FT-IR SPECTROSCOPY

# Spectrum One FT-IR Spectrometer

#### Introduction

PerkinElmer FT-IR spectrometers are built to the highest ISO-9001 manufacturing standards. This document presents confirmed performance specifications based on factory tests. All instruments will meet or achieve better than the confirmed specifications, under normal conditions of use as described in the user manual.

## **Optical system**

General	Sealed and desiccated optical unit. Vibration isolated baseplate.
Interferometer	Improved Michelson interferometer, self-compensating for dynamic alignment changes due to tilt and shear, incorporating high reflectivity first-surface aluminum-coated optics.
Source	Long-life source with proprietary hot-spot stabilization. User replaceable.
Beamsplitter	Proprietary optimized, multi-layer potassium bromide. An extended range cesium iodide beamsplitter is optional.
Detectors	Electrically, temperature-stabilized fast recovery deuterated triglycine sulfate (FR-DTGS) or lithium tantalate (LiTaO <sub>3</sub> ). A liquid nitrogen cooled mercury cadmium telluride (MCT) detector is optional as a second detector.

## **Optical performance**

	FR-DTGS Detector	LiTaO <sub>3</sub> Detector
Wavelength range	7,800 – 350 cm <sup>-1</sup> with KBr beamsplitter	7,800 – 350 cm <sup>-1</sup> with KBr beamsplitter 7,800 – 225 cm <sup>-1</sup> with CsI beamsplitter
Resolution	0.5 cm <sup>-1</sup> to 64 cm <sup>-1</sup>	0.5 cm <sup>-1</sup> to 64 cm <sup>-1</sup>
Wavelength accuracy	0.1 cm <sup>-1</sup> at 1,600 cm <sup>-1</sup>	0.1 cm <sup>-1</sup> at 1,600 cm <sup>-1</sup>
Signal to noise ratio – for KBr optics	30,000/1 rms, 6,000/1 p-p for a 5 second measurement and 100,000/1 rms, 20,000/1 p-p for a 1 minute measurement	7,500/1 rms, 1,500/1 p-p for a 5 second measurement and 26,000/1 rms, 5,000/1 p-p for a 1 minute measurement
Available OPD velocities	0.1, 0.2, 0.5, 1 and 2 cms <sup>-1</sup>	0.1, 0.2, 0.5, 1 and 2 cms <sup>-1</sup>



Data system	
Communication	TCP/IP interface allows direct connection or a Local Area Network (LAN). Instruments are given their own unique IP address and can be controlled over the internet.
Signal sampling	Over-sampling delta-sigma converter.
General	Windows® 2000 and Windows XP compatible.
Calibration transfer	Absolute Virtual Instrument (AVI) – actively standardizes instrument response to improve repeatability and protect data integrity.
Atmospheric compensation	Minimizes effect of atmospheric water and CO <sub>2</sub> on the sample spectra without the need for reference or calibration spectra.
Accessory recognition	Spectrum <sup>™</sup> One accessories and ATR top plates are automatically detected as soon as they are locked into the sampling area. Instrument parameters are optimized for the installed accessory.
Error trapping	All sample spectra are checked for common spectroscopic and sampling problems. Key instrument components are continuously monitored.
Productivity	Look-ahead function automatically detects when a sample is placed into the sample compartment. Data is collected while the operator is entering sample information.
Bench details	
Size	475 mm x 547 mm x 260 mm (W x D x H)
Weight	30 Kg
Software	
General	A single software platform incorporates all of the functions required for infrared analyses; instrument control, data manipulation and analysis, and flexible report utilities. A suite of optional software packages provide advanced capabilities or functions designed for specific application areas.
User interface	Password-protected user login function. Access to methods and routines, menu, toolbar and toolbox functions can be controlled by a supervisor.
Reports	Quick print facility for graphs, spectra and results windows. User defined templates can be created to enable custom printed and electronic reports.
Processing	1st - 4th derivative with a variable filter, smooth (Savitsky-Golay, moving average and triangular), difference, normalization, A, %T, %R, KM, LOG (1/R), ordinate modes, cm <sup>-1</sup> , nm and micron abscissa modes, +,-,*,/, difference, baseline correction, smooth, deconvolution, normalize, abex, interpolate, blank, Kramers-Kronig, ATR correction, peak table, peak height and peak area.
Materials testing	Patented COMPARE™ spectral comparison algorithm and Euclidean searching available. Spectral searching against commercially available or customer developed libraries.
Quantitative analysis	Single frequency, method development software. Spectrum includes Beer's Law, PLS and PCR quantitative prediction.

User training	Full multimedia tutorials CD guides users through operation of the instrument and its accessories, and provides both an overview and detailed training on the software. Accessory training is accompanied by multimedia testing and certification. HTML tutorials provide additional training for common maintenance and software operation. Context- sensitive help provides assistance throughout the software.	
Macros	IR Assistant guides users through analysis by selecting preferences from simple options presented to them. Spectrum Learn Mode allows custom procedures to be generated by development of a script or by recording mouse actions. These procedures can then be stored and repeated using a single mouse click.	
Validation	Data processing Validation and Suitability CD contains test algorithm descriptions, test data and results for all Spectrum algorithms. Comprehensive IQ/OQ documentation and services available.	
Optional software packages		
21 CFR Part 11	Spectrum Enhanced Security™ (ES) software meets the technical requirements for the FDA's 21 CFR Part 11.	
Macros	Advanced macro programming that provides access to instrument functionality through a graphical programming interface while also providing access to Microsoft®'s powerful Visual Basic® development environment.	
Materials testing	AssureID <sup>™</sup> – software designed for materials testing. Advanced features guide developers through building a robust reliable materials testing method. A customizable wizard-style interface provides a risk free environment for routine materials testing packages. OLE-DB compliant data storage.	
Quantitative analysis	Spectrum QuantC for curve fitting and Spectrum Quant+ for PLS and PCR quantitative method development. Includes Expert Assist for method troubleshooting.	



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