

Thermo Spectral ID[®] Library Collections

Aldrich Infrared Condensed Phase Libraries

Aldrich FTIR Collection - Edition II

A collection of over 18,000 of the most common chemicals found in the Aldrich Chemical catalog. These spectra were acquired by Aldrich and examined and processed at Thermo Electron and represent a wide range of functional groups. Aldrich Edition II libraries come complete with the Aldrich Library of FTIR Spectra - Edition II Reference books.

834-016200 Aldrich Edition II Condensed Phase Library - High Resolution (18,452 spectra)

Aldrich Edition II Material Specific Sub-Libraries

Sub-groups of the chemicals found in the Aldrich Edition II Condensed Phase Library are organized by chemical type. All Aldrich Edition II Material Specific Libraries are offered in the high resolution format only.

834-019500 Aldrich Hydrocarbons and Halogenated Hydrocarbons Library (1,199 spectra)

834-019600 Aldrich Alcohols and Phenols Library (1,200 spectra)

834-019700 Aldrich Aliphatic and Aromatic Aldehydes and Ketones Library (1,311 spectra)

834-019800 Aldrich Carboxylic Acids, Esters, Lactones and Anhydrides Library (1,653 spectra)

834-019900 Aldrich Dyes, Indicators, Alkynes, Nitro and Azo Compounds Library (1,229 spectra)

834-020000 Aldrich Phosphorus and Sulphur Containing Compounds Library (822 spectra)

834-020100 Aldrich Organometallic, Inorganic, Silane, Borane & Deuterium Compounds (1,523 spectra)

834-020200 Aldrich Polymers Library - High Resolution (466 spectra)

Aldrich FTIR Collection - Edition I

A collection of over 10,000 of the most common chemicals found in the original Aldrich Edition I chemical catalog. These spectra were acquired by Aldrich and examined and processed at Thermo Electron and represent a wide range of functional groups. Aldrich Edition I libraries do not come with any reference books.

834-018400 Aldrich Edition I Condensed Phase Library (10,505 spectra)

Aldrich Edition I Material Specific Sub-Libraries

Sub-groups of the chemicals found in the Aldrich Edition I Condensed Phase Library are organized by chemical type. All Aldrich Edition I Material Specific Libraries are offered in the deresolved format only.

834-004600 Aldrich Hydrocarbons and Halogenated Hydrocarbons Library (839 spectra)

834-004700 Aldrich Alcohols and Phenols Library (788 spectra)

834-004800 Aldrich Aliphatic and Aromatic Aldehydes and Ketones Library (834 spectra)

834-004900 Aldrich Carboxylic Acids, Esters, Lactones and Anhydrides Library (724 spectra)

834-005000 Aldrich Dyes, Indicators, Alkynes, Nitro and Azo Compounds Library (753 spectra)

834-005100 Aldrich Phosphorus and Sulphur Containing Compounds Library (671 spectra)

834-005200 Aldrich Organometallic, Inorganic, Silane, Borane & Deuterium Compounds (632 spectra)

834-005300 Aldrich Polymers Library (275 spectra)

Aldrich Infrared Condensed Phase Libraries (cont'd)

Aldrich FTIR Edition I Supplement Library

This library is a collection of the 7,949 spectra added to the Aldrich Edition 1 (10K) library to create the Aldrich Edition II (18K) library. This supplement library is ideal for customers who currently have the Aldrich Edition I library and want to add the additional 7,949 spectra found in the Aldrich Edition II library. The Aldrich Edition I Supplement library also includes the Aldrich Library of FTIR Spectra Edition II reference books.

834-018800 Aldrich Edition I FTIR Supplement Library (7,949 spectra)

Aldrich Condensed Phase Academic Sampler Library

This collection contains 1,000 spectra that are most likely to be observed in chemistry laboratories in colleges and universities. All of the spectra are from the Aldrich Condensed Phase Library and were chosen by a group of university professors. In addition, very basic chemicals, most likely to turn up in any other environment, particularly production, are also included.

834-009800 Condensed Phase Academic Sampler Library (1,000 spectra)

Nicolet Standard Collection of FTIR Spectra

The Nicolet Standard Collection of FTIR Spectra is a subset of the Aldrich FTIR Condensed Phase library. It provides 3,119 common spectra that are of general interest to the analytical laboratory customer.

