

Expanding FTIR Capabilities at SNOLAB: Building a Chemical and Materials Spectral Database

Utilizing FTIR Spectroscopy for Accurate Material Verification and Contamination Control at SNOLAB



Cameron Van Der Zyl
Analytical Chemistry Program Research Assistant

**Why FTIR at
SNOLAB?**

Why FTIR at SNOLAB?



The Environment at SNOLAB

- Ultra-clean, low-background science requires strict contamination control
- Need fast, accurate material verification
- FTIR = rapid, non-destructive, versatile
- Previously underused at SNOLAB
- My project: Unlock full potential + building spectral library



FTIR Basics

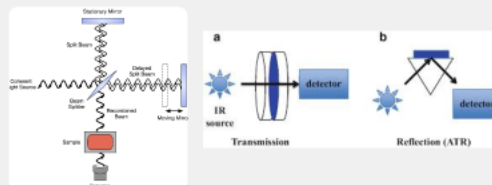
What it does:

- Identifies chemical bonds via IR absorption
- Each substance has a unique spectrum ("finger print")



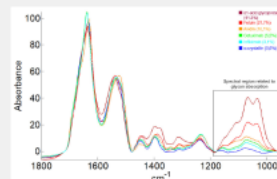
How it works:

- ATR: IR reflects through crystal, measures surface layers
- Transmission: IR passes through thin sample (less common at SNOLAB)



What Spectra Show

- X - axis = wavenumber ($1/\text{cm}$)
- Y - axis = Absorbance/Transmittance (But not limited)
- Peaks = Specific molecular vibrations (Functional Groups)
- Match to reference to ID materials/contaminants



A Quick Primer on FTIR

FTIR Basics

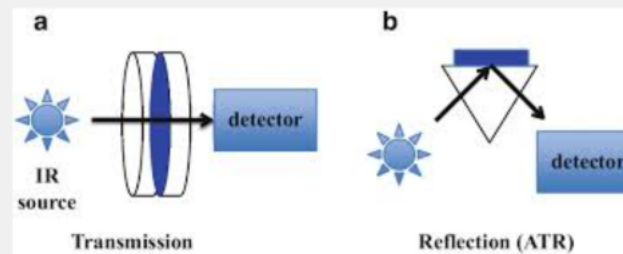
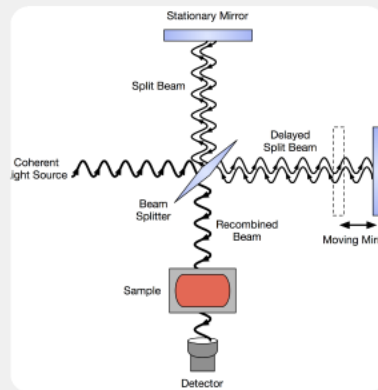
What it does:

- Identifies chemical bonds via IR absorption
- Each substance has a unique spectrum ("finger print")



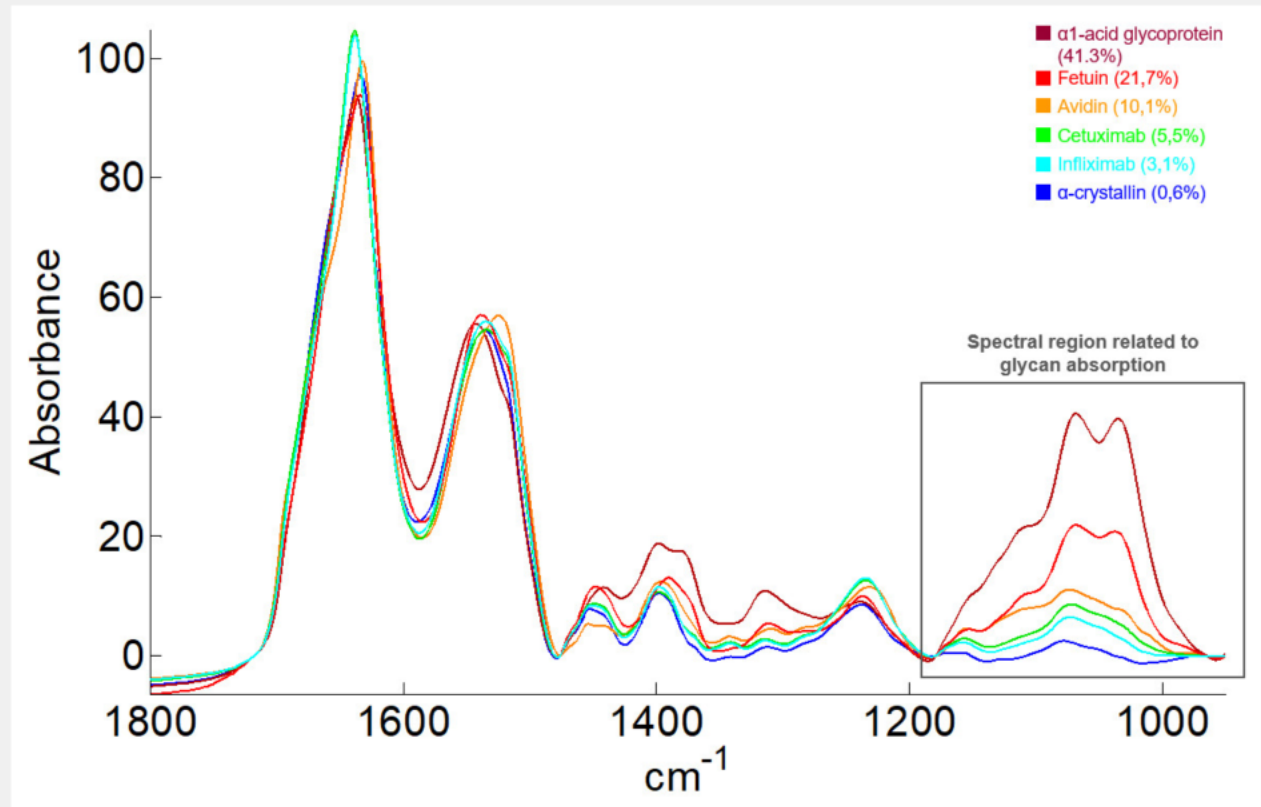
How it works:

- ATR: IR reflects through crystal, measures surface layers
- Transmission: IR passes through thin sample (less common at SNOLAB)



What Spectra Show

- X - axis = wavenumber ($1/\text{cm}$)
- Y - axis = Absorbance/Transmittance (But not limited)
- Peaks = Specific molecular vibrations (Functional Groups)
- Match to reference to ID materials/contaminants



Project Overview: Building a Spectral Reference Library

Creating a comprehensive spectral reference library is crucial for effective material verification at SNOLAB.

