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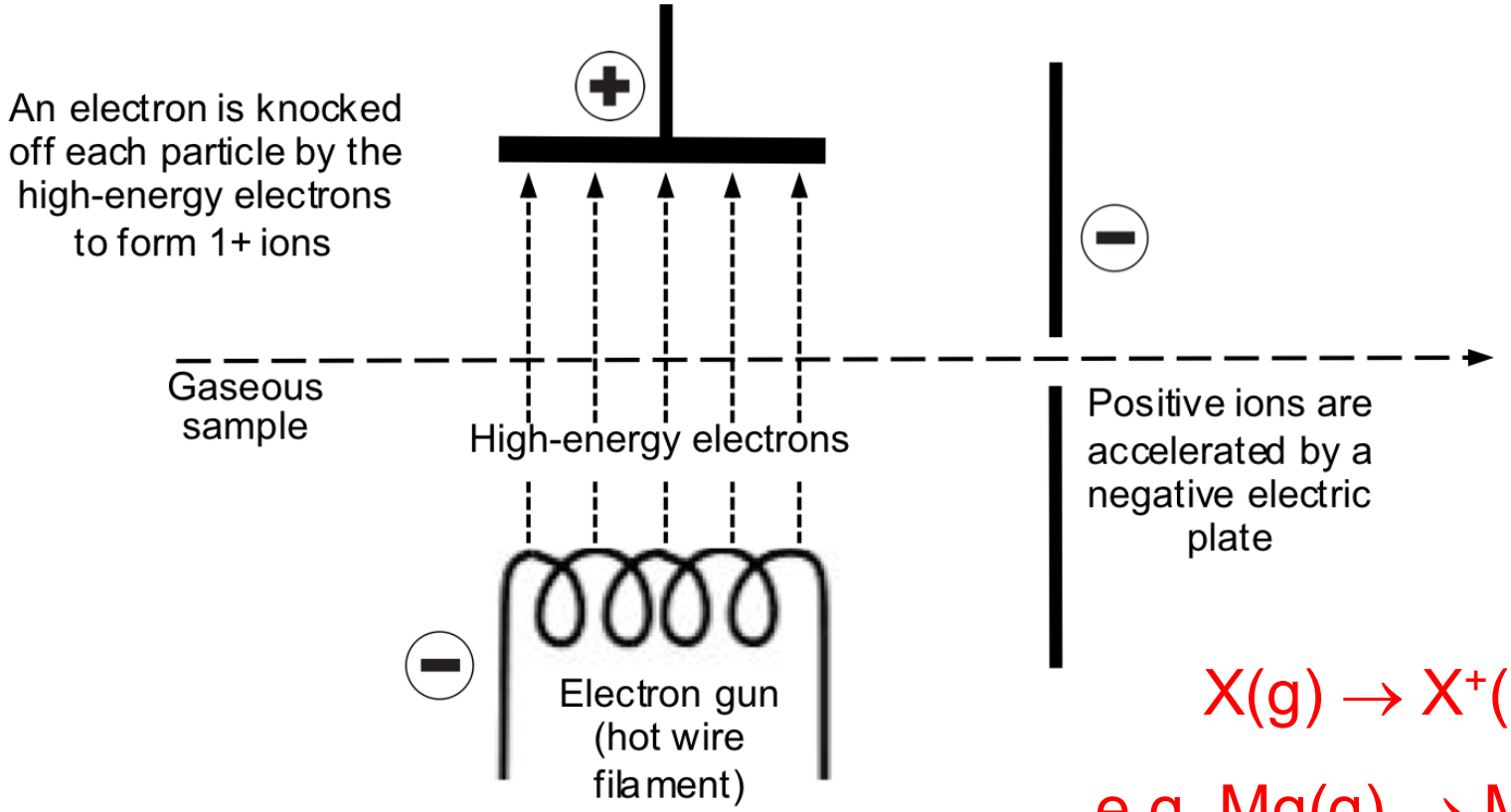
ToF MASS SPECTROMETRY

