

IR - Sadtler IR Reference Database (Organic and Polymeric)

Product Code - 426200

Spectra - 10,000

Description

This database contains a comprehensive collection of 9,700 IR spectra of pure organics, as well as 300 polymeric compounds found in industrial and academic laboratories. This compilation of spectra was gleaned from Bio-Rad's IR Standard collection which contains over 75,000 pure organic compounds and Bio-Rad's Comprehensive Monomers & Polymers collection. The spectra are representative of a broad range of chemical classifications from commercially available sources.

Technique

A variety of analysis methods were used depending on the nature of the compounds. Liquids were prepared by placing a small amount of sample between two infrared transparent windows. The crystals were pressed together to form a thin layer of the sample. The formulation of the sample determined which window material was used. For non-aqueous samples, the window material was KBr. For aqueous samples, KRS-5 was preferred. Solids presented a variety of challenges. The melting point of the sample pointed to which technique to was attempted first.

- For samples with a melting point less than 72° C, filming on a KBr window from a suitable solvent was initially attempted. If this was not successful due to a poor baseline or insolubility, a melt between two KBr windows was attempted. If this was not successful, the sample was tried as a KBr pellet.
- For samples with a melting point greater than 72° C, the technique of first choice was a KBr pellet. For polymer samples, filming the sample was attempted first, followed by a melt and then KBr pellet techniques.
- For samples with an unknown melting point, an examination of the crystallinity of the sample indicated which technique would be successful. Highly crystalline samples tend to yield good KBr pellets. For samples that exhibit low crystallinity, films and melts tend to give better spectra.

Other analysis methods were used as needed.

Additional Information Listed

Each spectrum is labeled with the chemical name or trade name of the product, a chemical description and physical data furnished by the manufacturer, the source of the sample, and the manner in which the product was examined.

Classifications

Pure Organic Compounds

Hydrocarbons

- A. Saturated Hydrocarbons
 - 1. Normal Alkanes
 - 2. Branched Alkanes
 - 3. Cyclic Alkanes
- B. Unsaturated Hydrocarbons
 - 1. Acyclic Alkenes
 - 2. Cyclic Alkenes
 - 3. Alkynes
- C. Aromatic Hydrocarbons
 - 1. Monocyclic (Benzenes)
 - 2. Polycyclic

Halogenated Hydrocarbons

- A. Fluorinated Hydrocarbons
 - 1. Aliphatic
 - 2. Aromatic
- B. Chlorinated Hydrocarbons
 - 1. Aliphatic
 - 2. Olefinic
 - 3. Aromatic
- C. Brominated Hydrocarbons
 - 1. Aliphatic
 - 2. Olefinic
 - 3. Aromatic

D. Iodinated Hydrocarbons

- 1. Aliphatic And Olefinic
- 2. Aromatic

Nitrogen Containing Compounds

- A. Amines
 - 1. Primary
 - a. Aliphatic And Olefinic
 - b. Aromatic
 - 2. Secondary
 - a. Aliphatic And Olefinic
 - b. Aromatic

Classifications (cont.)

- 3. Tertiary
 - a. Aliphatic And Olefinic
 - b. Aromatic
- B. Pyridines
- C. Quinolines
- D. Miscellaneous Nitrogen Heteroaromatics
- E. Hydrazines
- F. Amine Salts
- G. Oximes (-CH=N-OH)
- H. Hydrazones (-CH=N-NH₂)
- I. Azines (-CH=N-N=CH-)
- J. Amidines (-N=CH-N)
- K. Hydroxamic Acids
- L. Azo Compounds (-N=N-)
- M. Triazines (-N=N-NH-)
- N. Isocyanates (-N=C=O)
- O. Carbodiimides (-N=C=N-)
- P. Isothiocyanates (-N=C=S)
- Q. Nitriles (-C≡N)
 - 1. Aliphatic
 - 2. Olefinic
 - 3. Aromatic
- R. Cyanamides (≡N-C≡N)
- S. Thiocyanates (-S-C≡N)
- T. Nitroso Compounds (-N=O)
- U. N-Nitroso Compounds (=N-N=O)
- V. Nitrites (-O-N=O)
- W. Nitro Compounds (-NO₂)
 - 1. Aliphatic
 - 2. Aromatic
- X. N-Nitro-Compounds (=N-NO₂)
- Y. Nitrates (-O-NO₂)

Silicon Containing Compounds (Except Si-O)

Phosphorus Containing Compounds (Except P-O And P(=O)-O)

