

CHN ELEMENTAL ANALYSIS

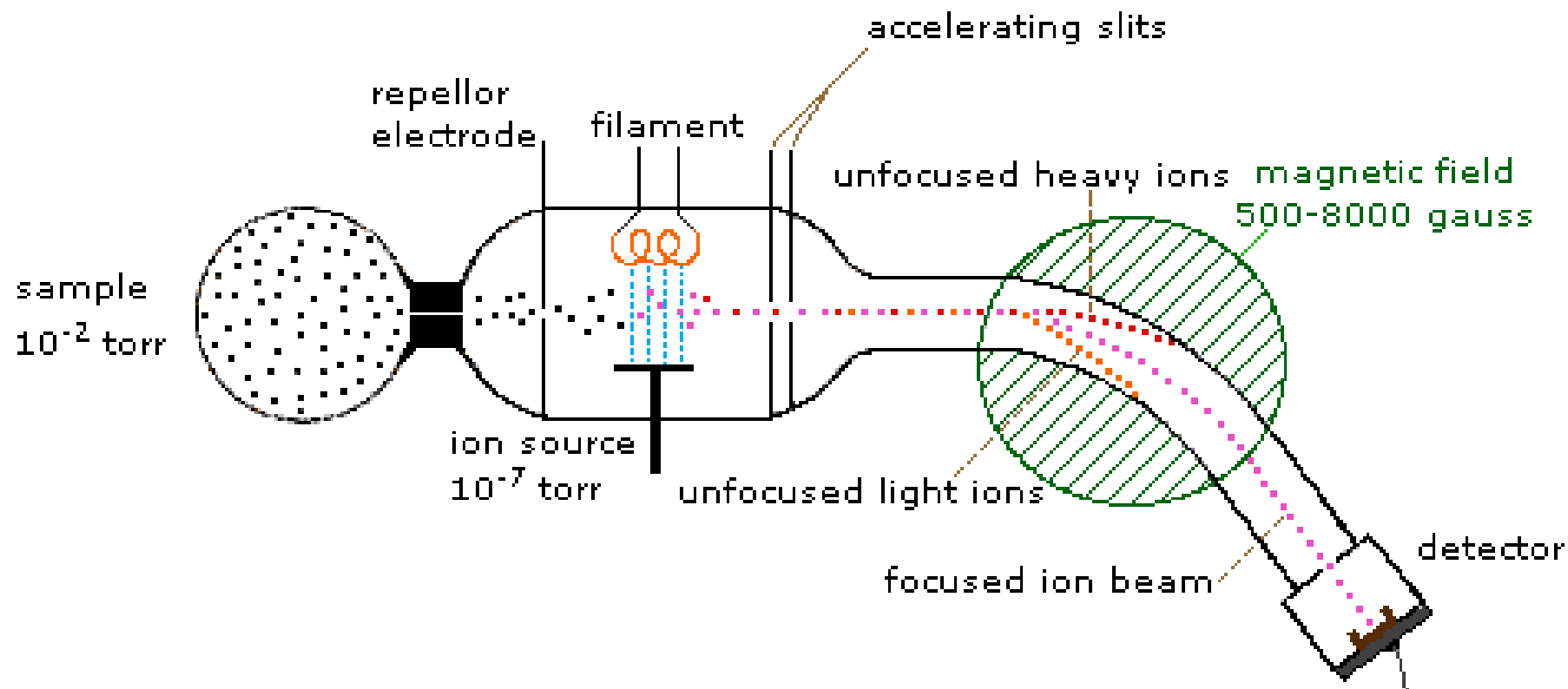
PRINCIPLE

The analytical method is based on the complete and instantaneous oxidation of the sample by “flash combustion”, which converts all organic and inorganic substances into combustion products. The resulting combustion gases pass through a reduction furnace and are swept into the chromatographic column by the carrier gas (helium), where they are separated and detected by a thermal conductivity detector (TCD), which gives an output signal proportional to the concentration of the individual components of the mixture.

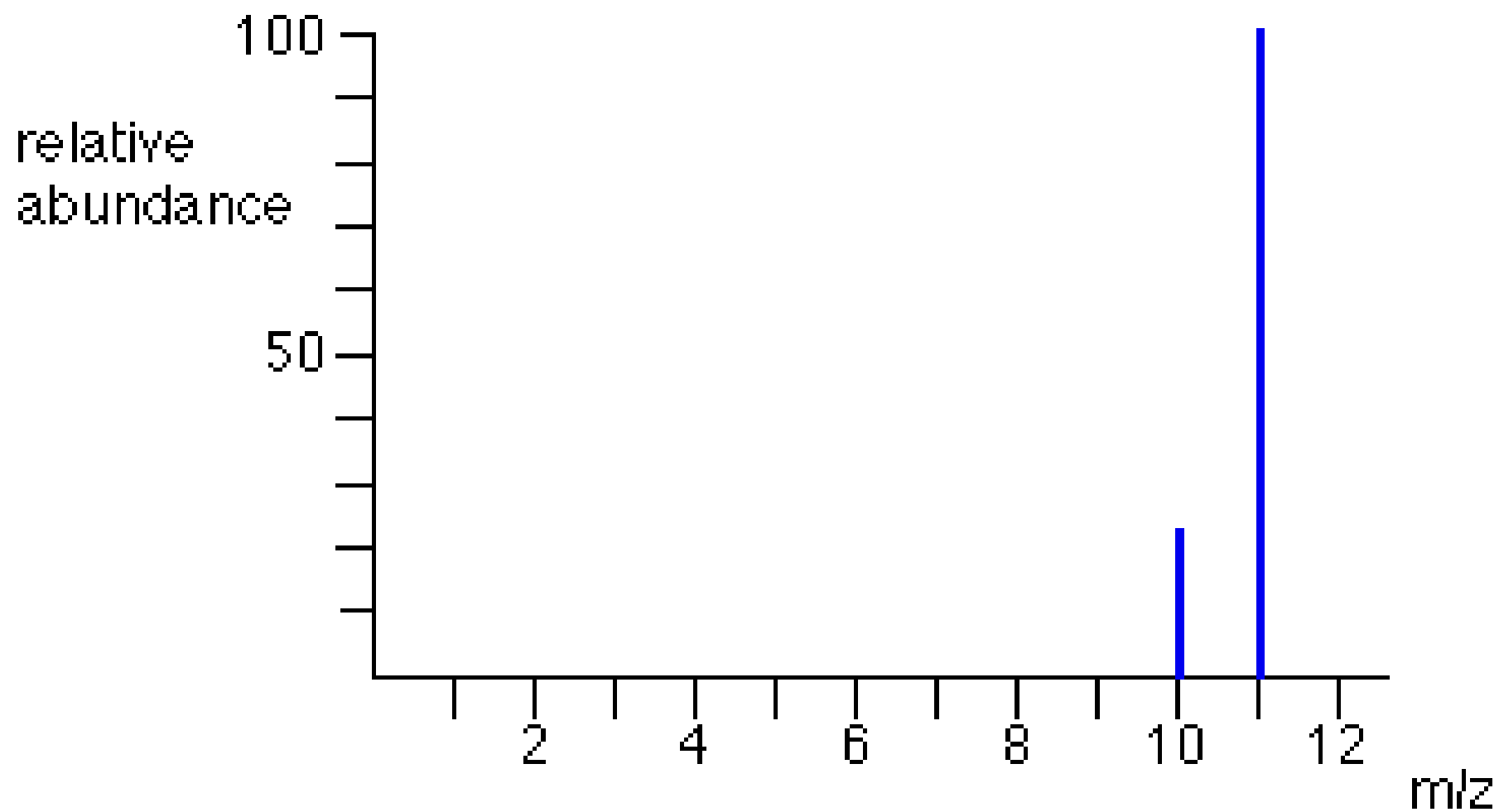
1. A 1.50 g sample of hydrocarbon undergoes complete combustion to produce 4.40 g of CO_2 and 2.70 g of H_2O . What is the empirical formula of this compound?

