

Additional information E-mail: info@anadis.nl , PH: +31(0)36 5214190, FX: +31(0)36 5214 428

Available databases

With S.T.Japan we provide a broad range of FTIR, ATR-FTIR, Raman, and NIR spectra. The databases are available as full collections or in specialized subsets in accordance with your application requirements.

- ATR-FTIR Spectra Databases
- FTIR Transmission Spectra Databases
- Raman Spectra Databases
- Hummel Infrared Standards
- Other Transmission Spectra Databases
- NIR Spectra Database

All spectra databases are available in the following spectral formats:

- A2 Technologies - MicroLab PC™
- ABB - Horizon MBTM™
- ACD/Labs - ACD/UV-IR Manager™, SpecManager™
- Agilent-Varian - Resolutions , Resolutions Pro™ v4.1 (and later versions)
- new Agiltron, Inc.
- new BaySpec, Inc.
- BioRad/Sadtler – KnowItAll™, SearchMaster™
- Bruker – Opus™
- B&W Tek Inc. - BWID™
- Enwave Optronics, Inc.
- new EssentialFTIR
- Galactic - Grams/32™, SpectralID™
- Horiba/Jobin Yvon – LabSpec™
- Jasco - Spectra Manager Suite™
- JEOL
- Kaiser Optical Systems - Grams32™
- LabCognition – Panorama, IRanalyze, RAMalyze
- LabControl – Spectacle™
- Lambda Solutions, Inc.
- Lumex – Spectralum™
- Mattson - WinFirst™
- Perkin Elmer - Spectrum Expert Search™
- Raman Systems, Inc. - RSIScan™
- Renishaw - WIRE™, Grams32™
- Shimadzu - IRSolution™, HyperIR™
- Smiths Detection Ltd. (SensIR) - Hazmat™, QualID™, PharmID™
- Thermo Nicolet – Omnic™, new Omnic Specta™

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ATR-FTIR Spectra Databases

In cooperation with Aldrich™, Smiths Detection™, and Nicodom we have enhanced our spectra collections and offer now one of the largest and most advanced collection of ATR-FTIR spectra databases unmatched in quality.

All spectra were collected of samples of highest purity produced by the Aldrich Chemical Company and Japanese fine chemical manufacturers. Therefore, the spectra are taken of important, chemically significant compounds, which make the databases ideal for investigative analysis and quality control applications:

- Specifically prepared for identifying unknowns measured by ATR-FTIR
- All spectra measured using one bounce Diamond ATR
- All data has been reviewed by trained spectroscopists
- Name, CAS number, molecular formula, and additional information with most spectra*
- Databases are delivered with resolutions compatible with your instrument software
- Lists of compounds/spectra in each database are available in pdf format

The complete collection comprises more than 31.000 ATR-FTIR spectra and is subdivided into dedicated databases meeting your individual application needs.

List of all available ATR-FTIR Spectral Databases:

ATR-FTIR Aldrich Spectra Database, P/N 10001

18.513 ATR-FTIR spectra of compounds from the Aldrich collection of the Sigma-Aldrich Company.

ICChem Spectra Database, P/N 20001

13.557 ATR-FTIR spectra of compounds from fine chemical manufacturers in Japan.

Aldrich-ICChem Package Spectra Database Volume 1-3, P/N 30001

36.639 ATR-FTIR spectra of compounds taken from either the Aldrich or the ICChem databases with no duplication.

ATR-FTIR Database Upgrade B, P/N 30101-1

9.121 ATR-FTIR spectra from database version B.

ATR-FTIR Database Upgrade C, P/N 30101-2

4.543 ATR-FTIR spectra from database version C.

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Aldrich Database Upgrade for ATR-FTIR Aldrich-Ichem Database 30001, P/N 30102
18.126 ATR-FTIR spectra of compounds in the IChem, Smiths Detection Ltd, and Nicodom database, which are not in the Aldrich Database P/N 10001. Please Note: Only available in combination with the Ichem Database P/N 20001.

