How to Select an Infrared Transmission Window

Currently, there are over a dozen different infrared window materials to choose from, each with its own characteristic properties. There are several factors that must be considered when choosing the optimum window material for your application needs. To select your window material, consider the spectral range to be studied, the chemical properties of the sample versus that of the window, the physical properties of the window, and finally the relative cost for the specific need.

The factors affecting the amount of energy through the transmission cell (exclusive of the sample) are: the transmission range of the window, the effective thickness of the window, the amount of energy lost due to reflection at the window surfaces, and the energy losses due to usage, such as marring and fogging. The useful transmission range that are listed below were established at the point where the transmission level falls off to 50% for a single window. Thin windows of the same material will transmit to lower wavenumbers. When using windows with a high refractive index, there will be significant energy losses due to reflections through the window, and there will be strong sinusoidal waves, called interference fringes. These interference fringes are caused by the reflection of infrared radiation within a cell that has window material that is plane parallel to the surface. The intensity of the fringes is dictated by the refractive index of the material, the greater the refractive index the stronger the fringes. The air gap between the windows of a cell defines the frequency of the fringes, a small gap (a 0.015 mm pathlength cell) gives a high frequency of fringes, a large gap (0.50 mm pathlength cell) gives a low frequency of fringes. The fringe pattern is very useful in calculating the pathlength of the cell (see *How to Calibrate Infrared Absorption Cells*).

An important factor to consider when choosing the appropriate windows for a specific application are the chemical properties of both the sample and windows. Samples that react with the windows in a cell will of course erode the inner surfaces. The relative water solubility, and the common samples or solvents that will erode the window surfaces is often listed in property charts. Solubility data is given in terms of the number of grams of the material that under equilibrium conditions will dissolve in 100 milliliters of water at room temperature. The solubility in water should not be confused with the degree to which a window material is hygroscopic. A material that is hygroscopic readily absorbs water from the atmosphere and will cause the window to fog or become opaque.

An ideal window material must also be compatible with the physical properties of the sample; such as hardness. With a very hard sample, soft window materials should not be used. To a large extent, the measures of hardness are empirical and comparative. Most methods of measuring hardness are based on pressing a material with a specified force with an indentor of a prescribed shape. The shape determines whether the method is called Brinell, Vickers, or Knoop. Hardness measurements can vary with applied load, duration of the load and speed of application and release. The variability depends on material properties of creep, cold flow, and stress relief by minute cracks. Some of the softer materials, such as potassium bromide and sodium chloride can be repolished by hand when they become etched or scratched. The very hard materials, such as silicon and sapphire resist scratching, but are extremely difficult to repolish by hand.

Two basic types of transmission cells can be selected; sealed cells with the appropriate holder, or demountable cells with the appropriate holder. A sealed cell has precision aligned windows and provides leakproof operation. It consists of one drilled window and one undrilled window sealed together. The windows are separated by a metal spacer that determines the pathlength, and are amalgam sealed together. Sealed cells have a shelf life of approximately 12 months, because of the amalgam seal. The windows are perfectly parallel and the pathlength is fixed, therefore the cell can easily be calibrated for quantitative measurements and other precision spectroscopic analyses. Sealed cells can be used with highly volatile samples, such as ethyl ether, without the risk of leakage.

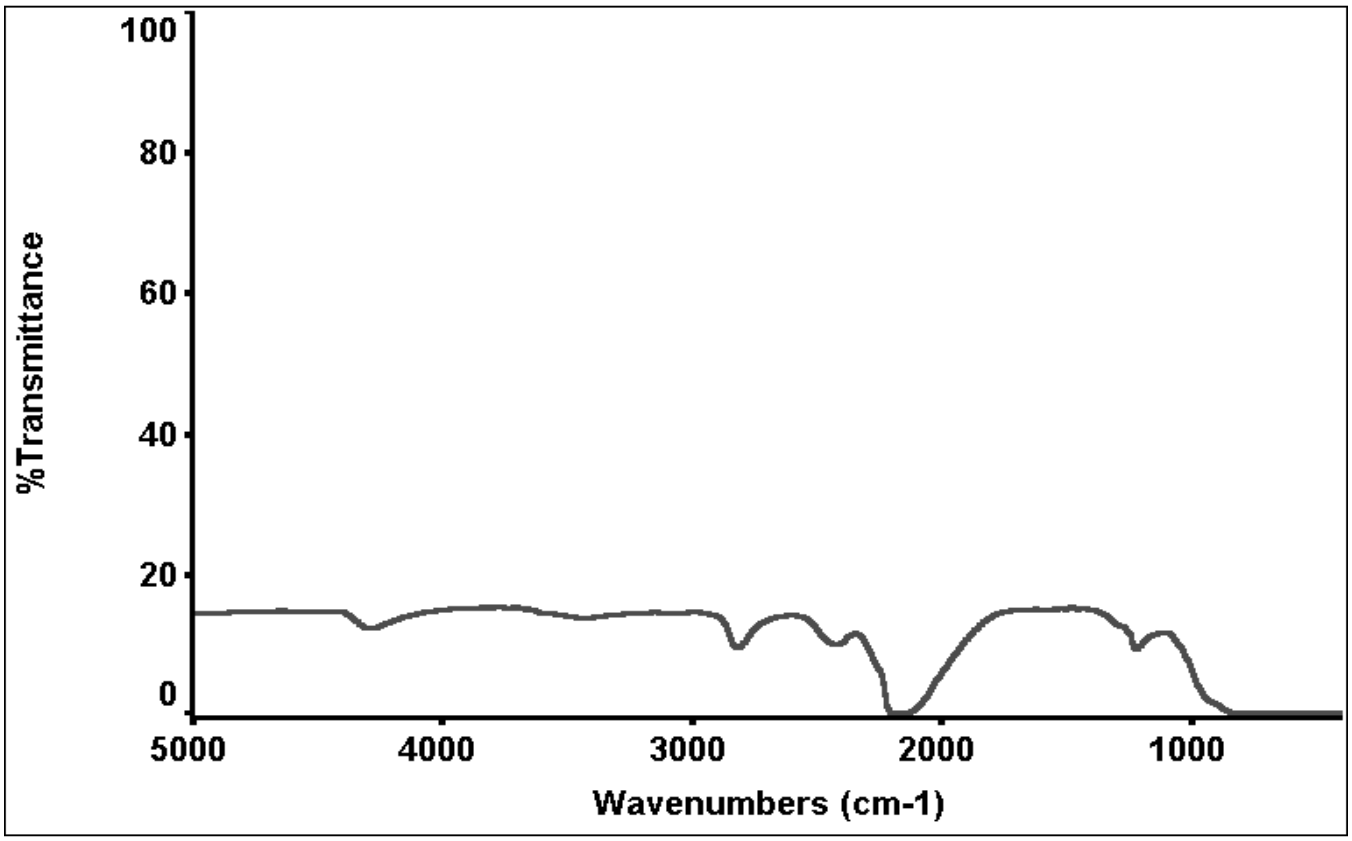
Demountable cells are a practical and economical alternative to sealed cells. Demountable refers to the ability to easily change, and polish the windows in the cell. These cells are composed of one drilled window, one undrilled window of the same size and material, a spacer (which is typically Teflon*), and a gasket. These cells are invaluable when used with viscous, or hard to clean samples, because they can be easily disassembled, cleaned and reassembled. A demountable cell should be used when the correct pathlength for a specific application is not known, and experimental determination is required. The pathlength of demountable cells can be altered by changing the spacer because they are not amalgamed together as in sealed cells.

* *Teflon is a registered trademark of Dupont Corporation.*

SpectraTech

Chalcogenide (AsSeTe Glass)

Chalcogenide is the best material for mid-Infrared Fiber Optics. The Chalcogenide fiber is composed of AsSeTe glass, is chemically inert and mid-infrared transmissive. The useful pH is 1-9.