2. A 0.2500 g sample of a compound known to contain carbon, hydrogen and oxygen undergoes complete combustion to produce 0.3664 g of CO_2 and 0.1500 g of H_2O . What is the empirical formula of this compound?

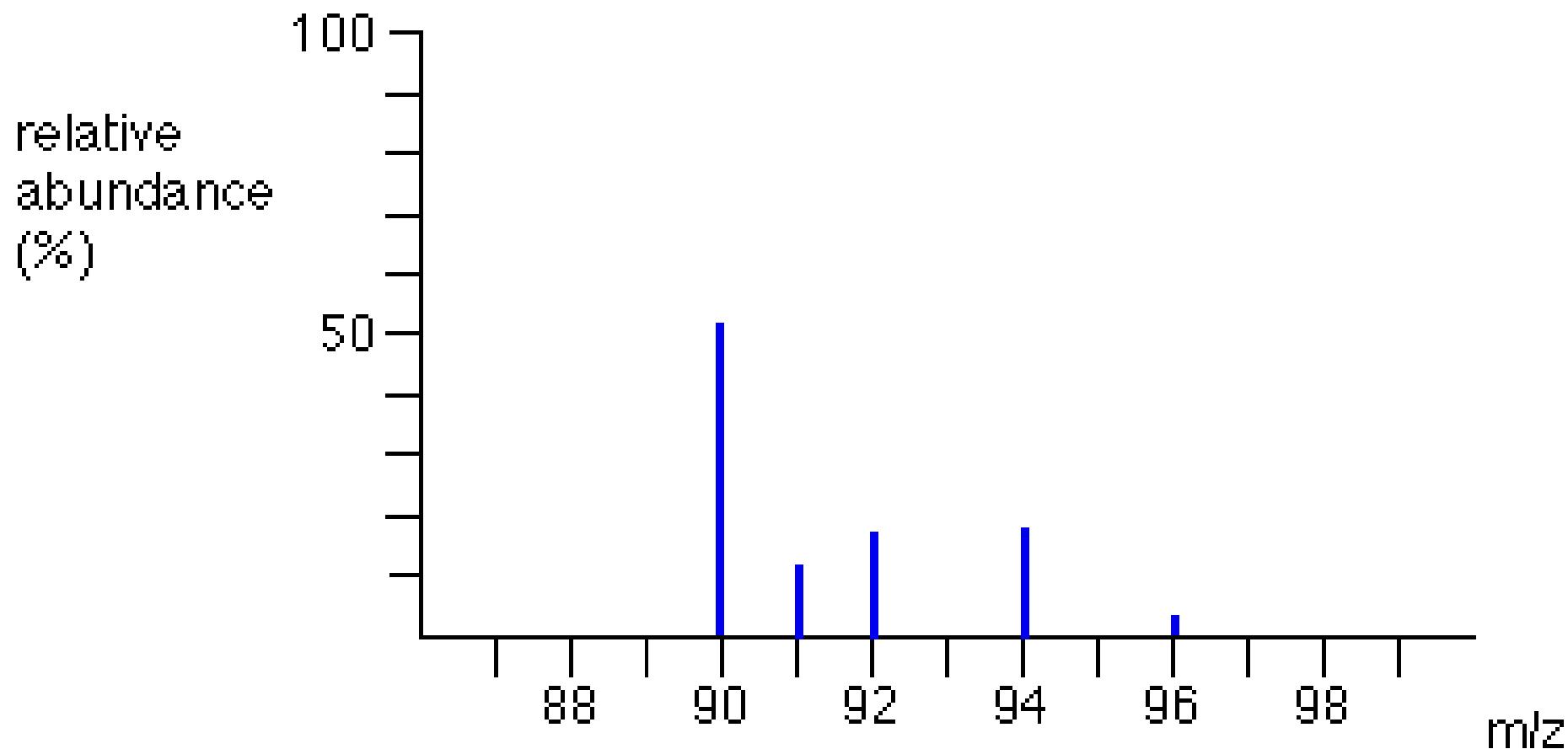
MASS SPECTROSCOPY



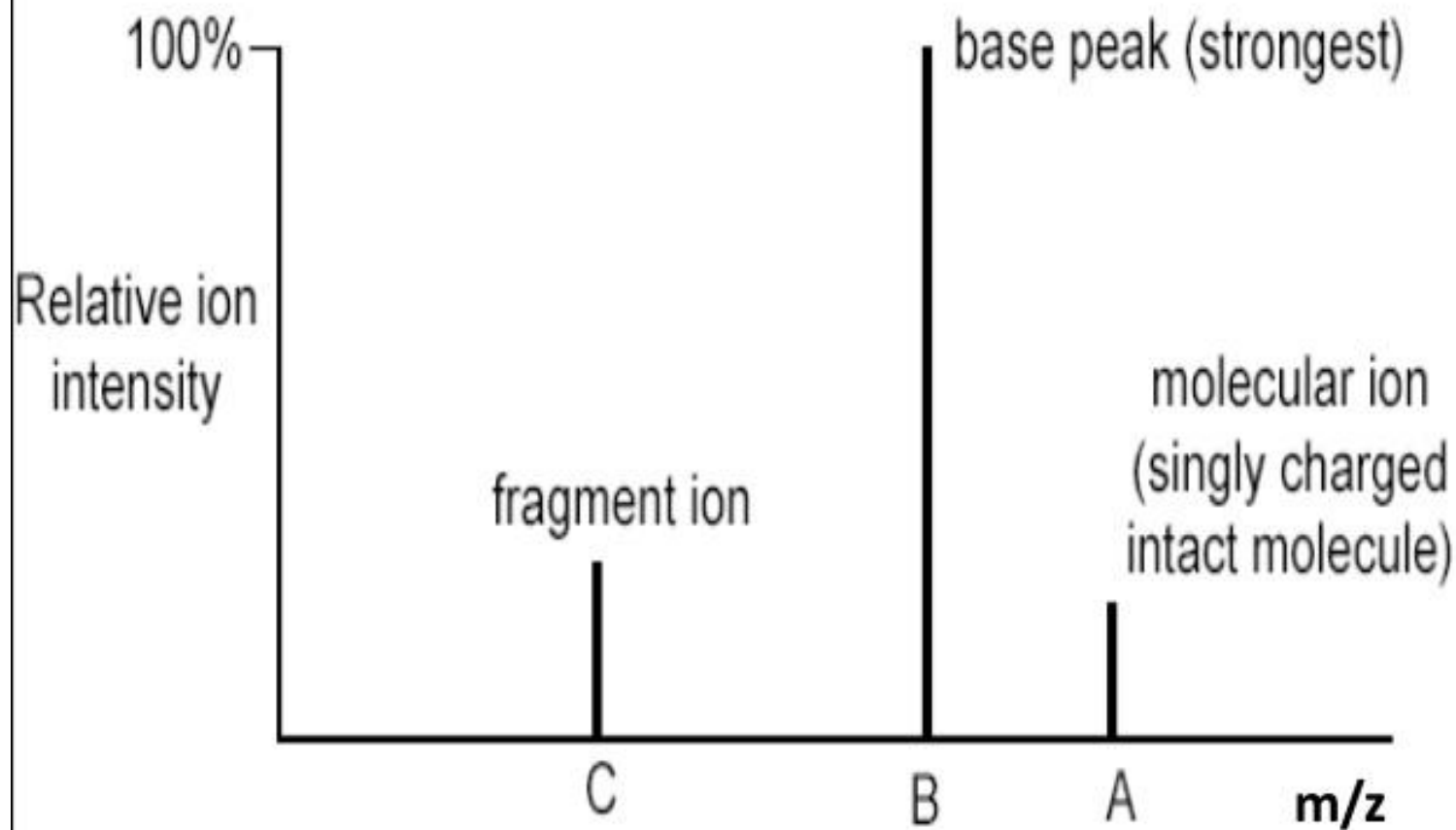
BORON



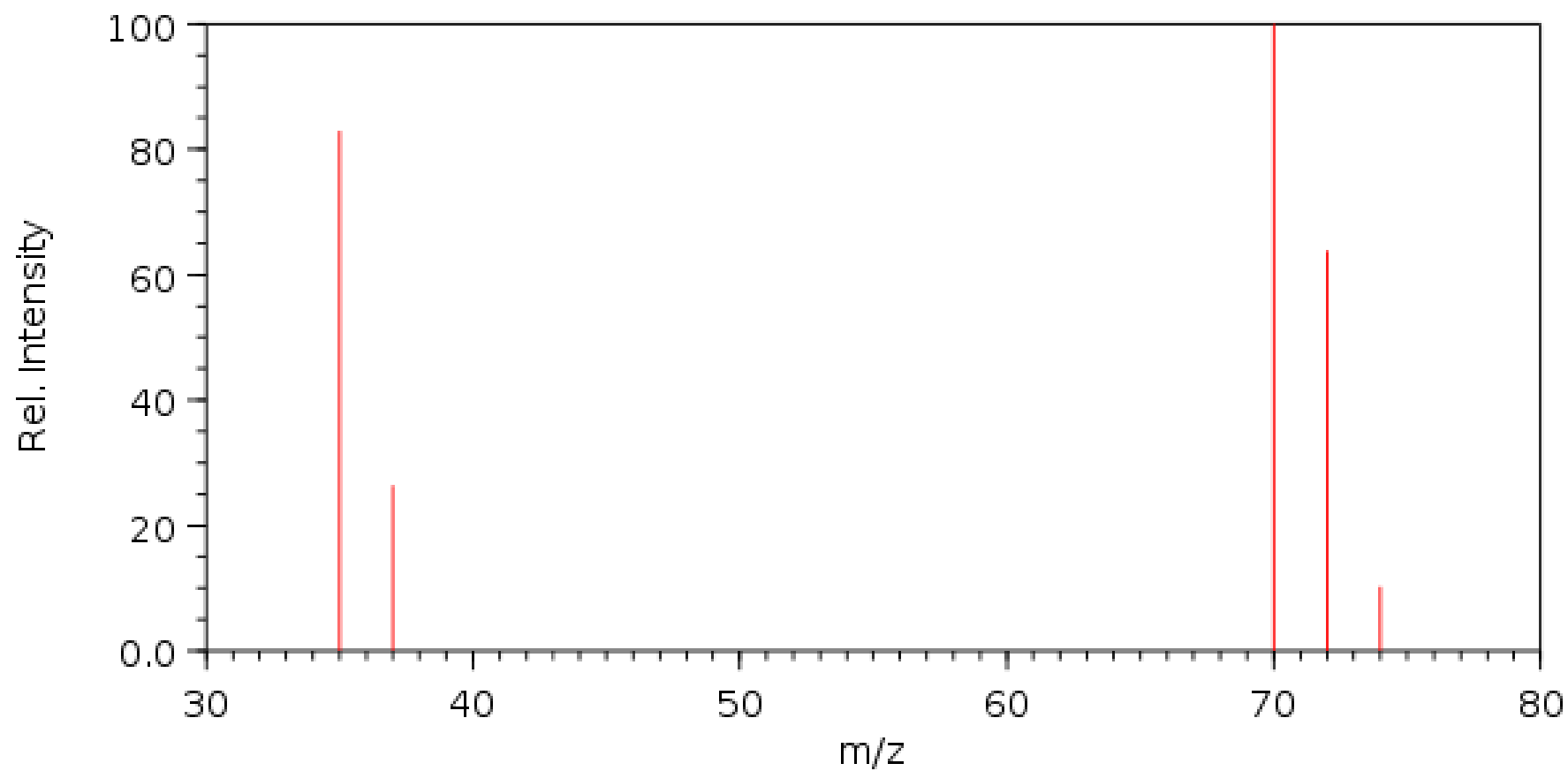
