

IR - Priority Pollutants - Bio-Rad Sadtler/ IR - Priority Pollutants (Vapor Phase) - Bio-Rad Sadtler

Spectra - 475

Description

This database is a convenient and practical spectral reference for those who analyze, monitor, control, or study environmental, physiological, or occupational pollutants and toxic substances.

It includes 475 spectra of hazardous or toxic chemical substances, selected from the EPA Priority Pollutants List, and the OSHA Category 1 List of Carcinogenic Substances. Also included is a list of hazardous compounds common to industry and of concern in interstate transportation. There are 300 condensed phase spectra, with the balance being the vapor phase spectra of selected compounds in the group.

The condensed phase spectra are typical of those obtained using standard laboratory sample handling techniques for condensed phase spectroscopy. The vapor phase spectra are representative of those one would obtain using GC/FT-IR analysis where the spectra are measured above ambient temperature in a heated optical cell. Condensed phase spectra for compounds that are gases at room temperature are not included; instead, a spectrum of the gas at 25°C is presented in addition to the vapor phase spectrum measured above ambient temperature. Also, some of the vapor phase spectra presented are for mixtures of compounds, such as the PCBs. These spectra are presented for band correlation purposes and are not spectra of pure compounds. Also included are compounds represented by a single spectrum. In these cases, the compounds are generally not suitable for gas chromatography analysis, i.e. inorganics.

Additional Information

Each compound is listed by its Chemical Abstracts name together with frequently used common names. The molecular formula, the structure, molecular weight, source of sample, melting point, boiling point, CAS Registry number, and NIOSH number are all given when the information is available. The sample preparation method is specified with the condensed phase spectra, and pertinent physical and instrumental data including cell temperature are presented with vapor phase spectra. Traces of impurities were found in a small number of the samples used to compile this collection.

Technique

In the condensed phase spectra, triangular apodization was used for all interferometrically measured spectra. Standard techniques, developed in Bio-Rad's Laboratories, ensure that the spectra are of the best possible quality, and are reproducible for comparison and identification purposes. The preferred sample preparation methods are the capillary cell for liquids and low-melting solids and the KBr wafer for solids. The KBr method is used for solids since it is a standard technique and requires only a small amount of sample for the preparation of good spectra, leaving the remainder for further analytical investigations. Since the KBr method cannot be used for solids which undergo ionic exchange with the KBr, these samples were mullied. Each spectrum is clearly labeled with sample preparation technique used.

All vapor phase spectra were determined at Bio-Rad Laboratories using a Digilab FTS-14 Fourier transform spectrometer in the spectral region 4000 cm^{-1} to 450 cm^{-1} with a nominal resolution of 4 cm^{-1} being maintained across the entire spectral region. A Sadtler CIRA 101 chromatographic infrared analyzer was used to vaporize and trap the compounds for examination. The carrier gas was helium. The compounds were examined at temperatures ranging 100 °C to 280 °C; the temperature used for each compound was based on the boiling point or melting point of the material and its chemical stability. Thermally sensitive compounds were always run at lower vaporization temperatures.

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 - 44
Halogenated Hydrocarbons - 76
Nitrogen Containing Compounds - 164
Amines - 94
Pyridines - 4
Quinolines - 4
Hydrazines 4
Azo Compounds (-N=N-) - 15
Triazenes (-N=N-NH-) - 3
Nitriles (-CN) - 8

Nitroso Compounds (-N=O) - 17
Nitro Compounds (-NO₂) - 35
Phosphorus Containing Compounds - 22
Sulfur Containing Compounds - 46
Oxygen Containing Compounds - 281
Ethers - 33
Alcohols (R-OH) - 71
Ketones (R-C(=O)-R) - 19
Aldehydes (R-C(=O)-H) - 11
Acid Halides (R-C(=O)-X) - 4

Anhydrides (R-C(=O)-O-C(=O)-R) - 4
Amides - 10
Imides (R-C(=O)-NH-C(=O)-R) - 1
Hydrazides (R-C(=O)-NH-NH₂) - 1
Ureas (R-NH-C(=O)-NH₂) - 3
Hydantoins, Uracils, Barbituates - 6
Carboxylic Acids (R-C(=O)-OH) - 58
Esters - 50
Inorganics - 10
Miscellaneous - 8