K-edge X-ray Absorption Near Edge Structure (XANES) Analysis Methodology: A Case Study on Thiophenic Sulfur Compounds

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The objective of this project is to determine the most efficient and accurate method, among peak fitting analysis (PFA), linear combination fitting analysis (LCF), and principal components analysis (PCA), of predicting specific compositions of unknown compounds given a set of raw X-ray Absorption Near Edge Structure (XANES) data. By understanding how to best interpret data from synchrotrons, currently an open problem, the researchers can better predict the chemical makeup of unknown materials. This project was executed with three different computational tools -- the computer language R, Microsoft Excel's built-in Solver, and Athena for XAS analysis. Each data set's background noise was subtracted and normalized using R. They were then processed through original LCF, PFA, and PCA programs in R, Excel, and Athena, respectively. Specifically, the LCF code utilized four interpolation methods, PFA used Lorentzian peak calculation and arctangent step functions, and PCA isolated four related components. Each resulting model was evaluated against the original unknown data using the residual sum of squares (RSS) method. RSS results indicated that the LCF method using local regression interpolation had the lowest error reading. The most accurate models consistently resulted from LCF calculations, which corroborates the popularity of LCF methods in the XANES research community. Outside of LCF, PFA was calculated to be marginally more accurate than PCA. However, the problem of XANES analysis remains an open one, and as this analysis was done on one specific set of sulfur compounds, it is not an absolute indication of the superiority of LCF.

Awards Won:

American Statistical Association: Certificate of Honorable Mention