ZIRCONIUM



MASS SPECTRUM

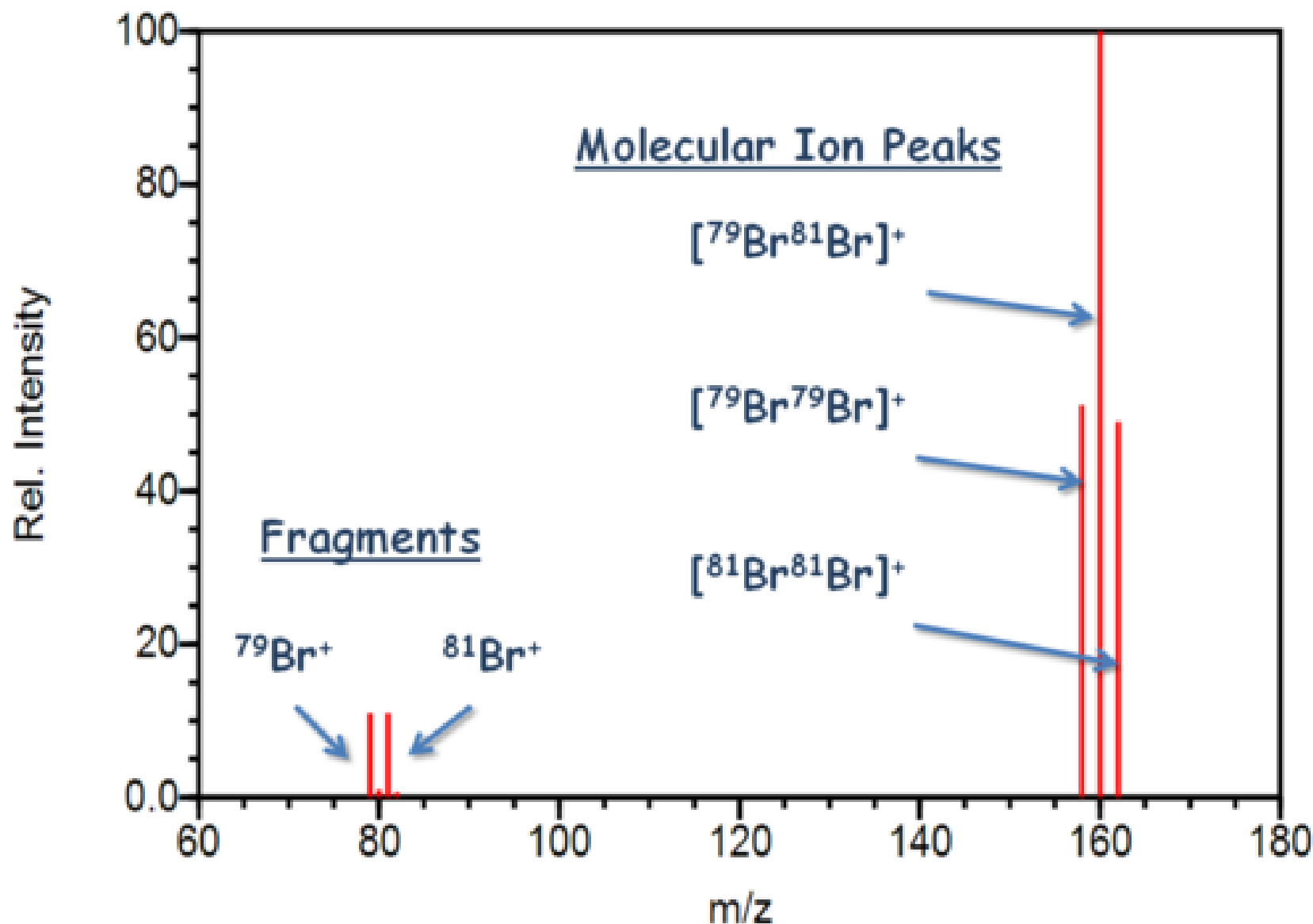


CHLORINE

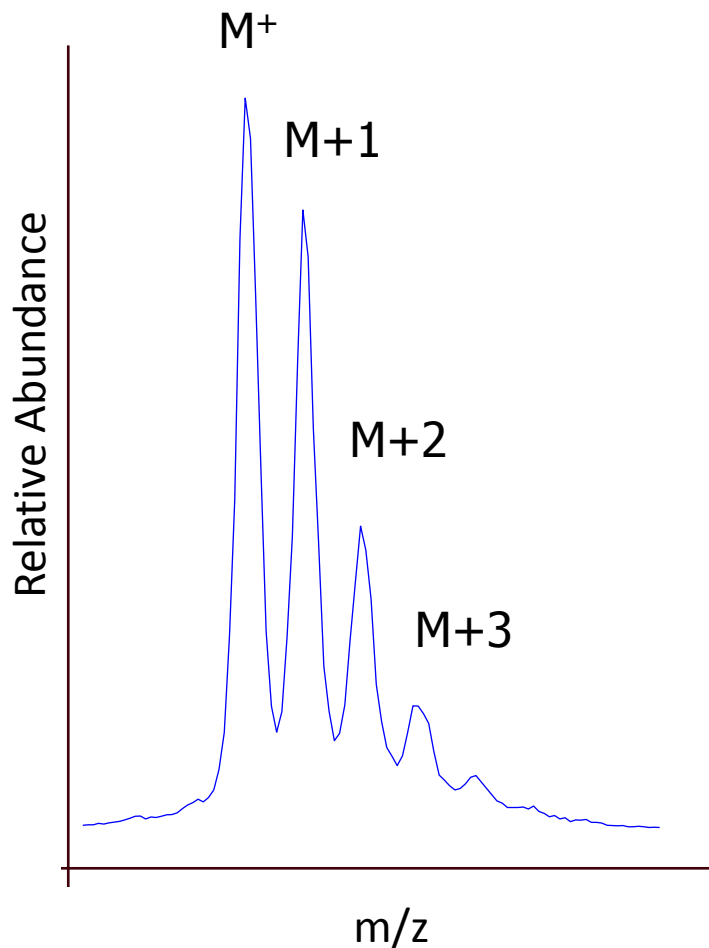


NIST Chemistry WebBook (<http://webbook.nist.gov/chemistry>)