Polymers and Polymer Additives Spectra Database, P/N 30002
4.520 selected ATR-FTIR spectra of polymers, plastics, polymer additives, plasticizers and packing materials.

Food Additives and Food Packaging Spectra Database, P/N 30003
2.762 ATR-FTIR spectra of substances added to food, including substances regulated by the FDA. Also spectra of indirect food additives: substances that come into contact with food such as packaging and processing substances.

Solvents Spectra Database, P/N 30004
667 ATR-FTIR spectra of solvents selected from the Aldrich and IChem Databases.

Organometallics and Inorganics Spectra Database, P/N 30005
2.149 ATR-FTIR spectra of Organometallic, Inorganic, Silanes, Boranes and Deuterium compounds selected from the Aldrich and IChem databases.

Biochemicals Spectra Database, P/N 30006
5.343 ATR-FTIR spectra of Biochemicals selected from Aldrich and IChem and including vitamins, resins, starches, glycerides, fatty acids, sugars, carbohydrates, proteins and peptides.

Aldehydes and Ketones Spectra Database, P/N 30007
3.482 ATR-FTIR spectra of Aliphatic and Aromatic Aldehydes and Ketones selected from the Aldrich and IChem databases.

Alcohols and Phenols Spectra Database, P/N 30008
2.671 ATR-FTIR spectra of Alcohols and Phenols selected from the Aldrich and IChem databases.

Esters and Lactones Spectra Database, P/N 30009-1
4.170 ATR-FTIR spectra of esters and lactones selected from the Aldrich and IChem databases.

Anhydrides and Carboxylic Acids Spectra Database, P/N 30009-2
5.718 ATR-FTIR spectra of Anhydrides and Carboxylic Acids selected from the Aldrich and IChem databases.

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Hydrocarbons Spectra Database, P/N 30010

1.175 ATR-FTIR spectra of Hydrocarbons and Halogenated Hydrocarbons selected from the Aldrich and IChem databases.

Flavors, Fragrances, and Cosmetic Ingredients Spectra Database, P/N 30011

2.716 ATR-FTIR spectra of flavors, fragrances, and ingredients used in the cosmetic industry.

Pesticides Spectra Database, P/N 30012

1.820 selected ATR-FTIR spectra of pesticides including insecticides, herbicides, algacides and fungicides

Semiconductor Chemicals Spectra Database, P/N 30013

919 selected ATR-FTIR spectra a of chemicals used in the Semiconductor industry.

Forensic Spectra Database, P/N 30014

3.579 ATR-FTIR spectra of compounds commonly of interest in the forensic laboratory.

Dyes, Pigments, and Stains Spectra Database, P/N 30015

2.867 ATR-FTIR spectra of selected dyes, pigments, stains and indicators.

Sulfur and Phosphorus Spectra Database, P/N 30016

5.336 ATR-FTIR spectra of sulfur and phosphorus containing compounds selected from the Aldrich and IChem databases.

Hazardous Chemicals Spectra Database, P/N 30017

3.730 ATR-FTIR spectra of chemicals included in the EPA Cameo Database for Chemical Emergencies and Responders and USCG Chris Hazardous Chemicals database.

Hazardous and Toxic Chemicals Spectra Database, P/N 30018

8.136 ATR-FTIR spectra of chemicals included in the EPA Cameo Database for Chemical Emergencies and Responders, the USCG Chris Hazardous Chemicals database, the NIOSH Guide to Chemical Hazards Databases and including chemicals regulated under the Toxic Substances Control Act.

Pharmaceuticals, Drugs, and Antibiotics Spectra Database, P/N 30020

2.715 ATR-FTIR spectra of active substances and aids commonly used in pharmaceutical industry.

High Production Volume (HPV) Chemicals Spectra Database, P/N 30021

1.315 ATR-FTIR spectra of substances included in the HPV Challenge Program Chemical List. The U.S. high production volume (HPV) chemicals are those, which are manufactured in or imported into the United States in amounts equal to or greater than one million pounds p.a.

