Chemistry 3.2
Molecular Spectroscopy

Introduction

Mass Spectrometry

Spectroscopy

- Spectroscopy uses the interaction of electromagnetic radiation with matter to obtain information about molecules (particularly organic compounds)
- There is a wide range of techniques and methods and we will only look at three of them
  - Mass Spectrometry **(MS)**
  - Infrared Spectroscopy **(IR)**
  - ^{13}C Nuclear Magnetic Resonance Spectroscopy **(^{13}C NMR)**

Mass Spectrometry (MS)

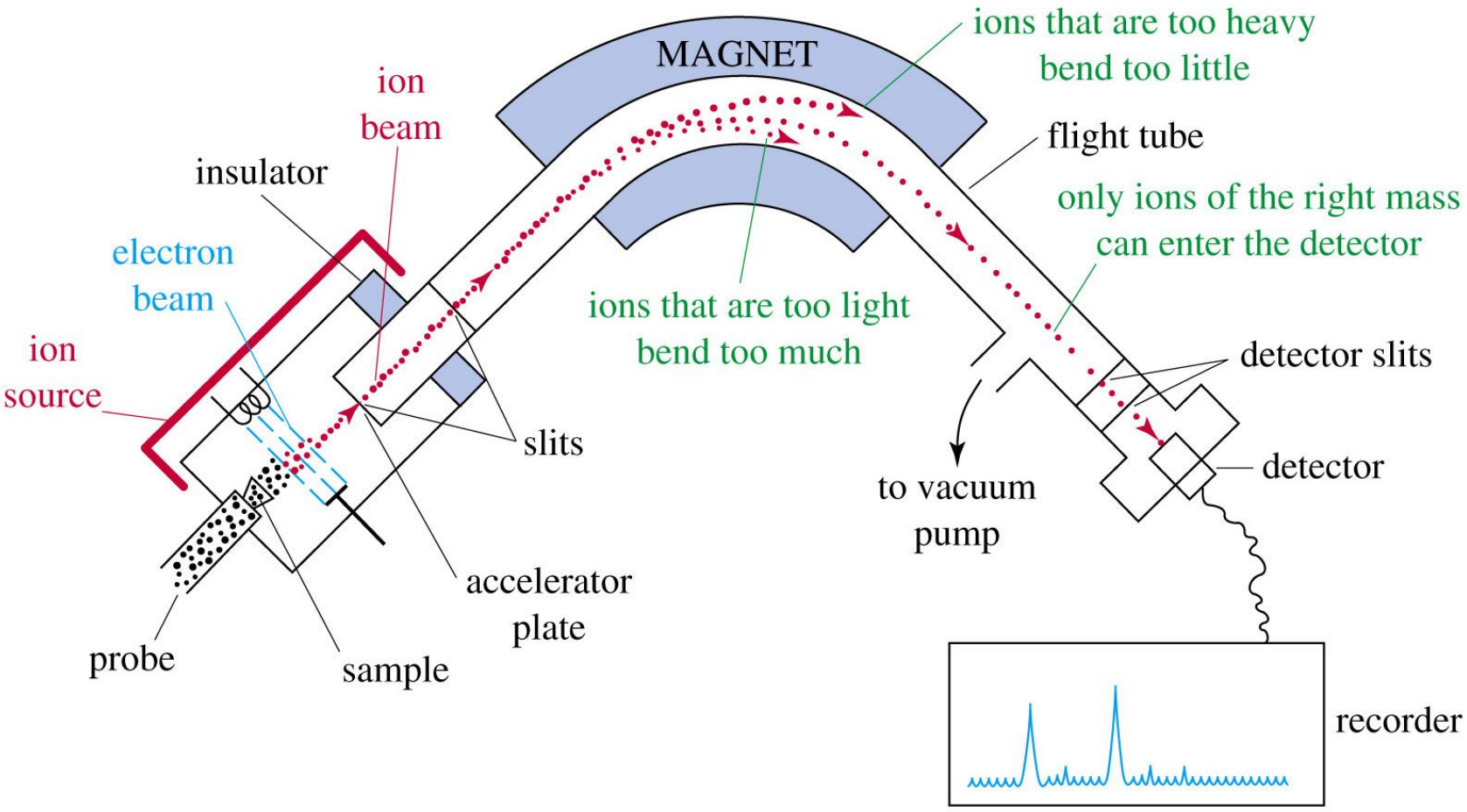
- This technique does not involve electromagnetic radiation
  - That's why it is spectrometry not spectroscopy
- The purpose for **MS** is to determine the **molecular mass** of the compound
- There are many different types of MS, but for level 3, we will focus on the technique called **Electron impact (EI MS)**

How does MS work?