BROMINE

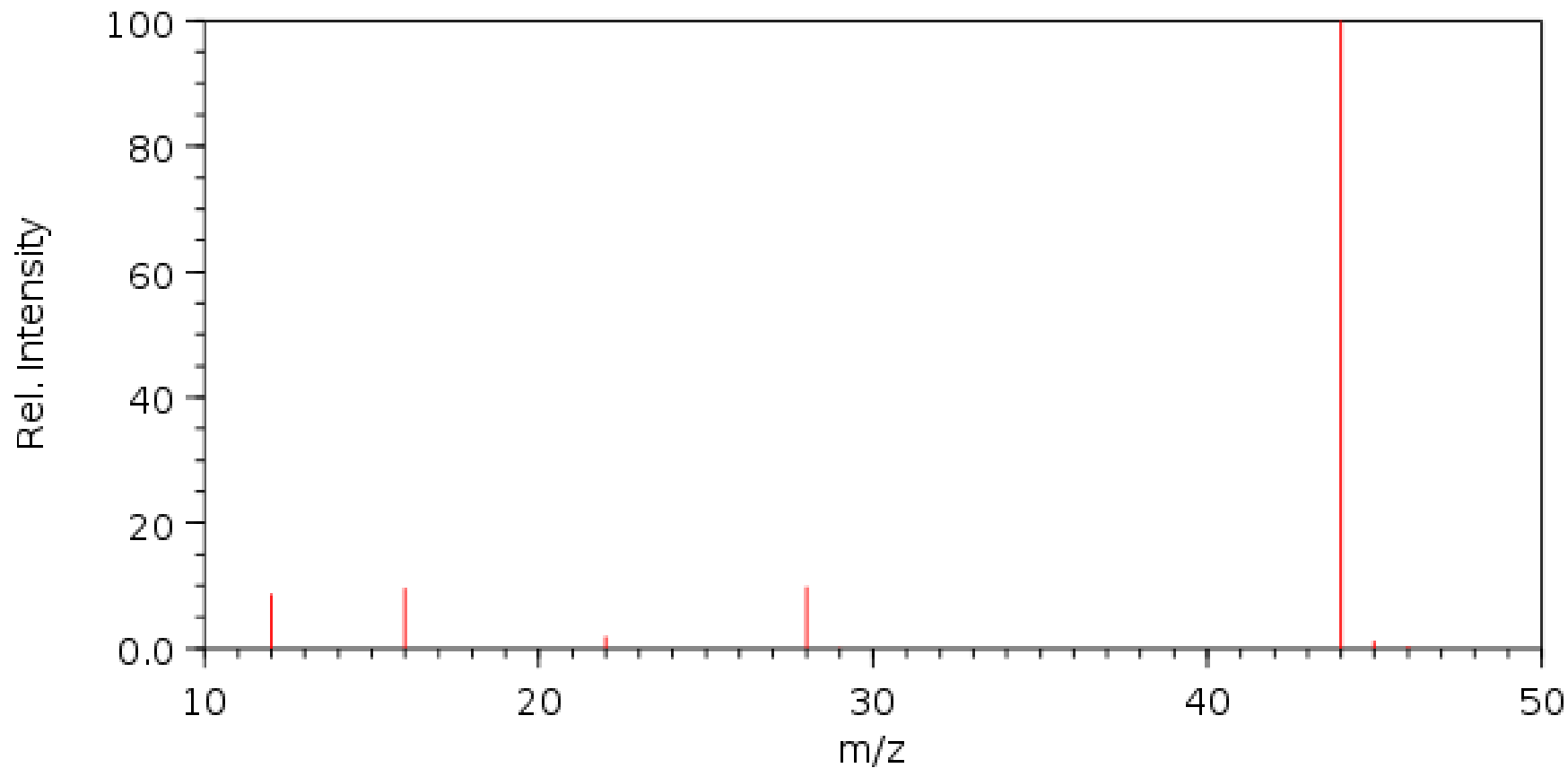


M+1 Peak



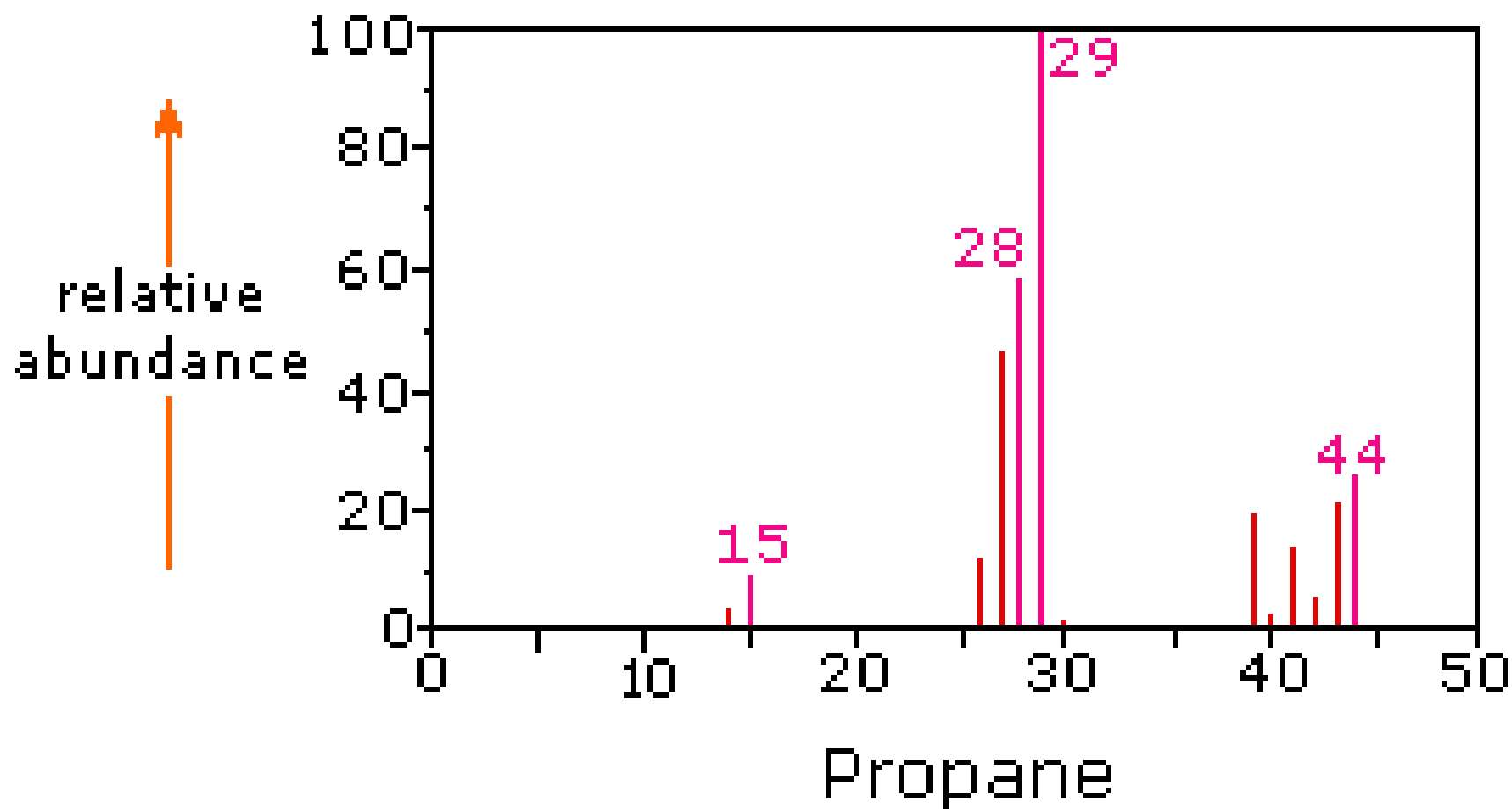
Here is the molecular ion peak(s) for a peptide containing 96 carbon atoms – note that the M+1 peak is almost as intense as the M⁺ peak

CARBON DIOXIDE



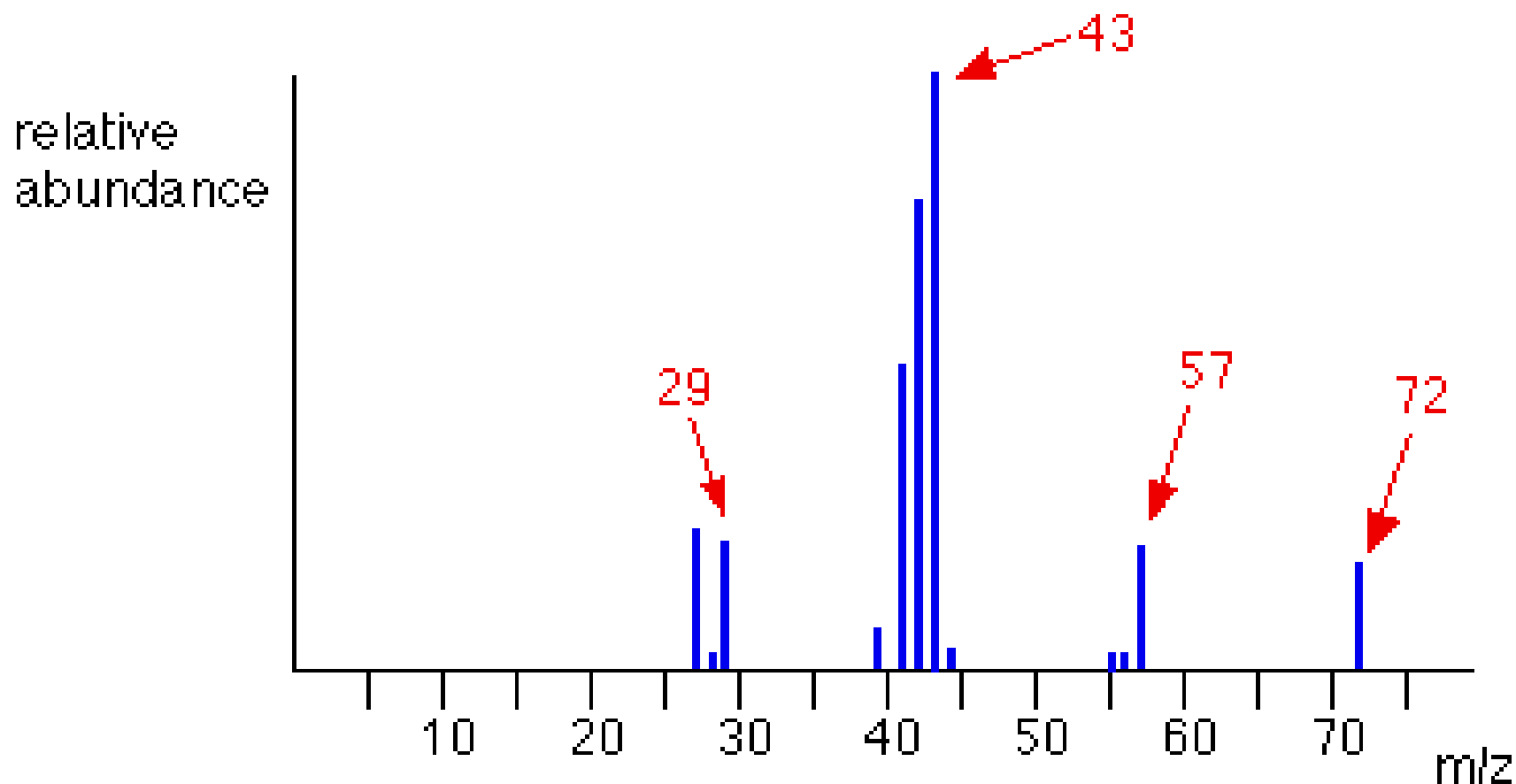
NIST Chemistry WebBook (<http://webbook.nist.gov/chemistry>)

