PIKE TECHNOLOGIES
Spectroscopic Creativity

Application Note - 0501

Calculating the Pathlength of Liquid Cells by FTIR

FTIR analysis of liquid samples is often done using either a sealed liquid cell or demountable liquid cell using a spacer of optimal thickness. When making comparisons of results from different cells, it is important to know the actual cell pathlength. The transparent windows have parallel sides and smooth surfaces and measurement of the FTIR spectrum from an empty cell will produce a well known "fringing effect"[1,2], which originates from constructive and destructive interference of the IR beam from the parallel surfaces of the cell. This effect is clearly seen in the FTIR spectrum (Figure 1) of an empty Demountable Liquid cell with 0.05 mm spacer installed.

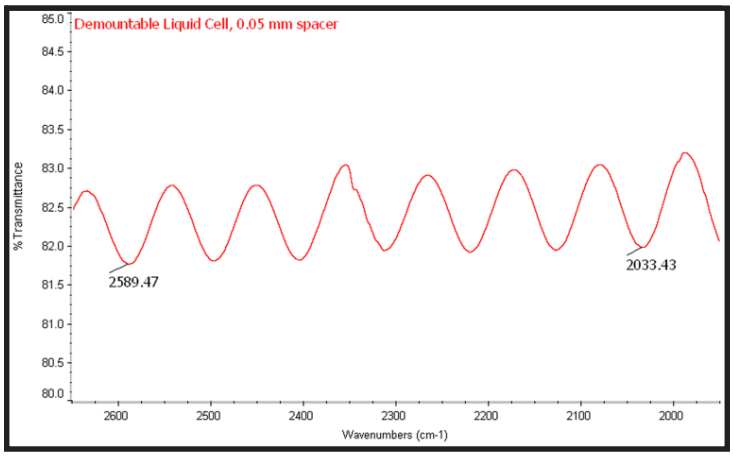

Figure 1. FTIR spectrum of an empty Demountable Liquid Cell with 0.05 mm spacer showing "fringing effect".

From this fringing effect we can calculate the pathlength of the liquid cell using the following equation;

$$b = 10\,N / 2\,(\upsilon_1 - \upsilon_2)$$

where;

b = pathlength of the cell in millimeters
N = number of fringes within a given spectral region
υ_1, υ_2 = start and end point in the spectrum in cm-1

In the spectrum shown in Figure 1, we selected starting and ending points in the spectrum of 2589.47 and 2033.43 cm-1 and counted the number of fringes within this spectral region as 6. To count the number of fringes, select starting and ending points both as minima or maxima of the spectrum and then count the number of opposing minima or maxima. In other words if we select minima values for starting and ending points in the spectrum, then we select maxima points to count the number of fringes.

Using these values in our equation, we calculate a cell pathlength of 0.0539 mm. This value is consistent with the expected pathlength of 0.05 mm, however, is more precise. This calculated value provides the ability to compare pathlength with other liquid cells and also to monitor and measure the pathlength of the cell over its lifetime.

A convenient way to perform the above calculations is by using PIKECalc software (PIKE Technologies part number; 007-0300). With this software package you can enter the values for N, υ_1, and υ_2 and the cell pathlength is calculated immediately.

References:

1. Griffiths, P. R., de Haseth, J. A., *Fourier Transform Infrared Spectrometry* (John Wiley & Sons, 1986).
2. Stuart, B., George, B., McIntyre P., *Modern Infrared Spectroscopy* (John Wiley & Sons, 1998).