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Application News

No. A637

Fourier Transform Infrared Spectrophotometer (FTIR)

Determination of Ethanol Content in and Simple Fail/Pass Judgment of Alcohol Hand Sanitizer by FTIR

Introduction

The effects of alcohol-based hand sanitizers are dependent on type of alcohol used and alcohol concentration. The Center for Disease Control and Prevention (CDC) has recommended sanitizers with 60 - 95% alcohol as the most effective composition of hand sanitizers.

Ethanol, which has bactericidal activity, is prepared at the optimal concentration level for a range of commercially available alcohol-based sanitizers. To measure alcohol concentration, the distillation method or gas chromatography (GC) is stipulated by the United States Pharmacopeia (USP). These methods require more than 20 minutes per sample for analysis. Pretreatment, such as dilution, is also required. In contrast, if the Fourier transform infrared spectrophotometer (FTIR) is used, the preparatory steps can be skipped and the ethanol content in alcohol sanitizers can quickly be determined in approximately one minute.

This report introduces a simple pass/fail judgment of ethanol concentration in a commercially available ethanol sanitizer using the photometric measurement function that comes as standard in LabSolutions™ IR.

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Experimental

Dehydrated ethanol was spiked with water to prepare the standards at concentrations of 70 vol% and 82 vol%. The samples were measured using IRSpirit™, a Fourier transform infrared spectrophotometer, equipped with QATR™-S (diamond crystal), a single-reflection ATR accessory, as shown in Fig. 1. The measurement conditions are shown in Table 1. First, 20 to 30 µL of the sample amount was placed onto the ATR crystal using a micropipette and, as shown in Fig. 2, covered immediately with a volatile cover to minimize evaporation, which could cause its concentration to change. Fig. 3 shows the IR spectra of ethanol standards. The figure shows that the heights of peaks from ethanol at 1086 cm^{-1} and 1044 cm^{-1} (green lines) and those from water at 3340 cm^{-1} and 1650 cm^{-1} (blue lines) are dependent on the concentration.

Table 1 Measurement Conditions

Instrument	: IRSpirit, QATR-S (Diamond)
Resolution	: 4 cm^{-1}
Accumulation	: 20
Apodization function	: Sqr-Triangle
Detector	: DLATGS

Fig. 1 IRSpirit™ FTIR with QATR™-S

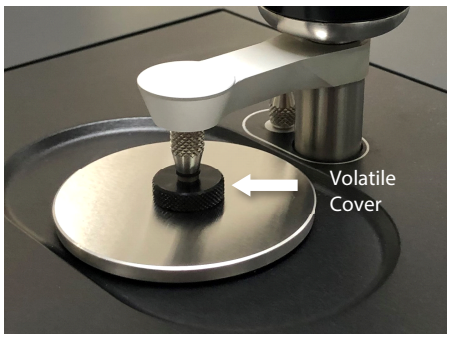

Fig. 2 QATR-S with Volatile Cover

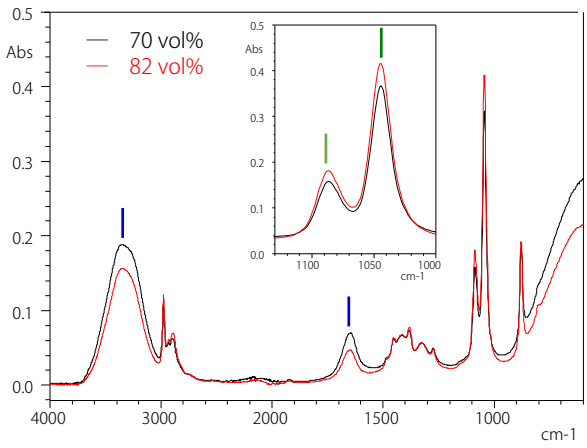

Fig. 3 IR Spectra of Ethanol Standards (70, 82 vol%)

Pass/Fail Judgment Using Labsolutions IR

To maintain the quality of alcohol sanitizers, it is important to control the concentrations of the constituents in these sanitizers. As a general rule, the spectra of a sample of known concentration and the sample to be controlled are analyzed to estimate the concentration of the sample to be controlled based on the height or area of the peak. Additionally, the obtained concentration should be judged by the analyzer as either pass or fail. These steps should be performed carefully because they not only require a lot of time but may also be affected by human error. The photometric measurement function installed as standard on LabSolutions IR can determine the absorbance or transmittance at specific wave numbers/wavelengths, and calculate these results using the formulas for pass/fail judgment. This makes it possible to reduce the operation time significantly.

