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

- 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. *Appl. Spec. 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: Crambe abyssinica seed oil, High percentage of fatty acids, particularly erucic acid [$CH_3(CH_2)_7CH{=}CH(CH_2)_{11}COOH$], 68956-68-3
- IUPAC name: n/a
- Synonyms: Crambe oil; Abyssinian Oil
- Physical properties: FW = n/a; mp = n/a; bp = n/a; ρ = 0.9 – 0.93 g/cm^3
- Supplier and stated purity: High Altitude Naturals, 100% (Lot # 10189-JE-1016600)
- Temperature of sample: 26 °C (+/-1 °C)
- Individual samples were measured at the following path lengths: MIR: 2.3, 7.2, 15.9, 20.2, 52.2, 111, 206 and 511 μm; NIR: 110, 203, 506, 942 and 3617 μm. Final data are a composite of these spectra.
- Sample cell window material is potassium bromide (KBr).
- Preparation: None

NIR Instrument Parameters:

- Bruker Vertex 70, purged with UHP nitrogen
- Spectral range: 10,000 to 3,000 cm^{-1} (1.0 to 3.33 microns)
- IR source: Quartz tungsten bulb
- Beamsplitter: Broadband Potassium bromide (KBr)
- Detector: DLTGS at room temperature
- Aperture: 3 mm
- Folding limits: 15801 to 0 cm^{-1}

MIR Instrument Parameters:

- Tensor 27, purged with UHP nitrogen
- Spectral range: 7800 to 400 cm^{-1} (1.282 to 25 microns)
- NIR source: Silicon carbide glow bar
- Beamsplitter: Broadband Potassium bromide (KBr)
- Detector: DLTGS at room temperature
- Aperture: 3 mm
- Folding limits: 15802 to 0 cm^{-1}

NIR/MIR Instrument Parameters:

- 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
- Interferogram zerofill: 4x
- Spectral interval after zerofilling: 0.4823 cm^{-1}

a) b)

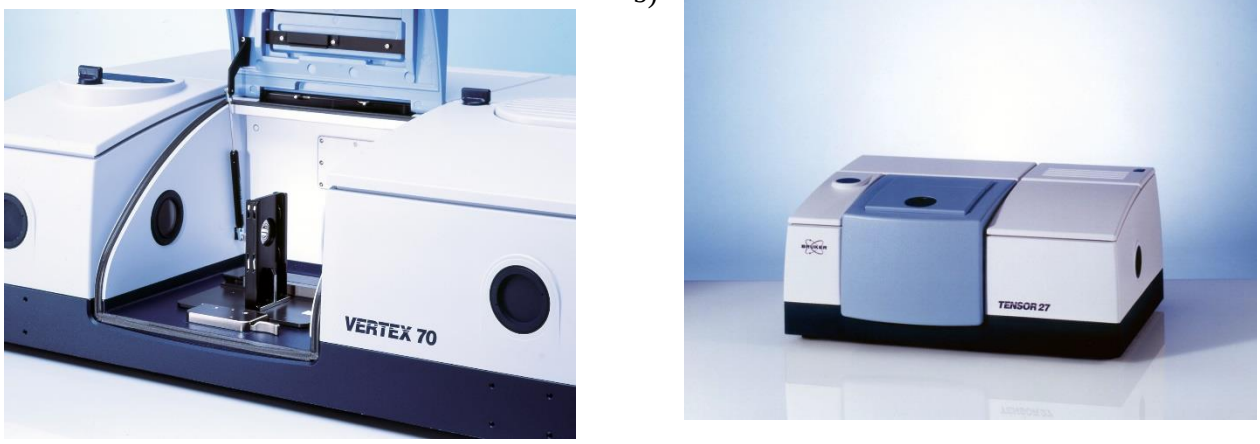

Figure 1: The Bruker Vertex 70 FTIR (a) and Tensor 27 FTIR (b).

Measured Refractive Index:

The refractive index for Crambe oil was measured at 25 °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 infrared viewer from Atago 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 = 1.476	486 nm: n = 1.4756	546 nm: n = 1.4715
589 nm: n = 1.44691	644 nm: n = 1.4671	656 nm: n = 1.4667
1550 nm: n = 1.45753		

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 points in our experimental spectra. For Crambe oil, the results were

n(7800 cm^{-1}) = 1.4585 at 25 °C for MIR data and
n(10,0000 cm^{-1}) = 1.4603 at 25 °C for NIR and merged data.

Post Processing and Related Parameters:
For the MIR, a composite spectrum was created from 8 absorbance spectra (base-10) taken at 8 path lengths: 2.3, 7.2, 15.9, 20.2, 52.2, 111, 206 and 511 micrometers (μm). For the NIR, a composite spectrum was created from 5 absorbance spectra (base-10) taken at 5 path lengths: 110, 203, 506, 942 and 3617 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 in which the NIR and MIR data were analyzed independently.

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. For the MIR, three composite vectors were created and merged by hand.
   a) The first *k* vector used the results from the 111 through 511 μm cells. This *k* vector determined the final values for the range from 7800 to 4000 cm^{-1}.
   b) The second *k* vector used the results from the 52 through 511 μm cells. This *k* vector determined the final values for the range from 4000 to 3100 cm^{-1}, 2800 to 1800 cm^{-1} and 550 to 400 cm^{-1}.
   c) The third *k* vector used the results from the 2 through 52 μm cells. This *k* vector determined the final values for the range from 3100 to 2800 cm^{-1} and 1800 to 550 cm^{-1}.
3) The resulting composite MIR *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) Frequency correction (already applied): $\tilde{\upsilon}$(corrected) = [$\tilde{\upsilon}$(instrument) * 0.99994+ .010722] as determined by comparing measured atmospheric spectral lines (H_2O and CO_2) to values from the Northwest Infrared Spectral Library Database.
4) For the NIR, two composite vectors were created and merged by hand.
   a) The first *k* vector used the results from the 506 through 3617 μm cells. This *k* vector determined the final values for the range from 10,000 to 4500 cm^{-1}.
   b) The second *k* vector used the results from the 110 through 3617 μm cells. This *k* vector determined the final values for the range from 4500 to 400 cm^{-1}.
5) The resulting composite NIR *k* vector and the refractive index at 10,000 cm^{-1} were used to create the real or *n* vector using the Kramers-Kronig relation, as per Bertie's program "LZZKTB."
   a) Frequency correction (already applied): $\tilde{\upsilon}$(corrected) = [$\tilde{\upsilon}$(instrument) * 0.999848 + .01072] as determined by comparing measured atmospheric spectral lines (H_2O and CO_2) to values from the Northwest Infrared Spectral Library Database.
6) Finally, the MIR data were mapped onto the NIR x-axis using an interpolation routine, i.e. the Make Compatible command in OPUS 5.5. Then, the composite MIR and NIR *k* vectors were merged by hand to generate a final composite k vector across the entire spectral range. The resulting composite *k* vector and the refractive index at 10,000 cm^{-1} were used to create the final *n* vector using the Kramers-Kronig relation, as per Bertie's program "LZZKTB.

Photograph of Sample Crambe oil:

Figure 2: Crambe oil in High Altitude Naturals container.