Learning Phase

- Mastered FTIR and OMNIC software
- Developed consistent scan parameters & cleaning SOP



Nicolet iS10
Rapid Sample Analysis and
Product Optimization



Nicolet 6700
Rational Development,
Analytical Support and R&D



OMNIC SOFTWARE



Nicolet iS5
Materials Inspection

What I needed to learn

★ Instrument capabilities

★ OMNIC tools

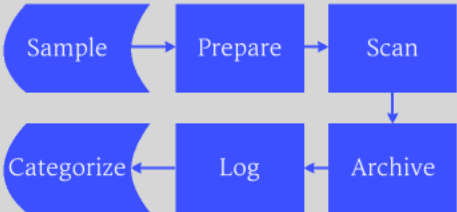
★ Background scanning

★ Scan setting

★ Sample contact/ATR cleaning

Library Build

- Scanned high-priority chemicals, materials, common contaminants
- Created structured folders + metadata system



■ Polyethylene	7/17/2025 3:08 PM
■ PVC Tubing (Polyvinyl Chloride)	7/17/2025 2:51 PM
■ Polypropylene	7/17/2025 2:41 PM
■ Nitrile Gloves	7/17/2025 2:32 PM
■ Krimble	7/17/2025 12:52 PM
■ Swab Tip	7/17/2025 11:56 AM
■ Sulfuric Acid	7/17/2025 11:20 AM
■ Nitric Acid	7/17/2025 11:19 AM
■ H2O-3, 240716, pH 11.84	7/14/2025 3:47 PM
■ H2O-2, 240806, pH 11, 240813	7/14/2025 3:46 PM
■ H2O-2, 240723, pH 11.85, 2024-07-30	7/14/2025 3:44 PM
■ H2O 240813	7/14/2025 3:03 PM
■ EDTA	7/11/2025 10:41 AM
■ Sodium Bicarbonate	7/6/2025 2:50 PM

Automation

- Python tool for functional group recognition

```
import numpy as np

def assign_functional_groups(wavenumber, shape, absorbance):
    matches = []
    partial_matches = []
    shape = shape.lower()
    for fg, wv_min, wv_max, shape, min_abs, max_abs in FUNCTIONAL_GROUPS:
        # Properly handle None for wv_min/wv_max
        if wv_min is not None and wv_max is not None:
            wv_match = wv_min < wavenumber < wv_max
        else:
            wv_match = False
        shape_match = shape in shapes or 'variable' in shapes
        absorbance_match = min_abs <= absorbance <= max_abs
        if wv_match and shape_match and absorbance_match:
            matches.append(fg)
        elif wv_match and shape_match:
            partial_matches.append(fg)
    return matches, partial_matches

# Strong absorbance (a > 0.35)
# Medium absorbance (a > 0.15 but < 0.35)
# Weak absorbance (a > 0.05 but < 0.15)

def make():
    n = int(input("How many peaks are being analyzed? "))
    except ValueError:
        pass

    # How many peaks are being analyzed? 3
    # Please enter the wavenumber (cm^-1), shape (sharp/broad), and absorbance (numeric) for each peak.
    # Peak 1:
    wavenumber (cm^-1): 1688
    Shape (Sharp, Broad, etc.): sharp
    Absorbance (numeric): 0.5

    # Peak 2:
    wavenumber (cm^-1): 1688
    Shape (Sharp, Broad, etc.): broad
    Absorbance (numeric): 0.3

    # Peak 3:
    wavenumber (cm^-1): 2555
    Shape (Sharp, Broad, etc.): sharp
    Absorbance (numeric): 0.7

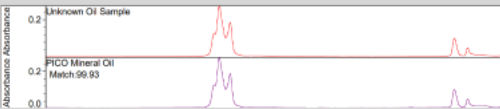
    # Peak Assignments with Shape/Absorbance Narrowing:
    Peak at 1688.0 cm^-1 (sharp, absorbance=0.5):
    Most likely functional groups:
    - Alkenes | Trisubstituted
    - Alkenes | Conjugated
    - Mononuclear Aromatics | C=C Ring Stretch
    - Ketones | Enol of 1,3-Diketone
    - Ketones | o - Hydroxy Aryl Ketone
    - Carboxylic Acids | Carboxylate Ion

    Peak at 1688.0 cm^-1 (broad, absorbance=0.3):
    No matching functional group found.

    Peak at 2555.0 cm^-1 (sharp, absorbance=0.7):
    Most likely functional groups:
    - Carboxylic Acids | Dimer
    - Amines | Ammonium Ion
```

Impact Assessment

- Faster, more consistent material verification with more accuracy and consistency



Index	Match	Compound Name
1	71	PICO Mineral Oil
2	32	POLY(ETHYLENE-PROPYLENE-DIENE)
3	637	Poly(ethylene-propylene:ethylenenorbornene)
4	629	Poly(ethylene-propylene:ethylenenorbornene)
5	252	Ethylene/propylene/diene terpolymer
6	107	Mineral oil
7	628	Poly(ethylene-propylene:diene)
8	758	Thermoplastic elastomer
9	1	TRIACONTANE, 99%
10	39	POLY(ETHYLENE-PROPYLENE)

CONCLUSION

Based on FTIR-ATR analysis, the unknown liquid sample from the PICO detector is conclusively identified as PICO's standard Mineral Oil, with a spectral similarity of 99.93%. There is no evidence of chemical deviation or contamination. The leak likely originated from the existing oil system used in the detector.