Stage 1 – IONISATION

Elements and low M_r compounds



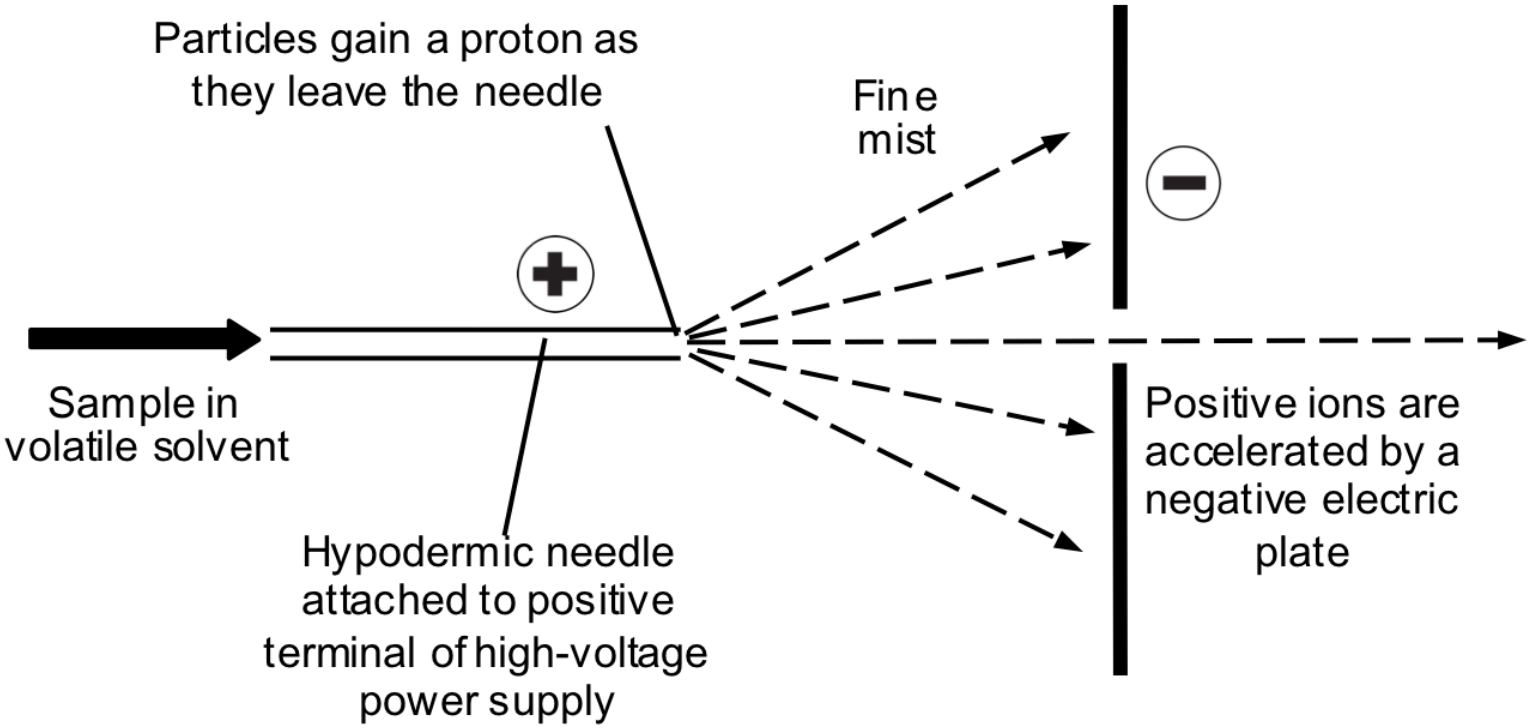
$X(g) \rightarrow X^+(g) + e^-$

e.g. $Mg(g) \rightarrow Mg^+(g) + e^-$

Loss of electron

Stage 1 – IONISATION

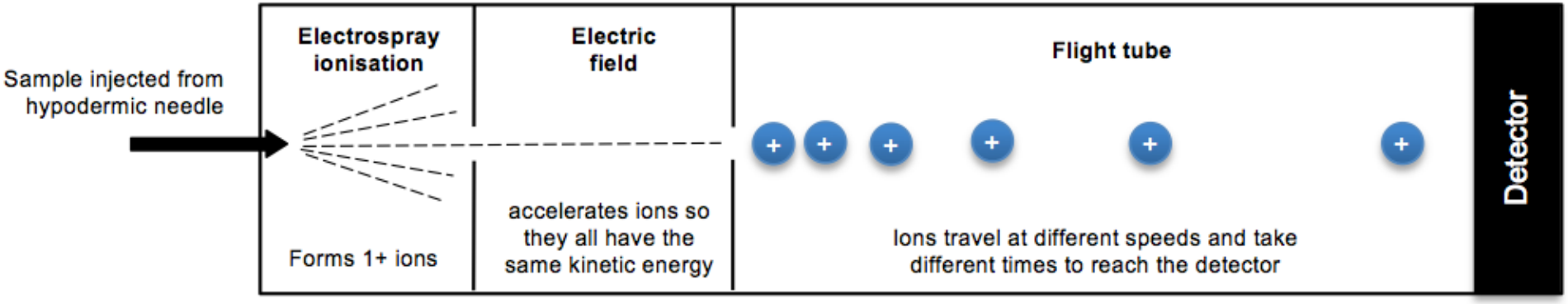
High M_r compounds (e.g. proteins)