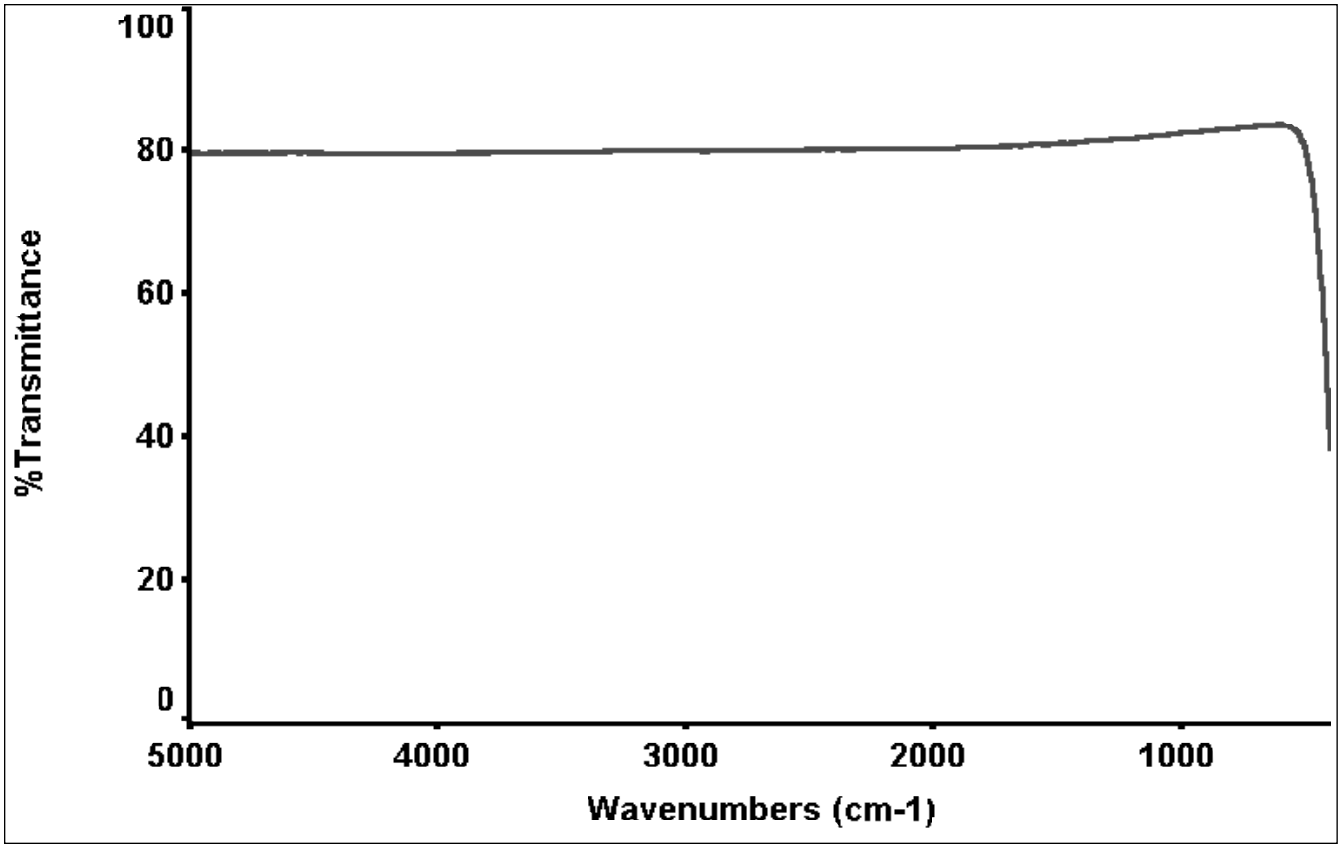
Specifications

CAS #	NA
Transmission Range	4,000-900 cm^{-1}
Refractive Index	2.8
% Transmittance (thickness)	15 (1.5m cable)
Cleaning Agents	water, Acetone, CH_2Cl_2
Solubility in Water (100g H_2O @25°C)	insoluble
Solvents which attack	strong acids, bases
Max Temp in Air °C	100
Melting Point °C	170
Hardness kg/mm^2 (Knoop #)	NA
Composition	Single Crystal
Crystal Class	Cubic

SPECTRA-TECH

Silver Chloride (AgCl)

Silver Chloride is a non-hygroscopic material. It darkens with prolonged exposure to UV light and is soft. Prolonged contact with base metals where moisture is present will cause corrosion. AgCl is malleable and will cold flow under pressure. It is insensitive to thermal and mechanical shock. Used for infrared transmission cell windows.



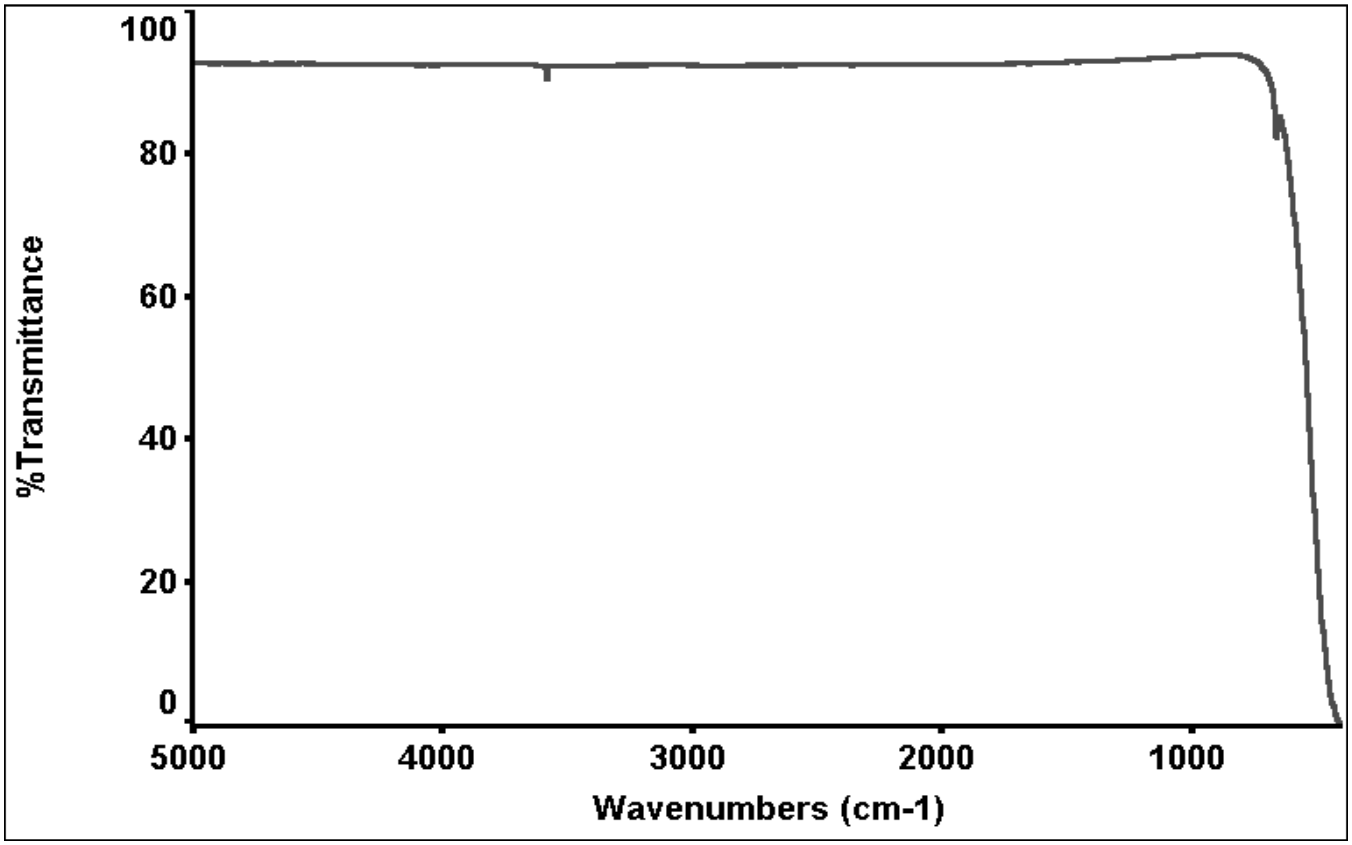
Specifications

CAS #	7783-96-2
Transmission Range	25,000-360 cm^{-1}
Refractive Index	1.98
% Transmittance (thickness)	84.0 (3mm)
Cleaning Agents	Acetone CH_2Cl_2
Solubility in Water (100g H_2O @25°C)	.00015 grams
Solvents which attack	Complexing Agents, NH_4OH
Max Temp in Air °C	200
Melting Point °C	457.7
Hardness kg/mm^2 (Knoop #)	9.5
Composition	Single Crystal
Crystal Class	Cubic, does not cleave

SPECTRA-TECH

Sodium Chloride (NaCl)

One of the most useful materials because of its useful spectral range and low cost. NaCl withstands thermal and mechanical stress fairly well and is easily polished. Major disadvantage: It is soluble in water. Used for infrared transmission cell windows.



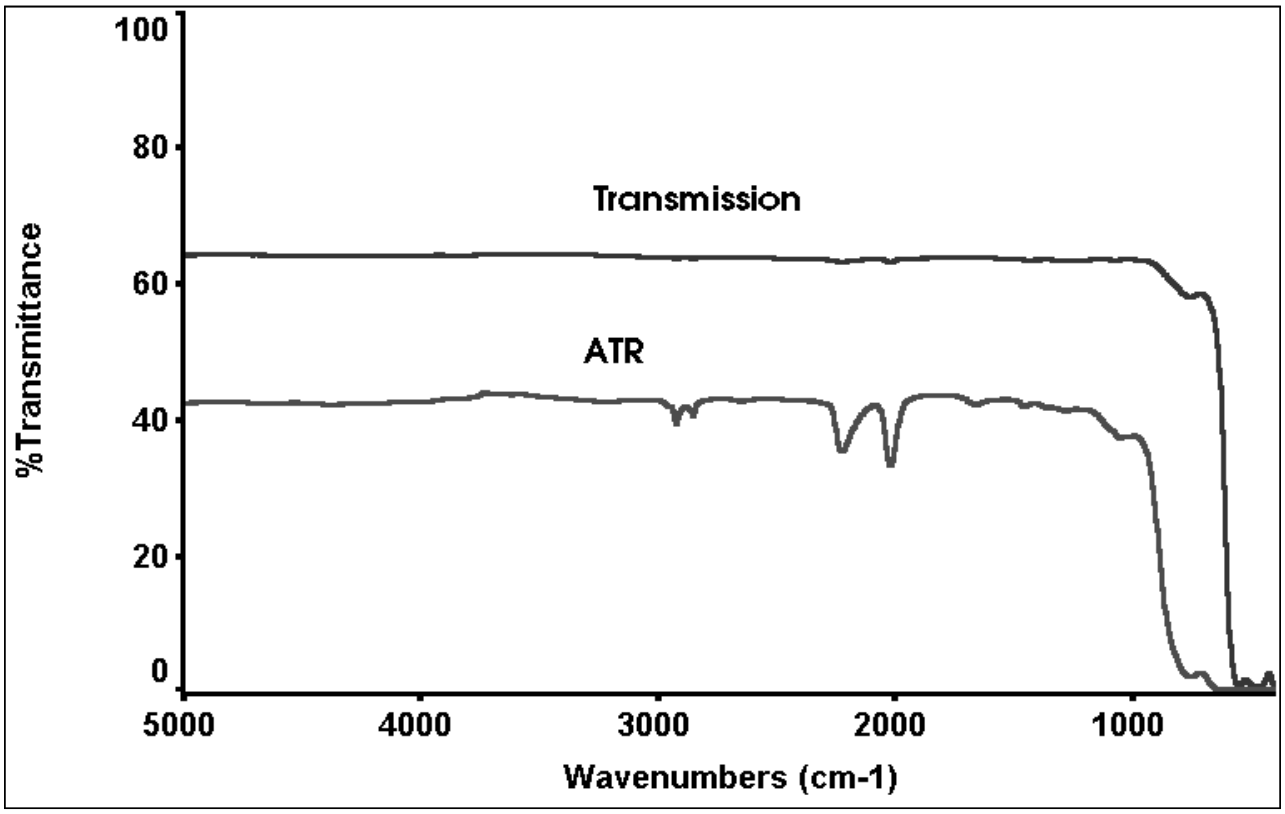
Specifications

CAS #	7647-14-5
Transmission Range	40,000-625 cm^{-1}
Refractive Index	1.49
% Transmittance (thickness)	91.5 (4.0mm)
Cleaning Agents	anhydrous solvents
Solubility in Water (100g H_2O @25°C)	35.7 grams
Solvents which attack	lower alcohols, wet solvents
Max Temp in Air °C	400
Melting Point °C	801
Hardness kg/mm^2 (Knoop #)	15
Composition	Single crystal
Crystal Class	Simple cubic, cleaves on (100) planes

