Molecular speciation of microparticles
: application of pattern recognition techniques to laser microprobe mass spectrometric data

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Attempts were made to enhance the ability of laser microprobe mass spectrometry (LAMMS) to identity molecular species in individual microparticles by applying pattern recognition methods. Principal component analysis (PCA) and canonical discriminat analysis were applied to LAMMS data for nickel-containing environmental particles. Detailed comparison of the two statistical methods demonstrated the utility oof PCA. The successful application was highly dependent on the use of approximate spectral normalization and feature extraction techniques prior to PCA. Although the test system involved only a small number of standard compounds, the LAMMS data were complicated by the effects of intra-particle heterogeneity common to environmental samples and by instrumental limitations. Pattern recognition techniques provided more accurate quantitative assignments of molecular species than were available by qualitative inspection of characteristic cluster ions or by simple spectral subtraction to compare particle data with a library compounds. Results were substantiated by comparison with bulk analysis studies using wet chemical techniques.

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