

IR - Sadtler Standards (Vapor Phase Selected Subset) - Wiley

Spectra - 485

Description

This database contains 485 vapor phase infrared reference spectra that have been measured and produced by Bio-Rad specifically as a companion work to the volume entitled *The Interpretation of Vapor Phase Infrared Spectra - Group Frequency Data* by Richard A. Nyquist, Ph.D. The spectra in the database are arranged in the same sequence as the chemical classes of the textbook, and the compounds listed have been carefully chosen by Dr. Nyquist to exemplify the principles described in his text. It is recommended that this database be used in conjunction with the group frequency data, since all the compounds appearing in this book are also listed in tables.

This collection provides a reference for spectroscopists identifying compounds in the vapor state from gas chromatography separations and to present high quality spectra for the evaluation and interpretation of vapor phase infrared spectra.

Additional information

Each spectrum is presented with the Chemical Abstracts name, molecular formula, molecular weight, and structural formula. Also, each spectrum shows the description and analytical data for the compound and the supplier of the sample together with the instrumental conditions applying to that spectrum. When a peak caused by a small impurity occurs in the spectrum, it becomes part of the spectrum.

The following information will also be also supplied when available: boiling point or melting point, CAS Registry number, vaporization temperature, cell volume, injection amount, path length, pressure, max./min., scale expansion, and source of sample.

The data is arranged in chemical class sequence to display similarities within a group.

Classifications

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| Straight Chain Aliphatic Hydrocarbons - 12 | Ketones - 24 | Sulfonyl Halides - 3 |
| Cyclic Aliphatic Hydrocarbons - 3 | Carboxylic Acid Esters - 46 | Sulfonates - 6 |
| Alkenes - 22 | Carbonates - 4 | Sulfoxides & Sulfones - 5 |
| Acetylenic Compounds - 6 | Carboxylic Acid Halides - 4 | Alkyl Borates - 2 |
| Propadienes - 1 | Chloroformates - 2 | Halogenated Hydrocarbons - 18 |
| Alcohols - 42 | Carbamates - 3 | Nitro Compounds - 12 |
| Phenols - 24 | Organic Ethers - 15 | Phosphorus Compounds - 18 |
| Oximes - 5 | Nitriles - 11 | Substituted Benzenes - 35 |
| Aliphatic Amines - 18 | Isothiocyanates - 2 | Pyridines - 18 |
| Arylamines - 37 | Isocyanates - 2 | Naphthalenes - 7 |
| Carboxylic Acids - 30 | Carbodiimides - 2 | Thiophenes & Furans - 7 |
| Carboxamides - 31 | Thiols - 6 | Water - 1 |
| Aldehydes - 11 | Sulfites And Sulfates - 4 | |

Technique

All spectra were measured 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 Coblenz 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, $1\text{ }\mu\text{l}$ 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.