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
Chemistry

Orthogonal Signal Correction -- Partial Least Squares Method for Simultaneous Spectrophotometric Determination of Nickel, Cobalt, and Zinc

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Abstract: The simultaneous determination of nickel, cobalt, and zinc mixtures by spectrophotometric method is a difficult problem in analytical chemistry, due to spectral interferences. By multivariate calibration methods, such as partial least squares (PLS) regression, it is possible to obtain a model adjusted to the concentration values of the mixtures used in the calibration range. Orthogonal signal correction (OSC) is a preprocessing technique used for removing the information unrelated to the target variables based on constrained principal component analysis. OSC is a suitable preprocessing method for partial least squares calibration of mixtures without loss of prediction capacity using spectrophotometric method. In this study, the calibration model is based on absorption spectra in the 450-600 nm range for 21 different mixtures of nickel, cobalt, and zinc. Calibration matrices were formed from samples containing 0.025-0.55, 0.025-0.50, and 0.025-0.50 $\mu\text{g mL}^{-1}$ for nickel, cobalt, and zinc, respectively. The RMSEP for nickel, cobalt, and zinc with OSC and without OSC were 0.0127, 0.0101, and 0.0145, and 0.0045, 0.0049, and 0.0058 $\mu\text{g mL}^{-1}$, respectively. This procedure allows the simultaneous determination of nickel, cobalt, and zinc in synthetic and real samples and good reliability of the determination was proved.

Key Words: Nickel, cobalt, zinc, determination, spectrophotometric, PLS, OSC

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