$X(g) + H^+ \rightarrow XH^+(g)$

gains a proton

Stage 2 – ACCELERATION



$$KE = \frac{1}{2}mv^2$$

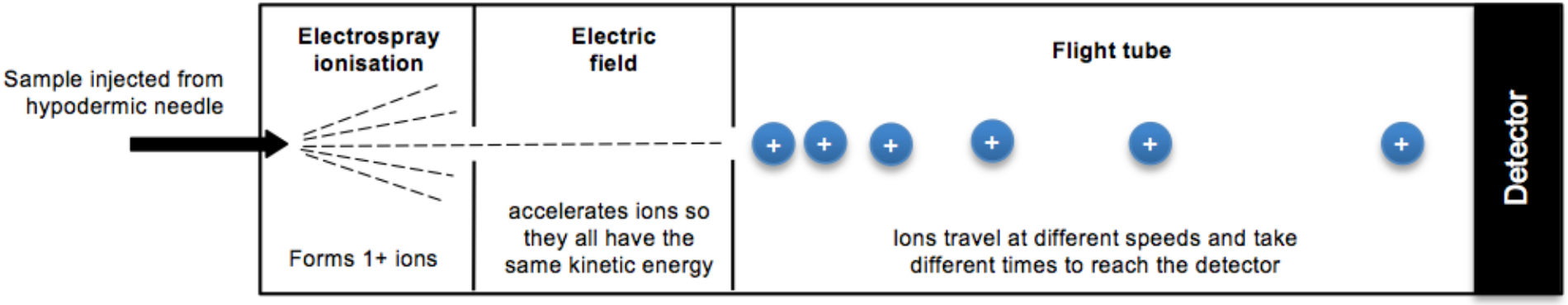
KE = kinetic energy of particle (J)

m = mass of the particle (kg)

v = velocity of the particle (m s^{-1})

$$v = \sqrt{\frac{2KE}{m}}$$

Stage 3 – FLIGHT TUBE



$$t = \frac{d}{v}$$

$$t = d\sqrt{\frac{m}{2KE}}$$

t = time of flight (s)

KE = kinetic energy of particle (J)

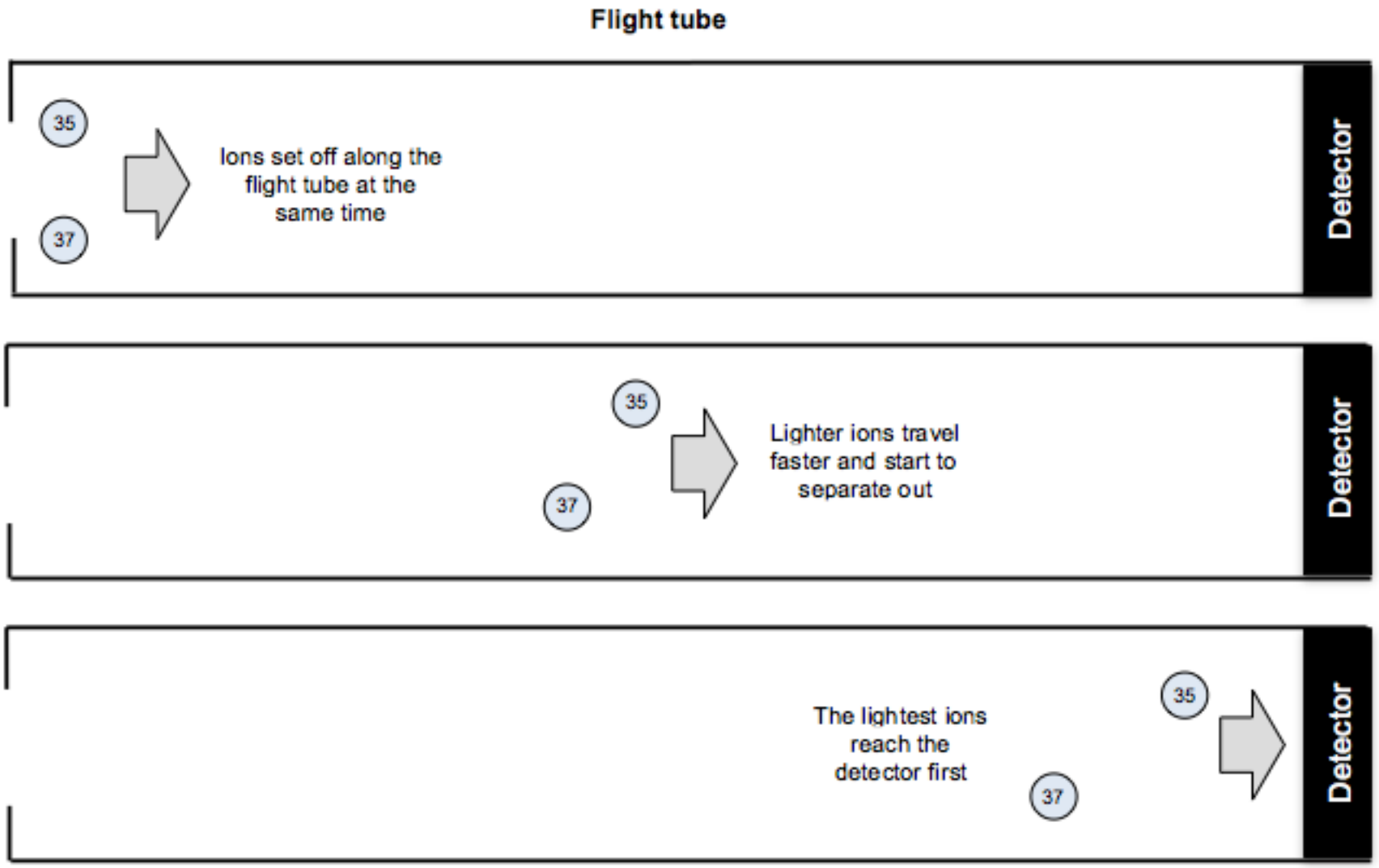
m = mass of the particle (kg)

v = velocity of the particle (m s^{-1})

d = length of flight tube (m)