*****Note a similarity of 100% is generally not attainable as factors as minimal as CO2 and H2O content in the air can cause deviations in spectral readings*****

Learning Phase

- Mastered FTIR and OMNIC software
- Developed consistent scan parameters & cleaning SOP

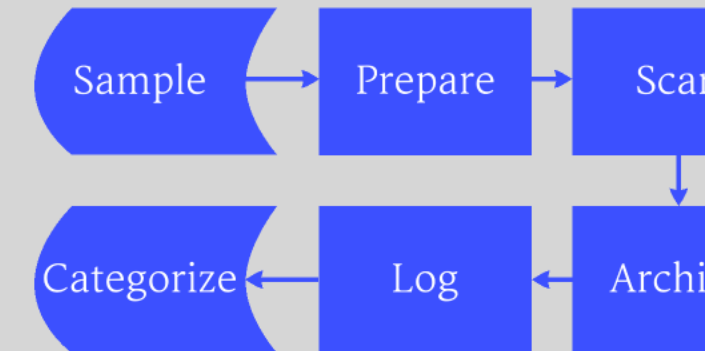


What I needed to learn

- ★ Instrument capabilities
- ★ Background scanning
- ★ Sample contact/ATR cleaning
- ★ OMNIC tools
- ★ Scan setting

Library Build

- Scanned high-priority chemical materials, common contaminants
- Created structured folders + metadata system



■ Polyethylene	7/17/2025 3:08 PM
■ PVC Tubing (Polyvinyl Chloride)	7/17/2025 2:51 PM
■ Polypropylene	7/17/2025 2:41 PM
■ Nitrile Gloves	7/17/2025 2:32 PM
■ Kimwipe	7/17/2025 12:12 PM
■ Swab Tip	7/17/2025 11:56 AM
■ Sulfuric Acid	7/17/2025 11:20 AM
■ Nitric Acid	7/17/2025 11:19 AM
■ HTiO-3, 240716, pH 11.84	7/14/2025 3:47 PM
■ HTiO-2, 240806, pH 11, 240813	7/14/2025 3:46 PM
■ HTiO-2, 240723, pH 11.85, 2024-07-30	7/14/2025 3:44 PM
■ HTiO 240813	7/14/2025 3:03 PM
■ EDTA	7/11/2025 10:41 AM
■ Sodium Bicarbonate	7/9/2025 2:50 PM

Training Phase

Mastered FTIR and OMNIC
Software
Developed consistent scan
parameters & cleaning SOP

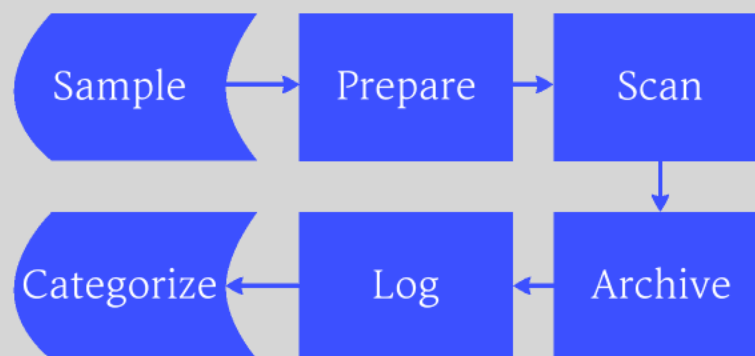


What I needed to learn

Instrument capabilities ★ OMNIC tools
Background scanning ★ Scan setting
Sample contact/ATR cleaning

Library Build

- Scanned high-priority chemicals, materials, common contaminants
- Created structured folders + metadata system



■ Polyethylene	7/17/2025 3:08 PM
■ PVC Tubing (Polyvinyl Chloride)	7/17/2025 2:51 PM
■ Polypropylene	7/17/2025 2:41 PM
■ Nitrile Gloves	7/17/2025 2:32 PM
■ Kimwipe	7/17/2025 12:12 PM
■ Swab Tip	7/17/2025 11:56 AM
■ Sulfuric Acid	7/17/2025 11:20 AM
■ Nitric Acid	7/17/2025 11:19 AM
■ HTiO-3, 240716, pH 11.84	7/14/2025 3:47 PM
■ HTiO-2, 240806, pH 11, 240813	7/14/2025 3:46 PM
■ HTiO-2, 240723, pH 11.85, 2024-07-30	7/14/2025 3:44 PM
■ HTiO 240813	7/14/2025 3:03 PM
■ EDTA	7/11/2025 10:41 AM
■ Sodium Bicarbonate	7/9/2025 2:50 PM

Automation

- Python tool for functional group recognition

```
import numpy as np

def assign_functional_groups(wavenumber, shape, absorbance):
    matches = []
    partial_matches = []
    shape = shape.lower()
    for fg, wn_min, wn_max, shapes, min_abs, max_abs in FUNCTIONAL_GROUPS:
        # Properly handle None for wn_min/wn_max
        if wn_min is not None and wn_max is not None:
            wn_match = wn_min <= wavenumber <= wn_max
        else:
            wn_match = False
        shape_match = shape in shapes or 'variable' in shapes
        absorbance_match = min_abs <= absorbance <= max_abs
        if wn_match and shape_match and absorbance_match:
            matches.append(fg)
        elif wn_match and shape_match:
            partial_matches.append(fg)
    return matches, partial_matches

# Strong absorbance is > 0.55
# Medium absorbance is > 0.15 but < 0.54
# Weak absorbance is > 0.00 but < 0.14

def main():
    try:
        n = int(input("How many peaks are being analyzed? "))
    except ValueError:
        pass

    # MONONUCLEAR AROMATICS
    # ALCOHOLS AND PHENOLS
    # ACETALS
    # ETHERS
```

Peak Assignments with Shape/Absorbance Narrowing:

Peak 1:
Wavenumber (cm⁻¹): 1600
Shape (sharp, broad, etc): sharp
Absorbance (numeric): 0.5

Peak 2:
Wavenumber (cm⁻¹): 3650
Shape (sharp, broad, etc): broad
Absorbance (numeric): 0.3

Peak 3:
Wavenumber (cm⁻¹): 2555
Shape (sharp, broad, etc): sharp
Absorbance (numeric): 0.7

Peak Assignments with Shape

Peak at 1600.0 cm⁻¹ (sharp)

Most likely functional

- Alkenes | Trisubstituted
- Alkenes | Conjugated
- Mononuclear Aromatic
- Ketones | Enol of 1,3-diketone
- Ketones | σ - Hydroxyketone
- Carboxylic Acids | Carboxylic Acid

Peak at 3650.0 cm⁻¹ (broad)

