All data taken at the Pacific Northwest National Laboratory
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Composite spectrum for: Sodium hypochlorite solution

- 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: Sodium hypochlorite solution, ClNaO, [7681-52-9]
- IUPAC name: Sodium hypochlorite
- Synonyms: Bleach; Antiformin; Chloride of soda
- Physical properties: FW = 74.44 g/mole; mp = -30 – -20 °C; bp = 111 °C; ρ = 1.206 g/cm^3
- Supplier and stated purity: Sigma-Aldrich, Chlorine 10-15% (Lot # MKBZ1666V)
- Temperature of sample: 26 °C (+/-1 °C)
- Individual samples were measured at the following path lengths: 5.38, 5.51, 13.8, 26.2, 57.9, 107, 204, 512 and 991 micrometers (μm). Final data are a composite of these spectra.
- Sample cell window material is zinc selenide (ZnSe).
- 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: 32
- 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 Sodium hypochlorite solution 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 = 1.381	486 nm: n = 1.3808	546 nm: n = 1.3776
589 nm: n = 1.3759	644 nm: n = 1.3741	656 nm: n = 1.373
1550 nm: n = 1.3555		

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 Methanol, the result was

$$n(7800\ \text{cm}^{-1}) = 1.3585 \text{ at } 27\ ^\circ\text{C}.$$

a) b)

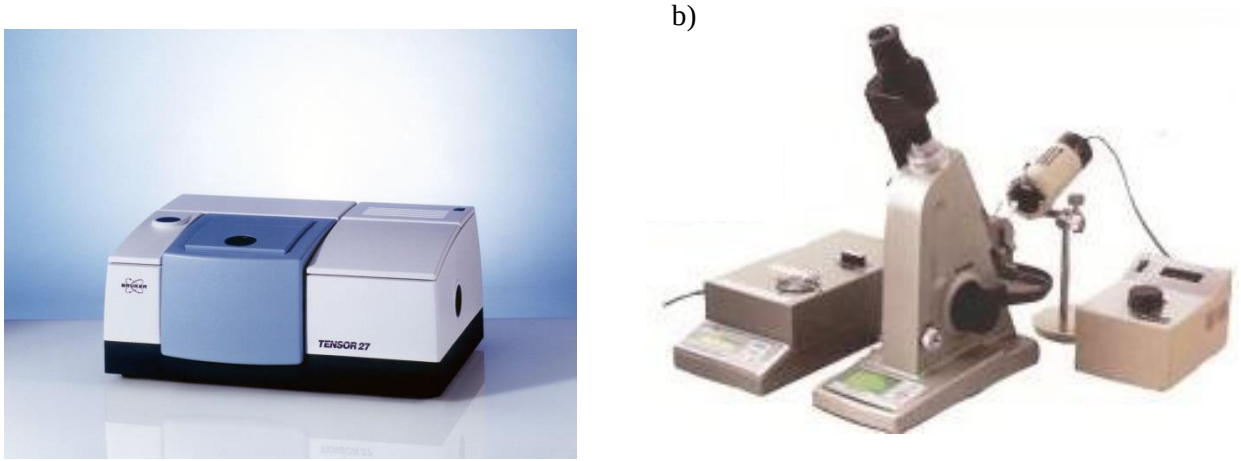

Figure 1: The Bruker Tensor 27 FTIR (a) and Abbe refractometer (b).

Post Processing and Related Parameters:
A composite spectrum was created from 5 absorbance spectra (base-10) taken at 5 path lengths: 5.38, 57.9, 107, 204 and 991 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. The large refractive index of ZnSe resulted in considerable fringing in the spectra. Absorption also increases for ZnSe at wavenumbers below 550 cm^{-1} resulting in increased noise; thus the data is truncated at 533 cm^{-1}. The spectra from the 5.51, 13.8, 26.2 and 512 μm cells were not used.

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 ZnSe 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. No composite vectors were created and merged by hand. In the entire region, the results from only a single cell were used.
   a) The single k vector result from the 991 μm cell was used to determine the final values for the range from 7800 to 5241 cm^{-1}.

b) The single *k* vector result from the 204 μm cell was used to determine the final values for the range from 5241 to 3735 cm^{-1}.
c) The single *k* vector result from the 107 μm cell was used to determine the final values for the range from 3735 to 3707 cm^{-1}.
d) The single *k* vector result from the 58 μm cell was used to determine the final values for the range from 3707 to 3681 cm^{-1}.
e) The single *k* vector result from the 5.38 μm cell was used to determine the final values for the range from 3681 to 534 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 Sodium hypochlorite solution:

Figure 2: Sodium hypochlorite solution in Sigma-Aldrich container.