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HIGH-RESOLUTION MASS SPECTROMETRY

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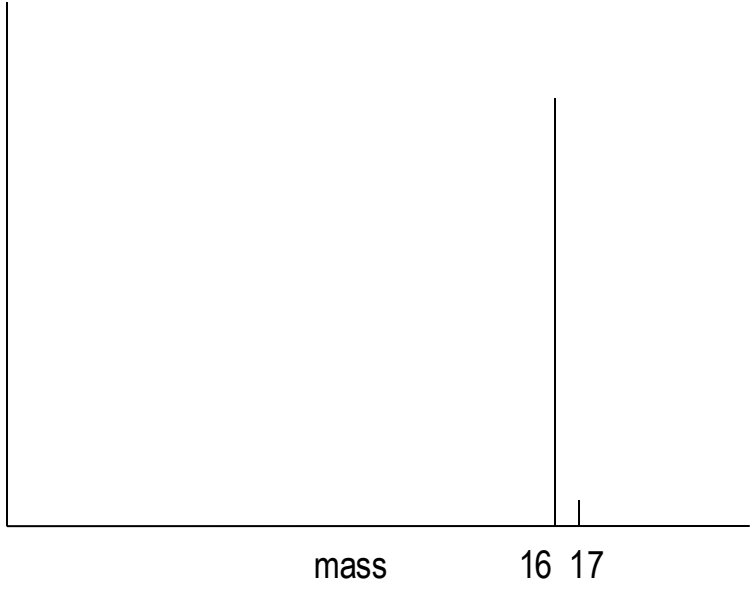
Agilent Technologies
Binary SL

	Electron impact	Electrospray ionisation
What it does	removes one electron to form M^+ ion $M(g) \rightarrow M^+(g) + e^-$	Adds one proton to form MH^+ ion $M(g) + H^+(g) \rightarrow MH^+(g)$
Which compounds	Compounds with low M_r	Compound with high M_r (e.g. proteins)
How is it done	High energy electrons (from an "electron gun" are fired at the sample).	The compound is dissolved in a volatile solvent and sprayed out into a fine mist via a hypodermic needle whose tip is connected to the positive terminal of a high voltage power supply.

^{2}H & ^{13}C

- Spectra measure the mass of individual ions – ions with ^{13}C / ^{2}H atom
- There is often a small peak with a value that is 1 greater than that for the molecular ion.