834-004300 Nicolet Standard Collection of FTIR Spectra

Sigma Biochemical Libraries

Sigma Biochemical Condensed Phase Library

A collection of over 10,000 of the most common chemicals found in the Sigma Chemical catalog. These spectra were acquired by Sigma and examined and processed at Thermo Electron and represent a wide range of functional groups of particular interest to those engaged in biochemical research or QC.

834-005500 Sigma Biochemical Library (10,411 spectra)

Sigma Steroids Library

A collection of over 3,000 spectra of steroids available from Sigma or provided to Sigma by the UK Medical Research Council.

834-008100 Sigma Steroids Library (3,011 spectra)

Sigma Material Specific Libraries

Subgroups of the chemicals found in the complete Sigma Condensed Phase library are organized by chemical type. All Sigma Material Specific Libraries are offered in the deresolved format only.

834-005700 Sigma Proteins and Peptides Library - Deresolved (747 spectra)

834-005800 Sigma Enzymes, Coenzymes, and Enzyme Substrates Library - Deresolved (485 spectra)

834-005900 Sigma Sugars and Carbohydrates Library - Deresolved (614 spectra)

834-006000 Sigma Dyes, Stains, and Natural Pigments Library - Deresolved (628 spectra)

834-006100 Sigma Fatty Acids, Glycerides, Oils, and Waxes Library - Deresolved (766 spectra)

Chemical Concepts Infrared Libraries

Chemical Concepts Fluka Infrared Spectral Collection

This collection of 2,680 FTIR spectra were measured using various methods like KBr tablet, Nujol suspension, ATR, etc. The spectra are accompanied by information such as Fluka catalog and CAS numbers, compound names, molecular formula, boiling point, melting point, density, refractive index, etc.

LBF1	Chemical Concepts Fluka Infrared Spectral Collection (2,680 spectra)
------	--

Chemical Concepts Near IR Spectra

This collection contains near infrared spectra for 1,900 common organic compounds. All spectra were measured at a spectral resolution of 2 cm⁻¹.

LBCN	Chemical Concepts Near IR spectra (3,800 spectra)
------	---

Chemical Concepts Pure Organic Compounds

A collection of 20,330 FTIR spectra for 17,770 common organic compounds.

LBCO	Chemical Concepts Basic Organic Sub-Library (1,000 spectra)
LBFT	Chemical Concepts Organic Compounds Infrared (20,800 spectra)

Polymer Libraries

Coatings Technology Library

Prepared in cooperation with the Federation of Societies for Coatings Technology, this library includes 2,507 spectra commonly used in the coatings industry. This library corresponds with the Infrared Spectroscopy Atlas published by the Federation. It includes the digitized library, an index and a copy of the Atlas.

834-010900	Coatings Technology Library -non member version (2,507 spectra)
834-010900M	Coatings Technology Library member version (Must provide proof of membership) (2,507 spectra)

Hummel Polymer Library

A collection of over 2,000 spectra of polymers, polymer additives, and chemicals related to the polymer industry acquired by Professor Dieter Hummel of the University of Cologne.

834-008600	Expanded Hummel Polymer Library (2,011 spectra)
------------	---

Industrial Coatings Library

A wide-ranging, current collection of spectra of monomers, polymers, plasticizers, extenders, solvents, pigments, and other additives that are of interest to commercial and industrial laboratories.

834-010600	Industrial Coatings Library (1,961 spectra)
------------	---

Polymers, Polymer Additives, and Plasticizers

A collection of 1,799 spectra of polymers, plastics and additives for polymers, rubbers, cosmetics, adhesives, sealants and plasticizers. Collected by Chemir/Polytech labs and Dr. John Kokosa. Includes a sequential index with additional data like manufacturer, chemical name, product name, chemical abstract number, and category name, if available.

834-008300	Polymer, Polymer Additives, and Plasticizers Library (1,799 spectra)
------------	--

Polymer Libraries (cont'd)

Rubber Compounding Materials Condensed Phase Library

This collection contains 350 spectra of materials used by the rubber and polymer industries and includes accelerators, extenders, plasticizers, curing agents and other processing aids.

