All data taken at the Pacific Northwest National Laboratory
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Composite spectrum for: tert-Butylamine
- First Column: Position in wavenumber (cm^{-1})
- Second column: Real refractive index $n(\tilde{v})$ (dispersion index)
- Third column: Imaginary refractive index, $k(\tilde{v})$ (absorption index per unit length in centimeters)

Where the complex refractive index $\hat{n} = n(\tilde{v}) + ik(\tilde{v})$

Following Bertie (in the references below) we define the absorbance as $A = - \log_{10}(I/I_0)$ and the linear absorption coefficient $K = A/d$, where d is the path length. The connection between the imaginary refractive index and the absorbance coefficient arises from the following: $2.303K = 4 \pi \tilde{v} k$

See the following references for a detailed description of terms and units:

1) Bertie, J. E., Zhang, S. L., Eysel, H. H., Baluja, S., & Ahmed, M. K. (1993). Infrared Intensities of Liquids XI: Infrared Refractive Indices from 8000 to 2 cm^{-1}, Absolute Integrated Intensities, and Dipole Moment Derivatives of Methanol at 25°C. *Applied Spectroscopy, 47*(8), 1100-1114. doi:10.1366/0003702934067973
2) Bertie, J. E., Zhang, S. L., & Keefe, C. D. (1995). Measurement and use of absolute infrared absorption intensities of neat liquids. *Vibrational Spectroscopy, 8*(2), 215-229. doi:10.1016/0924-2031(94)00038-i

Sample:
- Chemical name, formula and CAS number: tert-Butylamine, $C_4H_{11}N$, [75-64-9]
- IUPAC name: 2-Methylpropan-2-amine
- Synonyms: 2-Amino-2-Methylpropane; Trimethylaminomethane
- Physical properties: FW = 73.14 g/mole; mp = -67 °C; bp = 46 °C; $\rho = 0.696$ g/cm^3
- Supplier and stated purity: Aldrich, ≥99.5% (Lot # SHBG8066V)
- Temperature of sample: 26 °C (+/-1 °C)
- Individual samples were measured at the following path lengths: 0.748, 0.951, 3.81, 11.3, 15.9, 38.7, 55.5, 107, 206, 508 and 1042 micrometers (µm). Final data are a composite of these spectra.
- Sample cell window material is potassium bromide (KBr).
- Preparation: None.

Instrument Parameters:
- Bruker Tensor 27 FTIR, purged with UHP nitrogen
- Spectral range: 7800 to 400 cm^{-1} (1.282 to 25 microns)
- Instrument resolution: 2.0 cm^{-1}
- Number of interferograms averaged per single channel spectrum: 128
- Apodization: Norton-Beer, Medium
- Phase correction: Mertz
- Scanner velocity: 10 kHz
- Folding limits: 15802 to 0 cm^{-1}
- Interferogram zerofill: 4x
- Spectral interval after zerofilling: 0.4823 cm^{-1}
- IR source: Silicon carbide glow bar
- Beamsplitter: Broadband potassium bromide (KBr)
- Detector: DLTGS at room temperature
- Aperture: 3 mm

Measured Refractive Index:
The refractive index for tert-Butylamine was measured at 10 °C and 15 °C using an Atago model DR-M2/1550 Abbe refractometer. Notch filters were employed in front of a white light source to make measurements at multiple wavelengths. An InGaAs camera was used to detect signal at 1550 nm. The temperature was controlled to match that in the sample compartment of the FTIR using a heated circulating bath. The measurements at 15 C/10 °C were as follows:

480 nm:	$n = 1.3879/1.3911$	486 nm:	$n = 1.3867/1.3907$	546 nm:	$n = 1.3833/1.3869$
589 nm:	$n = 1.3815/1.3854$	644 nm:	$n = 1.3800/1.3836$	656 nm:	$n = 1.3789/1.3831$
1550 nm:	$n = 1.3714/1.3750$				

The average change in refractive index with increasing temperature (dn/dT) was calculated as -0.00075/°C using the measured values from 15 °C and 10 °C. This estimate of dn/dT was used to estimate the refractive index at 27 °C for each of the wavelengths. Then, the refractive index, n, vs. wavelength in microns, λ, was fit to an equation similar to that of Sellmeier:

$$n(\lambda) = \{a + b/(\lambda^2 - c)\}^{1/2}$$

The resulting best-fit equation was used to find the refractive index at the highest energy data point in our experimental spectra. For tert-Butylamine, the result was

$$n(7800 \text{ cm}^{-1}) = 1.3635 \text{ at } 27 \text{ °C.}$$

a) b)

Figure 1: The Bruker Tensor 27 FTIR (a) and Abbe refractometer (b).