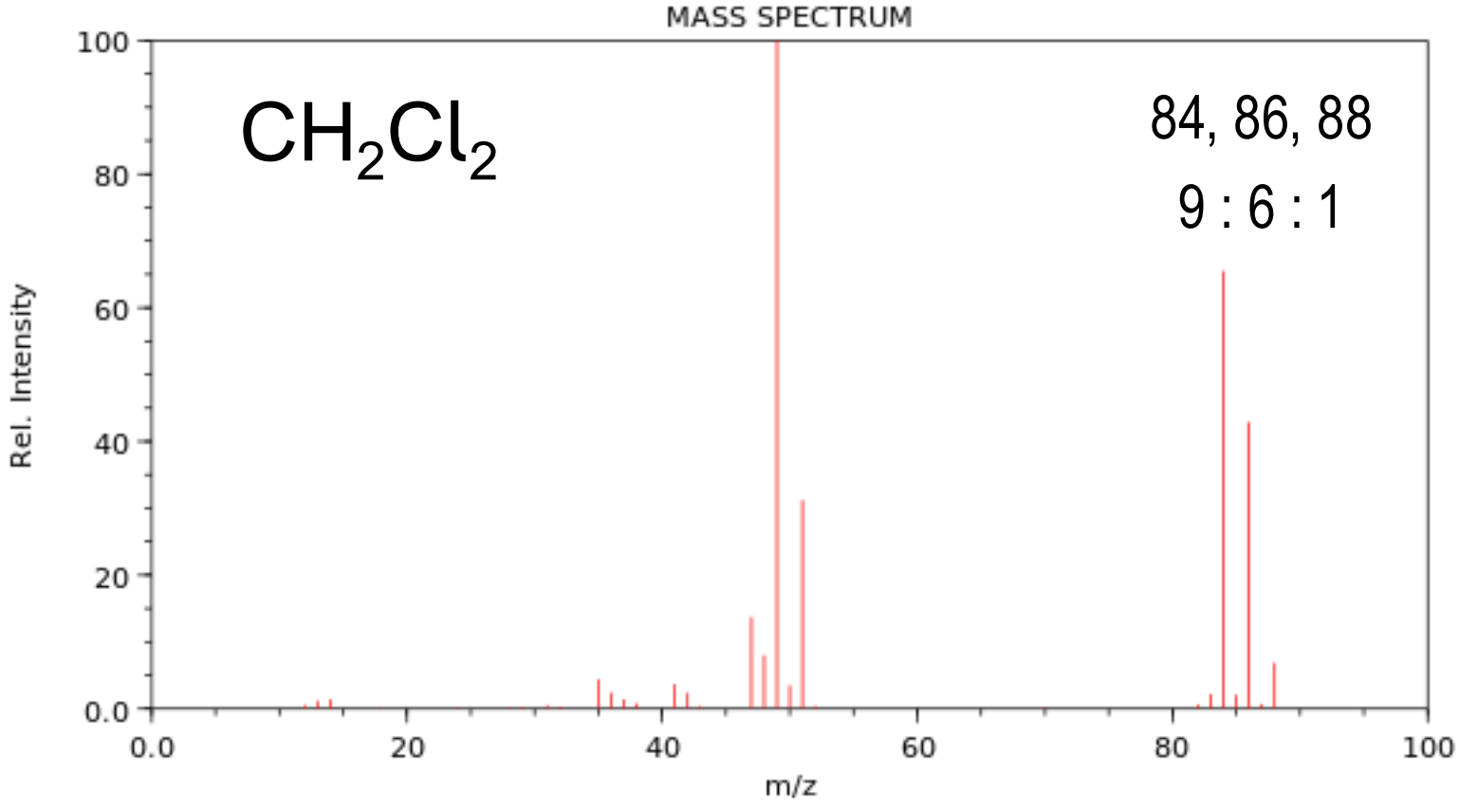
e.g. CH_4



Isotopes of Cl and Br

- Chlorine 75% ^{35}Cl & 25% ^{37}Cl
- Bromine 50% ^{79}Br & 50% ^{81}Br

Compound	Molecule	Mass	Probability		Mass spectrum peaks
CH_3Cl	$CH_3{}^{35}Cl$	50	$\frac{3}{4}$		2 signals @ 50, 52 in ratio 3:1
	$CH_3{}^{37}Cl$	52	$\frac{3}{4}$		
CH_2Cl_2	$CH_2{}^{35}Cl_2$	84	$\frac{3}{4} x \frac{3}{4} = \frac{9}{16}$		3 signals @ 84, 86, 88 in ratio 9:6:1
	$CH_2{}^{35}Cl{}^{37}Cl$	86	$\frac{3}{4} x \frac{1}{4} = \frac{3}{16}$	$\frac{6}{16}$	
	$CH_2{}^{37}Cl{}^{35}Cl$	86	$\frac{1}{4} x \frac{3}{4} = \frac{3}{16}$		
	$CH_2{}^{37}Cl_2$	88	$\frac{1}{4} x \frac{1}{4} = \frac{1}{16}$		



NIST Chemistry WebBook (https://webbook.nist.gov/chemistry)

type of mass spectrometer	low-resolution	high-resolution
resolution of M_r	nearest unit (e.g. 60)	0.0001 or better (e.g. 60.0211)
what it tell us	M_r to nearest unit	M_r to to high resolution molecular formula

Low resolution M_r	High resolution M_r	Molecular formula	Possible compounds	
60	60.0211	$C_2H_4O_2$	CH_3COOH	ethanoic acid
			$HCOOCH_3$	methyl methanoate
60	60.0575	C_3H_8O	$CH_3CH_2CH_2OH$	propan-1-ol
			$CH_3CH(OH)CH_3$	propan-1-ol
			$CH_3OCH_2CH_3$	methoxethane
60	60.0324	CH_4N_2O	H_2NCONH_2	urea