IR - Sadtler Standards (Vapor Phase Comprehensive) - Wiley

Spectra - 9,185

Description

This spectral database contains 9,185 vapor phase infrared spectra of common pure organic compounds and is helpful in identifying unknown compounds by GC-IR, TGA-IR, or other vapor phase methods of analysis. It is useful in pollution and toxicological identification and other relevant application areas.

Additional Iinformation

Each record is identified by Chemical Abstracts name and includes the following (when available): molecular formula, molecular weight, structural formula, source of sample, instrumental conditions, boiling, point, melting point. Molecular structures are also available with the database.

Technique

Sadtler data was run under controlled conditions. All spectra were measured at Bio-Rad Laboratories using either a Digilab FTS-14 or FTS-15 Fourier transform spectrometer in the spectral region 4000 cm^{-1} to 450 cm^{-1} with a nominal resolution of 4 cm^{-1} across the entire spectral region. A Sadtler CIRA 102 chromatographic infrared analyzer was used as the sampling device to measure all reference spectra. The carrier gas was helium.

All vapor phase reference IR spectra have been measured and recorded generally conforming to Coblentz specifications.

The compounds were examined at temperatures ranging from 25°C to 300°C depending on the vaporization temperature required for the particular compound and its chemical stability. Thermally sensitive compounds such as esters and acid chlorides were measured at the lowest possible cell temperature to reduce oxidation or thermal decomposition while the reference spectra were measured.

For liquid samples, 1µl of sample was injected into the CIRA at the selected injection port and cell temperature. For samples that were solids at ambient temperature approximately 1mg of sample was introduced into the system using the CIRA Solid Sampling Accessory.

This collection has been subject to the Sadtler Data Review Protocol™ to provide you with the highest standard in spectral data today. These rigorous qualifying procedures start at data acquisition and continue throughout the database development process.

Classifications

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 Olefinc
    - b. Aromatic
  - 2. Secondary
    - a. Aliphatic And Olefinic
    - b. Aromatic
  - 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. Triazenes (-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. alpha-Diketones and beta-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. Hydantroins, 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