Description

This IR spectral database contains spectra of pure organic chemical compounds, including simple aliphatic, aromatic, alicyclic, and heterocyclic compounds, as well as numerous complex materials.

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: 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

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.