All data taken at the Pacific Northwest National Laboratory
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Composite spectrum for: Benzene

- First Column: Position in wavenumber (cm^{-1})
- Second column: Real refractive index $n(\tilde{\upsilon})$ (dispersion index)
- Third column: Imaginary refractive index, $k(\tilde{\upsilon})$ (absorption index per unit length in centimeters)

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

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: $2.303K = 4\pi\tilde{\upsilon}k$

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: Benzene, C_6H_6, [71-43-2]
- IUPAC name: Benzene
- Synonyms: Benzol; Phene; Phenyl hydride; Cyclohexatriene
- Physical properties: FW = 78.11 g/mole; mp = 5.5 °C; bp = 80-80.2 °C; $\rho = 0.88$ g/cm^3
- Supplier and stated purity: Sigma-Aldrich, 99.8% (Lot #SHBG6315V)
- Temperature of sample: 26 °C (+/-1 °C)
- Individual samples were measured at the following path lengths: 0.64, 1.7, 2.3, 10.1, 12.9, 36.5, 91.7, 93.2, 197, 523, 1020 and 1233 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 benzene was measured at 27 °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.

480 nm: n = 1.5087	486 nm: n = 1.5076	546 nm: n = 1.4996
589 nm: n = 1.4958	644 nm: n = 1.4919	656 nm: n = 1.4912
1550 nm: n = 1.4767		

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 benzene, the result was

$$n(7800\ \text{cm}^{-1}) = 1.4781 \text{ at } 27\ ^\circ\text{C}.$$

a) b)

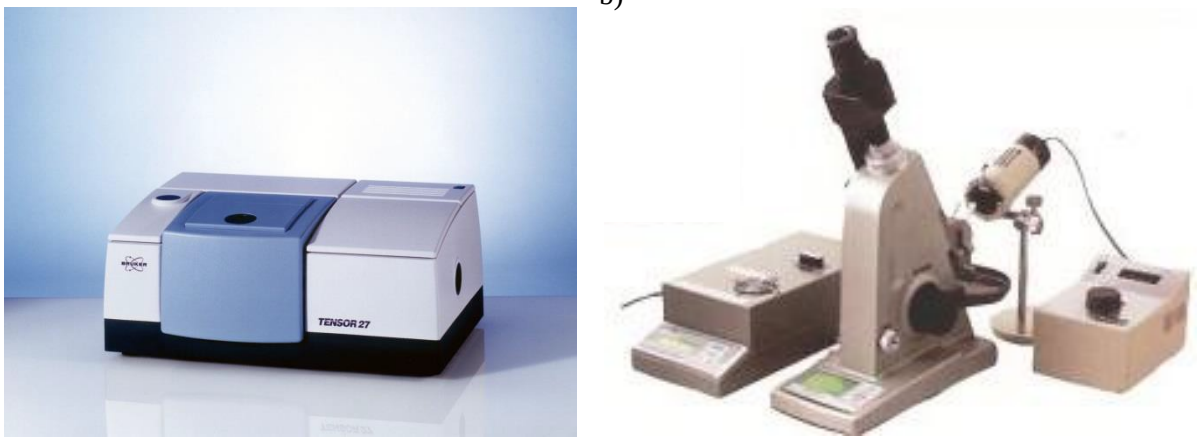

Figure 1: The Bruker Tensor 27 FTIR (a) and Abbe refractometer (b).

Post Processing and Related Parameters:
A composite spectrum was created from 12 absorbance spectra (base-10) taken at 12 path lengths: 0.6, 1.7, 2.3, 10.1, 12.9, 36.5, 91.7, 93.2, 197, 523, 1020 and 1233 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. Five composite vectors were created and merged by hand.
   a) The first k vector used the results from the 523, 1020 and 1233 μm cells. This k vector determined the final values for the range from 7800 to 4140 cm^{-1}.
   b) The second k vector used the results from the 37 through 197 μm cells. This k vector determined the final values for the range from 4140 to 3150 cm^{-1}.

c) The third *k* vector used the results from the 0.6 through 13 μm cells. This *k* vector determined the final values for the range from 3150 to 2950, 1660 to 1400 and 750 to 560 cm^{-1}.
d) The fourth *k* vector used the results from the 13 through 197 μm cells. This *k* vector determined the final values for the range from 2950 to 1600, 1400 to 1100 and 560 to 400cm^{-1}.
e) The fifth *k* vector used the results from the 2.3 through 37 μm cells. This *k* vector determined the final values for the range from 1100 to 750 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): $\tilde{\nu}$(corrected) = [$\tilde{\nu}$(instrument) * .99975 + .003891] 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 Benzene:

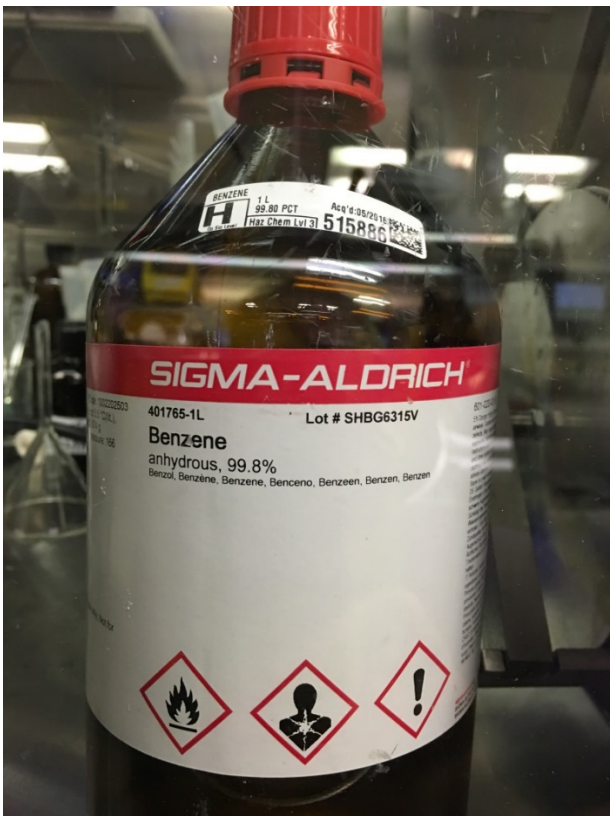

Figure 2: Benzene in Sigma-Aldrich container.