SPECTRA-TECH

AMTIR (GeAsSe Glass)

AMTIR-1 (Amorphous Material Transmitting Infrared Radiation) GeAsSe Glass is insoluble in water and very resistant to corrosion in acidic solutions. In case of long term exposure (one week), it will dissolve in alkaline solutions. It can be used to 300°C. Good ATR Material.



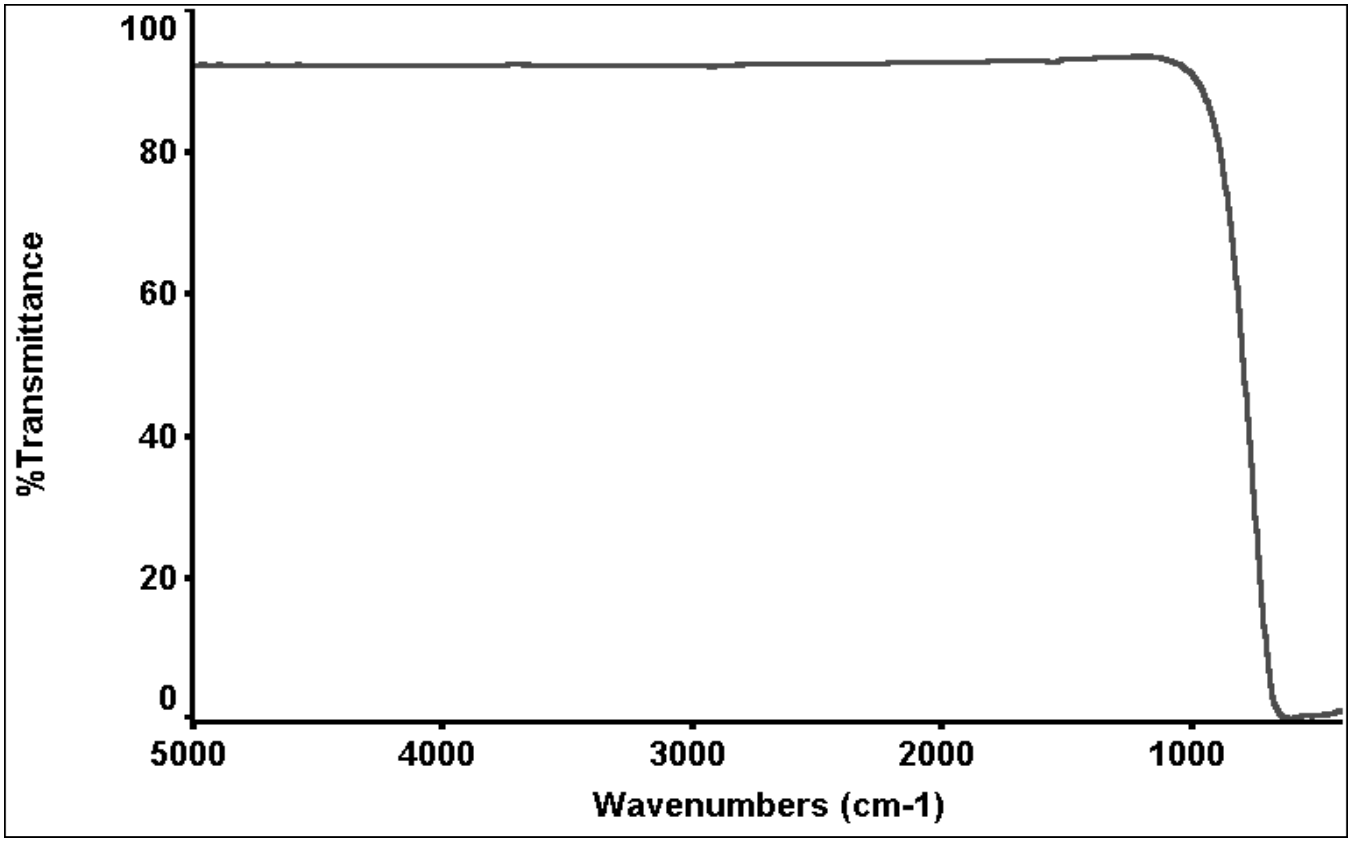
Specifications

CAS #	NA
Transmission Range	11,000-625 cm^{-1}
ATR Spectral Range (12 reflection crystal)	11,000-840 cm^{-1}
Refractive Index	2.5
% Transmittance (thickness)	68% (2mm)
Cleaning Agents	Alcohol, Acetone, H_2O
Solubility in Water ($100g\ H_2O$ @25°C)	insoluble
Solvents which attack	Alkalies
Max Temp in Air °C	300
Melting Point °C	370
Hardness kg/mm^2 (Knoop #)	170

SPECTRA-TECH

Barium Fluoride (BaF_2)

BaF_2 has greater transmission range than CaF_2. BaF_2 must be handled with care because it is easily cleaved by thermal or mechanical shock. The useful temperature range is narrower than for CaF_2 because BaF_2 reacts with air at 500°C and can be used only to 800°C in a dry atmosphere. It should not be used with solutions of ammonium salts. Used for infrared transmission cell windows.



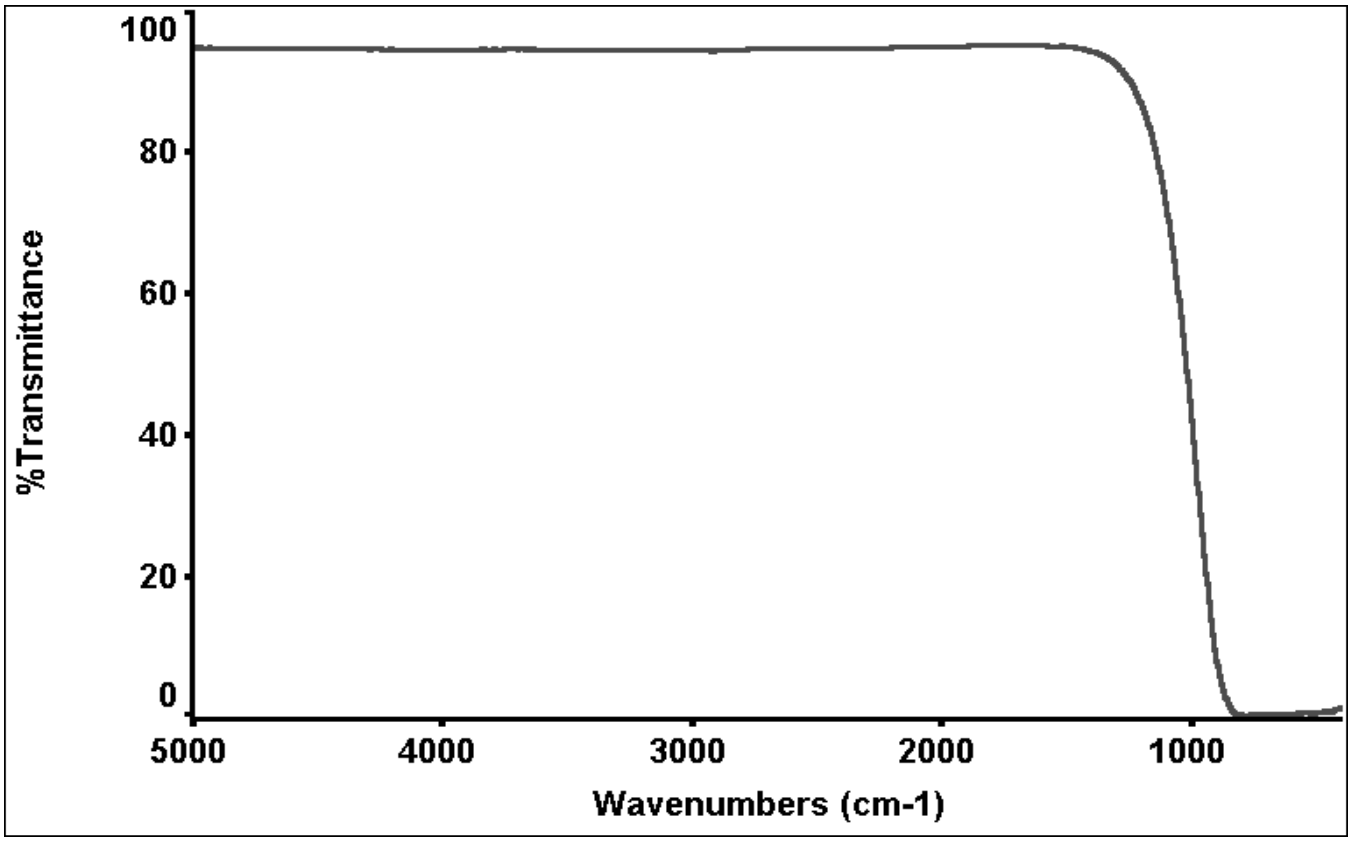
Specifications

CAS #	7787-32-8
Transmission Range	50,000-740 cm^{-1}
Refractive Index	1.42
% Transmittance (thickness)	90 (3.0mm)
Cleaning Agents	acetone, alcohol
Solubility in Water (100g H_2O @25°C)	0.17 grams
Solvents which attack	NH_4+ salts, acids
Max Temp in Air °C	500
Melting Point °C	1280
Hardness kg/mm^2 (Knoop #)	82
Composition	Single crystal
Crystal Class	Cubic

SPECTRA-TECH

Calcium Fluoride (CaF_2)

One of the hardest crystal materials, CaF_2 is particularly useful in high pressure cells. It resists most acids and alkalides. It is non-hygroscopic at room temperature but will react with air at elevated temperatures. If kept dry, crystal can be used to 900°C. CaF_2 should not be used with solutions of ammonium salts. Used for infrared transmission cell windows.