No matching functional

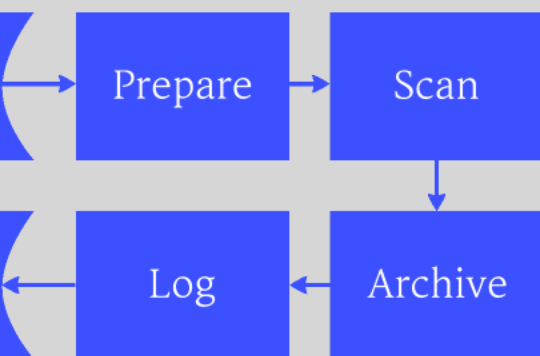
Peak at 2555.0 cm⁻¹ (sharp)

Most likely functional

- Carboxylic Acids | Dicarboxylic Acid
- Amines | Ammonium Ion

Build

high-priority chemicals,
common contaminants
structured folders +
system



lene	7/17/2025 3:08 PM
ing (Polyvinyl Chloride)	7/17/2025 2:51 PM
ylene	7/17/2025 2:41 PM
oves	7/17/2025 2:32 PM
	7/17/2025 12:12 PM
	7/17/2025 11:56 AM
Acid	7/17/2025 11:20 AM
id	7/17/2025 11:19 AM
240716, pH 11.84	7/14/2025 3:47 PM
240806, pH 11, 240813	7/14/2025 3:46 PM
240723, pH 11.85, 2024-07-30	7/14/2025 3:44 PM
0813	7/14/2025 3:03 PM
	7/11/2025 10:41 AM
Bicarbonate	7/9/2025 2:50 PM

Automation

- Python tool for functional group recognition

```
import numpy as np

def assign_functional_groups(wavenumber, shape, absorbance):
    matches = []
    partial_matches = []
    shape = shape.lower()
    for fg, wn_min, wn_max, shapes, min_abs, max_abs in FUNCTIONAL_GROUPS:
        # Properly handle None for wn_min/wn_max
        if wn_min is not None and wn_max is not None:
            wn_match = wn_min <= wavenumber <= wn_max
        else:
            wn_match = False
        shape_match = shape in shapes or 'variable' in shapes
        absorbance_match = min_abs <= absorbance <= max_abs
        if wn_match and shape_match and absorbance_match:
            matches.append(fg)
        elif wn_match and shape_match:
            partial_matches.append(fg)
    return matches, partial_matches

# Strong absorbance is > 0.55
# Medium absorbance is > 0.15 but < 0.54
# Weak absorbance is > 0.00 but < 0.14

def main():
    try:
        n = int(input("How many peaks are being analyzed? "))
    except ValueError:
        pass

    How many peaks are being analyzed? 3
    Please enter the wavenumber (cm^-1), shape (sharp/broad), and absorbance (numeric) for each peak.

    Peak 1:
    Wavenumber (cm^-1): 1600
    Shape (sharp, broad, etc): sharp
    Absorbance (numeric): 0.5

    Peak 2:
    Wavenumber (cm^-1): 3650
    Shape (sharp, broad, etc): broad
    Absorbance (numeric): 0.3

    Peak 3:
    Wavenumber (cm^-1): 2555
    Shape (sharp, broad, etc): sharp
    Absorbance (numeric): 0.7

    Peak Assignments with Shape/Absorbance Narrowing:
```

Peak Assignments with Shape/Absorbance Narrowing:

Peak at 1600.0 cm⁻¹ (sharp, absorbance=0.5):
Most likely functional groups:

- Alkenes | Trisubstituted
- Alkenes | Conjugated
- Mononuclear Aromatics | C=C Ring Stretch
- Ketones | Enol of 1,3-Diketone
- Ketones | σ - Hydroxy Aryl Ketone
- Carboxylic Acids | Carboxylate Ion

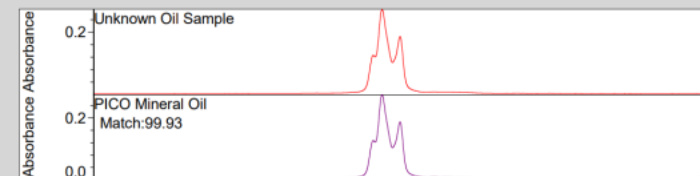
Peak at 3650.0 cm⁻¹ (broad, absorbance=0.3):
No matching functional group found.

Peak at 2555.0 cm⁻¹ (sharp, absorbance=0.7):
Most likely functional groups:

- Carboxylic Acids | Dimer
- Amines | Ammonium Ion

Impact Assessment

- Faster, more consistent material verification
more accuracy and consistency



	Index	Match	Compound Name
1	71	99.93	PICO Mineral Oil
2	32	92.36	POLY(ETHYLENE:PROPYLENE:DIENE)
3	637	91.93	Poly(ethylene:propylene:ethylidenetetracyclopentadiene)
4	629	91.30	Poly(ethylene:propylene:ethylidenetetracyclopentadiene)
5	252	88.72	Ethylene/propylene/diene terpolymer
6	107	87.43	Mineral oil
7	628	87.28	Poly(ethylene:propylene:diene)
8	758	87.26	Thermoplastic elastomer
9	1	87.11	TRIACONTANE, 99%
10	39	86.98	POLY(ETHYLENE:PROPYLENE)

CONCLUSION

Based on FTIR-ATR analysis, the unknown liquid sample from the PICO leak was conclusively identified as PICO's standard Mineral Oil, with a spectral similarity of 99.93%. There is no evidence of chemical deviation or contamination. The leak likely originated from the existing oil system used in the detector.

Note a similarity of 100% is generally not attainable as factors as minimal H2O content in the air can cause deviations in spectral readings

Note a similarity of 100% is generally not attainable as factors as minimal as CO2 and H2O content in the air can cause deviations in spectral readings

Project Overview: Building a Spectral Reference Library

Creating a comprehensive spectral reference library is crucial for effective material verification at SNOLAB.

