

## Interpret the IR spectra of polymer compounds.

KnowItAll's Analyzelt™ Polymer IR is an application developed to aid in the interpretation of the bands in an infrared spectrum specifically for polymeric compounds.

Selected Structure Fragment

Browse Knowledge Base by Functional Group

Notes

Summary: Classification, Group, Bond, Range, Intensity, Mode, Notes

Spectrum with Peak Ranges (Interpret a Spectrum)

S.	Classification	Group	Bond	Range	Intensity	Mode	Notes
1	Aliphatic Polyester-Polymer IR	Poly (vinyl acetate)	C-H	2975-2950	W	ASYM_STR	The relat
			CH2	2940-2915	W	ASYM_STR	
			CH	2990-2900	W	STR	
			CH3	2880-2865	W	SYM_STR	
			CH2	2870-2840	W	SYM_STR	
			C=O	1750-1725	VS	STR	
			-CH2-	1480-1440	W	DEF	
			CH3	1465-1440	W/M	ASYM_DEF	
			CH3	1390-1370	M	SYM_DEF	The relat
			C-O	1285-1225	VS	STR	
			C-O	1040-1000	M	STR	
			CH2	2975-2950	M	ASYM_STR	The par i
			CH2	2975-2950	M	ASYM_STR	The par i
			CH2	2940-2915	W	ASYM_STR	
			CH	2990-2900	W	STR	
			CH3	2885-2865	W	SYM_STR	
			CH2	2870-2840	W	SYM_STR	
			C=O	1750-1725	VS	STR	
			-CH2-	1480-1440	W	DEF	
			CH3	1465-1440	M	ASYM_DEF	
			CH3	1390-1370	W	SYM_DEF	The par i
			C-O	1275-1240	M	STR	
			C-O	1175-1155	S	STR	The par i
			CH2	2975-2950	S	ASYM_STR	The par i
			CH3	3010-2960	W/PT	ASYM_STR	In poly (n
			CH3	2990-2950	W/PT	ASYM_STR	The need-
			CH2	2960-2940	W/PT	ASYM_STR	The spec

### Benefits

- Useful in the identification of IR spectra of unknown polymers.
- Useful in classification/pattern characterization of polymers.
- Supplemental to other methods of spectral interpretation.

### Key Features

- Knowledge Base of 100 functional groups.
- Knowledge Base contains hundreds of interpretation frequencies.
- Import experimental spectral data.
- Intelligent "Suggest a Peak" feature.
- Summarize negative or positive interpretations.
- Browse Knowledge Base by chemical class.
- Peak overlay display.
- Displays & highlights structural bonds.
- View notes for functional groups when available.
- For those expert and non-expert in polymer interpretation alike.

### How does it work?

Simply load a spectrum and click on a peak of interest to compare to the Analyzelt Polymer IR Knowledge Base to generate a list of all functional groups possible at that position. You can also view each structural fragment, along with other regions where these fragments would contain peaks.

A summary of the most likely candidates (positive interpretations) is maintained to assist in narrowing the interpretation. The application even highlights the bonds involved in the vibrational frequency.



## About the Analyzelt Polymer IR Knowledge Base.

The Knowledge Base is comprised of the characteristic group frequency ranges and intensities along with associated bar charts and structural fragments of the IR functional groups of polymer compounds. It can provide clear and rapid verification and identification of functional groups in the mid-infrared. Analyzelt Polymer IR features over 100 functional groups and hundreds of interpretation frequencies. The main classifications are:

Alcohols	Celluloses and Derivatives	Polyesters	Resins
Aliphatic Acids	Copolymers	Polyethers	Silicones
Aliphatic Hydrocarbons (Saturated/Unsaturated)	Halogenated Polymers	Polyimides	Sulfides
Aromatic Hydrocarbons	Miscellaneous Polymers	Polyketones	Sulfones
Carbonates	Nitriles and Polyesters	Polyureas	
	Polyamides	Polyurethanes	

## Use with your current methods of polymer interpretation.

Spectral searching is a key tool to improve the polymer researcher's ability and efficiency in the identification and classification of polymer compounds. However, over the years of working with our polymer customers, we have found that there are many cases when more information is desired than can be provided by this tool. Often a key piece of desired information is the spectral-structure correlation.

Bio-Rad's Analyzelt Polymer IR software, in tandem with a Knowledge Base of polymer spectral-structure correlations, can help you to fill that gap.

### References

*The Knowledge Base used by the Analyzelt Polymer IR application currently has over 1300 band assignments, corresponding to functional groups, subdivided into over 100 polymer classes. The databases have been built for use with condensed phase compounds in the mid-IR region (4000-400 cm<sup>-1</sup>). The data were compiled from several sources, with most of the knowledge base prepared and reviewed by John M. Chalmers of VS Consulting.*

For those who also work with monomers....  
please ask us for information on our Analyzelt IR application.

**BIO-RAD**

**Bio-Rad  
Laboratories**

**Informatics Division**  
www.knowitall.com

**China**  
**Europe**  
**Japan, Korea, Taiwan**  
**Rest of World**  
**USA**

Phone: +1 267 322 6931 • E-mail: [informatics.china@bio-rad.com](mailto:informatics.china@bio-rad.com)  
Phone: +44 20 8328 2555 • E-mail: [informatics.europe@bio-rad.com](mailto:informatics.europe@bio-rad.com)  
Phone: +81 03 (6361) 7080 • E-mail: [informatics\\_jp@bio-rad.com](mailto:informatics_jp@bio-rad.com)  
Phone: +1 267 322 6931 • E-mail: [informatics.row@bio-rad.com](mailto:informatics.row@bio-rad.com)  
Phone: +1 267 322 6931 • 1 888 5 BIO-RAD (888-524-6723) • E-mail: [informatics.usa@bio-rad.com](mailto:informatics.usa@bio-rad.com)