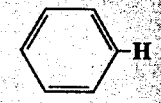
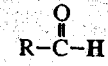
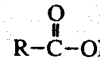




NOTE: THESE VALUES ARE ALL AVERAGE POSITIONS FOR "NORMAL" COMPOUNDS....

APPENDIX 2

Approximate ^{1}H Chemical Shift Ranges (ppm) for Selected Types of Protons[a]

$R-CH_3$		0.7 – 1.3
$R-CH_2-R$		1.2 – 1.4
R_3CH		1.4 – 1.7
		1.6 – 2.6
		2.1 – 2.4
		2.1 – 2.5
		2.1 – 3.0
		2.3 – 2.7
$R-C\equiv C-H$		1.7 – 2.7
$R-S-H$	var	1.0 – 4.0[b]
	var	0.5 – 4.0[b]
$R-O-H$	var	0.5 – 5.0[b]
	var	4.0 – 7.0[b]
	var	3.0 – 5.0[b]
	var	5.0 – 9.0[b]
		2.2 – 2.9
		2.0 – 3.0
		2.0 – 4.0
		2.7 – 4.1
		3.1 – 4.1
		ca. 3.0
		3.2 – 3.8
		3.5 – 4.8
		4.1 – 4.3
		4.2 – 4.8
		4.5 – 6.5
		6.5 – 8.0
		9.0 – 10.0
		11.0 – 12.0

[a] *For those hydrogens shown as*  *if that hydrogen is part of a methyl group (CH_3) the shift is generally at the low end of the range given, if the hydrogen is in a methylene group ($-CH_2-$) the shift is intermediate, and if the hydrogen is in a methine group*  *the shift is typically at the high end of the range given.*

[b] *The chemical shift of these groups is variable, depending not only on the chemical environment in the molecule, but also on concentration, temperature, and solvent.*

APPENDIX 7

Approximate ^{13}C Chemical-Shift Values (ppm) for Selected Types of Carbon

Types of Carbon	Range (ppm)	Types of Carbon	Range (ppm)	
$R-CH_3$	8–30	$C\equiv C$	65–90	ALKYNE
R_2CH_2	15–55	$C=C$	100–150	ALKENE
R_3CH	20–60	$C\equiv N$	110–140	NITRILE
C–I	0–40		110–175	AROMATIC
C–Br	25–65		155–185	ESTERS / ACIDS
C–N	30–65		155–185	AMIDES
C–Cl	35–80		160–170	ACID CHLORIDE
C–O	40–80		185–220	KETONE / ALDEHYDE