Lighter particles move faster and so have a shorter time of flight

Stage 3 – FLIGHT TUBE



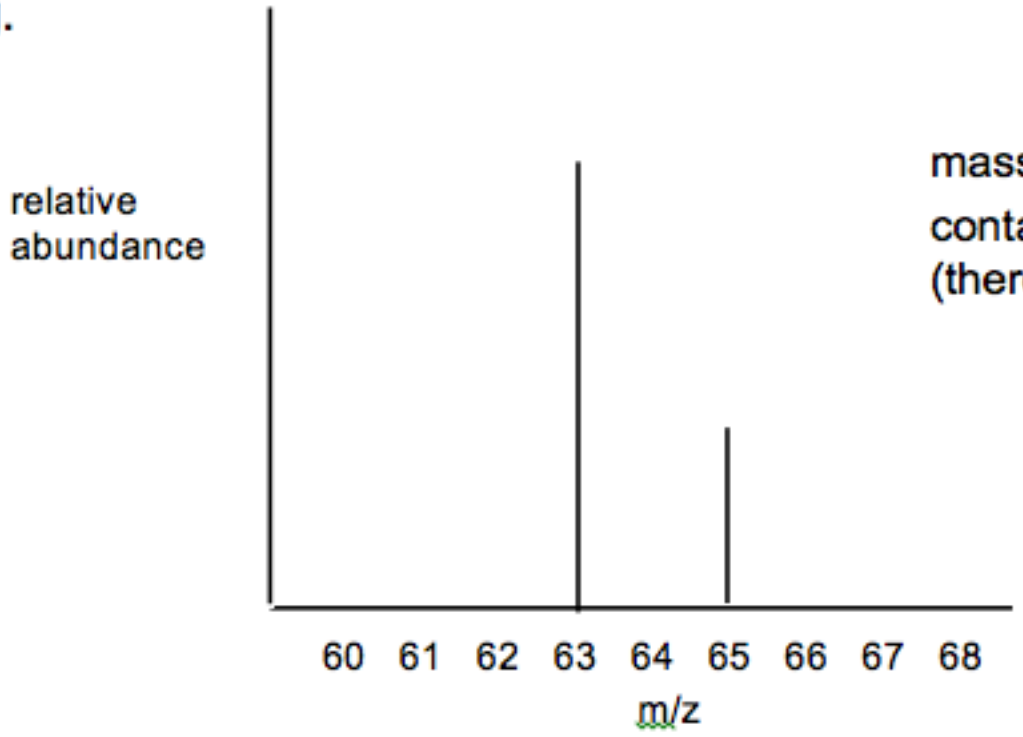
Stage 4 – DETECTION

- +ve ions hit –ve plate and produce electric current
- size of current proportional to number of ions

The Mass Spectrum

Copper

e.g.



mass spectrum of copper

contains two main isotopes: ^{63}Cu and ^{65}Cu
(there are more atoms of ^{63}Cu than ^{65}Cu)

Average mass

- 2 balls with mass 100 g
- 3 balls with mass 200 g
- 10 balls with mass 400 g

$$\text{average mass} = \frac{\text{total mass of all balls}}{\text{number of balls}}$$