- The sample is first vaporised then **bombarded by** a beam of high energy **electrons**

$$M + e^- \rightarrow M^{+\bullet} + 2e^-$$

- Ion produced will then be exposed under a magnetic field and their travel path will be altered depending on the strength of the magnetic field
- By altering the strength of the magnetic field, the mass of the ions that reach the detector can be recorded


MAGNET
ions that are too heavy
bend too little
ion
beam
flight tube
insulator
only ions of the right mass
can enter the detector
electron
beam
ions that are too light
bend too much
ion
source
detector slits
slits
detector
to vacuum
pump
accelerator
plate
probe
sample
recorder

Molecular ion

- $M^{+\bullet}$ ion, **the heaviest mass** corresponds to the **molecular mass (M_r)**
- However, **$M^{+\bullet}$ ion** is usually **unstable** and will **break down** to smaller ions to reach stability
- By **analysing** the **smaller ions**, chemist can gain good understanding of the nature of the sample molecule.

Nitrogen rule

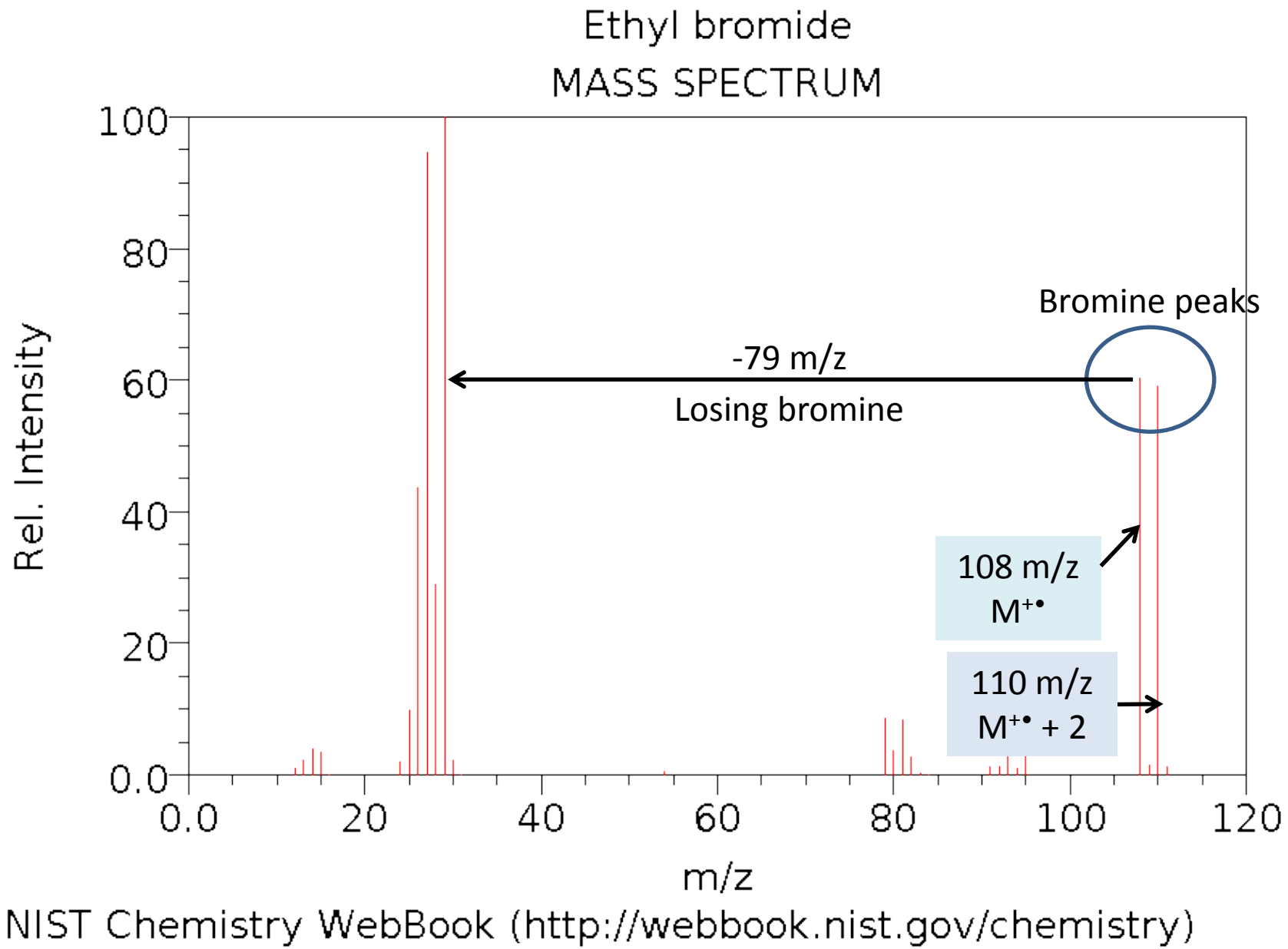
- A molecule with an **even molecular weight** must contain **no nitrogen** atoms or an **even number** of nitrogen atoms
- Another word, if the mass of $M^{+\bullet}$ is **odd number**, then an **odd number of N atoms** is present in the molecule