Using this function, we judged four commercially available ethanol sanitizers (A – D) shown in Table 2. The samples were analyzed without pretreatment and dilution.

The photometric measurement function screen is shown in Fig. 4. The formula for pass/fail judgment is set up in Equation tab (red box) as shown in Fig. 4. In this analysis, the height from baseline to peak at 1044 cm^{-1} (C-O stretching vibration) was used to calculate the ethanol concentration (baseline drawn at 1110 cm^{-1} - 1020 cm^{-1}). The formula for pass/fail judgment was set up so that samples at 70 vol% (height from baseline to peak: 0.301) - 82 vol% (height from baseline to peak: 0.348) are judged Pass and the others are judged Fail. After the measurement of sample spectra, the data are automatically added to the sample table (blue box) shown in Fig. 4 to judge the samples. As shown in Table 2, Samples A and B, for which the concentrations were lower than the set reference concentration, were judged Fail.

Table 2 Labeling and Pass/Fail Judgment of Commercially Available Ethanol Sanitizers

Sample	Ethanol content labeled on the product	Pass/fail judgment
A	58 vol%	Fail
B	65 vol%	Fail
C	70 vol%	Pass
D	76.9 ~ 81.4 vol%	Pass

The measurement results of IR spectra (magnified view) are shown in Fig. 5. Using the peak height from ethanol (black line), the ethanol concentration can also be estimated.

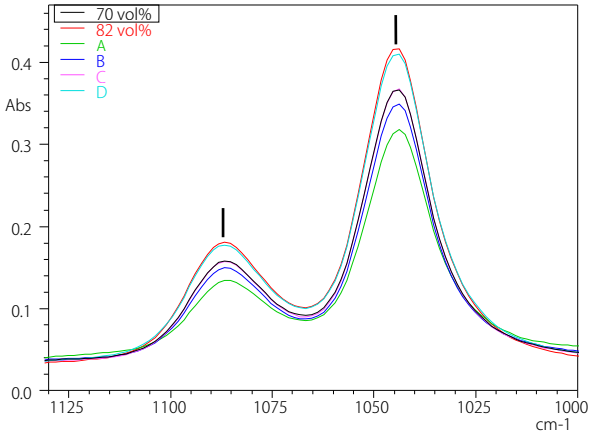

Fig.5 Measurement Results of IR Spectra (Magnified View)

Conclusion

With IRSpirit and QATR-S, ethanol content in sanitizers could be easily determined using just a single drop of sample. Additionally, the ethanol content could be easily and accurately judged for pass/fail by using the photometric measurement function of LabSolutions IR software. The use of this function can reduce the time required for analysis, including judgment. Concerns over product fraud or fake substances can be eliminated by controlling the quality of the major active ingredient (ethanol) in sanitizers.

For an example of quantitative analysis using the program installed as a standard function on LabSolutions IR, see also Application News No. A630 “Quick and Easy Analysis of Alcohol Content in Hand Sanitizer by FTIR Spectroscopy.”

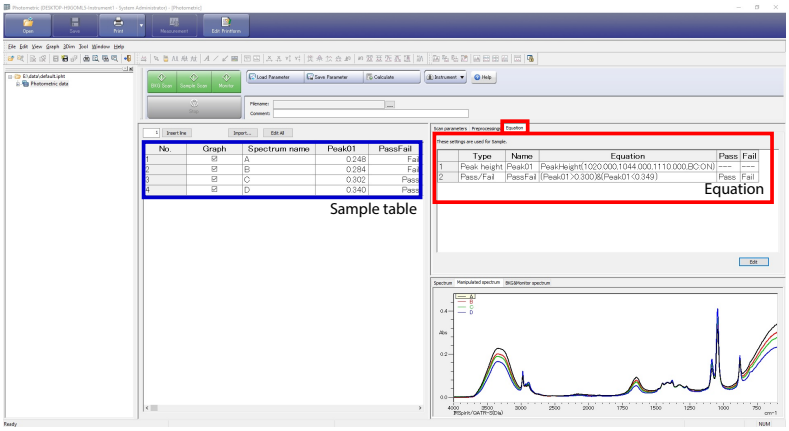

Fig. 4 Photometric Measurement Function Screen

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