834-012000 Rubber Compounding Materials
Condensed Phase Library (350 spectra)

Hummel Defined Polymers Library

Prof. Dieter Hummel's well-known Atlas of Polymer and Plastics Analysis is available in digital form. This unique library enables scientists to solve many analytical problems quickly and reliably in the various fields of polymer chemistry. All spectra were measured at a resolution of 2cm⁻¹.

LBHB Hummel Defined Polymers Basic
Sub-Library (1,040 spectra)
LBHD Hummel Defined Polymers Full
Collection (2,900 spectra)

Hummel Industrial Polymers Collection

Prof. Hummel's latest collection consists of three volumes of spectra for compounds that are actively used in the polymer industry. The spectra were collected directly from the manufacturers or from research laboratories responsible for their development. Volume 1 contains polymers, elastomers, and fibers. Volume 2 is a breakdown of the monomer classes. Volume 3 contains additives and auxiliaries, which are among the most important compounds used in the industry.

LBH1 Hummel Industrial Polymers V1
(1,915 spectra)
LBH2 Hummel Industrial Polymers V2
(1,570 spectra)
LBH3 Hummel Industrial Polymers V3
(1,520 spectra)
LBHA Hummel Industrial Polymers
3V Pkg (5,005 spectra)

Industry Specific Libraries

Aldrich Solvents Library

A collection of condensed and Vapor Phase Spectra of Solvents - a subcollection of the Aldrich Condensed and the Aldrich Vapor phase libraries.

834-008900 Aldrich Solvents Library
(246 spectra)

Commercial Materials Library

An aggregation of the Painter Mineral, the Polypropylene Additives, the Explosives, and the Epoxy libraries. High Resolution not available.

834-010100 Commercial Materials Library
Deresolved (212 spectra)

Food Additives Library

A collection of condensed phase spectra of compounds of interest to the food industry selected from the Aldrich and Sigma libraries. Many of these spectra in the vapor phase may be found in the Flavors and Fragrances library.

834-010300 Food Additives Library
(519 spectra)

Hazardous Chemicals Condensed Phase Library

A collection of 411 condensed phase spectra of toxic chemicals, pollutants and other contaminants of interest.

834-011400 Hazardous Chemicals Condensed
Phase Library (411 spectra)

Industry Specific Libraries (cont'd)

Inorganics Library of FTIR Spectra

The Inorganics library was produced at 2cm⁻¹ data spacing (4 cm⁻¹ resolution) and contains over 1,800 total spectra. This library contains four basic subgroups: Minerals (600 spectra), Borons (296 spectra), Inorganic Compounds (698 spectra) and Commercial Materials (211 spectra).

834-025800 Inorganic Library of FTIR Spectra
(1,803 spectra)

Minerals Spectral Library

This is a subset of the Inorganics Library of FTIR spectra. It contains 600 minerals from all over the world. Included with this library is information on the mineralogical name, chemical formulas, occurrence and color of the mineral.

834-025700 Minerals Library of FTIR Spectra
(600 spectra)

Lubricants and Oils Library

This is a international collection of over 1,500 spectra of motor oils, gear oils, electroinsulating oils, machinery oils, turbine oils, compressor oils, hydraulic oils, anticorrosion oils, steam cylinder oils, metal-cutting oils, natural oils, silicone oils, fuels, greases, and solvents. This library contains over 1,000 spectra measured by KBr transmittance, and over 550 spectra of ATR and ATR corrected data. The User's Guide contains an overview of oil analysis, list of the most common motor oil additives, and a table of characteristic compounds and bands.

834-016000 Lubricants and Oils
(1,576 spectra)

Near Infrared Pharmaceutical Reference Database

A reference database for near infrared users containing 385 pharmaceutical compounds of both active and inactive substances.

- ~ Solid samples were collected in reflectance using a SabIR fiber optics probe
- ~ Liquid samples were collected in transmittance using a 2 mm quartz cell

834-024300 Near-IR Pharmaceutical Reference
Database (385 spectra)

Paper Materials Library

The Paper Materials Library includes over 300 spectra of compounds and materials used in the production of paper products. The spectra were chosen to aid in the identification of impurities as well as to indicate the composition of completed paper products. The spectra were collected using a variety of techniques including transmission and ATR.