Learning Phase

- Mastered FTIR and OMNIC software
- Developed consistent scan parameters & cleaning SOP

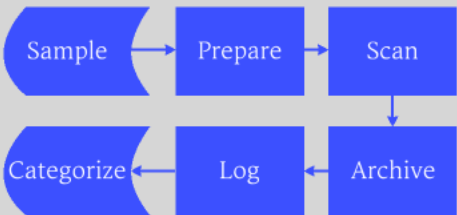


What I needed to learn

- ★ Instrument capabilities
- ★ OMNIC tools
- ★ Background scanning
- ★ Scan setting
- ★ Sample contact/ATR cleaning

Library Build

- Scanned high-priority chemicals, materials, common contaminants
- Created structured folders + metadata system



■ Polyethylene	7/17/2025 3:08 PM
■ PVC Tubing (Polyvinyl Chloride)	7/17/2025 2:51 PM
■ Polypropylene	7/17/2025 2:41 PM
■ Nitrile Gloves	7/17/2025 2:32 PM
■ Krimble	7/17/2025 12:52 PM
■ Swab Tip	7/17/2025 11:56 AM
■ Sulfuric Acid	7/17/2025 11:20 AM
■ Nitric Acid	7/17/2025 11:19 AM
■ H2O-3, 240716, pH 11.84	7/14/2025 3:47 PM
■ H2O-2, 240806, pH 11, 240813	7/14/2025 3:46 PM
■ H2O-2, 240723, pH 11.85, 2024-07-30	7/14/2025 3:44 PM
■ H2O 240813	7/14/2025 3:03 PM
■ EDTA	7/11/2025 10:41 AM
■ Sodium Bicarbonate	7/6/2025 2:50 PM

Automation

- Python tool for functional group recognition

```
import numpy as np

def assign_functional_groups(wavenumber, shape, absorbance):
    matches = []
    partial_matches = []
    shape = shape.lower()
    for fg, wv_min, wv_max, shape_min, max_abs in FUNCTIONAL_GROUPS:
        # Properly handle None for wv_min/wv_max
        if wv_min is not None and wv_max is not None:
            wv_match = wv_min < wavenumber < wv_max
        else:
            wv_match = False
        shape_match = shape in shapes or 'variable' in shapes
        absorbance_match = min_abs <= absorbance <= max_abs
        if wv_match and shape_match and absorbance_match:
            matches.append(fg)
        elif wv_match and shape_match:
            partial_matches.append(fg)
    return matches, partial_matches

# Strong absorbance (> 0.35)
# Medium absorbance (> 0.15 but < 0.35)
# Weak absorbance (> 0.05 but < 0.15)

def main():
    n = int(input("How many peaks are being analyzed? "))
    except ValueError:
        pass

    # How many peaks are being analyzed? 3
    # Please enter the wavenumber (cm^-1), shape (sharp/broad), and absorbance (numeric) for each peak.
    # Peak 1:
    # Wavenumber (cm^-1): 1688
    # Shape (sharp, broad, etc.): sharp
    # Absorbance (numeric): 0.5
    # Peak 2:
    # Wavenumber (cm^-1): 1688
    # Shape (sharp, broad, etc.): broad
    # Absorbance (numeric): 0.3
    # Peak 3:
    # Wavenumber (cm^-1): 2555
    # Shape (sharp, broad, etc.): sharp
    # Absorbance (numeric): 0.7

    # Peak Assignments with Shape/Absorbance Narrowing:
    # Peak at 1688.0 cm^-1 (sharp, absorbance=0.5):
    # Most likely functional groups:
    # - Alkenes | Trisubstituted
    # - Alkenes | Conjugated
    # - Mononuclear Aromatics | C=C Ring Stretch
    # - Ketones | Enol of 1,3-Diketone
    # - Ketones | o - Hydroxy Aryl Ketone
    # - Carboxylic Acids | Carboxylate Ion

    # Peak at 1688.0 cm^-1 (broad, absorbance=0.3):
    # No matching functional group found.

    # Peak at 2555.0 cm^-1 (sharp, absorbance=0.7):
    # Most likely functional groups:
    # - Carboxylic Acids | Dimer
    # - Amines | Ammonium Ion
```

Impact Assessment

- Faster, more consistent material verification with more accuracy and consistency



Index	Match	Compound Name
1	71	PICO Mineral Oil
2	32	POLY(ETHYLENE-PROPYLENE-DIENE)
3	637	Poly(ethylene-propylene:ethylenenorbornene)
4	629	Poly(ethylene-propylene:ethylenenorbornene)
5	252	Ethylene/propylene/diene terpolymer
6	107	Mineral oil
7	628	Poly(ethylene-propylene:diene)
8	758	Thermoplastic elastomer
9	1	TRIACONTANE, 99%
10	39	POLY(ETHYLENE-PROPYLENE)

CONCLUSION

Based on FTIR-ATR analysis, the unknown liquid sample from the PICO detector is conclusively identified as PICO's standard Mineral Oil, with a spectral similarity of 99.93%. There is no evidence of chemical deviation or contamination. The leak likely originated from the existing oil system used in the detector.
Note a similarity of 100% is generally not attainable as factors as minimal as CO2 and H2O content in the air can cause deviations in spectral readings

**Future of the
SNO-
Library(ies)**

Library Access

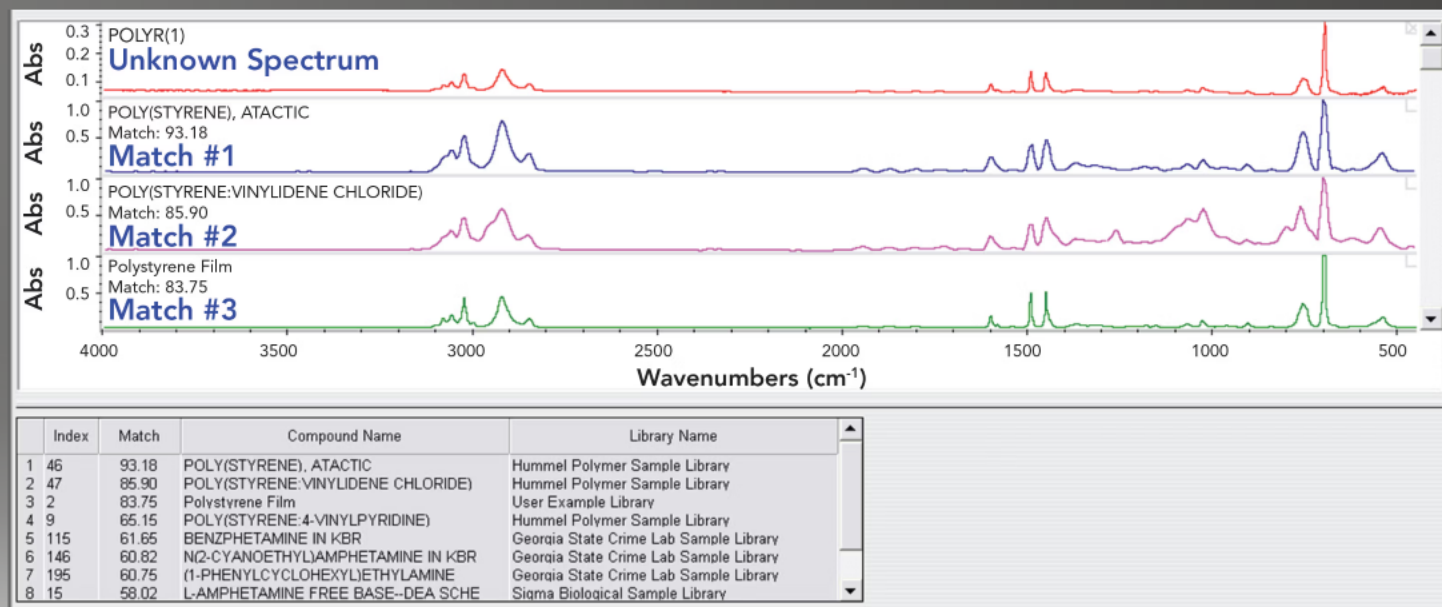
- Access to ~10 libraries
- Made in-lab + externally