Sulfur Containing Compounds

- A. Sulfides(R-S-R)
 - 1. Aliphatic
 - 2. Heterocyclic
 - 3. Aromatic
- B. Disulfides (R-S-S-R)
- C. Thiols
 - 1. Aliphatic
 - 2. Aromatic
- D. Sulfoxides (R-S(=O)-R)
- E. Sulfones (R-SO₂-R)
- F. Sulfonyl Halides (R-SO₂-X)
- G. Sulfonic Acids (R-SO₂-OH)
 - 1. Sulfonic Acid Salts (R-SO₂-O-M)
 - 2. Sulfonic Acid Esters (R-SO₂-O-R)
 - 3. Sulfuric Acid Esters (R-O-S(=O)-O-R)
 - 4. Sulfuric Acid Salts (R-OS(=O)-O-M)
- H. Thioamides (R-C(=S)-NH₂)
- I. Thioureas (R-NH-C(=S)-NH₂)
- J. Sulfonamides (R-SO₂-NH₂)
- K. Sulfamides (R-NH-SO₂-NH-R)

Oxygen Containing Compounds (Except -C(=O)-)

- A. Ethers
 - 1. Aliphatic Ethers (R-O-R)
 - 2. Acetals (R-CH(-O-R)₂)
 - 3. Alicyclic Ethers
 - 4. Aromatic Ethers
 - 5. Furans
 - 6. Silicon Ethers (R₃-Si-O-R)
 - 7. Phosphorus Ethers ((R-O)₃-P)
 - 8. Peroxides (R-O-O-R)
- B. Alcohols (R-OH)
 - 1. Primary
 - a. Aliphatic And Alicyclic
 - b. Olefinic
 - c. Aromatic
 - d. Heterocyclic
 - 2. Secondary
 - a. Aliphatic And Alicyclic
 - b. Olefinic
 - c. Aromatic
 - 3. Tertiary

- a. Aliphatic
- b. Olefinic
- c. Aromatic
- 4. Diols
- 5. Carbohydrates
- 6. Phenols

Compounds Containing Carbon To Oxygen Double Bonds

- A. Ketones (R-C(=O)-R)
 - 1. Aliphatic And Alicyclic
 - 2. Olefinic
 - 3. Aromatic
 - 4. α-Diketones And β-Diketones
- B. Aldehydes (R-C(=O)-H)
- C. Acid Halides (R-C(=O)-X)
- D. Anhydrides (R-C(=O)-O-C(=O)-R)
- E. Amides
 - 1. Primary (R-C(=O)-NH₂)
 - 2. Secondary (R-C(=O)-NH-R)
 - 3. Tertiary (R-C(=O)-N-R₂)
- F. Imides (R-C(=O)-Nh-C(=O)-R)
- G. Hydrazide (R-C(=O)-NH-NH₂)
- H. Ureas (R-NH-C(=O)-NH₂)
- I. Hydantoins, Uracils, Barbiturates
- J. Carboxylic Acids (R-C(=O)-OH)
 - 1. Aliphatic And Alicyclic
 - 2. Olefinic
 - 3. Aromatic
 - 4. Amino Acids
 - 5. Salts Of Carboxylic Acids
- K. Esters
 - 1. Aliphatic Esters Of Aliphatic Acids
 - 2. Olefinic Esters Of Aliphatic Acids
 - 3. Aliphatic Esters Of Olefinic Acids
 - 4. Aromatic Esters Of Aliphatic Acids
 - 5. Esters Of Aromatic Acids
 - 6. Cyclic Esters (Lactones)
 - 7. Chloroformates
 - 8. Esters Of Thio-Acids
 - 9. Carbamates
 - 10. Esters Of Phosphorus Acids

There are almost 50 classifications presented in the polymeric group of 300 IR reference spectra. The list includes:

Acrylic Copolymers
Acrylonitrile-Butadiene-Styrene Resins
Aliphatic Hydrocarbon Copolymers
Aminoplasts/Polyamines
Anhydrides Polymers
Butadiene-Acrylonitrile Copolymers
Carboxymethyl Cellulose & Salts
Cellulose Esters & Mixed Esters
Cellulose Esters
Chlorinated Hydrocarbon Resins
Coumarone-Indene Resins
Fluorocarbon Resins
Hydroxyethyl Celluloses
Ion Exchange Resins
Miscellaneous Polymers
Miscellaneous Vinyl Polymers
Modified Epoxy Resins

Modified Polyesters
Other Styrene Copolymers
Phenolic Resins
Polyacrylic & Polymethacrylic Acids & Salts
Polyacrylic & Polymethacrylic Esters
Polyamides
Polybutadienes
Polybutenes & Butyl Rubbers
Polycarbonates
Polyesters
Polyethers
Polyethylenes
Polyimides
Polypropylenes
Polystyrenes
Polysulfones
Polyterpene & Naphthene Resins

Polyurethane & Urethane Prepolymers
Polyvinyl Acetate Copolymers
Polyvinyl Esters
Polyvinylpyridines
Polyvinylpyrrolidones
Rosin & Rosin Derivatives
Silicone Polymers
Styrene-Acrylonitrile Copolymers
Styrene-Butadiene Copolymers
Sulfonated Polymers
Synthetic Polyisoprenes & Natural Rubbers
Thioplasts/Polysulfides
Unmodified Epoxy Resins
Vinyl Chloride Copolymers