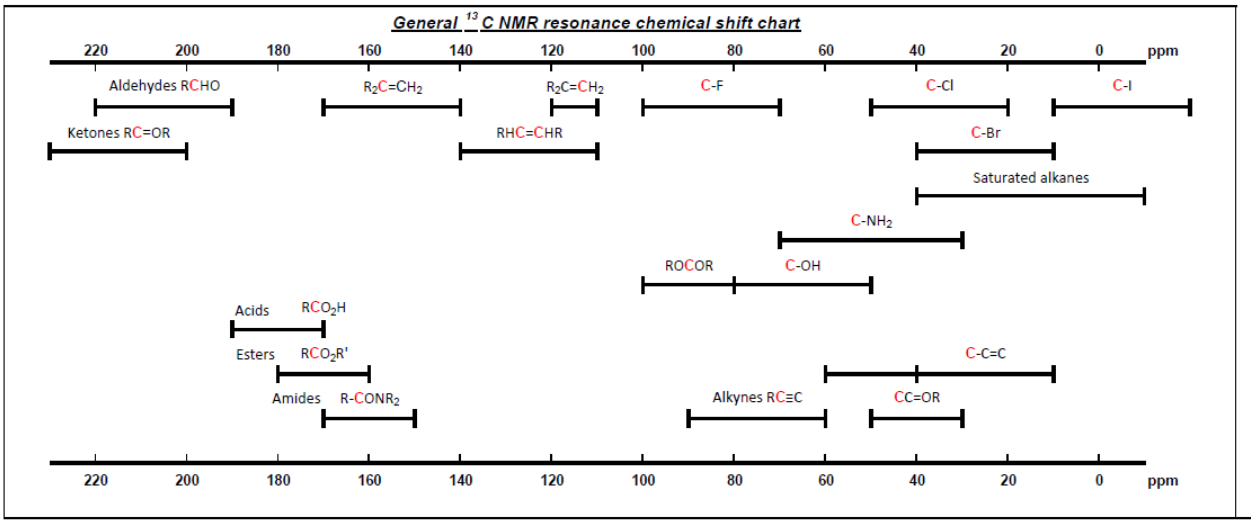
SPECTROSCOPY DATA SHEET

INFRARED SPECTROSCOPY

Functional group	Vibration	Wavenumber/ cm^{-1}
Alkane	C-H stretch	2950-2800 (s)
Alkene	C=C-H stretch	3100-3010 (s)
	C=C stretch	1690-1630 (m)
Alkyl halide	C-F stretch	1400-1000 (s)
	C-Cl stretch	785-540 (m-w)
	C-Br stretch	650-510 (s-m)
	C-I stretch	600-485 (s-m)
Alcohol	O-H stretch	3600-3300 (s)
	C-O stretch	1260-1000 (s)
Aldehyde	C=O stretch	1725 (s)
Ketone	C=O stretch	1715 (s)
Carboxylic acid	O-H stretch	3400 (s)
	C=O stretch	1730-1700 (s)
	C-O stretch	1320-1210 (s)
Acid chloride	C=O stretch	1810-1775 (s)
	C-Cl stretch	730-550 (s-m)
Ester	C=O stretch	1750-1735 (s)
	C-O stretch	1260-1160 (s)
Amine	N-H stretch (1 per bond)	3500-3300 (s-w)
	N-H bend	1640-1500 (s)
	C-N stretch	1200-1025 (s)
Amide	N-H stretch	3500-3200 (s)
	C=O stretch	1680-1630 (s)
	N-H bend	1640-1515 (s)

s = strong
m = medium
w = weak

^{13}C NMR RESONANCE SHIFTS

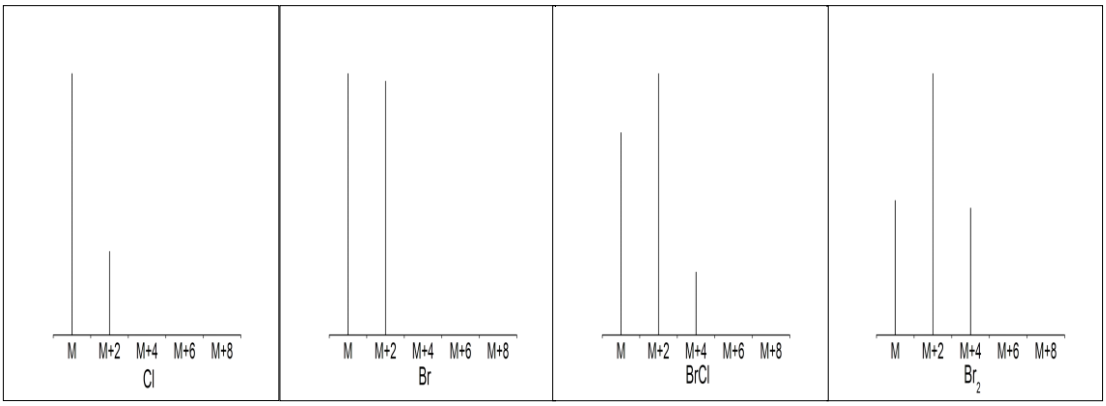


COMMON FRAGMENT IONS FOUND IN EI MS

All ions suggested are +1 charge, this list is suggestive and not exhaustive

m/z	Structural Inference	*m /z*	Structural Inference
15	CH_3	55	C_4H_7, CH_2=CHC=O
17	OH	57	C_4H_9, $CH_3(C=O)CH_2$
27	C_2H_3	59	$(CH_3)_2COH$, $C_2H_5OCH_2$, $C=OOCH_3$, CH_3OCHCH_3, CH_3CHCH_2OH, C_2H_5CHOH
29	C_2H_5, CHO	93	CH_2Br (+ 95), C_7H_9,
30	CH_2NH_2,	101	$COOC_4H_9$
31	CH_2OH, OCH_3	127	I
41	C_3H_5	141	CH_2I
43	$CH_3C=O$, C_3H_7		
44	$C=ONH_2$, $(CH_3)_2N$		
45	COOH, $(CH_3)CHOH$, $(CH_2)_2OH$, CH_2OCH_3		

ISOTOPIC DISTRIBUTION OF POLYHALOGENATED MOLECULES



Adapted from material supplied by Rob Keyzers and Peter Northcote from Victoria University of Wellington