Characteristic Bands in Infrared Spectrum

Func group	Organic molecule in which functional gp is found	Type of vibration	Characteristic Wavenumber/cm^{-1}
C–H	alkanes, alkenes	stretch	2 850–3 100
=C–H	alkenes	bending	675-1 000
C=C	alkenes	stretch	1 630–1 690
O–H	alcohols	stretch (H-bonded)	3 200–3 600
C–O	alcohols, esters	stretch	1 000–1 300
C=O	aldehydes, ketones, carboxylic acids, esters	stretch	1 670–1 780
C=O	acid chlorides	stretch	1 785–1 815
O–H	carboxylic acids	stretch	2 500–3 300
C=O	amides	stretch	1 630–1 700
N–H	amides	bending	1 550-1 640
C–N	amines	stretch	1 000–1 250
N–H	amines, amides	stretch	3 300–3 500
N–H	amines	bending	1 600
C-Cl	chloroalkanes	stretch	600-800
C-Br	bromoalkanes	stretch	500-600

Fragments in Mass Spectrum

Relative mass	Molecular ion, M^+
15	CH_3^+
17	OH^+
28	CO^+
29	$CH_3CH_2^+$ or CHO^+
31	CH_3O^+ or CH_2OH^+
43	$C_3H_7^+$
45	$COOH^+$

Characteristic Shifts in ^{13}C NMR spectrum

Carbon environment	Chemical shift (ppm)
C=O (in ketones)	205–220
C=O (in aldehydes)	190–200
C=O (in acids and esters)	170–185
C=C (in alkenes)	115–140
$RCO_2\underline{\mathbf{C}}H_2R'$ (esters)	60–80
RCH_2OH	50–65
RCH_2Cl	40–45
RCH_2Br	30–40
RCH_2NH_2	37–45
R_3CH	25–35
$\underline{C}H_3CO–$	20–30
R_2CH_2	16–25
RCH_3	10–15

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