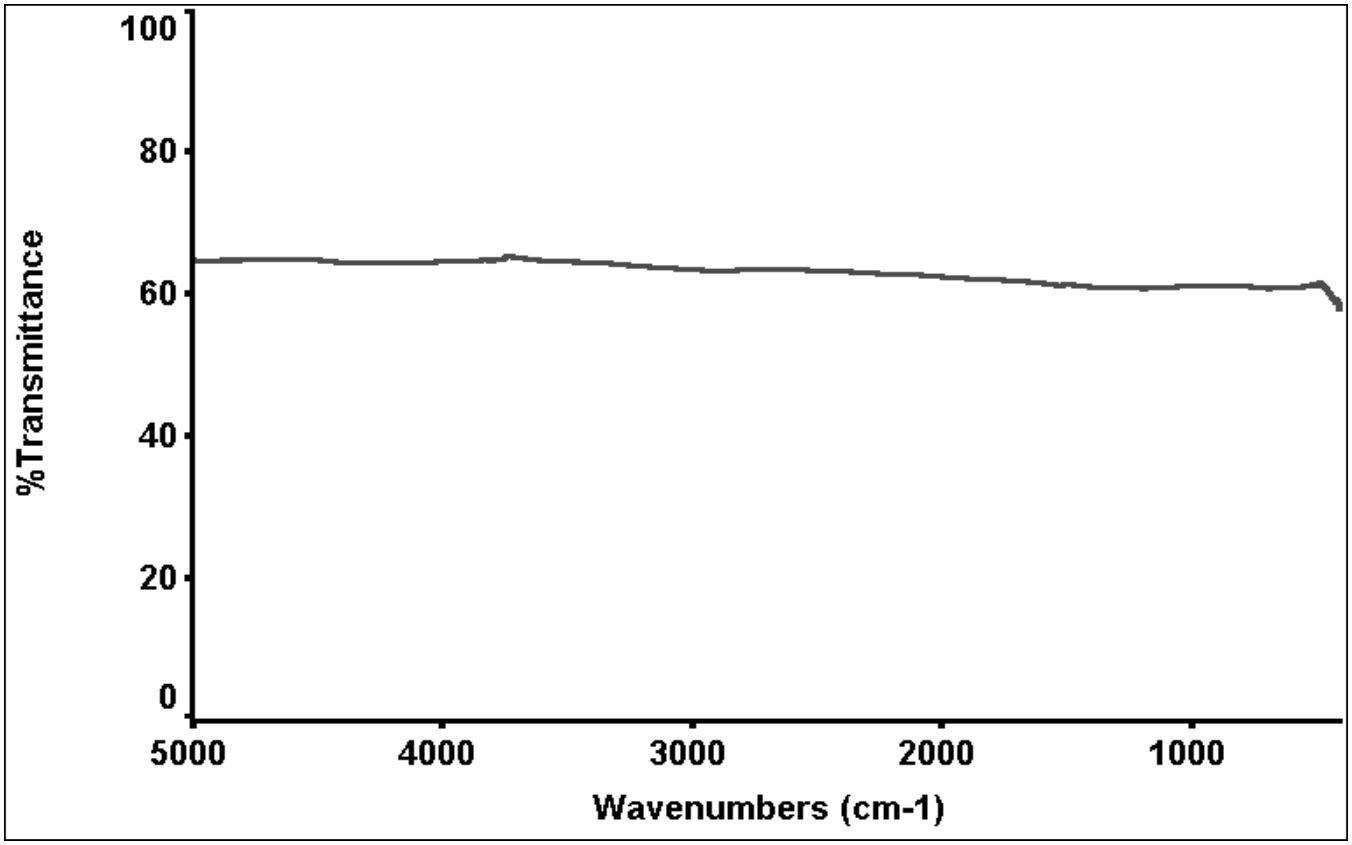
Specifications

CAS #	7789-75-5
Transmission Range	50,000-1,025 cm^{-1}
Refractive Index	1.4
% Transmittance (thickness)	90.0 (4.0mm)
Cleaning Agents	acetone, alcohol
Solubility in Water (100g H_2O @25°C)	0.0013 grams
Solvents which attack	NH_4+ salts, acids
Max Temp in Air °C	900
Melting Point °C	1360
Hardness kg/mm^2 (Knoop #)	158
Composition	Single crystal
Crystal Class	Cubic, cleaves on (111) plane

SPECTRA-TECH

Cadmium Telluride (CdTe)

Cadmium Telluride is attacked by Oxidizers and slightly soluble in acids. CdTe is softer than ZnS and ZnSe. Useful for infrared transmission windows and ATR material.



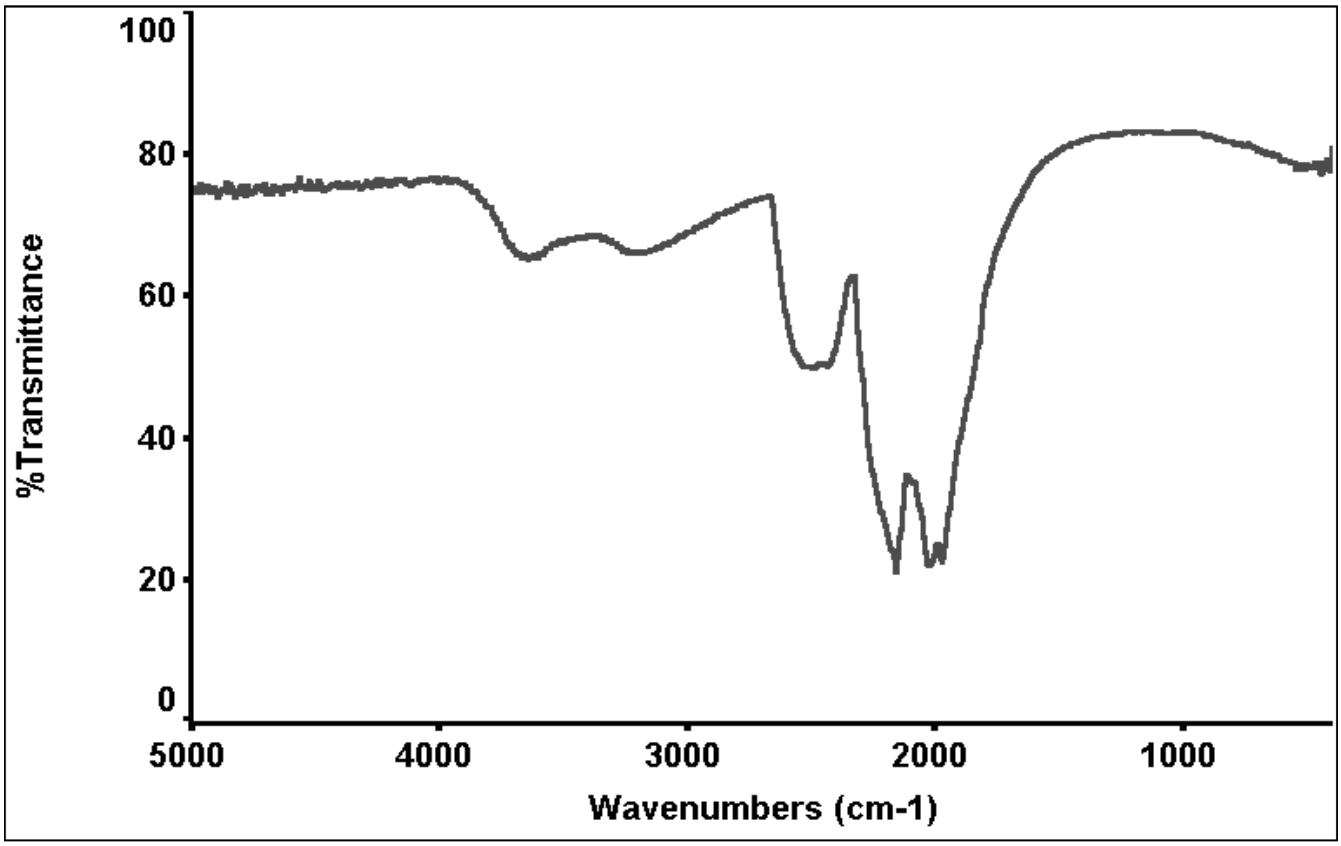
Specifications

CAS #	1306-25-8
Transmission Range	20,000-360 cm^{-1}
Refractive Index	2.67
% Transmittance (thickness)	40 (5mm)
Cleaning Agents	alcohol, acetone
Solubility in Water (100g H_2O @25°C)	insoluble
Solvents which attack	Acids, HNO^3
Max Temp in Air °C	300
Melting Point °C	1040
Hardness kg/mm^2 (Knoop #)	56
Crystal Class	Cubic

SPECTRA-TECH

Diamond

The Type IIa diamond has a transparency in the IR from 4000 to 400 cm-1 with spectral bands at 2600 to 1600 cm-1 with the fingerprint region clear. The bands are the phonon bands of the diamond. The diamond is especially useful for high pressure and corrosive work.



