PNNL INFRARED REFRACTIVE INDEX (*n*/*k*) DATASET FOR SEVEN PAH SOLIDS AT ROOM TEMPERATURE

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This readme file was generated on 2026-06-22 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 seven polycyclic aromatic hydrocarbon (PAH) solids. A list of the chemicals is available at the end of this readme file. These spectra consist of the optical constants, i.e., the real, $n(\nu)$, and imaginary, $k(\nu)$, refractive indices, over the spectral range from 7,800 to 400 cm^{-1} (1.28 – 25 µm). These data are reported as vacuum wavenumbers. 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 their application.

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Recommended Citation for Dataset

Jessica M Salcido, Jeremy D. Erickson, Ashley M. Bradley, Russell G. Tonkyn, Timothy J. Johnson and Tanya L. Myers. 2026. *PNNL INFRARED REFRACTIVE INDEX (n/k) DATASET FOR SEVEN PAH SOLIDS AT ROOM TEMPERATURE.* [Data Set] PNNL DataHub. DOI

License Information

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 tab-delimited three-column format (wavenumber, *n*, *k*)

File Naming Convention

Files follow a 7-field format separated by periods:

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

1) Type: An abbreviation used to characterize files that provide the measurement type or ancillary information (e.g., META) 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 = spectral datafile (cm^{-1}, *n*, *k*)
2) Domain: An abbreviation used to characterize the wavelength range of the spectral measurement. The field value in this dataset is:
    a. MIR = mid-infrared
3) Purity: An abbreviation used to characterize each sample by purity state. The field value in this dataset is:
    a. PUR = Pure
4) Chemical-Name: A recognizable name for the chemical. No spaces, parentheses or commas are used. Instead, a hyphen is used to represent a space, parenthesis or comma if needed. An example of a field value in this dataset is:
    a. Benzo-a-pyrene = Benzo[a]pyrene
5) Phase: Field used to identify the phase of the material. For this dataset, the field value is

a. KBr-PLT = KBr pellet

6) Supplier: Field used to identify the vendor or origin 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. SigmaAldrich = Sigma-Aldrich

7) LabID: 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. An example in this dataset is:

   a. PNNL346496

The first chemical in this dataset is Benzo[a]pyrene and the two associated files are:

1. META.MIR.PUR.Benzo-a-pyrene.KBr-PLT.SigmaAldrich.PNNL346496.pdf
2. NK.MIR.PUR.Benzo-a-pyrene.KBr-PLT.SigmaAldrich.PNNL346496.txt

Acknowledgements

The research is based upon work supported by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), via DOE DE-AC05-76RLO1830 under the PICARD program.

Jessica Salcido was supported by the Henry M. MacCracken Program and Dean's Doctoral Fellowship from New York University's Graduate School of Arts and Sciences, as well as the Violet Scholars in Physics Fellowship from New York University's Physics Department.

List of Chemicals

Sample Name	CAS #	Molecular Formula	# of Rings
Benzo[a]pyrene (B[a]P)	50-32-8	$C_{20}H_{12}$	5
Benzo[e]pyrene (B[e]P)	192-97-2	$C_{20}H_{12}$	5
Benzo[ghi]perylene (B[ghi]P)	191-24-2	$C_{22}H_{12}$	6
Coronene (COR)	191-07-1	$C_{24}H_{12}$	7
Naphthalene (NAP)	91-20-3	$C_{10}H_{8}$	2
Phenanthrene (PHE)	85-01-8	$C_{14}H_{10}$	3
Pyrene (PYR)	129-00-0	$C_{16}H_{10}$	4