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Excipients Spectra Database, P/N 30022

852 ATR-FTIR spectra of pharmaceutical and cosmetic excipients.

White Powders Spectra Database, P/N 30023

697 ATR-FTIR spectra of commercially available white powders and white chemical substances.

Lubricants Spectra Database, P/N 30024

1.682 ATR-FTIR spectra of lubricants and oils, including motor specific oils, such as gear and hydraulic oils, anticorrosion oils, fuels, but also natural oils and essential oils.

Coatings Spectra Database, P/N 30025

1.809 ATR-FTIR spectra of common coating materials. Various types of coating including binders, fillers, resins, pigments, dyes. Also typical types of enamels, primers, lacquers, powder coatings, stoving varnishes in fresh and cured form and many other compounds.

Paints Spectra Database, P/N 30026

2.507 ATR-FTIR spectra of art materials used in historical and modern paintings. This databases was developed especially for paintings renovators and conservators, art museums and for forensic purposes. It includes spectra of pigments (historical, inorganic, synthetic), fillers, binders, glues, varnishes, conservation materials, proteins, gums, oils, waxes, balsams, natural and synthetic resins, dispersions, dyes (natural, from plants and animals, synthetic), carbohydrates, and many other related compounds like typical solvents and polymers, cleaning agents, thickeners, retarders, chemicals and more.

Selected Pure Compounds Spectra Database, P/N 30027

5.000 ATR-FTIR spectra of selected pure compounds for educational institutions.

Explosives Spectra Database, P/N 30103

405 ATR-FTIR spectra of explosive materials such as nitrates esters, nitro-aromatics, nitramines, etc. (Spectra are not included in 30001)

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List of all available Transmission Spectral Databases:

FTIR KBr Spectra Database, P/N 40001

22.995 spectra measured using KBr sample prep methods.

FTIR Liquid Film Spectra Database, P/N 40004

7.018 spectra measured using Liquid Film sample prep methods.

FTIR Nujol Spectra Database, P/N 40005

21.127 spectra measured using Nujol sample prep methods (two volumes).

FTIR KBr Spectra Database Upgrade B (from database vers. B), P/N 40101-1

1.156 spectra measured using KBr sample prep methods.

FTIR KBr Spectra Database Upgrade C (from database vers. C), P/N 40101-2

775 spectra measured using KBr sample prep methods.

Polymer and Polymer Additives Spectra Database, P/N 50002

1.273 KBr & Liquid Film spectra of polymers, plastics and polymer additives.

Food Additives and Food Packaging Spectra Database, P/N 50003

1.684 KBr & Liquid Film spectra of substances added to food, including substances regulated by the FDA. Also spectra of substances that come into contact with food such as packaging and processing.

Solvents Spectra Database, P/N 50004

668 KBr & Liquid Film spectra of solvents.

Organometallics and Inorganics Spectra Database, P/N 50005

1.445 KBr & Liquid Film spectra of Organometallic, Inorganic, Silanes, Boranes and Deuterium compounds.

Biochemicals Spectra Database, P/N 50006

4.590 KBr & Liquid Film spectra of Biochemicals including vitamins, resins, starches, glycerides, fatty acids, sugars, carbohydrates, proteins and peptides.

Aldehydes and Ketones Spectra Database, P/N 50007

4.226 KBr & Liquid Film spectra of Aliphatic and Aromatic Aldehydes and Ketones.

Alcohols and Phenols Spectra Database, P/N 50008

2.744 KBr & Liquid Film spectra of Alcohols and Phenols.

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Esters and Lactones Spectra Database, P/N 50009-1
4.335 KBr & Liquid Film spectra of Esters and Lactones.

Anhydrides and Carboxylic Acids Spectra Database, P/N 50009-2
4.920 KBr & Liquid Film spectra of Carboxylic Acids and Anhydrides.

