PNNL LIQUIDS REFRACTIVE INDEX (*n*/*k*) DATASET FROM 1 TO 25 MICRONS

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This readme file was generated on 2025-09-15 by Tanya Myers.

Description

This dataset is an open-source repository of spectral data measured at Pacific Northwest National Laboratory (PNNL). This database provides quantitative values for the complex index of refraction for 111 liquids. A list of the chemicals is available at the end of this readme. These spectra consist of the optical constants, i.e., the real, *n*(v), and imaginary, *k*(v), refractive indices, over the spectral range from 10,000 to 400 cm^{-1} (1 – 25 µm). The conditions under which the individual data were acquired are described in the associated metadata files, and the user is strongly encouraged to read and understand this information to ensure the data are used appropriately for your application.

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File Organization

- Each material has its own folder named by its common chemical name. A list of the chemicals is available at the end of this readme.
- Each folder contains exactly two files:
    - PDF file: Complete metadata including sample details, photographs, and collection/analysis methods
    - Text file (.txt): Spectral data in a three-column format (wavenumber, *n*, *k*) ASCII files

File Naming Convention

Files follow this 7-field format separated by periods:

[Type].[Domain].[Purity].[Chemical-Name].[Phase].[Supplier].[LabID]

1) Type: Measurement Type (or other ancillary info type, e.g. META). An abbreviation used to characterize files that provide the measurement type or ancillary information associated with a particular sample that is in the first or left-most field. Field values in this dataset include:
    a. META = metadata associated with the file
    b. NK = datafile containing the liquids spectral data (cm^{-1}, n, k)
2) Domain: Measurement Wavelength Domain. An abbreviation is used to characterize the wavelength range of the spectral measurement. The field value in this dataset is:
    a. MIR = mid-infrared
3) Purity: Purity State Designation. An abbreviation is used to characterize each sample by purity state. The field values in this dataset are:
    a. PUR = Pure
    b. MIX = Mixture
4) Chemical-Name: A recognizable name for the chemical. No spaces or commas are used. Instead a hyphen is used to represent a space or comma if needed. An example of a field value is:
    a. 1-1-3-3-Tetramethylguanidine = 1,1,3,3-Tetramethylguanidine
5) Phase: This field is used to identify the phase of the material. For this dataset, the field value is
    a. LIQ = Liquid

6) Supplier: Sample Version or Origin. Characterize the supplier or creator of the sample. To limit the number of characters, camel case (i.e., CamelCase) is often used. An example of the field value is

    a. AlfaAesar = Alfa Aesar

7) LabID: Measurement Lab Designation. Identification of the lab making the measurement along with a six-number unique identifier. This identifier is usually the chemical management number used at PNNL for inventory purposes and is in the last or right-most field.

    a. PNNL123456

The first chemical in this dataset is Acetophenone and the two files are:

1. META.MIR.PUR.Acetophenone.LIQ.SigmaAldrich.PNNL563423.pdf
2. NK.MIR.PUR.Acetophenone.LIQ.SigmaAldrich.PNNL563423.txt

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Chemicals

Sample Name	CAS #	State
1,1,3,3-Tetramethylguanidine	80-70-6	Liquid
1,3-Dichlorobenzene	541-73-1	Liquid
1,4-Butanediol	110-63-4	Liquid
1-Bromo-2-chloroethane	107-04-0	Liquid
1-Octanol	111-87-5	Liquid
2,3-Butanediol	513-85-9	Liquid
2-Ethylhexyl acrylate	103-11-7	Liquid
2-Methylcylcohexanol	586-59-5	Liquid
3-Bromo-1-propyne	106-96-7	Liquid
3-Chlorotoluene	108-41-8	Liquid
3-Nitrotoluene	99-08-1	Liquid
4-Amino-1-benzyl-piperidine	50541-93-0	Liquid
4-Carvomenthenol	562-74-3	Liquid
4-Ethyltoluene	622-96-8	Liquid
6-Methyl-2-heptanone	928-68-7	Liquid
Acetone	67-64-1	Liquid

