IR - Sadtler EPA Vapor Phase - Wiley

Spectra - 3,235

Description

This database was created for the US Environmental Protection Agenc (EPA) from a list of selected compounds relevant to pollution and toxicological identification. It includes 3,235 IR vapor phase 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.

Additional Information

Each spectrum is presented with the Chemical Abstracts name and registry number, molecular formula, molecular weight, and structural formula. The boiling or melting point is listed whenever it is available. Each spectrum also includes a description and analytical data for the compound, supplier of the sample, and instrumental conditions applying to that spectrum.

Technique

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 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.

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 1 mg 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
Saturated Hydrocarbons
Unsaturated Hydrocarbons
Aromatic Hydrocarbons

HALOGENATED HYDROCARBONS
Fluoronated Hydrocarbons
Chlorinated Hydrocarbons
Brominated Hydrocarbons
Iodinated Hydrocarbons

INITROGEN CONTAINING COMPOUNDS
Amines
Pyridines
Quinolines
Miscellaneous Nitrogen Heteroaromatics
Hydrazines
Amines Salts
Oximes (-CH=N-OH)
Hydrazones (-CH=N-NH2)
Azines (-CH=N-N=CH-)
Amidines (-N=CH-N)
Hydroxamic Acids
Azo Compounds (-N=N-)
Triazenes (-N=N-NH-)
Isocyanates (-N=C=O)
Carbodiimides (-N=C=N-)
Isothiocyanates (-N=C=S)
Nitriles (-C*N)
Cyanamides (*N-C*N)
Thiocyanates (-S-C*N)
Nitroso Compounds (-N=O)
N-Nitroso Compounds (=N-N=O)
Nitrites (-O-N=O)
Nitro Compounds (-NO2)
N-Nitro Compounds (=N-NO2)
Nitrates (-O-NO2)

SILICON CONTAINING COMPOUNDS (EXCEPT Si-O)

PHOSPHORUS CONTAINING COMPOUNDS (EXCEPT P-O and P(=O)-O)

SULFUR CONTAINING COMPOUNDS
Sulfides (R-S-R)
Disulfides (R-S-S-R)
Thiols
Sulfoxides (R-S(=O)-R)
SulfonesS (R-SO2-R)
Sulfonyl Halides (R-SO2-X)
Sulfonic AcidsR-SO2-OH)
Thioamides (R-C(=S)-NH2)
Thioureas (R-NH-C(=S)-NH2)
Sulfonamides (R-SO2-NH2)
Sulfamides (R-NH-SO2-NH-R)

OXYGEN CONTAINING COMPOUNDS (EXCEPT -C(=O)-)
Ethers
Alcohols (R-OH)

COMPOUNDS CONTAINING CARBON TO OXYGEN DOUBLE BONDS
Ketones (R-C(=O)-R)
Aldehydes (R-C(=O)-H)
Acid Halides (R-C(=O)-X)
Anhydrides (R-C(=O)-O-C(=O)-R)
Amides
Imides (R-C(=O)-NH-C(=O)-R)
Hydrazides (R-C(=O)-NH-NH2)
Ureas R-NH-C (=O)-NH2)
Hydantoins, Uracils, Barbituates
Carboxylic Acids (R-C(=O)-OH)
Esters