Post Processing and Related Parameters:
A composite spectrum was created from 11 absorbance spectra (base-10) taken at 11 path lengths: 0.748, 0.951, 3.81, 11.3, 15.9, 38.7, 55.5, 107, 206, 508 and 1042 micrometers (μm). At each path length several spectra were measured and the results averaged for better signal to noise. The measured cell lengths were adjusted using Beer's law plots.

1) The imaginary part of the refractive index, or k vector, was determined for each absorbance file as per Bertie's program "RNJ46A" (see reference above). This takes into account the reflective losses due to the KBr windows.
2) A composite k vector is created via a classical, weighted, linear, least squares fit using the output files of program "RNJ46A": Intercept=0, slope is fitted, individual absorbance values weighted by T^2 (transmission squared), all absorbance values ≥ 2.5 are given zero weight. Six composite vectors were created and merged by hand although one of the k vectors was excluded. In addition, over a narrow spectral region, the results from a single cell were used.

a) The first *k* vector used the results from the 1042 and 508 µm cells. This *k* vector determined the final values for the range from 7800 to 4330 cm^{-1}, 4307 to 3411 cm^{-1}, 3122 to 3015 cm^{-1} and 2256 to 1695 cm^{-1}.

b) The second *k* vector used the results from the 508 and 206 µm cells. This *k* vector determined the final values for the range from 3015 to 3009 cm^{-1} and 1695 to 1633 cm^{-1}.

c) The third *k* vector used the results from the 107 and 55.5 µm cells. This *k* vector determined the final values for the range from 3411 to 3122 cm^{-1}, 3009 to 2986 cm^{-1}, 2360 to 2256 cm^{-1}, 1601 to 1374 cm^{-1} and 710 to 400 cm^{-1}.

d) The fourth *k* vector used the results from the 38.7 and 15.9 µm cells. This *k* vector determined the final values for the range from 2986 to 2977 cm^{-1}, 2948 to 2360 cm^{-1} and 778 to 710 cm^{-1}.

e) The fifth *k* vector used the results from the 11.3 and 3.81 µm cells. This *k* vector determined the final values for the range from 2977 to 2948 cm^{-1}, 1633 to 1601 cm^{-1} and 1374 to 778 cm^{-1}.

f) The sixth *k* vector used the results from the 0.951 and 0.748 µm cells. This *k* vector was not used.

g) Additionally, the single *k* vector result from the 508 µm cell was used to determine the values from 4330 to 4307 cm^{-1}.

3) The resulting composite *k* vector and the refractive index at 7800 cm^{-1} were used to create the real or *n* vector using the Kramers-Kronig relation, as per Bertie's program "LZZKTB."

a) Calculated and estimated errors: Type A = 0.7%.

b) Frequency correction (already applied): $\tilde{\upsilon}$(corrected) = [$\tilde{\upsilon}$(instrument) * .99977 - .01872] as determined by comparing measured atmospheric spectral lines (H_2O and CO_2) to values from the Northwest Infrared Spectral Library Database.

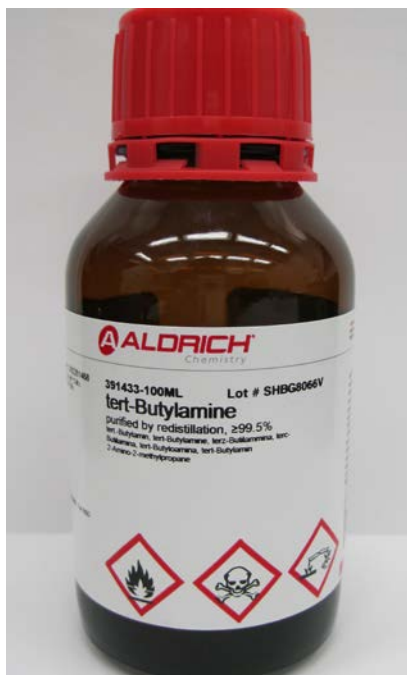c) Axis units: X = Wavenumbers (cm^{-1}); Y = Absorbance (base 10).

Photograph of Sample tert-Butylamine:

Figure 2: tert-Butylamine in Aldrich container.