$$= \frac{(2\text{x}100)+(3\text{x}200)+(10\text{x}400)}{2+3+10}$$

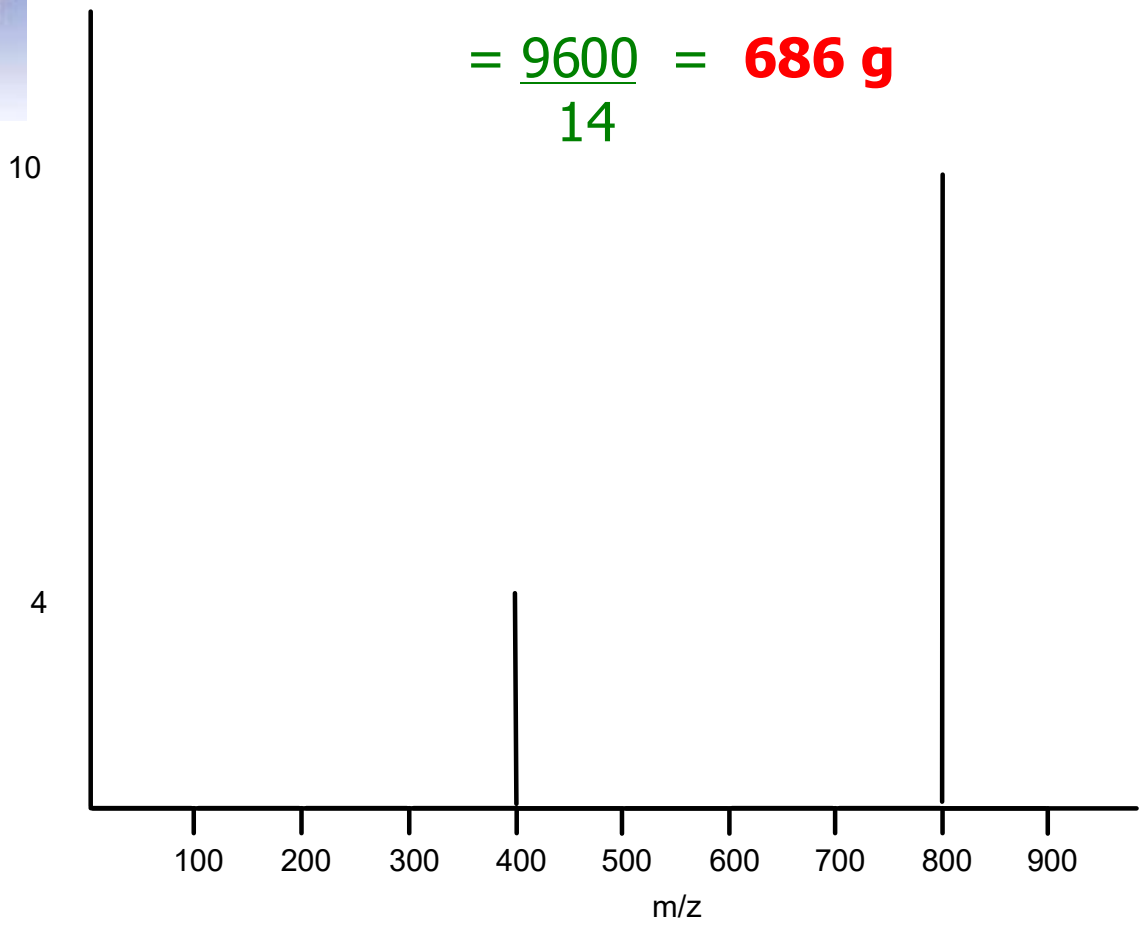
$$= \frac{4800}{15} = \mathbf{320\ g}$$

I have these loaves – what is the average mass?

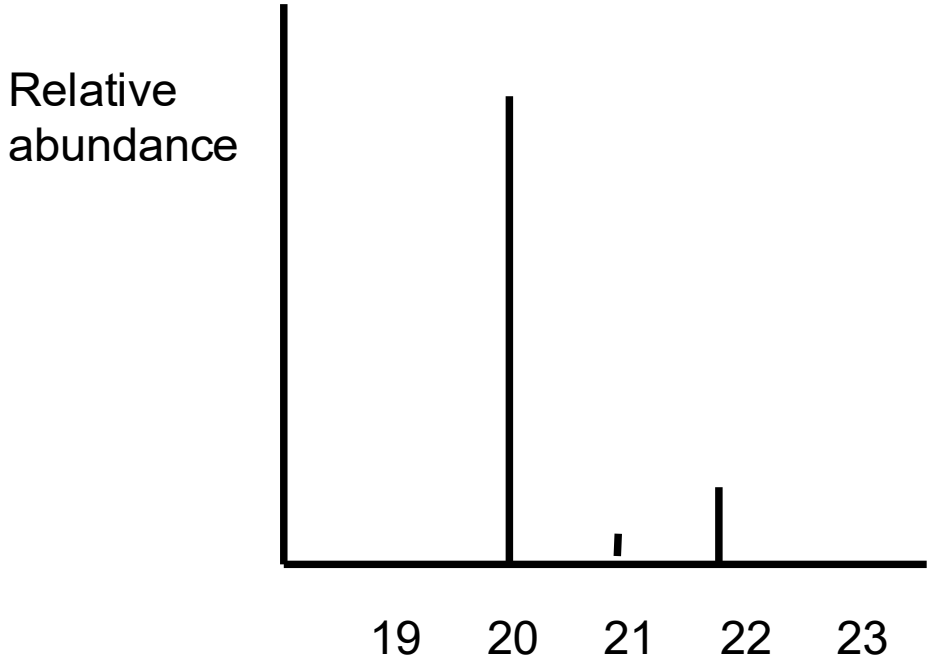
$$\text{average mass} = \frac{\text{total mass of all loaves}}{\text{number of loaves}}$$

$$= \frac{(4\times400)+(10\times800)}{4+10}$$

$$= \frac{9600}{14} = \mathbf{686\ g}$$



Neon



^{20}Ne 90.90 %

^{21}Ne 0.26 %

^{22}Ne 8.80 %

$$A_r = \frac{[\,(90.90 \times 20) + (0.26 \times 21) + (8.80 \times 22)\,]}{(90.90 + 0.26 + 8.80)} = 20.17$$

ISOTOPES

- Ions with different isotopes produce different signals.
- Most important for Br and Cl.

