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Spectral Databases

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IR – Vapor Phase FT-IR Library of Synthetic Cannabinoids – Wiley

Spectra – 225

This database is only available as part of the KnowItAll IR Spectral Library subscription

DESCRIPTION

Crime labs are in a constant race to identify substances, and with new drugs being synthesized every day it is difficult for researchers to reach conclusive analyses. Synthetic cannabinoids are a major category of designer drugs with rapid growth. This database has been designed in conjunction with forensics experts to enable chemists and toxicologists to identify in this ever-growing class of novel psychoactive substances.

- IR spectra in the database are applicable to both benchtop GC/IR and GC/MS/IR systems.
- For GC/MS, the infrared spectra from the detector provide an additional dimension of data that is essential for isomer determinations.
- Spectra are free from solid matrix effects like intermolecular actions, hydrogen-bonding, and polymorphism, and will prove useful for the identification of "unknown" synthetic cannabinoids.

ADDITIONAL INFORMATION

When it comes to spectral analysis, the more data you have the better. Wiley spectral databases provide much more information than simply the spectrum. Database records include the following valuable details when available:

- Chemical Structure
- IUPAC Name
- Chemical Name
- Lot Number
- CAS Registry Number
- Molecular Weight
- Catalog Number
- Purity
- DEA Properties
- Resolution
- Formula
- Source of Sample
- InChI/InChIKey
- Synonyms
- Instrument Parameters
- UVmax Data

TECHNIQUE

All spectra were collected using an HP 5890 Series II / HP 5965B GC/IRD system equipped with an HP 59970C IRD ChemStation. A cryogenic MCT wideband infrared detector (Judson Technologies, Montgomeryville, PA) was chosen, yielding a spectral range from 4000 cm^{-1} to 550 cm^{-1}.

All spectra were measured with a nominal resolution of 8 wavenumbers across the entire spectral region. The GC chromatogram was constructed in real time during the run using the Gram-Schmidt vector orthogonalization with a basis set of 8 vectors. Spectra were extracted from the finished chromatogram using chosen intervals of baseline and peak for averaged reference and sample interferograms. All spectra were measured with a velocity of 3 scans per second in a gold-coated pyrex lightpipe (120 mm L x 1 mm ID) at 285 °C.

All reference materials used in this collection were prepared as solutions either in methylene chloride or methanol, depending upon the solubility. One (1) µl of each solution was injected into the injection port at a temperature of 270 °C. The basic spectrometer component hardware used in this system (source, interferometer, lightpipe, and detector) basically have remained unchanged in comparison to the later Digilab/Bio-Rad/Varian IRD II and ASAP IRD II/IRD 3 systems. All have miniature optics matched to a 1 mm infrared beam from a 1400 °C ceramic source heated by a Platinum/Rhodium wire. This configuration, coupled with flow cell volume closely matching the effluent volume of a capillary column peak, results in noiseless spectra that are fractional in optical density in comparison to similar benchtop FT-IR vapor phase spectra.

TRUSTED DATA FROM A TRUSTED SOURCE

Wiley is the authoritative source for spectral data. Our renowned databases are processed according to rigorous protocols to ensure they are of the highest quality. Qualification procedures start at data acquisition and continue throughout the database development process. Any data acquired from trusted partners is thoroughly vetted before inclusion in our collections.

For additional information please visit **www.sciencesolutions.wiley.com**