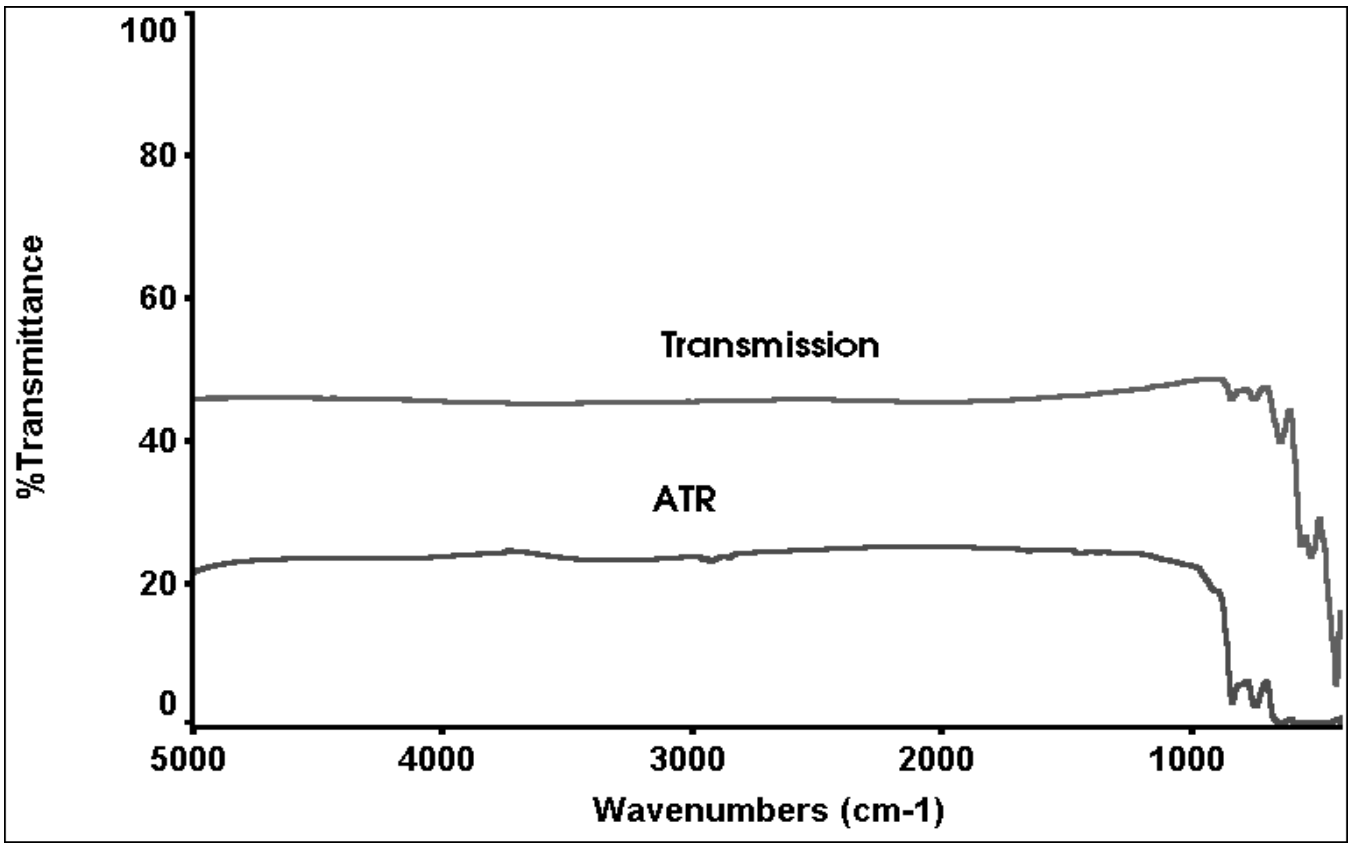
Specifications

CAS #	7782-40-3
Transmission Range	4,500-2,500 cm^{-1} & 1,667-33 cm^{-1}
Refractive Index	2.37
% Transmittance (thickness)	70 (1mm)
Cleaning Agents	alcohol, acetone, H_2O
Solubility in Water (100g H_2O @25°C)	insoluble
Solvents which attack	$K_2Cr_2O_7$, conc H_2SO_4
Max Temp in Air °C	750
Melting Point °C	3500
Hardness kg/mm^2 (Knoop #)	7000
Composition	Crystalline carbon, Single crystal

SPECTRA-TECH

Germanium (Ge)

Ge is a hard, brittle substance. It has low transmission levels due to high reflection losses. Ge is soluble in hot sulfuric acid and aqua regia, but insoluble in water. Good ATR material.



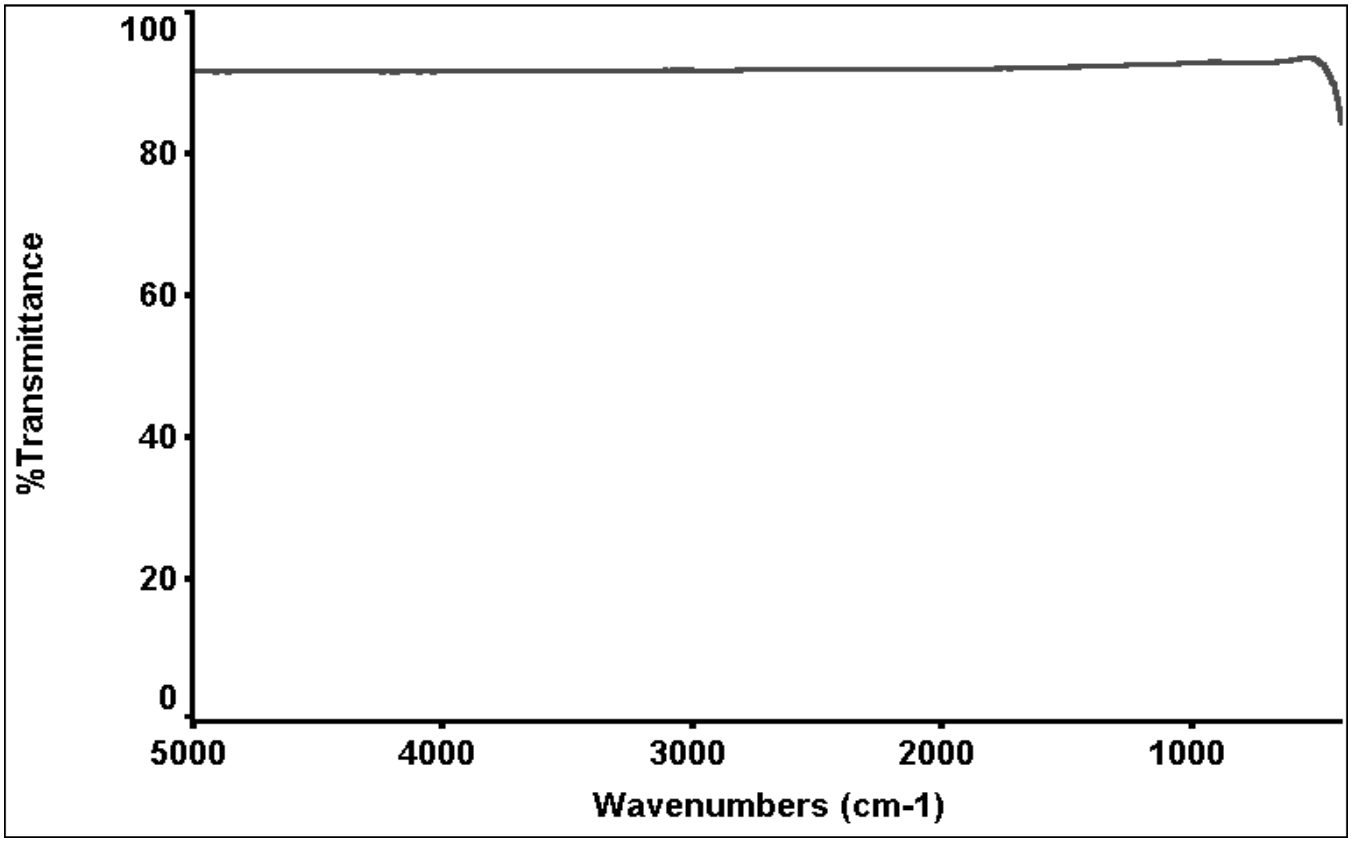
Specifications

CAS #	7440-56-4
Transmission Range	5,500-475 cm^{-1}
ATR Spectral Range	5,500-675 cm^{-1}
Refractive Index	4.0
% Transmittance (thickness)	50 (2mm)
Cleaning Agents	alcohol, acetone, H_2O
Solubility in Water (100g H_2O @25°C)	insoluble
Solvents which attack	hot H_2SO_4, aqua regia
Max Temp in Air °C	125
Melting Point °C	936
Hardness kg/mm^2 (Knoop #)	550
Composition	Single crystal
Crystal Class	Cubic

SPECTRA-TECH

Potassium Bromide (KBr)

A very useful material because it covers a wider spectral range than NaCl. KBr offers good resistance to thermal and mechanical shock. KBr windows are easy to polish but are more hygroscopic than NaCl.
Used for infrared transmission cell windows.



