

A Selection of Spectroscopic Data

Infrared Absorption Data

Bond	Compound Type	Wavenumber/cm ⁻¹
C-H	Alkanes	2960-2850(s) stretch
C=C	Alkenes	1680-1640(m,w) stretch
C-O	Alcohols, Ethers, Carboxylic acids, Esters	1260-1000(s) stretch
C=O	Aldehydes, Ketones, Carboxylic acids, Esters	1760-1670(s) stretch
O-H	Alcohols, Phenols	3640-3160(s,br) stretch
O-H	Carboxylic acids	3000-2500(b) stretch
N-H	Amines	3500-3300(m) stretch
		1650-1580 (m) bend

Typical Chemical Shifts in ¹³C NMR Spectra

Carbon	Compound Type	Typical Chemical Shift, δ/ppm
<u>C</u> =O	Ketone	205-220
<u>C</u> =O	Aldehyde	190-200
<u>C</u> =O	Carboxylic acids, Esters	170-185
<u>C</u> -C	Arene	125-150
<u>C</u> =C	Alkenes	115-140
R <u>C</u> H ₂ OH	Alcohols	50-65
R <u>C</u> H ₂ NH ₂	Amines	37-45
R <u>C</u> H ₂ Cl	Halogenoalkanes	40-45
R ₃ <u>C</u> H	3° Alkanes	25-35
<u>C</u> H ₃ CO-	Ketone, Aldehyde, Carb. Acid, Ester	20-30
R ₂ <u>C</u> H ₂	2° Alkanes	16-25
R <u>C</u> H ₃	1° Alkanes	10-15
TMS	Reference	0

Typical Chemical Shifts in ¹H NMR Spectra

Hydrogen	Compound Type	Typical Chemical Shift, δ/ppm
R- <u>C</u> H ₃ , R ₂ - <u>C</u> H ₂ , R ₃ - <u>C</u> H	Alkane	0.8-1.5
C= <u>C</u> H	Alkene	4.6-5.9
Ar- <u>H</u>	Aryl	6.5-8.5
R <u>C</u> H ₂ Cl, R <u>C</u> H ₂ Br	Haloalkane	3-4.3
R- <u>C</u> H ₂ O	Alcohol, ether, ester	3.4-4.3
R- <u>O</u> H*	Alcohol	0.5-5*
R- <u>N</u> H ₂ *	Amine	0.5-5*
R- <u>C</u> H-CO-R	Ketone	2-3
R- <u>C</u> HO	Aldehyde	9-10
R-CON <u>H</u> R	Amide	5-9
R-COO <u>H</u>	Carboxylic Acid	>10
TMS	Reference	0

* -OH & -NH protons can appear almost anywhere in the spectrum. They often appear very broad. Sometimes they can be split by neighbouring protons into multiplets and sometimes not. This depends upon the conditions; especially how dry the sample is.