Spectra Access

- 100+ spectra scanned in-lab + added to library
- 1000+ overall spectra

Future?

- Ability to create new libraries
- Ability to add to current libraries
 - International collaboration opportunity???



- Thermo Nicolet high quality commercial collections of FT-IR and Raman Spectral Libraries encompassing some 258,000 compounds are available

Future of the SNO- Library(ies)

Library Access

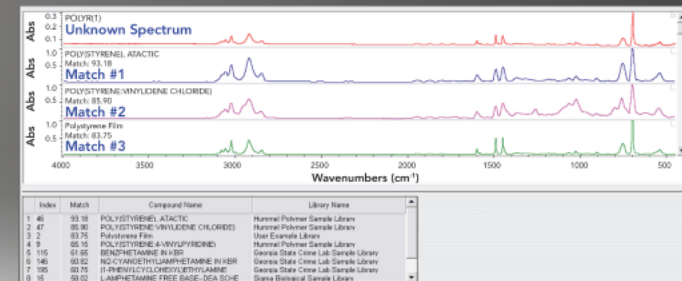
- Access to ~10 libraries
- Made in-lab + externally

Spectra Access

- 100+ spectra scanned in-lab + added to library
- 1000+ overall spectra

Future?

- Ability to create new libraries
- Ability to add to current libraries
- International collaboration opportunity???



- Thermo Nicolet high quality commercial collections of FT-IR and Raman Spectral Libraries encompassing some 258,000 compounds are available

- Input peak wavenumber, shape, absorbance
- Script matches to functional groups
- Flags full and partial matches

How many points are being analyzed?

Peak 1:

WaveNumber (cm⁻¹):

Shape (sharp, broad, etc):

Absorbance (numeric):

How many points are being analyzed? 1

Please enter the wavenumber (cm⁻¹), shape (sharp/broad), and absorbance (numeric) for each peak.

Peak 1:

Wavenumber (cm⁻¹): 3000

Shape (sharp, broad, etc): Sharp

Absorbance (numeric): 0.8

Peak Assignments with Shape/Absorbance Handwriting:

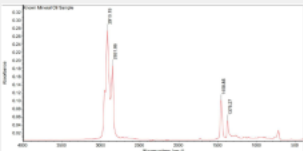
Peak at 3000.0 cm⁻¹ (sharp, absorbance=0.8)
best fit(s) to functional group:
Alcohol(s) and Phenol(s) | Free OH

Alcohol(s) and Phenol(s) | Secondary/tertiary Alcohol(s)

- Simple prompts, no programming skills needed
- Reduces learning curve for FTIR users
- Clear, readable results

[illegible]

- Faster unknown identification
- Consistent, reproducible analysis



```

Peak at 1450.0 eV x1 (sharp, abundance=0.12):
Next likely functional groups:
- Monocyclic Aromatics | C=O Ring Stretch
- Phosphorus Compounds | P=O
- Phosphorus Compounds | P=OR

```

```

Peak at 1370.4 eV x1 (sharp, abundance=0.05):
Next likely functional groups:
- Iodoarenes
- Silicon Compounds | SiOR
- Silicon Compounds | SiOR2

```

```

Peak at 285.0 eV x1 (sharp, abundance=0.1):
Next likely functional groups:
- Alkenes
- Alkenynes | Alkyl
- Alkenynes | Amino | Secondary
- Alkenes | Amino | Tertiary
- Alkenes | Amino | Sulfonamide

```

```
import numpy as np

def assign_functional_groups(wavenumber, shape, absorbance):
    matches = []
    partial_matches = []
    shape = shape.lower()
    for fg, wn_min, wn_max, shapes, min_abs, max_abs in FUNCTIONAL_GROUPS:
        # Properly handle None for wn_min/wn_max
        if wn_min is not None and wn_max is not None:
            wn_match = wn_min <= wavenumber <= wn_max
        else:
            wn_match = False
        shape_match = shape in shapes or 'variable' in shapes
        absorbance_match = min_abs <= absorbance <= max_abs
        if wn_match and shape_match and absorbance_match:
            matches.append(fg)
        elif wn_match and shape_match:
            partial_matches.append(fg)
    return matches, partial_matches
```

```
#Strong absorbance is > 0.55
#Medium absorbance is > 0.15 but < 0.54
#Weak absorbance is > 0.00 but < 0.14
```

```
def main():
    try:
        n = int(input("How many peaks are being analyzed? "))
    except ValueError:
        print("Invalid number. Exiting.")
        return
```

```
peaks = []
print("Please enter the wavenumber (cm^-1), shape (sharp/broad), and
for i in range(n):
    print(f"\nPeak {i+1}:")
    while True:
        try:
            wn = float(input(" Wavenumber (cm^-1): "))
            break
        except ValueError:
            print(" Please enter a valid number for wavenumber.")
    shape = input(" Shape (sharp, broad, etc): ").strip().lower()
    while True:
        try:
            absorbance = float(input(" Absorbance (numeric): "))
            break
        except ValueError:
```

Automating Functional Group Recognition with Python

Streamlined Data Analysis

- Input peak wavenumber, shape, absorbance
- Script matches to functional groups
- Flags full and partial matches

How many peaks are being analyzed?