Hydrocarbons Spectra Database, P/N 50010
1.417 KBr & Liquid Film spectra of Hydrocarbons and Halogenated Hydrocarbons.

Flavors, Fragrances, and Cosmetic Ingredients Spectra Database, P/N 50011
1.912 KBr & Liquid Film spectra of flavors, fragrances, and ingredients used in the cosmetic industry.

Pesticides Spectra Database, P/N 50012
958 KBr & Liquid Film spectra of pesticides including insecticides, herbicides, algacides and fungicides.

Semiconductor Chemicals Spectra Database, P/N 50013
664 KBr & Liquid Film spectra of chemicals used in the Semiconductor industry.

Forensic Spectra Database, P/N 50014
1.555 KBr & Liquid Film spectra of compounds commonly of interest in the forensic laboratory.

Dyes, Pigments, and Stains Spectra Database, P/N 50015
1.473 KBr & Liquid Film spectra of selected dyes, pigments, stains and indicators.

Sulfur and Phosphorus Spectra Database, P/N 50016
5.025 spectra of sulfur and phosphorus containing compounds

Hazardous Chemicals Spectra Database, P/N 50017
2.664 KBr & Liquid Film spectra of chemicals included in the EPA Cameo Database for Chemical Emergencies and Responders and USCG Chris Hazardous Chemicals database

Hazardous and Toxic Chemicals Spectra Database, P/N 50018
6.604 KBr & Liquid Film spectra of chemicals included in the EPA Cameo Database for Chemical Emergencies and Responders, the USCG Chris Hazardous Chemicals database, the NIOSH Guide to Chemical Hazards Databases and including chemicals regulated under the Toxic Substances Control Act.

Pharmaceuticals, Drugs, and Antibiotics Spectra Database, P/N 50020
2.806 KBr & Liquid Film spectra of active substances and aids commonly used in pharmaceutical industry.

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High Production Volume (HPV) Chemicals Spectra Database, P/N 50021
1.123 KBr & Liquid Film spectra of substances included in the HPV Challenge Program
Chemical List. The US high production volume chemicals are those, which are manufactured in
or imported into the US in amounts equal to or greater than one million pounds p.a.

Excipients Spectra Database, P/N 50022
438 Transmission spectra of pharmaceutical and cosmetic excipients.

Takayama Plastics Additives Spectra Database, P/N 70101
650 Transmission spectra of antioxidants, plasticizers, lubricants, UV absorbers, light
stabilizers, fillers, etc produced by Japanese chemical manufacturers

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Raman Spectra Databases

This Raman Spectra Database contains 8.694 searchable Raman spectra. The spectra were measured at the National Institute of Advanced Industrial Science and Technology (AIST) in Japan and by our scientists at S.T. Japan, Inc.

Specifications:

- Highest sample purity
- All spectra have been reviewed and evaluated
- Spectral range 4000 cm⁻¹ to 200 cm⁻¹
- Databases can be chosen by spectral resolution: 1 cm⁻¹, 2 cm⁻¹, and 4 cm⁻¹
- Excitation laser wavelength for most spectra: 532 nm or 488 nm
- Name, CAS number, molecular formula, and additional information with most spectra*
- Lists of compounds/spectra in each database are available in pdf format

List of all available Raman Spectral Databases:

Raman Spectra Database, P/N 60001
Complete collection of 8.694 Raman spectra.

Raman Database Upgrade B, P/N 60101-1
4.694 Raman spectra from database version B.

Raman Database Upgrade C, P/N 60101-2
2.152 Raman spectra from database version C.

Polymer and Polymer Additives Spectra Database, P/N 60002
929 Raman spectra of polymers, plastics and polymer additives.

Food Additives and Food Packaging Spectra Database, P/N 60003
1.075 spectra of substances added to food, including substances regulated by the FDA. Also spectra of indirect food additives: substances that come into contact with food such as packaging and processing.

