

Spectroscopy Data Sheet for AS91388

IR Spectra

Stretching Vibrations			
Functional Group	Range (cm ⁻¹)	Intensity	Assignment
Alkanes	2850-3000	med-str	C-H, 2 or 3 peaks
Haloalkanes	600-800	str	C-Cl
	500-600	str	C-Br
Alkenes	3020-3100	med	=C-H & =CH ₂ (usually sharp)
	1630-1680	var	C=C (symmetry reduces intensity)
Alcohols	3200-3550	str	O-H (H-bonded), usually broad
	970-1250	str	C-O
Amines & Amides	3300-3500	wk - med	N-H (1° amines) N-H (amides) - 2 peaks. N-H (2° amines)
	1000-1250	med	C-N
Aldehydes & Ketones	2690-2840	med	C-H, 2 peaks (aldehyde C-H)
	1720-1740	str	C=O (saturated aldehyde)
	1710-1720	str	C=O (saturated ketone)
Carboxylic Acids & Derivatives	2500-3300 (c.acids) overlap C-H	str	O-H (very broad)
	1705-1720 (c.acids)	str	C=O (H-bonded)
	1210-1320 (c.acids)	med	O-C (sometimes 2-peaks)
	1785-1815 (acid chlorides)	str	C=O
	1735-1750 (esters)	str	C=O
	1000-1300	str	O-C (2-peaks)
	1630-1695 (amides)	str	C=O
Bending Vibrations			
Functional Group	Range (cm ⁻¹)	Intensity	Assignment
Amines & Amides	2850 - 3000	med	N-H (1° amine)
	1550 - 1640	str	N-H (1°-amine)
	1590 - 1650	med	N-H (amide)
Alkane	1450 - 1470	med	C-H
Carboxylic acids	910 – 950	med	O-H
Alkene	650 - 1000	med-str	=C-H

Str = strong, med – medium, wk = weak, var = variable

Approximate Values of Chemical Shifts in ^{13}C NMR spectrum

Carbon environment	Chemical shift (ppm)
$\underline{\text{C}}=\text{O}$ (in ketones)	205–220
$\underline{\text{C}}=\text{O}$ (in aldehydes)	190–200
$\underline{\text{C}}=\text{O}$ (carboxylic acids, acid chlorides, amides and esters)	160–185
$\text{C}=\text{C}$ (in alkenes)	115–140
$\text{RCO}_2\underline{\text{C}}\text{H}_2\text{R}'$ (esters)	60–80
$\text{R}\underline{\text{C}}\text{H}_2\text{OH}$ ($\underline{\text{C}}-\text{OH}$ between 50-90)	50–70
$\text{R}\underline{\text{C}}\text{H}_2\text{Cl}$	40–45
$\text{R}\underline{\text{C}}\text{H}_2\text{Br}$	30–40
$\text{R}\underline{\text{C}}\text{H}_2\text{NH}_2$	35–45
$\text{R}\underline{\text{C}}\text{H}(\text{NH}_2)\text{R}$	30–60
$\text{R}_3\underline{\text{C}}\text{H}$	25–60
$\underline{\text{C}}\text{H}_3\text{CO}$	20–30
$\text{R}-\underline{\text{C}}\text{H}_2-\text{R}$	15-50
$\text{R}-\underline{\text{C}}\text{H}_3$	8-35

Fragments in Mass Spectrum

Relative mass	Molecular ion, M^+
15	CH_3^+
17	OH^+
28	CO^+
29	CH_3CH_2^+ or CHO^+
30	CH_2NH_2^+
31	CH_3O^+ or CH_2OH^+
43	C_3H_7^+ or CH_3CO^+
44	CONH_2^+
45	COOH^+ or CH_3CHOH^+ or $\text{CH}_3\text{CH}_2\text{O}^+$
57	C_4H_9^+

Molar mass / g mol^{-1}

H=1, C=12, N=14, O=16, Cl=35.5, Br=80