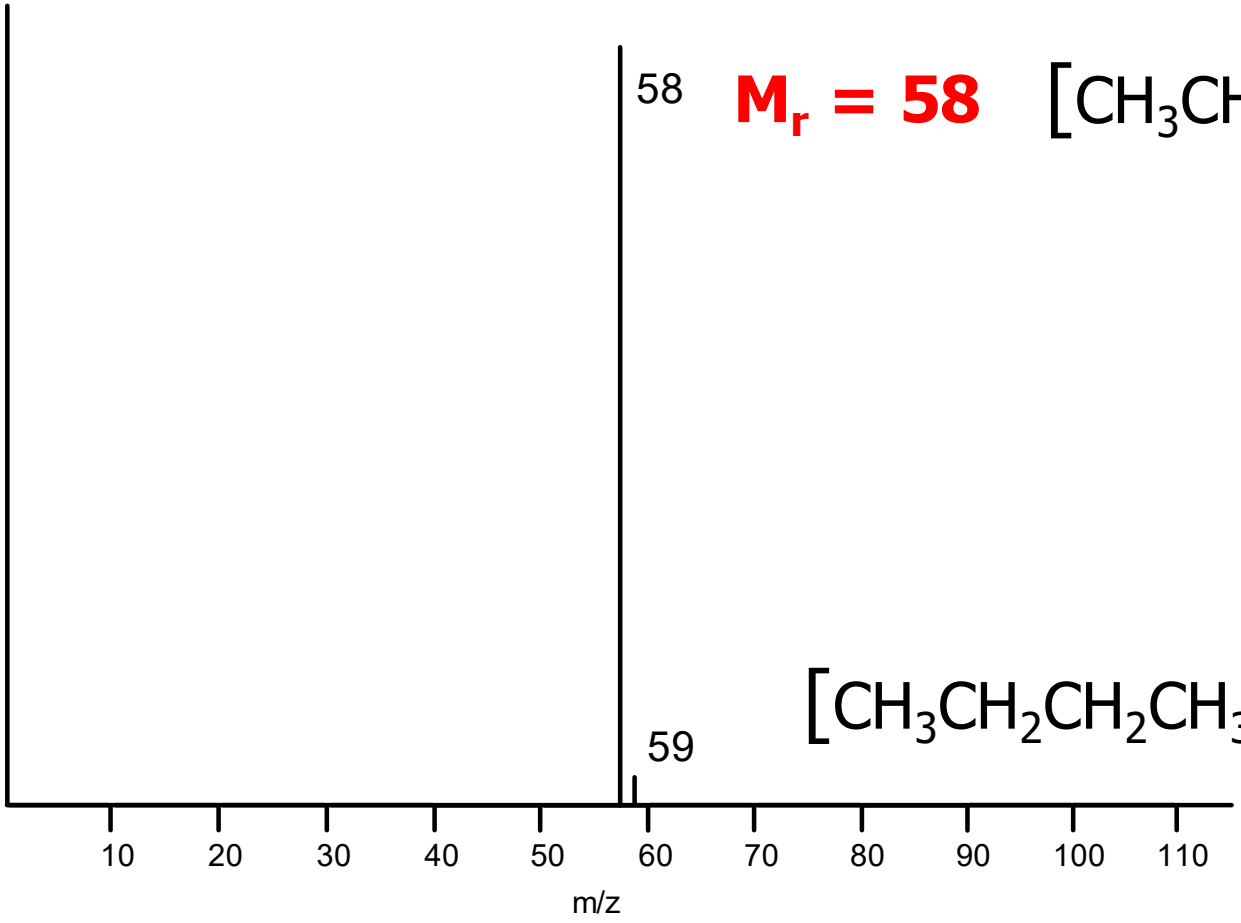
Br: 50% ^{79}Br 50% ^{81}Br

Cl: 75% ^{35}Cl 25% ^{37}Cl

- If two or more Br/Cl atoms, then spectrum is more complicated.
- Often small peaks at m/z + 1 due to ^{2}H and ^{13}C.

