

6.9: High vs Low Resolution

Two common categories of mass spectrometry are high resolution mass spectrometry (HRMS) and low resolution mass spectrometry (LRMS). Not all mass spectrometers simply measure molecular weights as whole numbers. High resolution mass spectrometers can measure mass so accurately that they can detect the minute differences in mass between two compounds that, on a regular low-resolution instrument, would appear to be identical.

The reason is because atomic masses are not exact multiples of the mass of a proton, as we might usually think.

- An atom of ^{12}C weighs 12.00000 amu.
- An atom of ^{16}O weighs 15.9949 amu.
- An atom of ^{14}N weighs 14.0031 amu.
- An atom of ^1H weighs 1.00783 amu.

As a result, on a high resolution mass spectrometer, 2-octanone, $\text{C}_8\text{H}_{16}\text{O}$, has a molecular weight of 128.12018 instead of 128. Naphthalene, C_{10}H_8 , has a molecular weight of 128.06264. Thus a high resolution mass spectrometer can supply an exact molecular formula for a compound because of the unique combination of masses that result.

- In LRMS, the molecular weight is determined to the nearest amu. The type of instrument used here is more common because it is less expensive and easier to maintain.
- In HRMS, the molecular weight in amu is determined to several decimal places. That precision allows the molecular formula to be narrowed down to only a few possibilities.

HRMS relies on the fact that the mass of an individual atom does not correspond to an integral number of atomic mass units.

? Exercise 6.9.1

Calculate the high-resolution molecular weights for the following formulae.

- $\text{C}_{12}\text{H}_{20}\text{O}$ and $\text{C}_{11}\text{H}_{16}\text{O}_2$
- $\text{C}_6\text{H}_{13}\text{N}$ and $\text{C}_5\text{H}_{11}\text{N}_2$

Answer

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