

Error analysis in the UV-vis experiment

1. From the standard line you obtain the slope at each measured wavelength, which is equal to the extinction coefficient, ϵ_λ . Each extinction coefficient has an associated standard error s_e that comes from the linear least square fitting. When reporting the extinction coefficient in a table we would like to see the error (usually in parentheses to indicate that it is a standard error and not a 95% confidence limit).
2. There is an error associated with the measurement of the absorbance. This can be estimated from replicates (3 or more) or from an analysis of the noise on the spectra. To obtain the noise on the spectra you would select a flat region of the spectrum and then determine the width of the Gaussian noise by taking the average and standard deviation.
3. The equation for the calculation of concentration uses two equations and two unknowns, c_1 and c_2 .

$$\begin{aligned}A_1 &= \epsilon_{11}c_1 + \epsilon_{12}c_2 \\A_2 &= \epsilon_{21}c_1 + \epsilon_{22}c_2\end{aligned}$$

Therefore,

$$c_1 = \frac{\epsilon_{22}A_1 - \epsilon_{12}A_2}{\epsilon_{11}\epsilon_{22} - \epsilon_{12}\epsilon_{21}}$$

$$c_2 = \frac{\epsilon_{11}A_2 - \epsilon_{21}A_1}{\epsilon_{11}\epsilon_{22} - \epsilon_{12}\epsilon_{21}}$$

The error propagation of error in this equation is

$$\sigma(c_1) \approx \frac{\sqrt{(\epsilon_{22})^2\sigma(A_1)^2 + (\epsilon_{12})^2\sigma(A_2)^2 + (A_1)^2\sigma(\epsilon_{22})^2 + (A_2)^2\sigma(\epsilon_{12})^2}}{\epsilon_{11}\epsilon_{22} - \epsilon_{12}\epsilon_{21}}$$

$$\sigma(c_2) \approx \frac{\sqrt{(\epsilon_{11})^2\sigma(A_2)^2 + (\epsilon_{21})^2\sigma(A_1)^2 + (A_2)^2\sigma(\epsilon_{11})^2 + (A_1)^2\sigma(\epsilon_{21})^2}}{\epsilon_{11}\epsilon_{22} - \epsilon_{12}\epsilon_{21}}$$