butane

$CH_3CH_2CH_2CH_3$

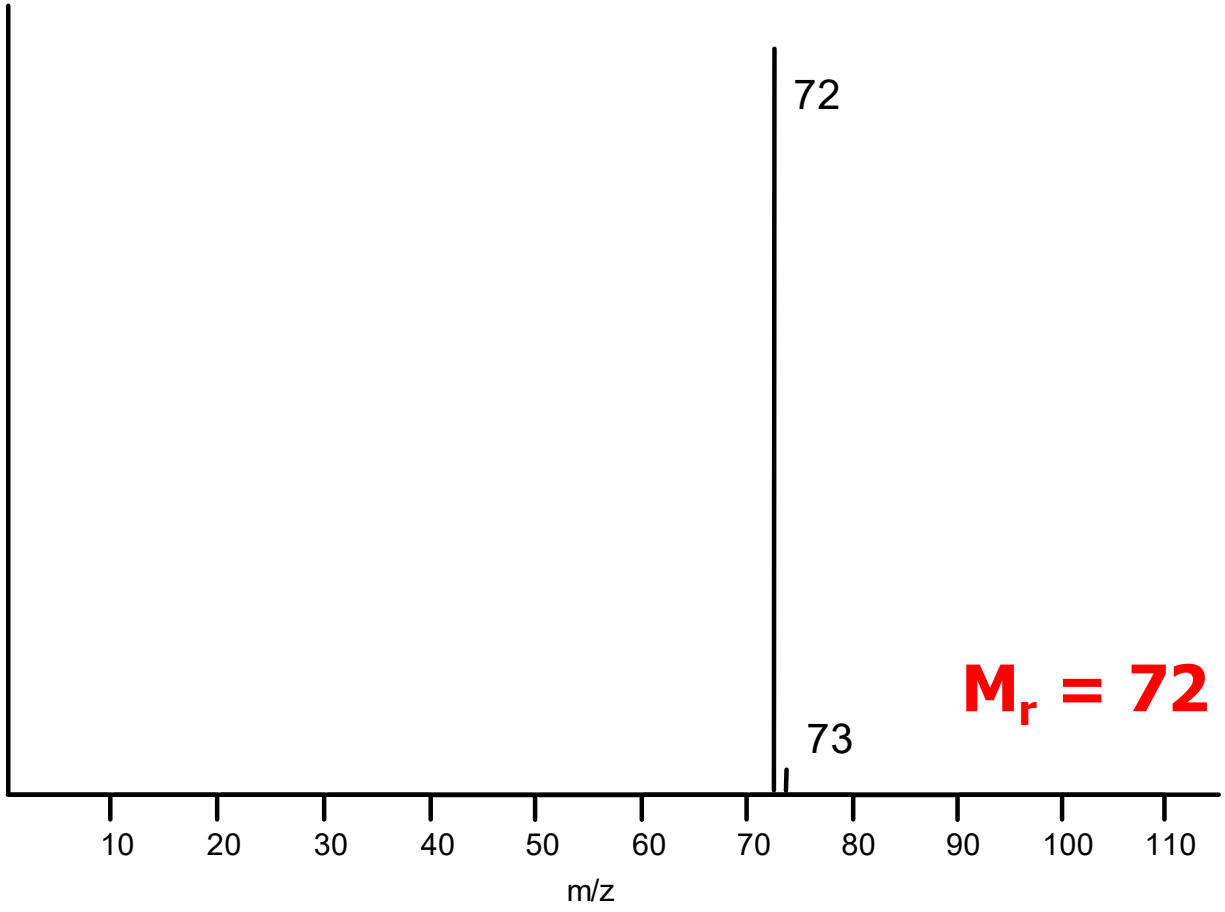


M_r = 58 $[CH_3CH_2CH_2CH_3]^+$

$[CH_3CH_2CH_2CH_3]^+$ with 1 x $^2H/^{13}C$

butanone