Solvents Spectra Database, P/N 60004
469 Raman spectra of solvents.

Biochemicals Spectra Database, P/N 60006
1.900 Raman spectra of Biochemicals partly including vitamins, resins, starches, glycerides, fatty acids, sugars, carbohydrates, proteins and peptides.

Aldehydes and Ketones Spectra Database, P/N 60007
1.079 Raman spectra of Aliphatic and Aromatic Aldehydes and Ketones.

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Alcohols and Phenols Spectra Database, P/N 60008
891 Raman spectra of Alcohols and Phenol.

Esters, Lactones, and Anhydrides Spectra Database, P/N 60009
2.935 Raman spectra of Carboxylic Acids, Esters, Lactones and Anhydrides.

Hydrocarbons Spectra Database, P/N 60010
565 Raman spectra of Hydrocarbons and Halogenated Hydrocarbons.

Flavors, Fragrances, and Cosmetic Ingredients Spectra Database, P/N 60011
1.030 Raman spectra of flavors, fragrances, and ingredients used in the cosmetic industry.

Pesticides Spectra Database, P/N 60012
468 Raman spectra of pesticides including insecticides, herbicides, algacides and fungicides.

Semiconductor Chemicals Spectra Database, P/N 60013
371 Raman spectra of chemicals used in the Semiconductor industry.

Forensic Spectra Database, P/N 60014
748 Raman spectra of compounds commonly of interest in the forensic laboratory.

Dyes, Pigments, and Stains Spectra Database, P/N 60015
300 Raman spectra of selected dyes, pigments, stains and indicators.

Sulfur and Phosphorus Spectra Database, P/N 60016
977 Raman spectra of sulfur and phosphorus.

Hazardous Chemicals Spectra Database, P/N 60017
1.361 Raman spectra of chemicals included in the EPA Cameo Database for Chemical Emergencies and Responders and USCG Chris Hazardous Chemicals database.

Hazardous and Toxic Chemicals Spectra Database, P/N 60018
3.035 Raman spectra of chemicals included in the EPA Cameo Database for Chemical Emergencies and Responders, the USCG Chris Hazardous Chemicals database, the NIOSH Guide to Chemical Hazards Databases and including chemicals regulated under the Toxic Substances Control Act.

Pharmaceuticals, Drugs, and Antibiotics Spectra Database, P/N 60020
1.172 Raman spectra of active substances and aids commonly used in pharmaceutical industry.

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High Production Volume (HPV) Chemicals Spectra Database, P/N 60021
697 Raman spectra of substances included in the HPV Challenge Program Chemical List. The U.S. high production volume (HPV) chemicals are those, which are manufactured in or imported into the United States in amounts equal to or greater than one million pounds p.a.

Minerals and Inorganic Materials Spectra Database, P/N 60022
1.419 Raman spectra of minerals and inorganic materials. (Spectral range 1500 – 200 cm⁻¹)

Minerals Spectra Database, P/N 60022-1
454 Raman spectra of minerals, extracted from database 60022. (Spectral range 1500 – 200 cm⁻¹). Spectra are not included in 60001.

Inorganic Materials Spectra Database, P/N 60022-2
965 Raman spectra of inorganic materials, extracted from database 60022. (Spectral range 1500 – 200 cm⁻¹). Spectra are not included in 60001.

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Hummel Infrared Standards

We also offer the renowned spectra libraries edited by Prof. D. Hummel grouped by class: Industrial Polymers, Defined Polymers, Surfactants and Organic Compounds.