Peak 1:

Wavenumber (cm⁻¹):

Shape (sharp, broad, etc):

Absorbance (numeric):

How many peaks are being analyzed? 1

Please enter the wavenumber (cm⁻¹), shape (sharp/broad), and absorbance (numeric) for each peak.

Peak 1:

Wavenumber (cm⁻¹): 3650

Shape (sharp, broad, etc): Sharp

Absorbance (numeric): 0.5

Peak Assignments with Shape/Absorbance Narrowing:

Peak at 3650.0 cm⁻¹ (sharp, absorbance=0.5):

Most likely functional groups:

- Alcohols and Phenols | Free OH
- Alcohols and Phenols | Intramolecular Bonded (weak)

Increased Accessibility

- Simple prompts, no programming skills needed
- Reduces learning curve for FTIR users
- Clear, readable results

```
# ISOTHIOCYANATES (RNCS) $
('Isothiocyanates | Alkyl', 1990, 2360, ['sharp'], 0.55, 14.0),
('Isothiocyanates | Alkyl', 650, 720, ['sharp'], 0.15, 0.54),
('Isothiocyanates | Aromatic', 2050, 2320, ['sharp'], 0.55, 14.0),
('Isothiocyanates | Aromatic', 900, 970, ['sharp'], 0.15, 0.54),

# NITRO COMPOUNDS $
('Nitro Compounds | Aliphatic', 1520, 1580, ['sharp'], 0.55, 14.0),
('Nitro Compounds | Aliphatic', 1320, 1400, ['sharp'], 0.15, 0.54),
('Nitro Compounds | Aromatic', 1510, 1570, ['sharp'], 0.55, 14.0),
('Nitro Compounds | Aromatic', 1315, 1400, ['sharp'], 0.15, 0.54),
('Nitro Compounds | Conjugated', 1500, 1560, ['sharp'], 0.55, 14.0),
('Nitro Compounds | Conjugated', 1290, 1385, ['sharp'], 0.15, 0.54),
('Nitro Compounds | Nitramine', 1575, 1625, ['sharp'], 0.55, 14.0),
('Nitro Compounds | Nitramine', 1275, 1350, ['sharp'], 0.55, 14.0),

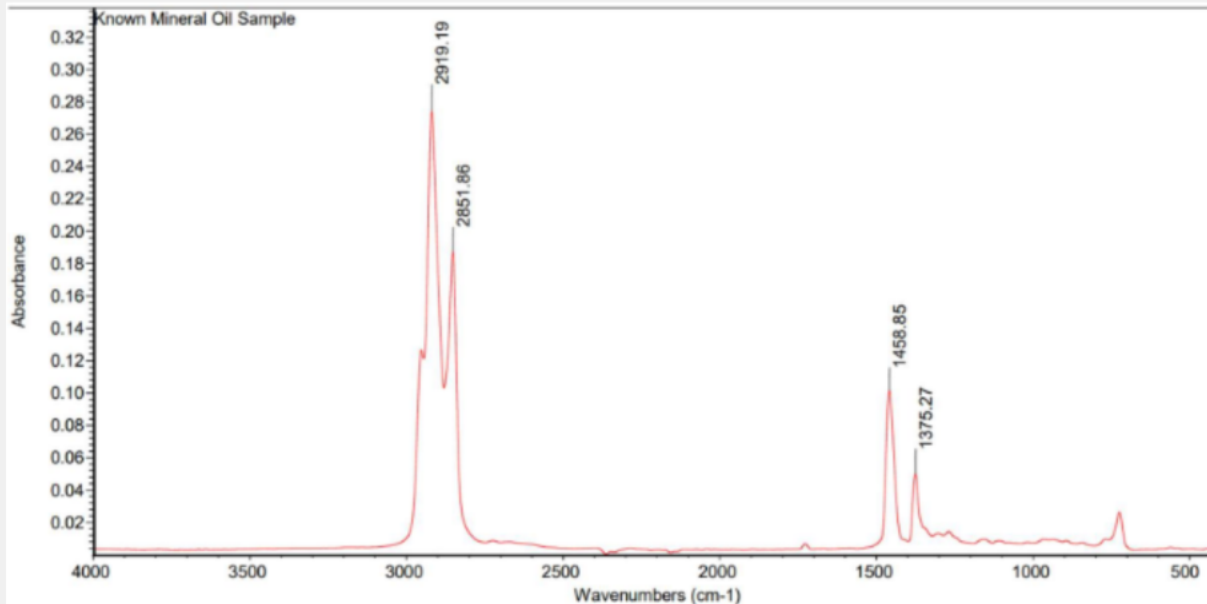
# NITROSOAMINES $
('Nitrosoamines | Vapor', 1515, 1595, ['sharp'], 0.55, 14.0),
('Nitrosoamines | Liquid', 1505, 1585, ['sharp'], 0.55, 14.0),

# NITRATES (RONO2) $
('Nitrates', 1600, 1680, ['sharp'], 0.55, 14.0),
('Nitrates', 1200, 1310, ['sharp'], 0.55, 14.0),
('Nitrates', 800, 870, ['sharp'], 0.55, 14.0),
```

Enhanced Efficiency in Research

- Faster unknown identification

- Consistent, reproducible analysis



Peak at 1458.0 cm⁻¹ (sharp, absorbance=0.12):

Most likely functional groups:

- Mononuclear Aromatics | C=C Ring Stretch
- Phosphorus Compounds | PCH₃
- Phosphorus Compounds | PC₆H₅

Peak at 1375.0 cm⁻¹ (sharp, absorbance=0.08):

Most likely functional groups:

- Isocyanates
- Silicon Compounds | SiCH₃
- Silicon Compounds | SiCH₂

Peak at 2919.0 cm⁻¹ (sharp, absorbance=0.3):

Most likely functional groups:

- Alkanes
- Aldehydes | Alkyl
- Aldehydes | Aromatic - Conjugated
- Amines | Amine Salts Primary
- Amines | Amine Salts Secondary

Peak at 2851.0 cm⁻¹ (sharp, absorbance=0.2):


Most likely functional groups:

- Alkanes
- Aldehydes | Alkyl
- Aldehydes | Aromatic - Conjugated
- Amines | Amine Salts Primary
- Amines | Amine Salts Secondary

FTIR's Growing Significance in SNOLAB's Workflows

FTIR's capabilities are now fully realized at SNOLAB, enabling rapid chemical identification, QA/QC assurance, and unknown material analysis with minimal sample prep.