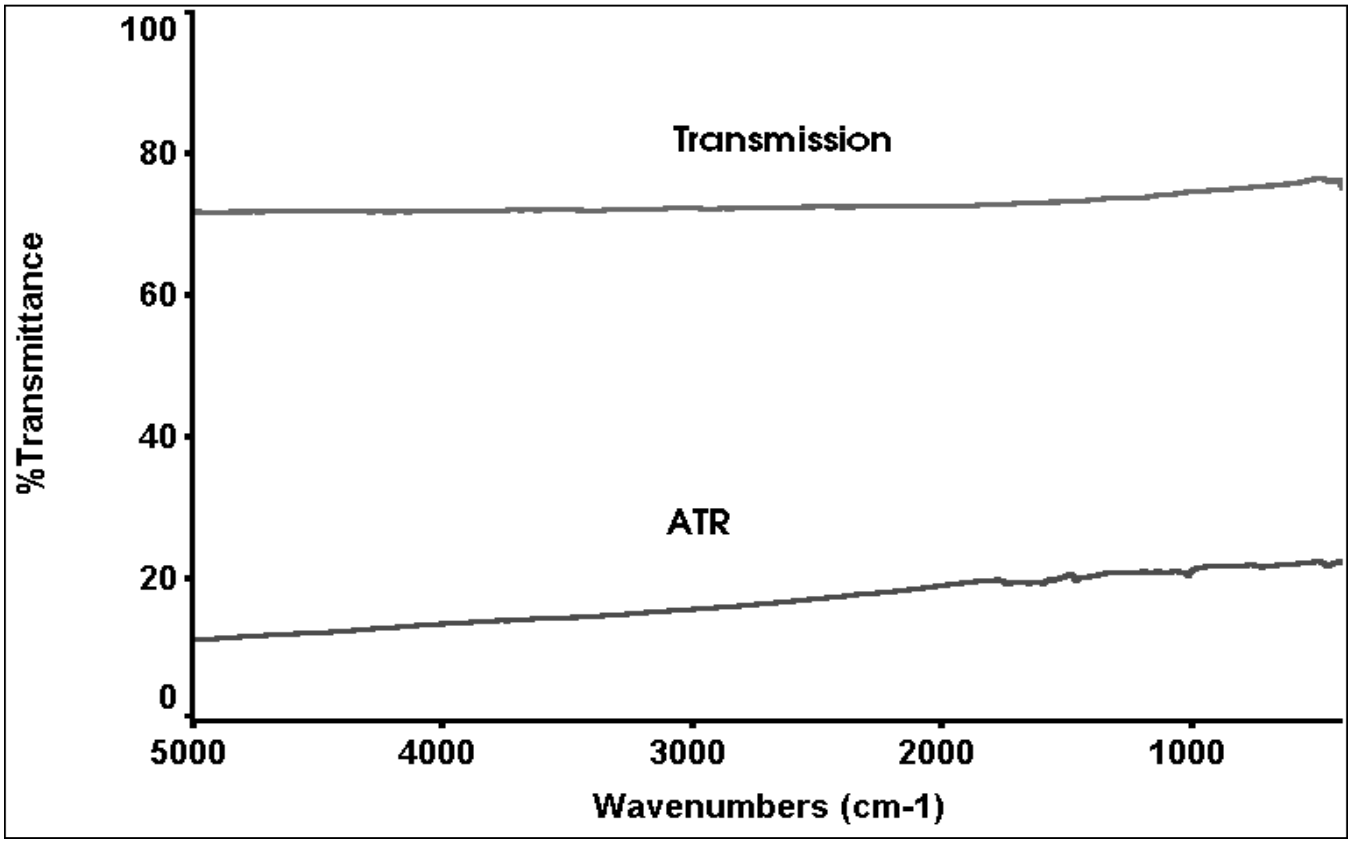
Specifications

CAS #	7758-02-3
Transmission Range	40,000-400 cm^{-1}
Refractive Index	1.52
% Transmittance (thickness)	90.5 (4.0mm)
Cleaning Agents	anhydrous alcohols
Solubility in Water (100g H_2O @25°C)	53.5 grams
Solvents which attack	lower alcohols, wet solvents
Max Temp in Air °C	300
Melting Point °C	730
Hardness kg/mm^2 (Knoop #)	7
Composition	Single crystal
Crystal Class	Cubic, cleaves on (100) planes

SPECTRA-TECH

Thallium Bromide-Iodide (KRS-5)

KRS-5 is used frequently for ATR crystals because it has a wide spectral range, high refractive index and does not easily fracture. It is slightly soluble in water, soluble in bases and insoluble in acids. This material should not be used with solutions of ammonium salts. KRS-5 is toxic, but only if the dust is ingested or absorbed into a cut. Used as an ATR material.



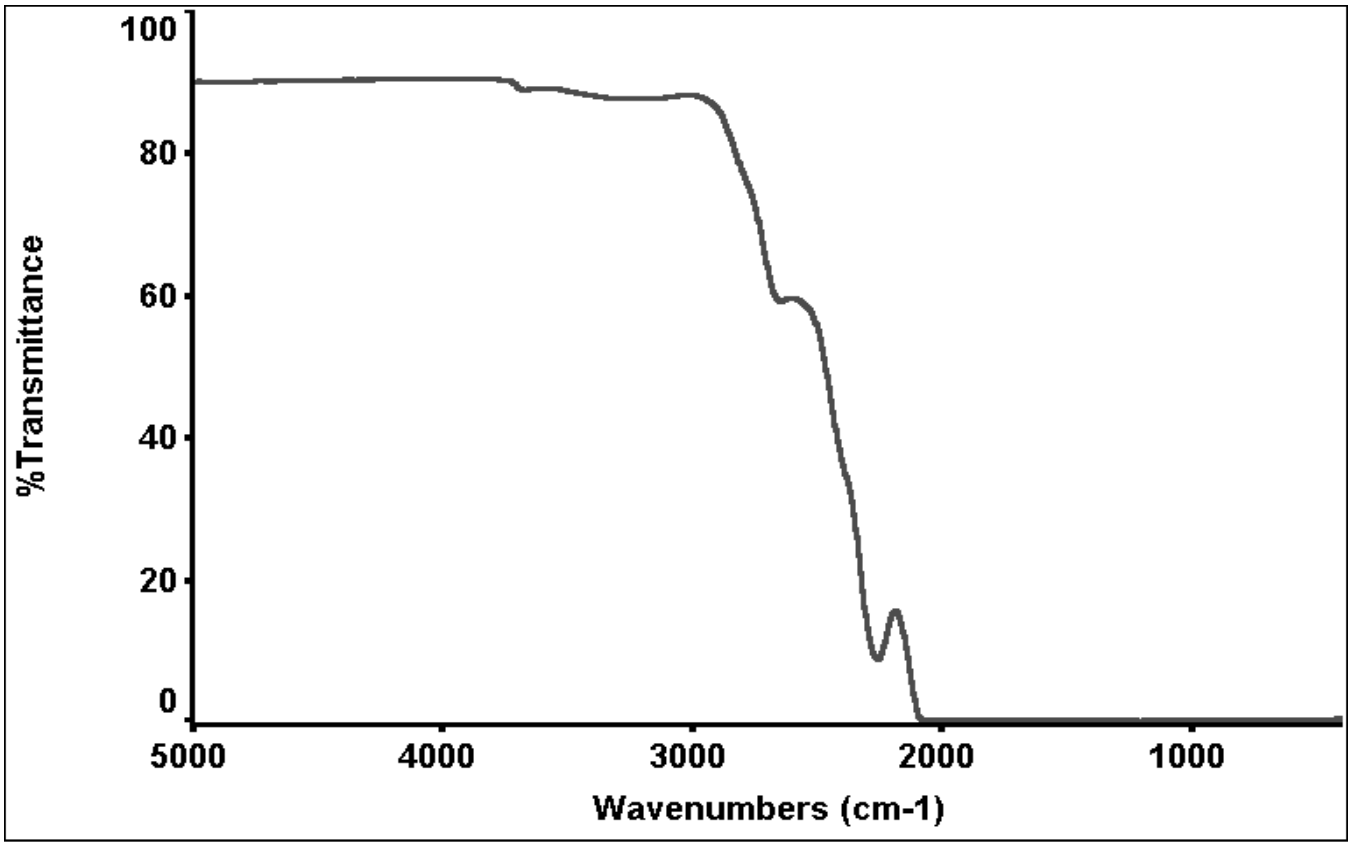
Specifications

CAS #	7758-02-3
Transmission Range	20,000-250 cm^{-1}
ATR Spectral Range	20,000-400 cm^{-1}
Refractive Index	2.37
% Transmittance (thickness)	70 (2.0mm)
Cleaning Agents	MEK
Solubility in Water (100g H_2O @25°C)	0.05 grams
Solvents which attack	complexing agents
Max Temp in Air °C	200
Melting Point °C	414.5
Hardness kg/mm^2 (Knoop #)	40
Composition	Mixed crystal
Crystal Class	Cubic, Does not cleave

SPECTRA-TECH

Quartz (SiO_2)

Quartz is mostly used in the UV-Vis and NIR spectral regions. Infrared Quartz is of high purity with minimal OH content. Quartz is water insoluble.