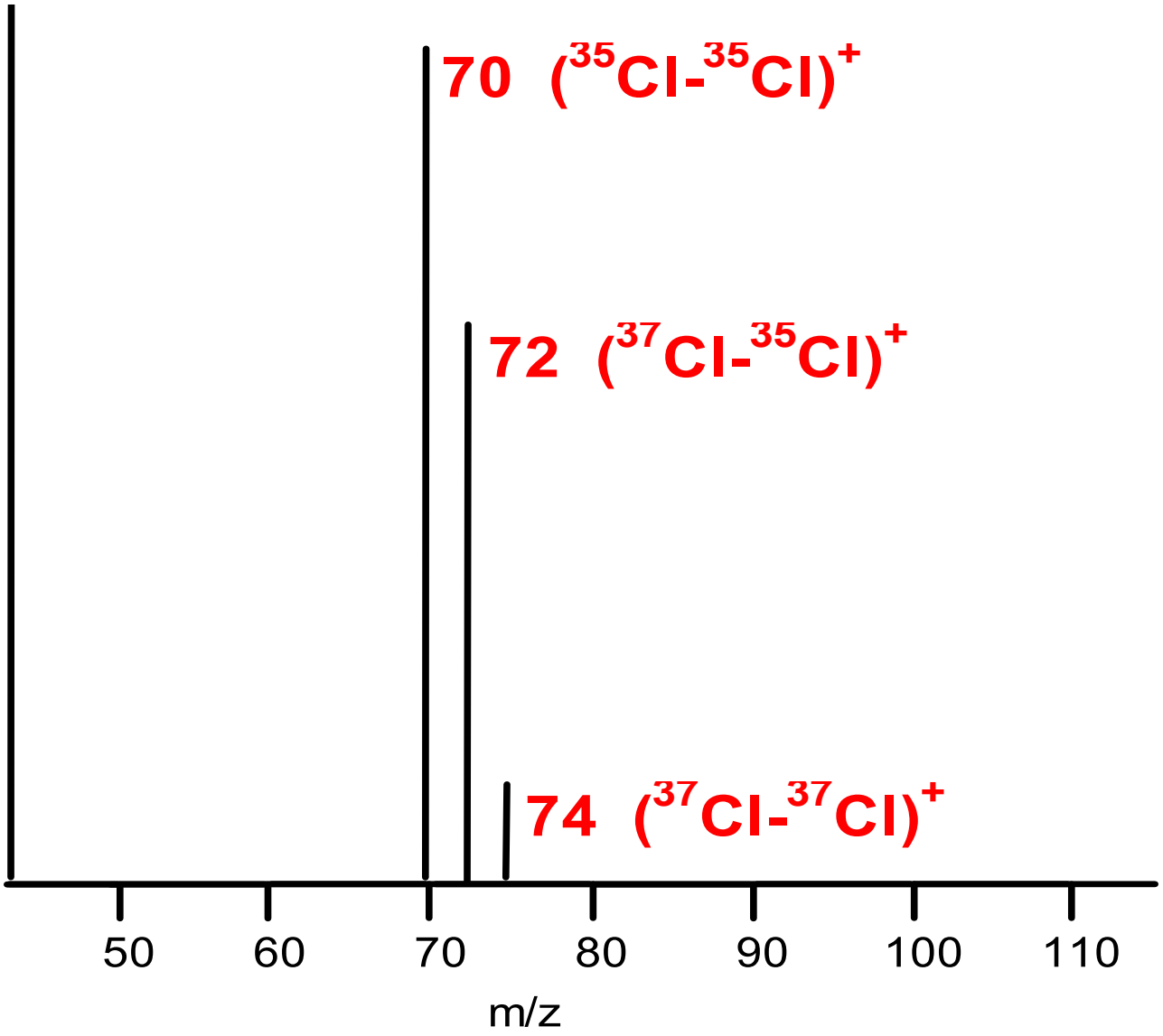
$CH_3CH_2COCH_3$



M_r = 72

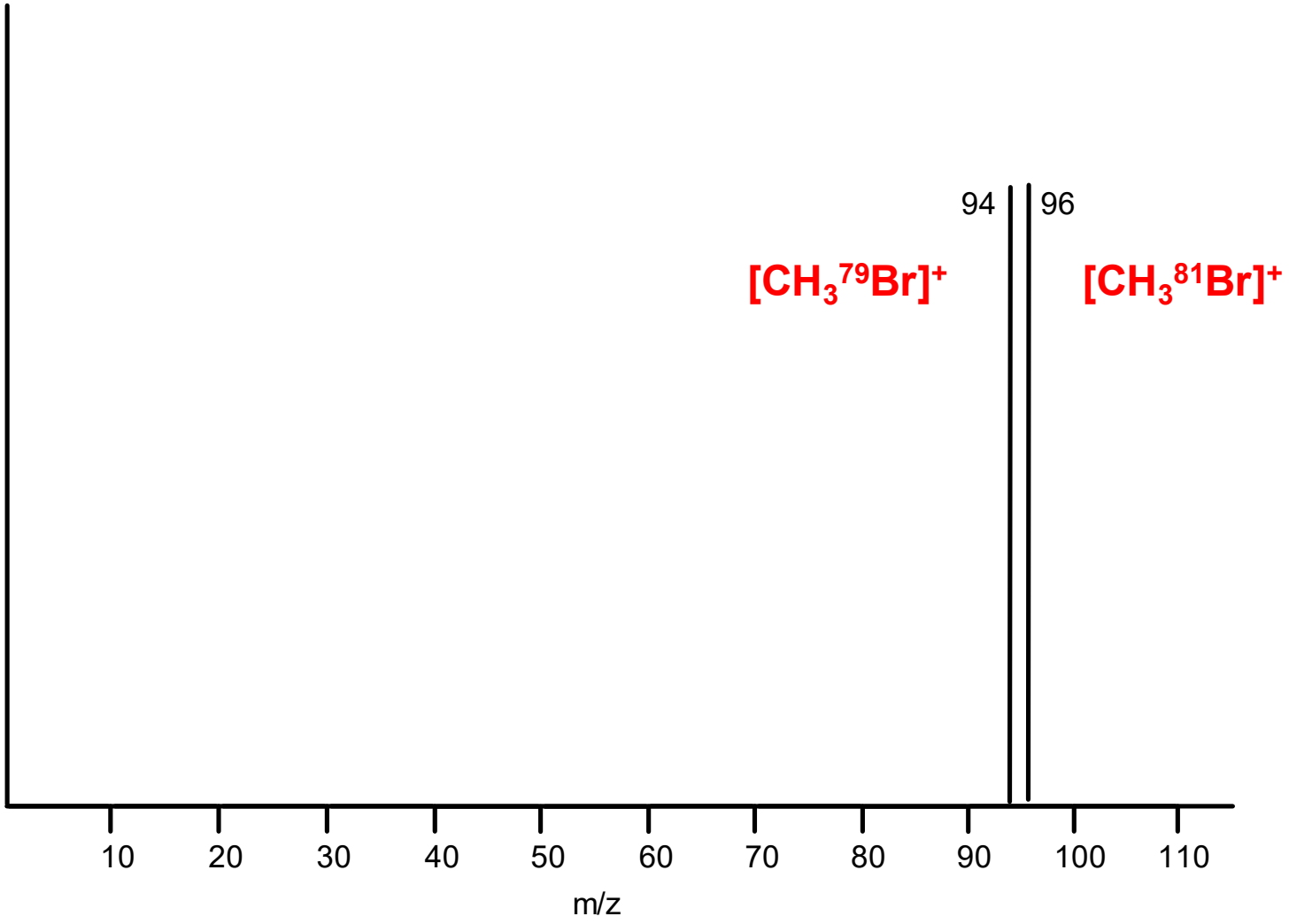
chlorine

Cl_2



bromomethane

CH_3Br



chloromethane

CH_3Cl