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## **Spectral Databases**

From the leader in spectral data



ATR-IR - Sigma-Aldrich Library of ATR-IR Spectra - Wiley

Spectra - 19,500

This database is available as part of the KnowltAll IR Spectral Library Collection subscription.



#### **Description**

The Sigma-Aldrich Library of ATR-IR Spectra is a world-class collection of ATR-IR spectra sourced from the laboratories of Sigma-Aldrich\* by Merck KGaA Darmstadt, Germany.

Featuring over 18,000 pure compounds and over 19,500 spectroscopic records, this collection includes the Sigma-Aldrich catalog number, ensuring quick and accurate ordering of standards from Sigma-Aldrich.



## **Applications**

- Clinical research
- Forensics
- Food safety

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#### **Additional information**

The Sigma-Aldrich Library of ATR-IR Spectra includes compound properties (molecular formula, mass, compound class) and ATR-IR spectroscopic data, which has been evaluated by Wiley and third-party experts.

- Chemical names
- Chemical structures
- Sigma-Aldrich catalog numbers
- CAS Registry numbers
- InChIs and InChIKeys

- Molecular formulas
- Molecular weights
- Purities
- Synonyms



#### Compound coverage

- 5-membered aromatic heterocycles and fused aromatic heterocycles
- 6-membered aromatic heterocycles and fused aromatic heterocycles
- Alkynes
- Aromatic compounds: acid halides, alcohols and phenols, aldehydes, amides, amines, amino acids and acid salts, anhydrides, carboxylic acids, esters and lactones, ethers, halogenated hydrocarbons, hydrocarbons, ketones, mercaptans and sulfides, nitriles & cumulated double bonds, nitro and nitroso compounds, phosphorus compounds, sulfur-oxygen compounds
- Boranes
- Coordination and complex compounds
- Deuterated compounds
- Heterocyclic N-oxides
- Mineral acids
- Non-aromatic compounds: acid halides, acid salts, alcohols, aldehydes, amides, amines, amino acids, amino acids, anhydrides, carboxylic acids, esters and lactones, ethers, acetals and epoxides, halogenated hydrocarbons, hydrocarbons, ketones, mercaptans and sulfides, nitriles & cumulated double bonds, nitro and nitroso compounds, phosphorus compounds, sulfur-oxygen compounds
- Non-metallic inorganics
- Organometallic and arsenic compounds
- Oximes
- Polymers
- · Schiff bases, azobenzenes, indicators & dyes
- Silanes
- · Steroids and indole alkaloids



#### **Library specifications**

ATR-IR spectra: 19,503

Distinct Sigma-Aldrich catalog

numbers: 19,503

 Searchable chemical structures: 18,910 • Unique compounds: >18,500

• Structures with InChl Key: 18,910

• CAS Registry numbers: 19,286



#### **Technique**

Featured spectra were measured in the spectral range of 4000 to 625 cm<sup>-1</sup>.



### Compatibility

For full compatibility information, please visit <a href="mailto:sciencesolutions.wiley.com/compatibility">sciencesolutions.wiley.com/compatibility</a>.



#### 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.