HIGH RESOLUTION MASS SPECTROMETRY

TASK 1 – Molecular ion peaks

Compound	Molecule	Mass	Probability	Mass spectrum peaks
CH_3Br	$CH_3{}^{79}Br$	94	$\frac{1}{2}$	2 signals @ 94, 96 in ratio 1:1
	$CH_3{}^{81}Br$	96	$\frac{1}{2}$	
CH_2Br_2	$CH_2{}^{79}Br_2$	172	$\frac{1}{2} x \frac{1}{2} = \frac{1}{4}$	3 signals @ 172, 174, 176 in ratio 1:2:1
	$CH_2{}^{79}Br\,{}^{81}Br$	174	$\frac{1}{2} x \frac{1}{2} = \frac{1}{4}$	
	$CH_2{}^{81}Br\,{}^{79}Br$		$\frac{1}{2} x \frac{1}{2} = \frac{1}{4}$ $\quad \frac{2}{4}$	
	$CH_2{}^{81}Br_2$	176	$\frac{1}{2} x \frac{1}{2} = \frac{1}{4}$	
CH_2BrCl	$CH_2{}^{79}Br{}^{35}Cl$	128	$\frac{1}{2} x \frac{3}{4} = \frac{3}{8}$	3 signals @ 128, 130, 132 in ratio 3:4:1
	$CH_2{}^{79}Br{}^{37}Cl$	130	$\frac{1}{2} x \frac{1}{4} = \frac{1}{8}$	
	$CH_2{}^{81}Br{}^{35}Cl$		$\frac{1}{2} x \frac{3}{4} = \frac{3}{8}$ $\quad \frac{4}{8}$	
	$CH_2{}^{81}Br{}^{37}Cl$	132	$\frac{1}{2} x \frac{1}{4} = \frac{1}{8}$	
CCl_4	$C^{35}Cl_4$	152	$\frac{3}{4} x \frac{3}{4} x \frac{3}{4} x \frac{3}{4} = \frac{81}{256}$	5 signals @ 152, 154, 156, 158, 160 in ratio 81 : 108 : 54 : 12 : 1
	$C^{35}Cl_3{}^{37}Cl$	154	$4\,ways\ x \frac{3}{4} x \frac{3}{4} x \frac{3}{4} x \frac{1}{4} = \frac{108}{256}$	
	$C^{35}Cl_2{}^{37}Cl_2$	156	$6\,ways\ x \frac{3}{4} x \frac{3}{4} x \frac{1}{4} x \frac{1}{4} = \frac{54}{256}$	
	$C^{35}Cl{}^{37}Cl_3$	158	$4\,ways\ x \frac{3}{4} x \frac{1}{4} x \frac{1}{4} x \frac{1}{4} = \frac{12}{256}$	
	$C^{37}Cl_4$	160	$\frac{1}{4} x \frac{1}{4} x \frac{1}{4} x \frac{1}{4} = \frac{1}{256}$	

TASK 2 – High-resolution mass spectrometry problems

1) How could high-resolution mass spectroscopy be used to distinguish propane and ethenol?

M_r of propane CH_3-CH_2-CH_2 = 44.0624

M_r of ethenol CH_2=CH-OH = 44.0261

Measure the M_r to 4 dp and see if it is 44.0624 or 44.0261

2) A compound is found to have an accurate relative formula mass of 46.0417. It is thought to be either CH_3CH_2OH or $H_2NCH_2NH_2$. Calculate the M_r of each compound to 4 decimal places to work out which one it is.

CH_3CH_2OH **46.0417**

$H_2NCH_2NH_2$ **46.0530**

Molecular formula = **C_2H_6O**

3) High-resolution mass spectroscopy showed the M_r of difluoromethane to be 52.0124. The only stable isotope of fluorine is ^{19}F. Calculate the mass of one atom of ^{19}F to 4 decimal places.

52.0124 – 12.0000 – 2(1.0078) = 37.9968

Mass of ^{19}F = $\frac{37.9968}{2}$ = 18.9984

4) Calculate the accurate mass to 4 decimal places of the two molecular ion peaks in the high-resolution mass spectrum of chloroethane.

Peak 1 **64.0079**

Peak 2 **66.0049**

5) Analysis of an organic compound showed that its relative formula mass is 102. High resolution mass spectroscopy showed it to be 102.0678.

a) Calculate the M_r to 4 decimal places of each of these molecular formulas (which have M_r = 102) and then determine the correct molecular formula.

$C_5H_{14}N_2$ **102.1154**

$C_5H_{10}O_2$ **102.0678**

$C_3H_6N_2O_2$ **102.0428**

Molecular formula = **$C_5H_{10}O_2$**

b) Identify two possible compounds that have M_r = 102.0678

any 2 of these (there are other possibilities)