

IR - Sadtler Flavors & Fragrances - Wiley

Product Code - This database is available only as part of the KnowItAll IR Spectral Library
Spectra - 590

Wiley is the leading producer of IR and Raman spectral databases with their Sadtler Spectral Databases, known for their high-quality.

Description

This IR spectral database provides scientists with a representative collection of 590 spectra of compounds used in the manufacture of flavors and fragrances, natural product oils, synthesized fragrance compounds, etc. It includes compounds approved by the Flavor and Extracts Manufacturers' Association of the United States (FEMA) and the FEMA number is listed when available.

Additional Information

The following information is supplied for each record when available: name, synonyms, CAS Registry Number, catalog number, lot number, source of spectrum, source of sample, instrument name, technique, melting point, boiling point, flash point, density, sample type, physical state, purity, storage requirements, molecular weight, and molecular formula. Molecular structures are also 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 Laboratories.

All spectra were run using a Bruker Tensor 27FT-IR spectrometer. A number of different techniques were employed: Neat, Melt, Film, KBr0 and KBr1.

- The Neat technique was used for liquids, pastes and oils.
- The Melt technique was used for compounds with melting points < 45 °C.
- The Film technique was used for compounds with melting points < 72 °C. It should only be used if the Melt technique and KBr0 were unsuccessful.
- For solids, KBr0 and KBr1 techniques were used.

Samples were checked to ensure that non-linearity was avoided to maximize reproducibility and provide for the best subtraction of reference spectra. Any spectra with evidence of decomposition, impurities, or reaction with sampling apparatus were rejected.

Each spectrum was then reviewed independently 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.

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.