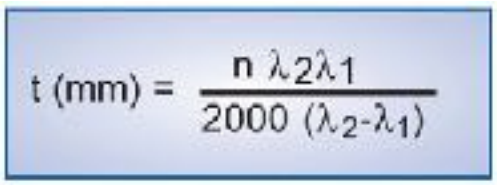
# CELL CALIBRATION

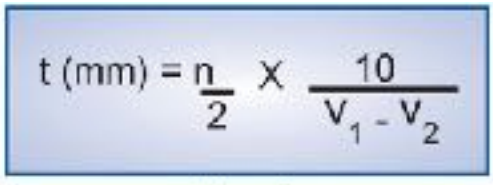
Most FTIR spectrophotometers have a cell calibration function. However, when working with a dispersive instrument, it is necessary to calibrate cells manually and it is prudent to check all FTIR instruments against manual calibrations from time to time.

The distance between the windows of a sealed cell is known as its pathlength. On most spectrophotometers, the pathlength can be measured by the interference fringe method for cells from .015 to 1.0mm. The pathlength can be calculated using either of the following equations:



$$t\,(mm) = \frac{n\,\lambda_2\lambda_1}{2000\,(\lambda_2-\lambda_1)}$$

Fig. 1



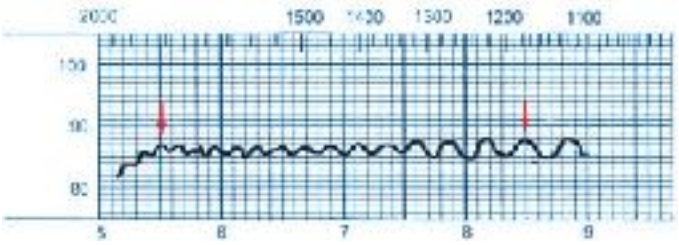
$$t\,(mm) = \frac{n}{2} \times \frac{10}{v_1 - v_2}$$

Fig. 2

**In these formulae:**
n = the number of fringes
t = the thickness of the space between windows (the pathlength)
**I2 and I1 = the wavelengths of the maxima (do not count the minima)**
**v1 and v2 = the frequencies (cm-1) of the maxima (do not count the minima)**

Below (Fig. 3) are fringes from an empty cell with a 0.1mm nominal pathlength run on a dispersive spectrophotometer. Applying the formula in Fig. 1 above using wavelengths, the pathlength is calculated as 0.1091. Note that when counting fringes or waves the starting or first maxima is ignored while the last maxima is counted regardless of whether working in microns or cm-1. In this case we started at 5.5 microns and counted 14 maxima to an end point at 8.5 microns.

To get accurate calibrations on a dispersive spectrophotometer with chart paper, it is important to start and finish counting the fringes on maxima that are bisected at the midpoint by a vertical line along the Y axis (ordinate) that intersects on the abscissa scale (x axis) with an identifiable wavelength. In the example of Fig. 3, we started counting maxima at 5.5 microns and ended at 8.5 microns because the maxima at these wavelengths were bisected at the midpoint.




**WAVENUMBER CM-1**

**WAVELENGTH IN MICRONS**

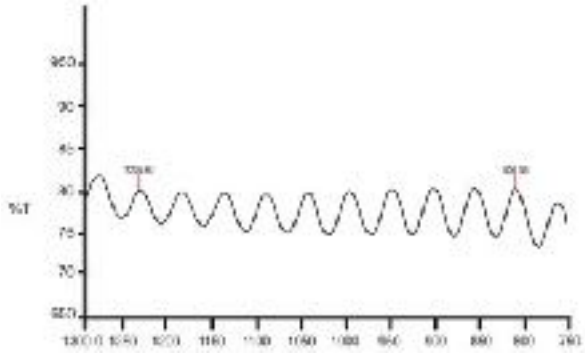
**Figure 3**

Cell calibrations will almost certainly vary from instrument to instrument. This occurs for several reasons, including (a) variations in both abscissa and ordinate scale accuracy from instrument to instrument, (b) infinitesimal variations in spacer thickness and window curvature at different points within the cell cavity, and (c) variations in exact location of the interface of the beam and the cell from instrument to instrument.

**For Figure 3, the pathlength is computed as follows:**

$$t = \frac{14\ (5.5 \times 8.5)}{2000\ (5.5\text{-}8.5)} = 0.10908$$

Below (Fig. 4), are fringes from an empty cell mounted in an FTIR spectrophotometer. Applying the pathlength formula for wave numbers (Fig. 2), V1 is 1235.67 cm-1, V2 is 806.98 cm-1 and n is 9 as we again count only maxima (not minima), and ignore the first maxima.




**WAVENUMBER CM-1**

**Figure 4**

**For Figure 4, the pathlength is computed as follows:**

$$t = \frac{9}{2} \times \frac{10}{1235.67 - 806.93} = 0.1050 \text{ mm}$$

There are many reasons why fringes may be difficult to produce. For example, cells with pathlengths of 1 mm and larger and cells with wedged windows (designed to reduce fringing), do not produce dramatic fringes. In these cases, calibration against a standard is useful. At ICL we use Benzene, which produces a useful peak at about 2650 cm-1. To calculate the pathlength of a cell with an unknown pathlength, the Benzene absorbance at 2650 cm-1 of the cell with a known pathlength is compared to the Benzene absorbance of a cell with the unknown pathlength at that wavenumber. A cell with a known pathlength of 1.0340mm produces the Benzene absorbance shown in Fig. 6 at 2650 cm-1. The Benzene absorbance (0.7635) is the difference between the absorbance units shown on the ordinate scale at the trough of the peak (0.2315) and the absorbance units shown on the ordinate scale at apex of the peak (0.9950). The cell with the unknown pathlength is shown in Fig. 7 and the Benzene absorbance at 2650 cm-1 is 0.7885. Applying the formula in Fig. 5, the pathlength of the unknown cell is 1.0679mm.

$$t = \frac{(Ab)\, t_{std}}{Ab_{std}}$$

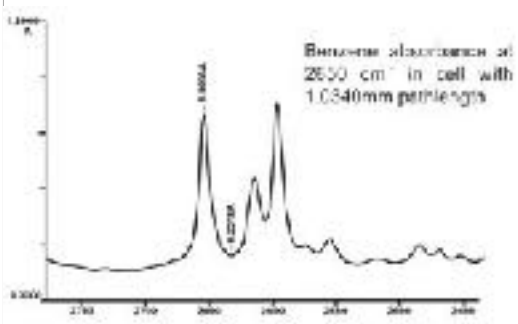
t = pathlength

Ab = absorbance of the unknown cell

$Ab_{std}$ = absorbance of the standard cell with the known pathlength

$t_{std}$ = the known pathlength of the standard cell

**Figure 5**




**WAVENUMBER CM-1**

**Figure 6**

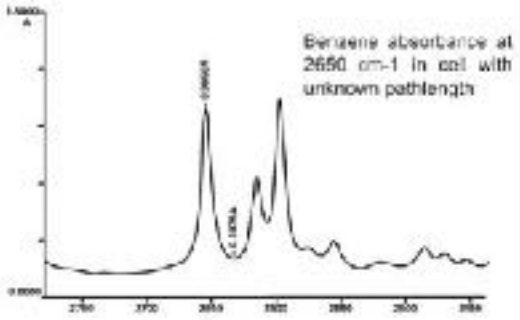



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**Figure 7**

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