List of all available Hummel Spectral Databases:

IR Hummel Industrial Polymers Volume 1-3, P/N 70001

Each compound in Volume 1 is identified by its IUPAC or common names. Volumes 2 and 3 additionally contain the chemical structure. All Associated legends quote references, inform about the origin and the synthesis of the polymers as well as the sample preparation. Each compound is identified by its IUPAC or common names and chemical structure.*

IR Hummel Industrial Polymers Volume 1, P/N 70002

1.910 IR spectra collection of polymers, elastomers and fibers consists of spectra of natural and synthetic construction polymers, natural and synthetic fibers, elastomers, miscellaneous resins like natural resins, paint and finishing resins, impregnation and casting resins, dispersion, moulding and printing inks, oils, fats, waxes, tars, inorganic compounds, adhesives, putties, cements, protective colloids, curing agents, initiators and activators, accelerators and modifiers.

IR Hummel Industrial Polymers Volume 2, P/N 70003

1.570 spectra: The following is a breakdown of the monomer classes presented in the database: Vinyl monomers, pyrolyzates, alcohols, phenols carboxylic acids and their salts, esters, anhydrides, amides, hydrazides, urethanes, cyanates, fulminates, heterocycles, amino and thiocarboxylic acids, sulphonamides, technical solvents and more.

IR Hummel Industrial Polymers Volume 3, P/N 70004

The database contains 1.520 FT-IR spectra within the following classes: antioxidants, stabilizer (including PVC stabilizer), light stabilizer, coloring agents, brightening agents, fillers, plasticizers, elasticators, extenders, processing agents, textile auxiliaries, vulcanization agents and rubber auxiliaries.

IR Hummel Defined Polymers, P/N 70011

2.900 polymer spectra with extensive sample information.

IR Hummel Defined Polymers, Basic Collection, P/N 70012

1.140 selected infrared spectra from the collection "Defined Polymers."

IR Hummel Infrared Surfactants Collection, P/N 70021

This database contains 1.020 spectra of surfactants. It has been compiled by Professor Dieter Hummel, University of Cologne in co-operation with Chemical Concepts.

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IR Industrial Organic Chemicals, P/N 70031

20.330 Infrared spectra of 17.770 common organic compounds produced by chemical companies. 5,600 of these spectra are taken from literature spectra and recalculated from peak tables. In addition to the molecular structure, in most cases the following information is available: Chemical name, Purity, Melting point, Boiling point, Density, Molecular formula, Molecular weight, CAS-No, Measurement conditions, Resolution. (Please note that the availability of sample information is depending on the spectrum format/the search software you are using!)

Other Transmission Spectra Databases

Essential third-party spectra collections of transmittance spectra.

List of all available 3rd party Spectral Databases:

Nicodolm Kidney Stone Spectra Database, P/N 70051

1.668 transmission spectra of human kidney stones and related chemicals. This is a collection of compounds found in human kidney such as different types of oxalates, phosphates, urates, other minerals and their mixtures as well as stones of drug or organic origin.

Toronto Forensic Spectra Database, P/N 70061

This extensive library is one of the most widely-used collections of its kind for forensic scientists and investigators. The Toronto Forensic Library contains 3.800 FT-IR spectra of illegal and legal drugs, drug precursors and reagents used to prepare them and other substances encountered in forensic analysis. The major divisions of substances are organic, inorganic, and natural and commercial products. (Please note: The spectra of this database were measured at the Forensic Laboratories of the Canadian Department of Health and Welfare in Toronto. (Spectral Range: 4000 cm⁻¹ to 650 cm⁻¹, Resolution: 2 cm⁻¹ or 4 cm⁻¹))

NIR Spectra Database

Near Infrared Spectra, P/N 70041

The Near Infrared Spectrum collection contains 1.900 common organic compounds each coming along with two spectra in the range of 3.800 – 7.200 cm⁻¹ and 6.300 - 10.500 cm⁻¹. All spectra have been recorded on a Bruker IFS 88 spectrometer at a spectral resolution of 2 cm⁻². Chemical structures and additional information are included: Chemical name, purity, melting point, boiling point, density, molecular formula, molecular weight, CAS-No, manufacturer's article number, path length. (Please note that the availability of sample information is depending on the spectrum format/the search software you are using!)