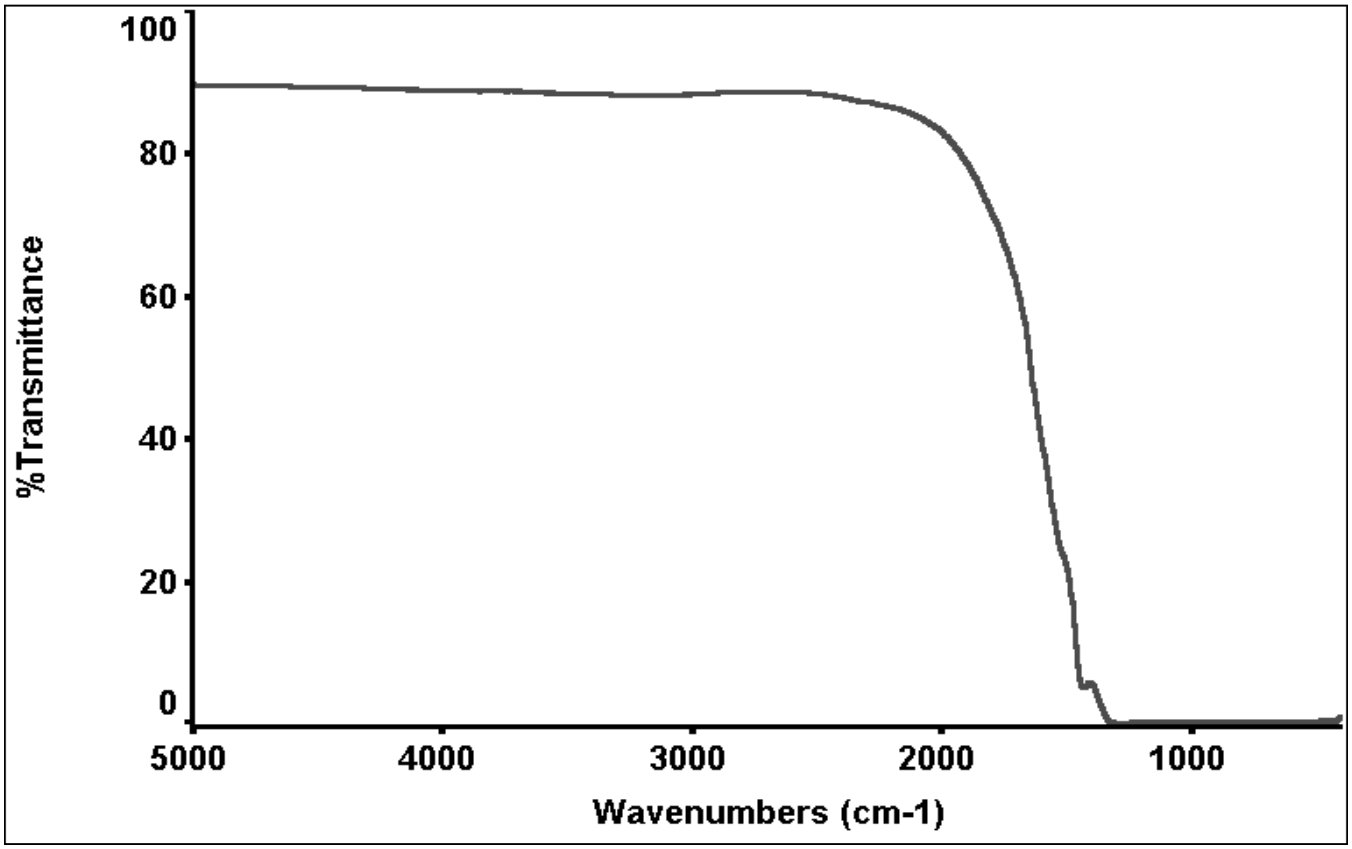
Specifications

CAS #	7631-86-9
Transmission Range	25,000-2,200 cm^{-1}
Refractive Index	1.4
% Transmittance (thickness)	90 (3mm)
Cleaning Agents	alcohol, acetone, H_2O
Solubility in Water (100g H_2O @25°C)	insoluble
Solvents which attack	
Max Temp in Air °C	1100
Melting Point °C	1470
Hardness kg/mm^2 (Knoop #)	174
Composition	Natural crystal
Crystal Class	Hexagonal (birefringent)

SPECTRA-TECH

Sapphire (AL_2O_3)

Sapphire, single crystal aluminum oxide, is a very hard material, chemically inert and is birefringent. It is attacked by concentrated acids and bases.



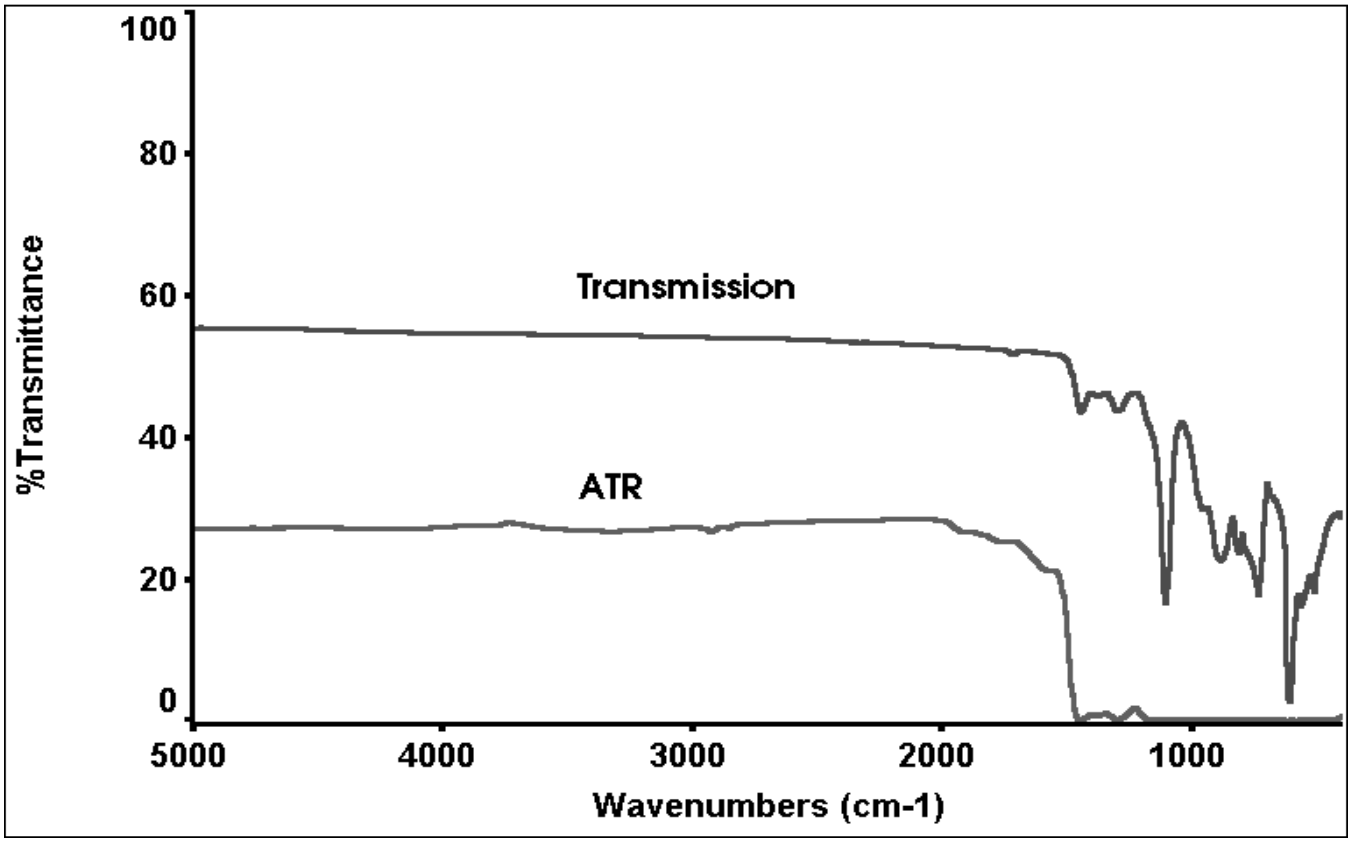
Specifications

CAS #	1344-28-1
Transmission Range	50,000-1,525 cm^{-1}
Refractive Index	1.5
% Transmittance (thickness)	
Cleaning Agents	alcohol, acetone, H_2O
Solubility in Water ($100g\ H_2O$ @25°C)	insoluble
Solvents which attack	slightly in acids and alkalis
Max Temp in Air °C	1800
Melting Point °C	2030
Hardness kg/mm^2 (Knoop #)	1370
Composition	Single crystal
Crystal Class	Hexagonal

SPECTRA-TECH

Silicon (Si)

Optical grade Si is very similar to Ge, but has better resistance to mechanical and thermal shock. Si is soluble in a hydrofluoric and nitric acids mixture. Used as an ATR material and for infrared transmission cell windows.