834-013900 Nicolet Paper Materials Library
(300 spectra)

Pharmaceutical Excipients Library

This spectral library contains 300 matched IR and Raman spectra collected using Thermo Electron FTIR and FT-Raman spectrometers. Customers may purchase the library as an IR only, Raman only or a matched IR/Raman library. It includes a textbook with an explanation of spectroscopy techniques and the spectra of pharmaceutical excipients for reference use.

834-019200 Pharmaceutical Excipients IR Library
(300 spectra)
834-020300 Pharmaceutical Excipients Matched
IR/Raman Library
(300 IR/300 Raman spectra)

Surfactants Library

A comprehensive collection of carefully characterized surfactant spectra organized by trade name and formula.

834-009100 Surfactants Library (637 spectra)

Hummel Surfactants Library

This library contains 1,020 spectra of surfactants, which has been compiled by Prof. Dieter Hummel (University of Cologne) in co-operation with Chemical Concepts.

LBHS Hummel Surfactants Library
(1,020 spectra)

Industry Specific Libraries (cont'd)

US Geological Survey Mineral Library

A collection of carefully characterized minerals acquired by the USGS.

829-412400 US Geological Survey Library
Deresolved (78 spectra)

Forensic Analysis Libraries

Georgia State Crime Drug Library

A collection of illicit and licit drugs acquired in the condensed phase by the Georgia Bureau of Investigation.

834-007500 Georgia State Crime Lab Drug
Library (1,940 spectra)

Synthetic Fibers Library

Of interest to forensic labs and others who do fibers work. Samples were acquired from the National Bureau of Standards, and were run on a microscope. High Resolution not available.

834-011100 Synthetic Fibers Library
Deresolved (376 spectra)

Toronto Forensic Library

A collection of illicit and licit drugs in various morphologies, physical states, and salt forms, as well as drug precursors, diluents and contaminants. It is supplemented by chemical reagents and spectra of other substances encountered as physical evidence.

834-007800 Toronto Forensic Library
(3,549 spectra)

Vapor Phase Libraries

Aldrich FTIR Vapor Phase Library

These spectra were collected by Aldrich at 1cm-1 resolution on a Thermo Electron FTIR spectrometer with a GC interface, enabling acquisition of chromatographically pure samples. The GC interface also greatly reduces the likelihood of decomposition, a problem when vapor phase spectra are obtained by heating the liquids in a conventional gas cell.

834-006300 Aldrich Vapor Phase Library
(5,010 spectra)

Nicolet Vapor Phase Library

All the spectra from the Aldrich Vapor Phase Library augmented with spectra from Hannover University, University of Wurzburg and Thermo Electron's applications scientists to total 8,654 spectra.

834-006600 HR Nicolet Vapor Phase Library
(8,654 spectra)

TGA Vapor Phase Libraries

This collection contains 460 spectra of compounds most likely to evolve during heating, drawn from the Nicolet Vapor Phase Library.

834-007200 TGA Vapor Phase Library (460 spectra)

E.P.A. Vapor Phase Libraries

This is a collection of 3,300 spectra acquired by the EPA in the late 1970s and early 1980s. The spectra were not run on a CG/FTIR.

834-006900 E.P.A. Vapor Phase Library
(3,300 spectra)

Vapor Phase Libraries (cont'd)

Hazardous Chemicals Vapor Phase Library

A collection of 304 vapor phase spectra of toxic chemicals, pollutants and other contaminants of interest.

834-011700 Hazardous Chemicals Vapor Phase Library (304 spectra)

Flavors and Fragrances

A collection of vapor phase spectra of compounds of interest to the flavors and fragrance industry selected from the Aldrich and Sigma libraries.

834-009400 Flavors and Fragrances Library (667 spectra)

Raman Libraries

Aldrich Raman Condensed Phase Library

The Aldrich Raman Library consists of 14,033 Raman spectra of various substances, most of which are pure organic or inorganic compounds. To create this library, the compounds in the Aldrich FTIR Condensed Phase library were excited with an Nd:YVO₄ laser (1064 nm) using laser powers between 400 - 600mW, measured at the sample. A Nicolet Raman 950 spectrometer (with a Ge detector) was used to collect the Raman spectra. The spectra were then saved in Raman Shift format. All of the spectra were originally measured at a resolution of 2 cm⁻¹ and then mathematically deresolved during conversion to the Nicolet library format.

