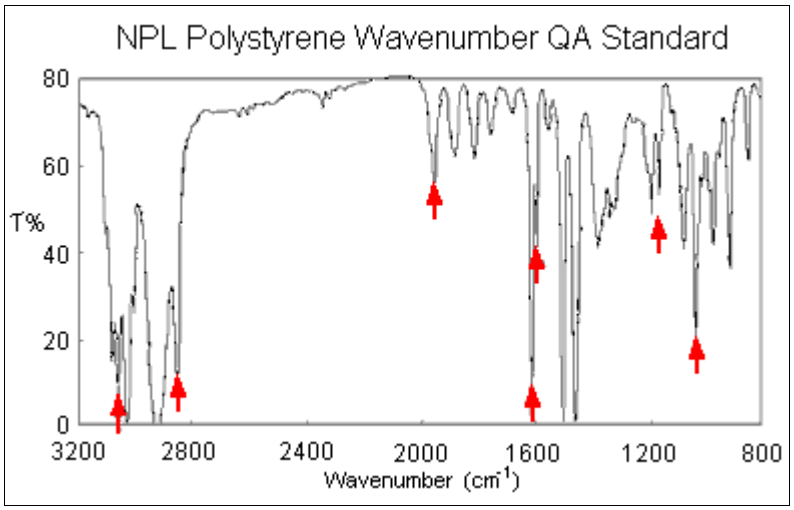
IR Wavenumber Calibration QA Standard

Each transfer standard is individually calibrated at NPL and consists of a selected polystyrene film, matt finished on both surfaces and nominally 35 µm thick, mounted in a cardboard frame with a circular window about 25 mm in diameter. The material of the standard is a wavenumber calibration device that has been improved in several respects over those available in the UK prior to 1992. In particular the matt finish eliminates interference ("channel") fringes for wavenumbers above about 2000 cm^{-1} and reduces them with progressively decreasing effectiveness in the region from 2000 cm^{-1} downwards. The card mount is 50 mm wide to fit the standard guide rails found in infrared spectrophotometers and 93 mm high so that it does not foul the lid of the sample compartment in certain instruments.



The transmittance minima (absorption peaks) calibrated are at nominal wavenumbers of around 3060, 2850, 1944, 1601, 1583, 1154 and 1028 cm^{-1}.

Purpose and use in Quality Assurance

The NPL wavenumber calibration transfer standard has been introduced to allow routine checking of the wavenumber scales of mid-infrared spectrophotometers for Quality Assurance purposes. It is far more convenient than using absorption lines of gases in sealed cells or from the atmosphere, and hence the procedure of inserting the standard in the usual 3" by 2" plate guides at regular intervals of, say, once a week is likely to be carried out in actual practice. Of course, gas absorption lines should be used for more accurate calibration in a particular critical spectral region.

Anadis Instuments Benelux B.V., Guadeloupestraat 30, 1339ME, Almere, The Netherlands,
PH +31(0)36 5214190, FX +31(0)36 5214428, E-mail: info@anadis.nl, Web: www.anadis.nl

Prior to July 1992 NPL was unwilling to calibrate the polystyrene films that were procurable, which were conventional films with glossy surfaces and were 50 µm or more in thickness: the IUPAC reference data refer to a film of 70 µm for most of the absorption peaks cited. The combined effects of the existence of full strength channel fringes, of their periodicity, and of the transmittance levels involved could cause a shift of up to 1.5 wavenumbers in the location of the transmittance minima in the worst case. Such a shift may vary between instruments, and vary slowly with time. However, the improved material now available has reduced the effects of channel fringes to a small fraction of a wavenumber and this allows credible calibration and use over an extended period.

The calibration of the NPL spectrophotometer makes use of a considerable number of gas absorption lines[1,2] using sealed cells containing suitable mixtures of methane with nitrogen, ammonia with nitrogen and nitric oxide with nitrogen, as well as water vapour and carbon dioxide in the atmosphere.

Polystyrene film has significant thermochromic effects, including shifts in wavenumbers of the transmittance minima. The uncertainties of calibration cited have been deliberately expanded to allow for the range of 30°C ±10°C in the temperature of the portion of film actually sampled that can occur in practical use.

The uncertainty of calibration at the 95% confidence level cited in a Certificate is ±0.4 wavenumber for the transmittance minima about 3060, 2850 1154 and 1028 cm^{-1}, ±0.5 wavenumber for the transmittance minima about 1601 and 1583 cm^{-1} and ±0.6 wavenumber for the transmittance minima about 1944 cm^{-1}. The calibrations will be fully valid for all resolutions of 4 wavenumbers or better, and will only be marginally affected by use of a resolution of 8 wavenumbers. Resolutions of worse than 8 wavenumbers will involve some increase in uncertainties.

References

1. Tables of wavenumbers for the calibration of infrared spectrophotometers. Second edition, edited by A. R. H. Cole, IUPAC, Pergamon Press, 1977.
2. The HITRAN database. Editions dated 1982, 1986, 1991, 1992, 1996. Purchasable from US Air Force Geophysics Laboratory, Hanscom Air Force Base, Mass. 01731, USA.