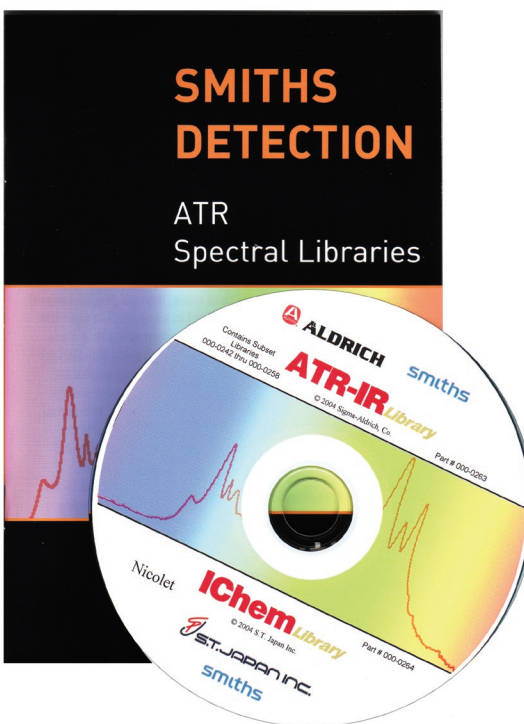


ATR Spectral Libraries

HIGH QUALITY GENERAL PURPOSE DATABASES



Feature Highlights

- Over 25,000 unique ATR spectra
- Subset libraries available
- Compatible with most current FT-IR applications software

Other Formats Available:

- Nicolet
- Perkin-Elmer
- Bruker
- Advanced Chemical Design (ACD)

Until now FT-IR users have been forced to search unknowns against Transmittance Libraries, due to the fact that large ATR Search Libraries were not available. Although transmission libraries can be useful for identifying materials analyzed by ATR, the most reliable identification is obtained when using ATR libraries.

Comparing samples analyzed with ATR to ATR Spectral library databases is the most accurate method of library searching because of the analogous parameters by which the spectra were obtained. Results are not only more reliable but more beneficial when

qualifying samples or identifying unknowns.

Smiths Detection in conjunction with Aldrich Chemical Company and ST Japan have created two ATR spectral libraries. Both libraries are high quality general-purpose databases comprised of spectra, which were collected using Smiths Detection's patented diamond ATR technology.

The libraries contain Organics, Inorganics, Organometallics, Polymers, Biochemicals and Reagents making them ideal for identifying unknowns. Additionally Smiths Detection has made available subsets of these libraries.

ATR Spectral Libraries

Technical Data

General Specifications

The IChem ATR spectral library from ST Japan

The IChem library contains over 12,000 ATR spectra. This library was produced with a 2cm^{-1} data resolution and a spectral range of 4000- 400 cm^{-1} .

Spectral Specifications

Spectral Label: Includes Name, CAS Registry # and Molecular Formula.
Data Resolution: 2cm^{-1}
Spectral Range: 4000 - 400 cm^{-1}
16-bit ordinate precision

Operating System Requirements

Windows NT, ver. 4.0
Windows 2000
Windows XP

Smiths Detection -Aldrich ATR spectral library

The Smiths Detection - Aldrich library contains 18,000 ATR spectra. This library was produced with a 2cm^{-1} data resolution and a spectral range of 4000 to 650 cm^{-1} . All spectra have been verified by other disciplines making all spectra traceable.

Spectral Specifications

Spectral Label: Includes Name, CAS Registry #, Molecular Formula, Aldrich catalog number and chemical structures.
Data Resolution: 2cm^{-1}
Spectral Range: 4000 - 650 cm^{-1}
16-bit ordinate precision

Operating System Requirements

Windows NT, ver. 4.0
Windows 2000
Windows XP

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The Benefits of ATR Spectral Libraries

The simplicity of the diamond ATR technique makes it an ideal tool for rapidly identifying unknown materials. With its unscratchable surface, minimal sample preparation and corrosion resistance, diamond ATR has quickly become the method of choice for analyzing samples.

Smiths Detection Subset ATR Libraries

Subset Library Name:	#of Spectra
ICHEM ATR Database	12,706
Common Chemicals Library	3,302
Aldrich ATR Database	18,513
Aldrich-ICHEM Package Database	25,470
Aldrich-ICHEM Package Database Vol.1	12,735
Aldrich-ICHEM Package Database Vol.2	12,735
Aldrich Database Supplement	9,062
Aldehydes and Ketones Library	2,021
Alcohols and Phenols Library	2,249
Organometallics and Inorganics Library	1,045
Biochemicals Library	4,669
Flavors, Fragrances and Cosmetic Ingredients Library	2,302
Dyes, Pigments and Stains Library	980
Esters, Lactones and Anhydrides Library	3,379
Food Additives and Food Packaging Library	2,083
Forensic Library	1,533
Hazardous Chemicals Library	2,579
Hazardous and Toxic Chemicals Library	6,765
Hydrocarbons Library	1,129
Pesticides Library	1,216
Polymers and Polymer Additives Library	1,635
Semiconductor Chemicals Library	684
Solvents Library	630
Sulfur and Phosphorous Compounds Library	4,070