834-004000 Aldrich Raman Condensed Phase Library (14,033 spectra)

Raman Polymer Library

A convenient sample library for an introduction to the Raman analytical technique for polymer application. The polymer reference samples were prepared by scientific polymer products.

834-014100 Raman Polymer Library (99 spectra)

Pharmaceutical Excipients Raman Library

This spectral library contains 300 matched IR and Raman spectra collected using Thermo Electron FTIR and Raman spectrometers. Customers may purchase the library as an IR only, Raman only or a matched IR/Raman library. It includes a textbook with an explanation of spectroscopy techniques and the spectra of pharmaceutical excipients for reference use.

834-019300 Pharmaceutical Excipients Library (300 spectra)

834-020300 Pharmaceutical Excipients Matched IR/Raman Library (300 IR/300 Raman spectra)

Raman Forensics Library

A collection of common drug compounds, excipients, precursors, and metabolites that are frequently encountered in the course of Forensic Science.

834-014200 Raman Forensics Library (175 spectra)

Raman Organic Chemical Library

Includes spectra at common organic chemicals.

834-004400 Raman Organic Chemical Collection (1,000 spectra)

Nicolet Standard Collection of Raman Spectra

834-004100 Nicolet Standard Collection of Raman Spectra (3,161 spectra)

Mass Spectra Libraries

NIST 2002 Mass Spectra Library

The NIST 2002 collection is the world's most widely used mass spectral reference library. It consists of 174,948 carefully reviewed spectra with molecular structures. This represents a 35% increase in coverage from the previous (NIST 1998) collection.

LBO2 NIST 2002 Library (174,948 spectra)

Wiley Registry of Mass Spectra, 7th Edition

The Wiley Registry is the largest, commercially available collection of mass spectra. The 7th edition contains 33800 spectra chosen and reviewed by Prof. Fred McLafferty, Cornell University. This collection is especially useful for scientists involved in clinical toxicology, drug development and screening, endocrinology, forensics, natural products, etc.

LBW7 Wiley Registry 7e (338,000 spectra)

Chemical Concepts Mass Spectra, 4th Edition

This collection contains reference spectra for more than 40,000 compounds. The main part of the library comes from the Industrial Chemicals Collection of Prof. Henneberg, at the Max-Planck-Institut für Kohlenforschung.

LBC4 Chemical Concepts Mass Spectra 4e (40,000 spectra)

Androstanes, Oestrogens, and Other Steroids

A collection of 2,500 mass spectra of androgens and estrogens and their trimethylsilyl-, o-methoxyoxime- and acetal derivatives. Because of the therapeutic importance of steroids, this library is of particular interest to the pharmaceutical industry.

LBCA Chemical Concepts Androstanes
Oestrogens Other Steroids
(2,500 spectra)

Drugs under Control / Designer Drugs 2003

This library contains 1,400 chemical compounds and 1,700 mass spectra. All new designer drugs that appeared on the market up to February 2003 are included. In reaction to recent terrorist activities, about 100 chemical warfare agents (Sarin, Tabun, etc.) have been added.

LBCD Chemical Concepts Designer Drugs
(1,200 spectra)

Drugs, Pharmaceuticals, and Metabolites

A collection of 2,200 mass spectra for drugs, narcotics, and drug metabolites that are subject to drug trafficking laws.

LBCP Chemical Concepts Drugs Pharmaceuticals
Metabolites (2,200 spectra)

Geochemicals, Petrochemicals, & Biomarkers, 2nd Edition

This reference collection contains 1,100 mass spectra covering a wide range of components relevant to the geochemical and petrochemical fields. Substance classes include saturated, unsaturated and aromatic hydrocarbons, aromatic and non-aromatic sulphur and oxygen compounds, terpenes, steroids and their degradation products.

LBCG Chemical Concepts Geochemicals, Petrochem
Biomarkers 2e (1,000 spectra)

Volatile Compounds in Food, 2nd Edition

This collection covers the whole range of volatile compounds in food. It includes mass spectra for a large number of natural, nature-identical, and artificial flavors and aromas. There are also spectra for food additives and solvents, pesticides, and veterinary pharmaceutical compounds, which are frequently found as residues. Derivatives of non-volatile compounds such as sugars or polyhydroxyphenols are also included.

LBCV Chemical Concepts Volatile Compounds
Food 2e (1,600 spectra)