IR - Sadtler Standards (Comprehensive) - Wiley

Spectra - 75,545

Description

This infrared spectral database contains spectra of 75,545 organic chemical compounds, including most simple aliphatic, aromatic, alicyclic, and heterocyclic compounds, as well as numerous complex materials. It also offers access to series of homologous compounds that range in complexity.

The database can be used a reference in the identification, verification, and classification of unknown compounds. It is also useful in the establishment of complex chemical classes of undocumented commercial compounds with similar structures.

Additional Information

The following information is supplied for each record when available: source of sample, technique, melting point, boiling point, molecular weight, and molecular formula. Molecular structures are available with the database.

Technique

Every effort is made to maintain the highest standard of accuracy for spectra placed in the Sadtler collections. Each compound was prepared under standard conditions at Bio-Rad Laboratories, Informatics Division using equipment manufactured by leading instrument makers. Samples were checked to ensure that non-linearity is avoided to maximize reproducibility and provide for the best subtraction of reference spectra. Wherever possible, Bio-Rad chemists verified every infrared spectrum by checking the corresponding NMR and UV spectra. Any spectra with evidence of decomposition, impurities, or reaction with sampling apparatus were rejected. Each spectrum was then reviewed by an independent consultant before inclusion in the database. These quality control procedures provide the best sample purity and structural formula confirmation available for the broad range of compounds in the collection.

With regard to the spectra of the collection, consideration should be given to the manner in which the compound was prepared for examination. A compound prepared by most preparative procedures fails to yield an infrared absorption spectrum which is ideal in all respects. Although a compound prepared for examination by a particular procedure yields a reproducible spectrum, the same compound prepared by two different methods does not, necessarily, yield identical spectra. For most compounds, a change in physical state or a change in solvent for solution spectra cause shifts in absorption band locations, changes in absorption band contours, and a splitting or coalescence of absorption bands. Furthermore, the use of solvents for solution spectra and the use of liquid media for mulls tend to confound the spectrum of the compound with their own unique absorption characteristics. However, each method of preparing a sample for examination has certain advantages and merits. The information desired from a spectrum largely determines how the compound is to be prepared for examination.

A compound in the crystalline state generally yields a spectrum which has more absorption bands than the spectrum of the same compound when examined in the liquid state or in solvent solution. The absorption bands in the spectrum of a solid compound, examined in the crystalline state, or a liquid compound, examined in the pure concentrated form (neat), are found, usually, at lower frequencies than the absorption bands in the spectrum of the same compound when it is examined in the vapor state or in solvent solution. The degree of absorption band shifts depends upon the presence or absence of intermolecular and intramolecular forces. For qualitative examinations involving empirical comparison of spectra, the spectrum of the sample should be obtained in a manner which is the same as that used for obtaining the spectrum of the reference compound. Identification established through empirical comparison of spectra should always be supported with physical or chemical data. The greatest obstacle to obtaining a spectrum of a sample which will match a reference spectrum of a pure compound is the lack of sameness in the composition of the sample.

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.