# Structural analysis (CH-314)

## Week 2

### Definitions & Formulas

1. Mass resolution:
$$R = \frac{m/z}{FWHM}$$
where FWHM is the full width at half maximum of the peak at m/z.
2. Resolving power:
$$RP = \frac{m/z}{\Delta m/z}$$
where $\Delta m/z$ is the minimum difference between $m/z$ of two peaks of the same intensity resolved with 10% valley. Assuming a gaussian peak shape, $\Delta m/z \approx 1.8 \cdot FWHM$, and therefore, $1.8 \cdot RP \approx R$.
3. Absolute mass accuracy is the difference between the measured and calculated $m/z$ values:
$$\Delta m/z \; = \; m/z_{exp} - m/z_{calc}$$
4. Relative mass accuracy is the absolute mass accuracy divided by the $m/z$ value it is determined for:
$$\delta m/m = \frac{\Delta m/z}{m/z}$$
5. Charge state (z) can be calculated using an isotopic distribution:
$$z \approx {}^{1}/_{\Delta({}^{m}/_{z})}$$
6. Average mass (m) can be calculated using an isotopic distribution:
$$M \approx \frac{\sum I_k \cdot m_k}{\sum I_k}$$
7. Charge state (z) and average mass (M) can be calculated from charge state distribution. If two protonated ions (two charge states of the same species) in a mass spectrum are separated by k peaks (in increasing order of m/z ratio) and have measured m/z ratios of $m_1$ and $m_2$, respectively, then the charge state of the first peak and the average mass can be determined as follows:
$$z = \frac{(k+1)(m_2 - m_p)}{(m_2 - m_1)}$$
$$M = z(m_1 - m_p)$$
8. Table of monoisotopic masses:

| Element | Monoisotopic mass (Da) |
|---|---|
| H | 1.007 825 |
| C | 12.000 000 |
| N | 14.003 074 |
| O | 15.994 915 |

9. Masses of an electron and of a proton:
$$m_e = 0.000549 \text{ Da}$$
$$m(H^+) = 1.007276 \text{ Da}$$