With a growing spectral library and functional group automation, FTIR is becoming a foundational tool across research, operations, and contamination control.



Sample Date: July 17th 2025
Date of Analysis: July 22nd 2025

Data For: Shane Meister
Email: shane.meister@snolab.ca
Project: PICO
Analyst: Cameron Van Der Zyl

Unknown PICO leak Sample (OSA#2111)



Sample Date: May 29th 2025
Date of Analysis: May 29th 2025

Data For: Angela Hesketh | Olivia Conrad
Email: ahesketh@snolab.ca | oonrad@snolab.ca
Project: SNOLAB
Analyst: Cameron Van Der Zyl

Particle Counter – Lab A Surface Facility Sample



Sample Date: Late May | To surface June 6th 2025
Date of Analysis: June 9th 2025

Data For: Regan Picotte
Email: rpicotte@snolab.ca
Project: CUTE
Analyst: Cameron Van Der Zyl

CUTE Unknown Waste Sample (OSA#2094)



Sample Date: May 20th 2025
Date of Analysis: May 26th 2025

Data For: Ashley Mathewson
Email: ashley.mathewson@snolab.ca
Project: PICO

PICO Chiller Samples (OSA-2083)



Future Prospects of FTIR at SNOLAB

Exploring advanced applications in material verification and contamination analysis.

Applications

- Fingerprint more materials and reagents

Quantitative use:

- Verify supplier quality
- Degredation of chemicals with time



Enhanced Contamination Forensics

- Build signature database from past incidents



Training

- With the help of intuitive workflows, guided procedures, and the functional group recognition script, new users can be trained faster and with fewer errors.
- This lowers the barrier for entry and empowers researchers, technicians, and students alike to use FTIR as a standard tool in their investigations.



Applications

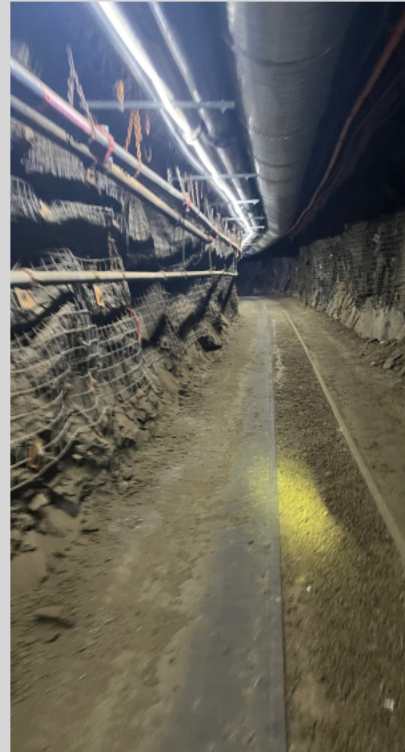
Enhanced

- Fingerprint more materials and reagents

Quantitative use:

- Verify supplier quality
- Degredation of chemicals with time

- Build signature d



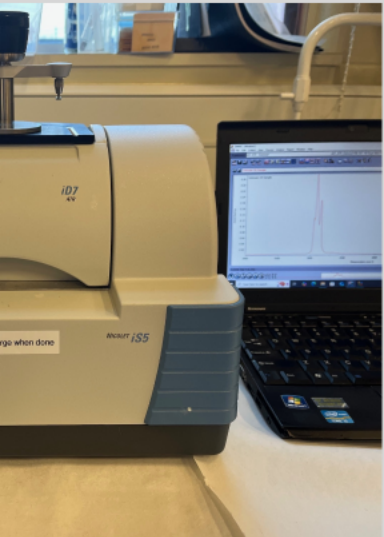
Enhanced Contamination Forensics

Reagents

- Build signature database from past incidents

- With the help of interdisciplinary functional group recognition, faster and with fewer reagents
- This lowers the barrier to entry for technicians, and students in their investigations.

me



- With the help of intuitive workflows, guided procedures, and the functional group recognition script, new users can be trained faster and with fewer errors.
- This lowers the barrier for entry and empowers researchers, technicians, and students alike to use FTIR as a standard tool in their investigations.





Future Prospects of FTIR at SNOLAB

Exploring advanced applications in material verification and contamination analysis.

Applications

- Fingerprint more materials and reagents

Quantitative use:

- Verify supplier quality
- Degredation of chemicals with time



Enhanced Contamination Forensics

- Build signature database from past incidents



Training

- With the help of intuitive workflows, guided procedures, and the functional group recognition script, new users can be trained faster and with fewer errors.
- This lowers the barrier for entry and empowers researchers, technicians, and students alike to use FTIR as a standard tool in their investigations.



The Indispensable Role of FTIR in Clean Science

The Indispensable Role of FTIR in Clean Science

FTIR spectroscopy has become a cornerstone in the pursuit of ultra-clean environments at SNOLAB. Its ability to rapidly identify trace-level contaminants, verify materials, and provide non-destructive analysis ensures that cleanliness is not just maintained — it is provable, repeatable, and continuously improvable.

By transforming a previously underutilized tool into a reliable frontline technique, FTIR empowers both research integrity and operational excellence. It bridges the gap between chemistry and contamination control, offering real-time insight where precision matters most.

As SNOLAB continues to push the boundaries of low-background physics, FTIR now stands as a guardian of purity — enabling cleaner science and stronger discoveries.





Applications Inquiry

Curious about how FTIR fits into your research or lab work? Let's talk use cases.



Results Discussion

Want to dive deeper into spectral interpretation or the script's logic? (maybe email me about this or pull me for a chat later on!)



Future Prospects

Interested in where FTIR could go next at SNOLAB or in clean science more broadly?



Q&A Session

Expanding FTIR Capabilities at SNOLAB: Building a Chemical and Materials Spectral Database

Utilizing FTIR Spectroscopy for Accurate Material Verification and Contamination Control at SNOLAB



Cameron Van Der Zyl
Analytical Chemistry Program Research Assistant