Acetonitrile	75-05-8	Liquid
Acetophenone	98-86-2	Liquid
Ammonium hydroxide soln	1336-21-6	Liquid
Aniline	62-53-3	Liquid
Benzaldehyde	100-52-7	Liquid
Benzene	71-43-2	Liquid
Bis-2-ethylhexyl sebacate	122-62-3	Liquid
Bromochloromethane	74-97-5	Liquid
Butyl stearate	123-95-5	Liquid
Butyraldehyde	123-72-8	Liquid
Carvone	99-49-0	Liquid
Chloroform	67-66-3	Liquid
Crambe oil	68956-68-3	Liquid
Cumin seed oil	8014-13-9	Liquid
Cyclohexane	110-82-7	Liquid
Cyclohexanol	108-93-0	Liquid
Cyclohexanone	108-94-1	Liquid
Deuterium oxide	7789-20-0	Liquid
Diazinon	333-41-5	Liquid
Dibromomethane	74-95-3	Liquid
Dibutyl phosphate	107-66-4	Liquid
Dibutyl phthalate	84-74-2	Liquid
Diethyl malonate	105-53-3	Liquid
Diethyl methylphosphonate	683-08-9	Liquid
Diethyl phthalate	84-66-2	Liquid
Diethyl pimelate	2050-20-6	Liquid
Diethyl sebacate	110-40-7	Liquid
Dimethyl sulfoxide	67-68-5	Liquid
DIMP	1445-75-6	Liquid
Di-n-octyl phthalate	117-84-0	Liquid
Dioctyl phthalate	117-81-7	Liquid
Dipentene	138-86-3	Liquid
Dimethyl-methylphosphonate	756-79-6	Liquid
Ethanol	64-17-5	Liquid
Ethyl 2-cyanoacrylate	7085-85-0	Liquid
Ethyl benzene	100-41-4	Liquid
Ethylene glycol	107-21-1	Liquid
Furfural	98-01-1	Liquid
Gasoline	8006-61-9	Liquid

Glycerol	56-81-5	Liquid
Glyceryl triacetate	102-76-1	Liquid
Hexane	110-54-3	Liquid
Isoamyl acetate	123-92-2	Liquid
Isopropanol	67-63-0	Liquid
Kerosene	8008-20-6	Liquid
Malathion	121-75-5	Liquid
Mesitylene	108-67-8	Liquid
Methanol	67-56-1	Liquid
Methyl anthranilate	134-20-3	Liquid
Methyl decanoate	110-42-9	Liquid
Methyl laurate	111-82-0	Liquid
Methyl paraoxon	950-35-6	Liquid
Methyl salicylate	119-36-8	Liquid
Methyl undecanoate	1731-86-8	Liquid
Methyl-2-cyanoacrylate	137-05-3	Liquid
Mineral oil	8042-47-5	Liquid
m-Xylene	108-38-3	Liquid
N,N-Dimethylaniline	121-69-7	Liquid
N,N-Dimethylformamide	68-12-2	Liquid
Nitrobenzene	98-95-3	Liquid
n-Octane	111-65-9	Liquid
Oleic acid	112-80-1	Liquid
Olive oil	8001-25-0	Liquid
o-Xylene	95-47-6	Liquid
Parathion	56-38-2	Liquid
Permethrin	52645-53-1	Liquid
Phenethyl alcohol	60-12-8	Liquid
2-Phenylethylamine	64-04-0	Liquid
(+)-β-Pinene	19902-08-0	Liquid
Phenylacetaldehyde	122-78-1	Liquid
Propylene glycol	57-55-6	Liquid
p-Xylene	106-42-3	Liquid
Pyridine	110-86-1	Liquid
Safrole	94-59-7	Liquid
Silicone oil	63148-62-9	Liquid
Soybean oil	10026-04-7	Liquid
Squalene	111-02-4	Liquid
Styrene oxide	96-09-3	Liquid

tert-Butylbenzene	98-06-6	Liquid
Tetraethylene glycol	112-60-7	Liquid
Tetraglyme	143-24-8	Liquid
Toluene	108-88-3	Liquid
trans-1,2-Dichloroethene	156-60-5	Liquid
Tribromofluoromethane	353-54-8	Liquid
Tributyl citrate	77-94-1	Liquid
Tributyl phosphate	126-73-8	Liquid
Trichloroethylene	79-01-6	Liquid
Tridecane	629-50-5	Liquid
Triethanolamine	102-71-6	Liquid
Triethyl phosphate	78-40-0	Liquid
Trimethyl phosphate	512-56-1	Liquid
Trioctyl trimellitate	3319-31-1	Liquid
Tris(2-ethylhexyl)phosphate	78-42-2	Liquid
Tropane	529-17-9	Liquid
γ-Valerolactone	108-29-2	Liquid