APPLICATION NOTE

Measurements of Ethanol Content in Alcoholic Beverages with the LSP-T Series Diamond ATR FTIR Analyzer

We investigated the use of the multiple reflection ATR technique for the quantification of the ethanol content of alcoholic beverages. We found that the higher effective pathlength provided by multiple reflections provides a robust platform for the quantification. We also found that this platform permitted the use of a highly reduced set of standards that are easily prepared using the standard volumetric technique.

INTRODUCTION

The two main ingredients in alcoholic beverages are water and alcohol (ethanol) and the alcohol content must be displayed on the label. Alcohol content is easily measured by ATR-FTIR spectroscopy.

Multiple reflection ATR spectroscopy used to be very popular for a large variety of spectroscopic measurements but was lately almost completely displaced by singe reflection ATR. While single reflection ATR is particularly well suited to investigations of solids and powders, multiple reflection ATR, with its higher effective pathlength, is in most cases a superior technique for the analysis of liquids. In this Application Note we investigated the use of multiple reflection diamond ATR spectroscopy for the analysis of ethanol content in alcoholic beverages.

We also wanted to see if a reduced set of prepared ethanol-water solutions with known ethanol content could be utilized as standards for the PLS based chemometric procedure instead of the more commonly used set of standards prepared from a large and diverse collection of alcoholic beverages with ethanol content determined by a reference technique.

STANDARDS

For the standards we used ethanol-water mixtures in the following concentrations: 4%, 10%, 20%, 30%, 40%, 50% and 60%. The PLS model was then created and verified by the standard technique of leaving one of the standards out of the set, creating a PLS model and then calculating the ethanol concentration for the left out standard. This model was then used to predict the ethanol content of a number of off the shelf alcoholic beverages.

EXPERIMENTAL

All the samples were analyzed using the Durasens LSP-T-9 Diamond ATR FTIR Analyzer (Figure 1) that features a built in multiple reflection diamond ATR. The resolution was set to 4 cm-1 and the number of spectra averaged was 32. After the PLS model was created it was imported into the Durasens Analyzer Software that allows straightforward sample spectrum acquisition and analysis.

Figure 1: Durasens LSP-T Series Diamond ATR FTIR Analyzer

RESULTS AND DISCUSSION

The resulting spectra are shown in Figure 2. The portion of the spectrum in the 2500 cm^{-1} to 2000 cm^{-1} region was replaced with a straight line due to the absorbance of diamond in that region.

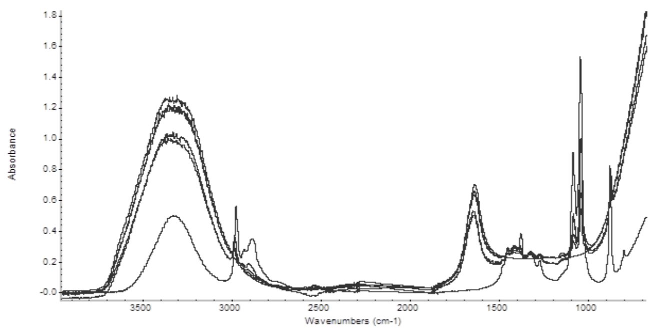


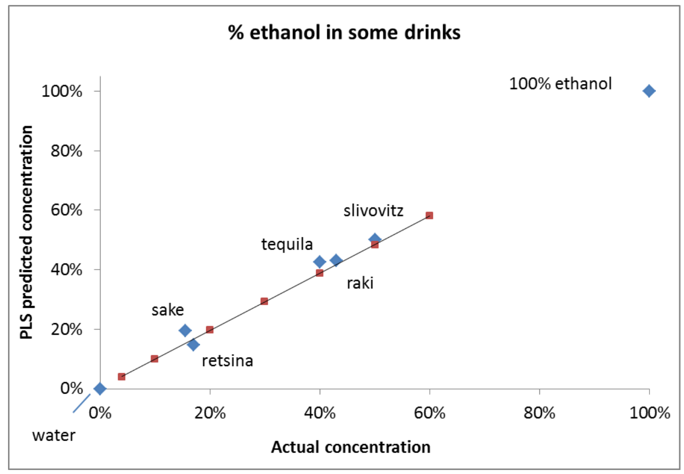
Figure 2: Spectra of the five alcoholic beverages analyzed. Also, shown are spectra of pure water and ethanol.

The results of the above described procedure are summarized in Table 1.

Sample	% ethanol on label	Predicated % ethanol
Ethanol	100%	100.0%
Raki	43%	43.1%
Retsina	17%	14.8%
Sake	15.50%	19.5%
Slivovitz	50%	50.10%
Tequila	40%	42.6%
Water	0%	0.0%

Table 1: Concentrations of alcohol shown on the labels and concentrations predicated using our PLS model.

The results of the analysis are displayed as diamonds in Graph 1. The concentrations of standards were calculated by the same PLS model and displayed in the graph as squares. Linear interpolation to the calculated values of standards is also displayed to help gauge the linearity of the model as applied to the standards. One sees that although some deviations from the label concentrations are encountered, the overall agreement is good. Particularly surprising is the model's prediction for pure ethanol which was perfect when rounded to whole percentages. The prediction for water was also perfect.



Graph 1: Actual vs. PLS Predicated concentrations of ethanol in a set of five samples of alcoholic beverages. Also shown are Actual vs. PLS Predicated concentrations of ethanol in water and 100% ethanol.

CONCLUSION

The above results demonstrate that multiple reflection ATR is exceptionally well suited to the analysis of ethanol content in alcoholic beverages even when using a reduced set of ethanol-water standards for the development of the PLS model.

This conclusion is, however, not restricted to ethanol in alcoholic beverages. It extends to any other solute dissolved in water, such as aqueous solutions of sucrose and other sugars.

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