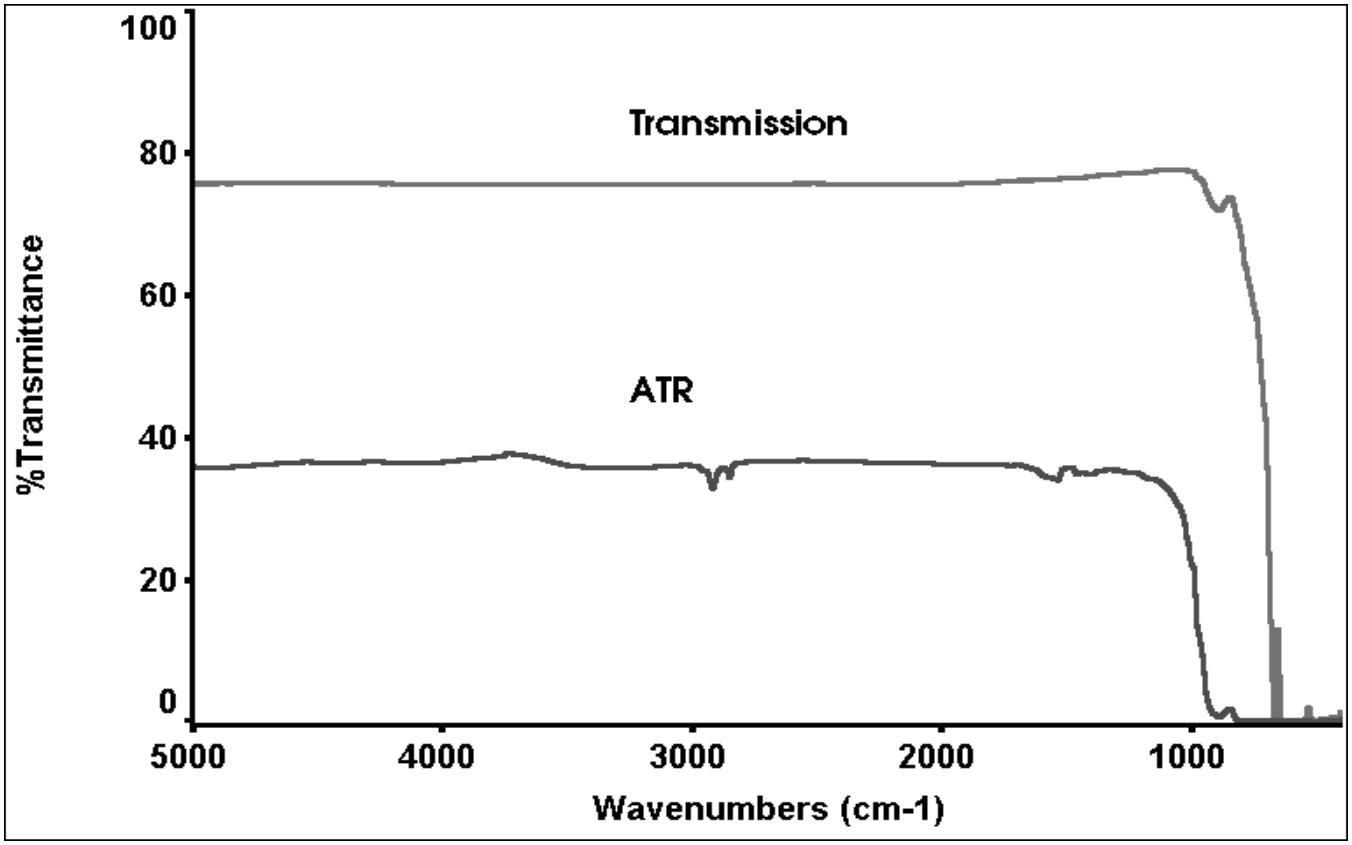
Specifications

CAS #	7440-21-3
Transmission Range	8,300-660 cm^{-1} & 360-70 cm^{-1}
ATR Spectral Range	8300-1500 cm^{-1} & 360-70 cm^{-1}
Refractive Index	3.4
% Transmittance (thickness)	55 (2.5mm)
Cleaning Agents	alcohol, acetone, H_2O
Solubility in Water ($100g\ H_2O$ @25°C)	insoluble
Solvents which attack	HF & HNO3
Max Temp in Air °C	300
Melting Point °C	1420
Hardness kg/mm2 (Knoop #)	1150
Composition	Polymorphic
Crystal Class	Cubic

SPECTRA-TECH

Zinc Sulfide (ZnS)

There are two kinds of Zinc Sulfide material. The first is chemical vapor deposited ZnS, which has a water band at 1640 cm-1. This will interfere with ATR work. The second kind is used for ATR and CIR (Cylindrical Internal Reflection) crystals, because it does not have a water absorption band. Zinc Sulfide is insoluble in water but can be attacked by strong oxidizing agents. It offers good resistance to thermal and mechanical shock.



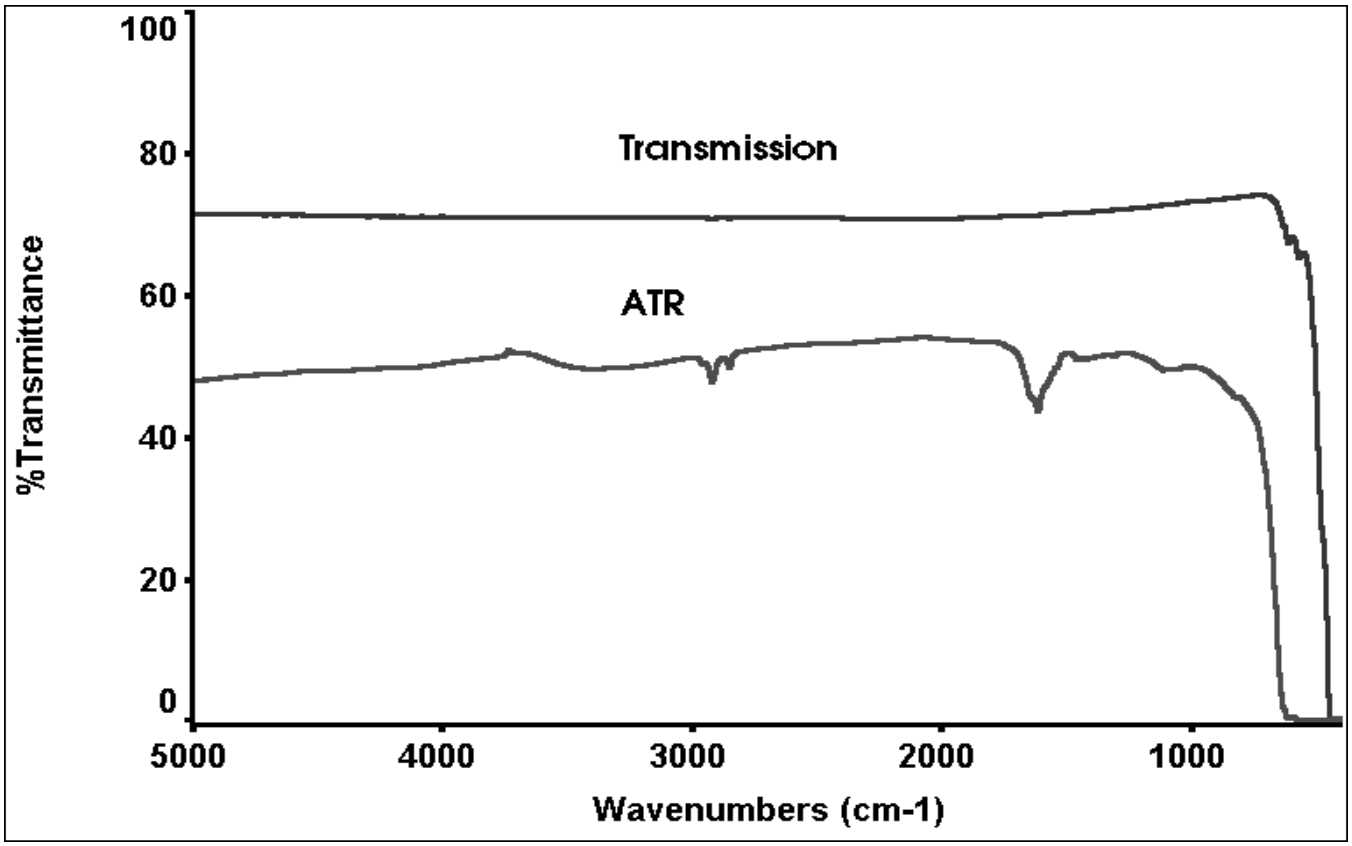
Specifications

CAS #	1314-98-3
Transmission Range	17,000-720 cm^{-1}
ATR Spectral Range	17,000-950 cm^{-1}
Refractive Index	2.2
% Transmittance (thickness)	70 (1.0mm)
Cleaning Agents	alcohol, acetone
Solubility in Water ($100g\ H_2O$ @25°C)	insoluble
Solvents which attack	acids
Max Temp in Air °C	300
Melting Point °C	1830
Hardness kg/mm^2 (Knoop #)	178
Crystal Class	Cubic

SPECTRA-TECH

Zinc Selenide (ZnSe)

Zinc Selenide (ZnSe) is a good window material because it is insoluble in water and very resistant to most solvents which attack. It is only slightly soluble in acids. Because of its low reflection losses in the infrared, it is a good material for ATR and CIR crystals.



Specifications

CAS #	1315-09-9
Transmission Range	20,000-454 cm^{-1}
ATR Spectral Range	20,000-650 cm^{-1}
Refractive Index	2.4
% Transmittance (thickness)	65 (1.0mm)
% Transmittance (ATR min.)	15 +
Cleaning Agents	alcohol, acetone, H_2O
Solubility in Water ($100g\ H_2O$ @25°C)	insoluble
Solvents which attack	acids, strong alkalies
Max Temp in Air °C	300
Melting Point °C	1520
Hardness kg/mm^2 (Knoop #)	137
Crystal Class	Cubic

SPECTRA-TECH

How to Calibrate Infrared Absorption Cells

One of the easiest ways to calculate the pathlength of a cell is by the interference fringe method. This can be done in any spectrometer. The interference fringe is caused by two parallel smooth surfaces in close proximity (less than 1mm) to each other.

Fringe Method

1. Collect a background file with the sample compartment empty.
2. Place the empty cell in the FTIR spectrometer on the usual sample slide.
3. Collect a sample file.
4. Display spectra in %Transmittance
5. Calculate the cell thickness by one of the following equations:

To calculate using wavenumbers:

$$L \text{ (in mm)} = \frac{n\,(10)}{2(W_1 - W_2)}$$

where L = cell thickness (in mm)
W_1 = starting wavenumber (cm^{-1})
W_2 = ending wavenumber (cm^{-1})
n = number of fringes between W_1 and W_2

To calculate using µm (microns):

$$L \text{ (in mm)} = \frac{n\,W_1 W_2}{2(W2 - W1)(1000)}$$

where L = cell thickness (in mm)
W_1 = starting wavelength (in µm)
W_2 = ending wavelength (in µm)
n = number of fringes between W_1 and W_2

Sample Calculation:
Data from the spectrum below
n = 10, W1 = 3640 W2 = 1370
Using the formula, calculate using wavenumbers, the thickness can be calculated by substituting the numbers.

$$L = \frac{n\,(10)}{2(W_1 - W_2)} \qquad \frac{10\,(10)}{2\,(3640 - 1370)}$$

$$L = \frac{100}{2\,(2270)}$$

L = 0.022 mm = 22 microns