PROPANE

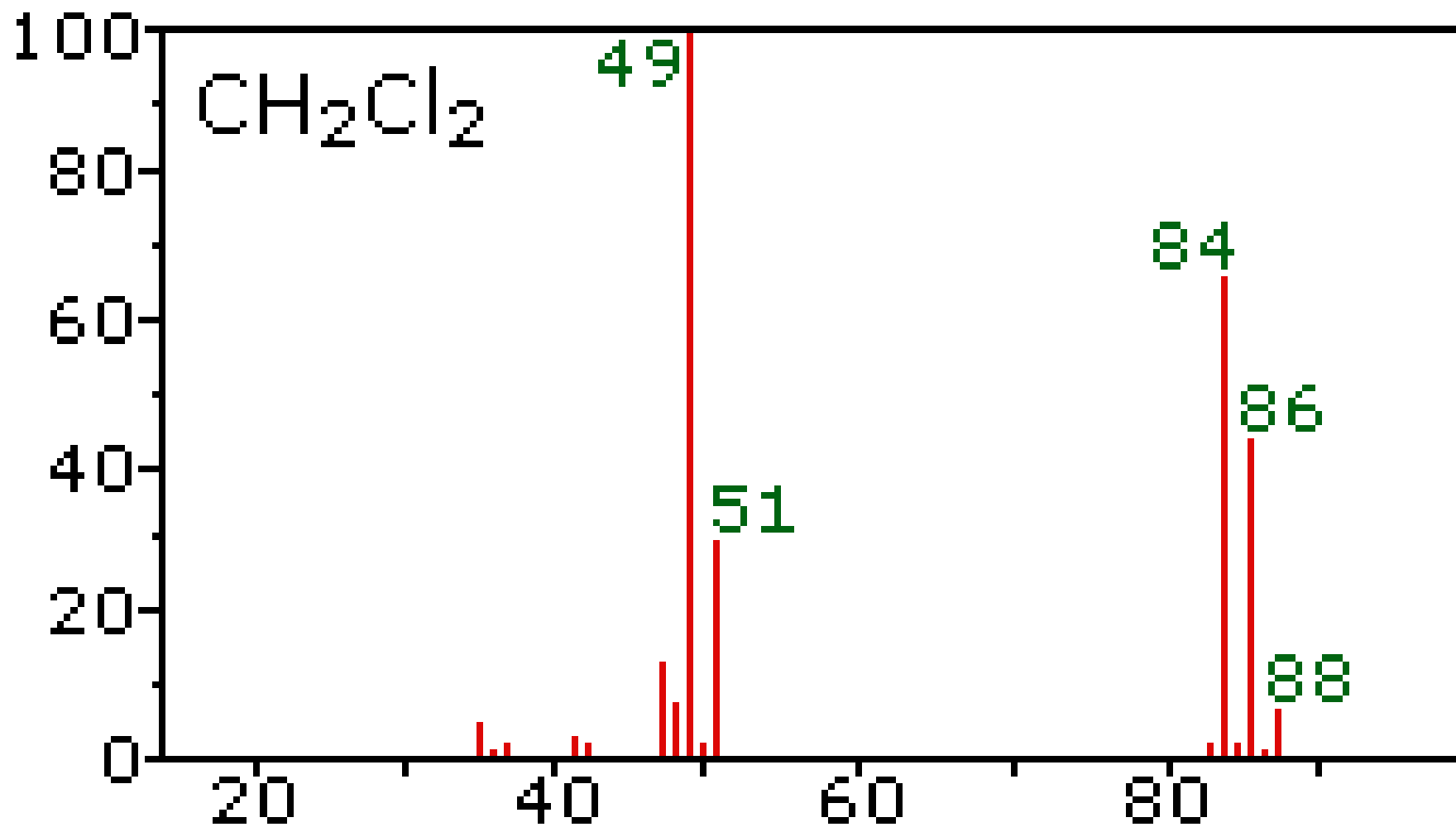


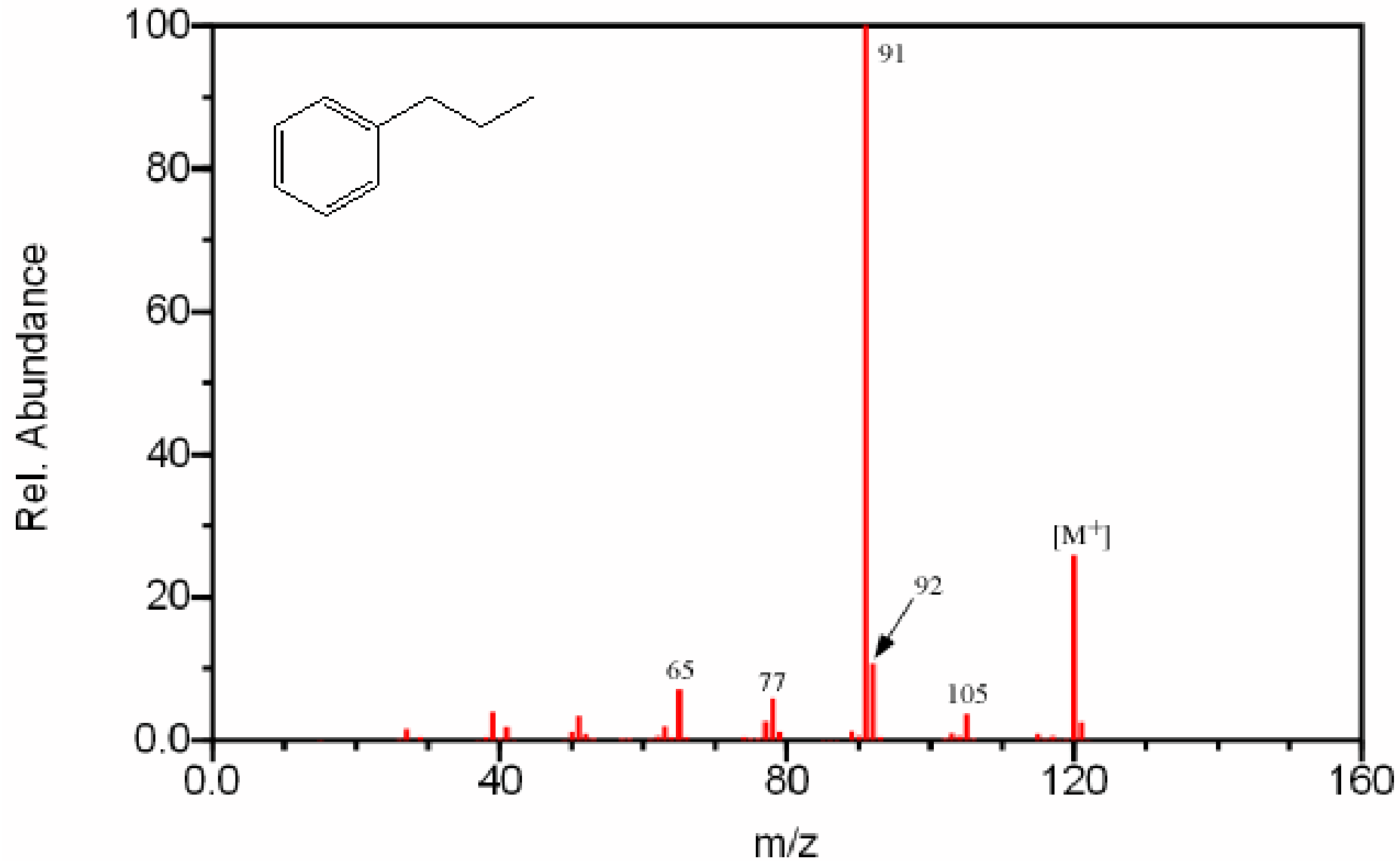
PENTANE

simplified mass spectrum of pentane - $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$

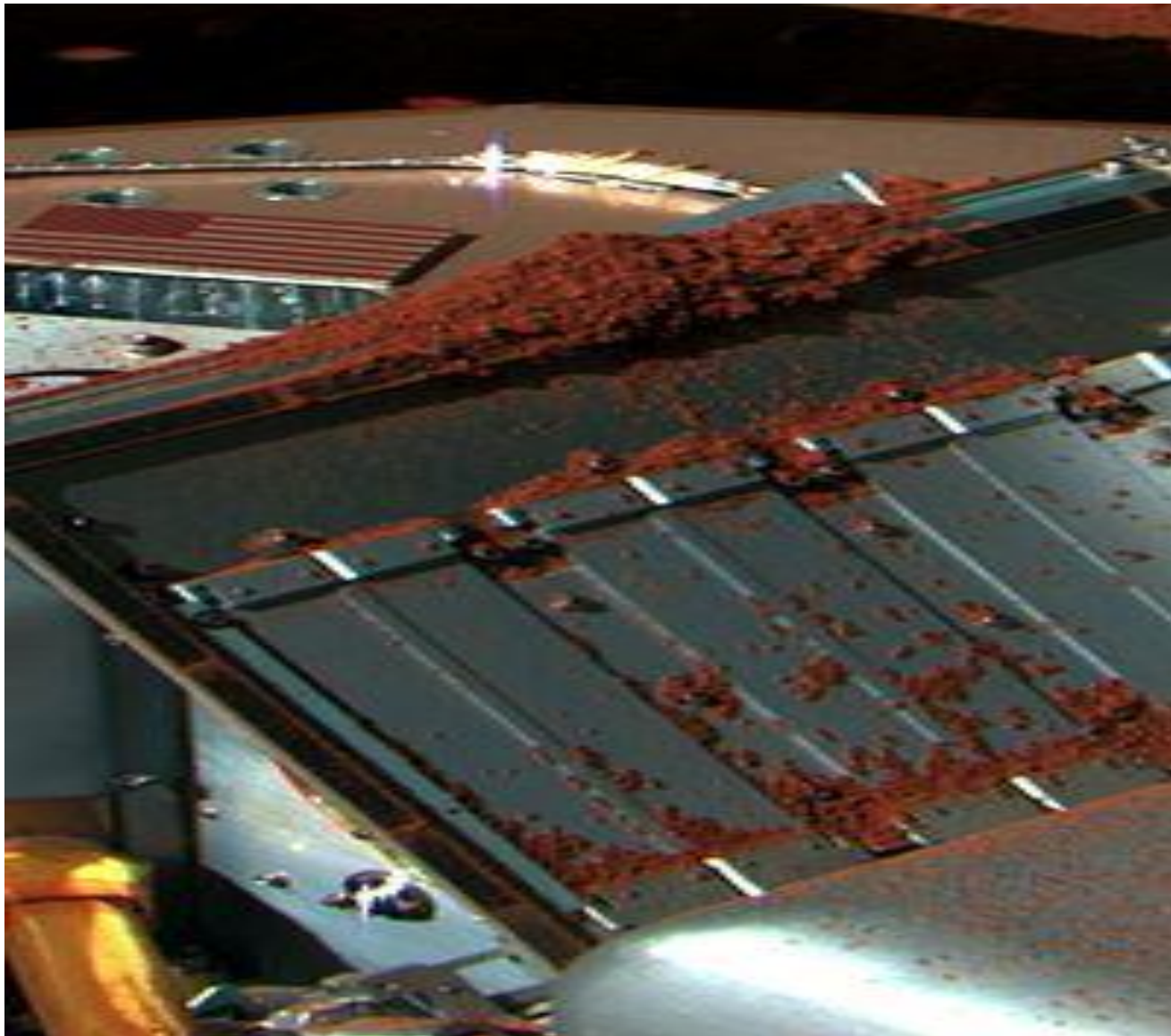


METHYLENE CHLORIDE





PHOENIX



PROBLEMS

1. An organic compound (**A**) is composed of carbon, hydrogen and nitrogen, with carbon constituting just over 60% of the mass. It shows a molecular ion at $m/z=112$ amu in the mass spectrum. Answer the following questions

- a) Write a plausible **Molecular Formula** for compound A
- b) How many **Rings + Double Bonds** must be present in compound A?

2. Another compound, **B**, composed only of carbon, hydrogen and oxygen, also shows a molecular ion at $m/z=112$ amu. Write a plausible **Molecular Formula** for compound B, assuming it has **three double bonds and no rings**.

3. The problem:

$m/z = 120$ (M; 100%),

$m/z = 121$ (9.8%), and

$m/z = 122$ (.42%)

4. An unknown substance shows a molecular ion peak at $m/z = 170$ with a relative intensity of 100. The $M + 1$ peak has an intensity of 13.2, and the $M + 2$ peak has an intensity of 1.00. What is the molecular formula of the unknown?