Bromine Isotopes

- Bromine- There are two major natural isotopes for bromine;

^{79}Br (50.7%) and ^{81}Br (49.3%)

- Therefore is an ion containing bromine, it will appear in two peaks that are two mass apart with similar height
- Also because Br is large and unstable, therefore there usually a peak in high intensity 79 mass unit below the $M^{+\bullet}$ peak



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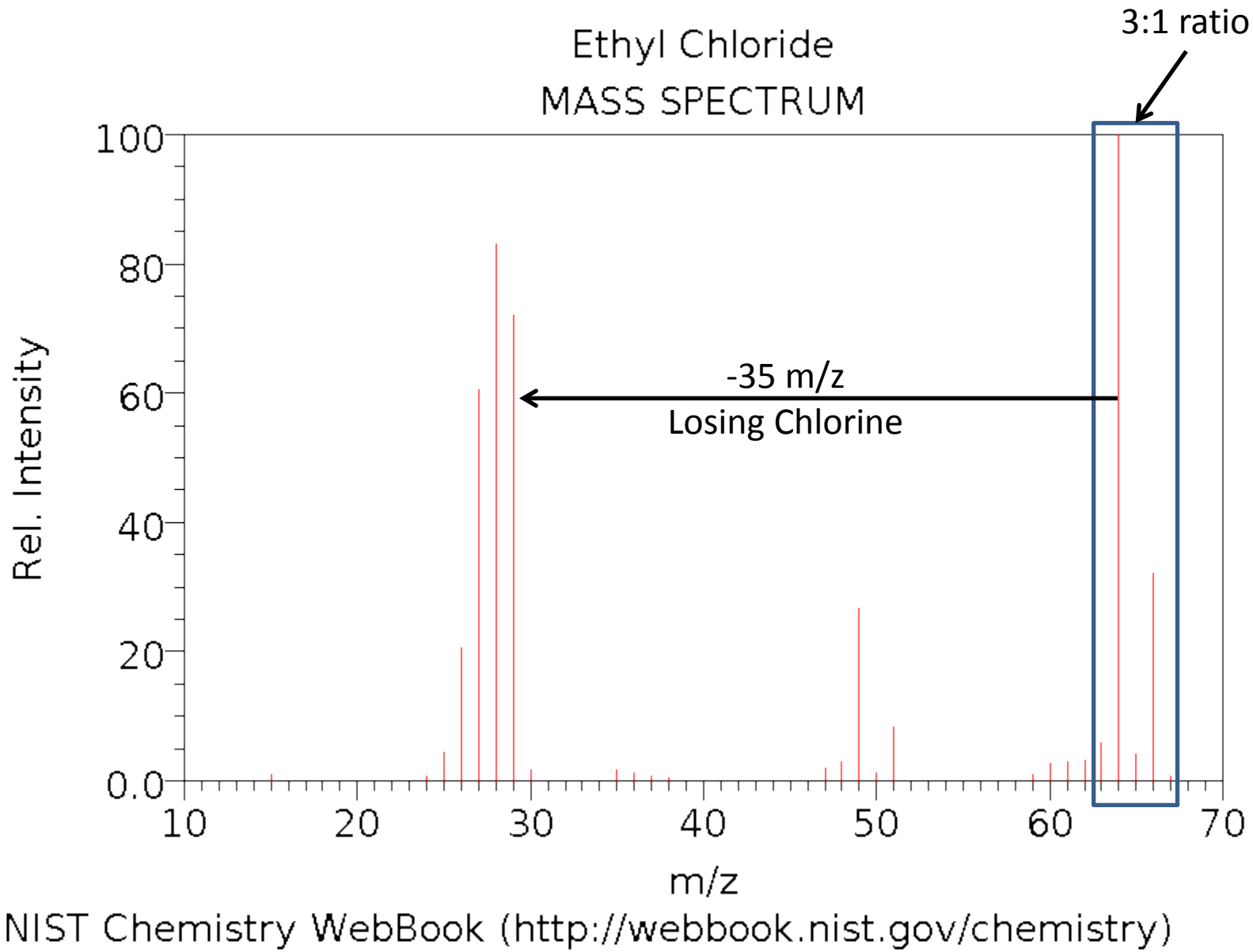
Chlorine Isotopes

- Similar to bromine, chlorine has two major isotopes

  ^{35}Cl (75.8%) and ^{37}Cl (24.2%)

- Therefore is an ion containing chlorine, it will appear in two peaks that are two mass apart with 3 : 1 height ratio
- Similar to Br, Cl is rather unstable and usually a peak with high intensity 35 mass unit below the $M^{+\bullet}$ peak



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