

Quantitative Analysis Using Raman Spectroscopy

RA-TN05

ELEMENTAL ANALYSIS

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Rapid, Non-Destructive Analysis of Liquid and Solid Samples

Abstract

Raman spectroscopy is well known as a powerful analytical method for qualitative chemical analysis. Less well known is that under certain conditions Raman spectroscopy can also be an effective method for quantitative analysis. Here we demonstrate that capability for quantitative analysis with concentrated aqueous solutions of guanidine hydrochloride.

Keywords

Raman spectroscopy, quantitative analysis, peak fitting, guanidine hydrochloride, MacroRAM, macroRaman

Introduction

Raman spectroscopy is generally recognized as a powerful analytical technique that is used to study the chemical composition of materials within the context of qualitative analysis. Nevertheless, under certain conditions Raman spectroscopy can also be an effective method for quantitative analysis in both liquid and solid samples.

With liquid samples, Raman spectroscopy allows one to perform rapid, non-destructive, quantitative analysis with minimal sample preparation. Quantitative analysis can be performed on solutions of high concentration without the need for dilution. Raman spectroscopy provides direct chemical information about the analyte in addition to quantitative information. Furthermore, the development of compact, low-cost, benchtop Raman spectrometers has made it possible to perform such analyses in a variety of locations from an undergraduate chemistry lab to an industrial environment.

Method

Raman spectra were measured using the MacroRAM Raman spectrometer from HORIBA Instruments Inc. of guanidine hydrochloride dissolved in water, which is a commonly used denaturant, with systematically varying concentrations. Each spectrum was collected using 785 nm excitation over 2 seconds and 2 accumulations. Spectra were collected from 3 separately prepared samples for each concentration in order to report the standard deviation.

Results

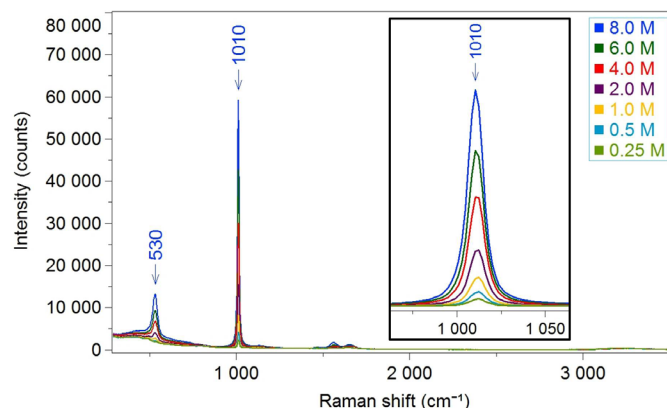


Figure 1: Raman spectra from 0.25, 0.50, 1.0, 2.0, 4.0, 6.0, and 8.0 M guanidine hydrochloride. Inset shows a zoomed-in area of the 1010 cm^{-1} peak that was used for peak fitting.

A series of Raman spectra were collected from guanidine hydrochloride at the following concentrations: 0.25, 0.50, 1.0, 2.0, 4.0, 6.0, and 8.0 M (Figure 1). The 1010 cm^{-1} Raman peak from each spectrum was processed and fitted and the peak areas were calculated using the LabSpec 6 software suite. The peak areas averaged from three sets of measurements were plotted as a function of the concentration.

As shown in Figure 2, a linear dependence of the Raman peak area on the concentration was obtained from the measurements, with reproducible peak area values for each concentration. The standard deviation amongst the three sets of peak areas was found to be extremely small compared to the difference in value between data points, thus yielding a reliable concentration plot. The values for the standard deviations of the intensities were typically less than 1/10th of the values of the average peak areas.

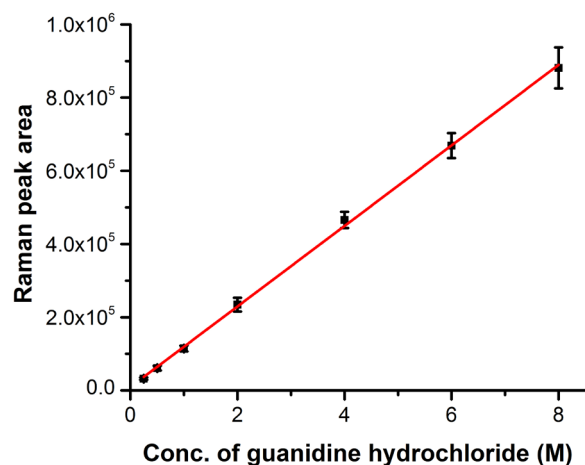


Figure 2: Average Raman peak area of 1010 cm^{-1} peak from 3 sets of measurements plotted as a function of guanidine hydrochloride concentration. Error bars represent standard deviation over 3 measurements per data point.

Summary

In this study, the potential of Raman spectroscopy to do rapid, non-destructive, quantitative analysis of liquid samples is shown, with guanidine hydrochloride as the example. A series of samples with systematically varying concentrations yielded a set of spectra, whose peaks could be fitted in order to obtain a linear relationship between the peak values and the concentration. Such a linear relationship can in principle be used to determine the concentration of analytes in liquid solutions.

References

1. Raman Spectroscopy for the Undergraduate Teaching Laboratory: Quantification of Ethanol Concentration in Consumer Alcoholic Beverages and Qualitative Identification of Marine diesels Using a Miniature Raman Spectrometer. D. Cleveland et al., *Spectroscopy Letters*, 40: 903-924, 2007.



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