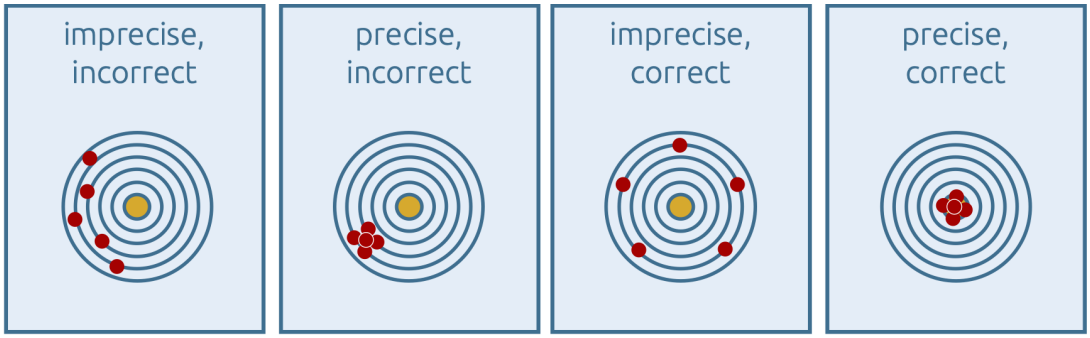
Referencing

The referencing of spectra is one of the most important steps in the pre-processing of spectra, as the aim is to measure precisely and correctly. Once spectra have been recorded in insufficient quality or incorrectly referenced, improvement is not possible even with mathematical methods. The results of chemometric and machine learning methods also become invalid if gross errors have already occurred in the spectra recording.



Precision and correctness

All electronic detectors have a noise that is thermally or electronically induced. This noise is often referred to in the respective software as 'background', 'dark image', 'detector reference' or 'dark reference'. This noise is subject to a drift that depends on the (mains) voltage and the ambient or detector temperature. If this background correction does not take place, the measurements will be imprecise. In some cases, the background of the device, i.e. the characteristics of the radiation source and all optical components, are also included in the background measurement.

In other cases, the measurement of the device background can also be found separately in the measurement of the 'white reference' or simply 'reference measurement'. For all reflection methods, it is advisable to measure a reflection standard with known reflection (as a rule, standards with consistently high, practically complete (100 %) reflection over the entire spectral range are used). In practice, gold, aluminum, silicon or PTFE standards are used for this purpose. There are certified white standards whose absorptions/reflections are precisely known. For transmission measurements, the substrate or solvent can be removed directly from the sample spectrum in this way. If the measurement of the device background or reference is omitted, incorrect spectra are obtained which are not comparable. In general, referencing can be calculated in the spectra data as follows (I Intensity):

$$I_\lambda = \frac{(I_{\lambda,\ measured} - I_{\lambda,\ dark\ reference})}{I_{\lambda,\ white\ reference}}$$

Wavelength referencing should also be carried out from time to time. Certified wavelength standards based on rare earths, for example, are available for this purpose, but materials with a known spectrum (stored in a database or literature) can also be used as a wavelength reference. Incorrect wavelength assignment also leads to incorrect spectra. For MCT detectors, spectral

interpolation of the faulty pixels of the detector is also necessary.

Revision #4
Created 7 August 2024 21:00:03 by Admin
Updated 10 August 2024 11:15:19 by Admin