Multi-energy calibration (MEC) applied to laser-induced breakdown spectroscopy (LIBS)

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Consider the following relationships for two standards:

$$I(\lambda_i)^{Sam+Std} = m(C^{Sam} + C^{Std}) \quad \textbf{\textit{(eqn. 1)}}$$

$$I(\lambda_i)^{Sam} = mC^{Sam} \quad \textbf{\textit{(eqn. 2)}}$$

where $I(\lambda_i)^{Sam}$ ***and*** $I(\lambda_i)^{Sam+Std}$ ***are the instrument responses at a certain wavelength (i) for pellet 1 and pellet 2, respectively; m is a proportionality constant; and*** C^{Sam} ***and*** C^{Std} ***are the analyte concentrations in the sample and in the standard added to sample, respectively. If one considers the same instrumental conditions, and the same matrix since both***

solutions have 50% m m^{-1} sample, Eqs. (1) and (2) may be combined (Eq. (3)) and rearranged (Eq. (4)):

$$\frac{I(\lambda_i)^{Sam}}{C^{Sam}} = \frac{I(\lambda_i)^{Sam + Std}}{C^{Sam} + C^{Std}} \quad \textit{(eqn. 3)}$$

$$I(\lambda_i)^{Sam} = I(\lambda_i)^{Sam + Std}\left[\frac{C^{Sam}}{C^{Sam} + C^{Std}}\right] \quad \textit{(eqn. 4)}$$

By plotting $I(\lambda_i)^{Sam}$ (from pellet 2) on the y-axis vs. $I(\lambda_i)^{Sam + Std}$ (from pellet 1) on the x-axis, with instrument responses recorded at several different wavelengths (λ_1, λ_2, …, λ_n), the slope of that plot's linear regression will be:

$$Slope = \frac{C^{Sam}}{C^{Sam} + C^{Std}} \quad \textit{(eqn. 5)}$$

Because C^{Std} is known, the analyte concentration in the sample can then be easily determined by rearranging Eq. (5):

$$C^{sample} = \frac{slope \cdot C^{Standard}}{(1 - slope)} \quad \textit{(eqn. 6)}$$

Reference 32 of the manuscript: A. Virgilio, D. A. Gonçalves, T. McSweeney, J. A. Gomes Neto, J. A. Nobrega and G. L. Donati, Anal. Chim. Acta, 2017, 982, 31-36.

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