Mid-IR and Far-IR Spectroscopy

## Frontier FT Mid-IR and Far-IR System



Frontier<sup>™</sup> IR/FIR System

## Introduction

The PerkinElmer Frontier<sup>™</sup> IR/FIR is a combined FT-IR spectrometer, covering the mid-infrared and far-infrared spectral ranges. The system combines optimum performance in both the Mid-IR and Far-IR regions with sampling versatility in a single instrument.

Software-driven switch-over between the Mid- and Far-IR spectral configurations, combined with fast purge operation enables rapid changeover between the ranges.

This configuration enables a busy analytical or research laboratory to access the broadest scope of applications. The system's research-grade performance and flexibility enable advanced experiments – from kinetics measurements to externally synchronized experiments, in Mid- and Far-IR.

PerkinElmer<sup>®</sup> Frontier FT Mid-IR/Far-IR spectrometers are built to the highest ISO-9001 manufacturing standards. This document presents technical information and performance specifications based on recent factory tests.

As expected with advanced PerkinElmer infrared spectrometers, a full suite of sophisticated built-in instrument standardization and validation functions are included with the standard instrument configuration, to ensure the utmost confidence in your results.



OPTICAL PERFORMANCE		
Mid-IR (KBr) beamsplitter spectral range	8,300-350 cm <sup>-1</sup>	Other beamsplitter materials/ranges available on request
Far-IR (grid beamsplitter) spectral range	700-30 cm <sup>-1</sup>	
Spectral resolution	0.4-64 cm <sup>-1</sup>	For the 3028 cm <sup>-1</sup> band in Methane Software allows intermediate values to be selected in increments of 0.1 cm <sup>-1</sup> . Variable J-stop iris setting is automatically optimized for selected resolution and given frequency.
Wavelength repeatability	$\pm 0.02$ cm <sup>-1</sup> at 1,600 cm <sup>-1</sup>	$\pm 0.008$ cm <sup>-1</sup> achievable
Wavelength accuracy	$\pm 0.1 \text{ cm}^{-1}$ at 1,600 cm $^{-1}$	±0.02 cm <sup>-1</sup> achievable
Signal-to-noise	11,100:1 peak-peak (>50,000:1 RMS) 38,000:1 peak-peak (>174,000:1 RMS)	5 seconds, 4 cm <sup>-1</sup> , transmission measurement 1 minute, 4 cm <sup>-1</sup> , transmission measurement
Available OPD velocity range	0.1, 0.2, 0.5, 1, 2 and 4 cms <sup>-1</sup>	

OPTICAL SYSTEM	
General	Sealed and desiccated optical unit. Vibration isolated baseplate. All beamsplitter, output beam and detector switchovers performed under motorized control. No manual realignment following beamsplitter change.
Interferometer	Improved rotary Michelson interferometer for fast scanning, self-compensating for dynamic alignment changes due to a tilt and shear, incorporating high reflectivity first-surface gold-coated optics.
Optics	Kinematically mounted, zero alignment optics.
Mirrors	High reflectivity gold-coated optics incorporating low-angle off axis design.
Source	Proprietary Mid- / Far-IR long-life source with hot spot stabilization. Source is user-replaceable. External source option. (see External Beam Ports)
Variable J-stop	Software controlled variable Jaquinot stop (J-stop) allows user-control of beam divergence through interferometer and sample focus image size. Iris size automatically optimized for resolution and J-stop wavenumber settings.
Optical filter wheel	7-position software controlled optical filter wheel. User-replaceable filters.
Automated Range Switching (ARS)	Fully motorized beamsplitter, source and beam-switching mirrors under full software control, with auto-optimization provides simple range switchover via graphical PC interface.
External windows	Quick-fit external windows providing rapid window changeover. Desiccated area available for storage of four spare optical windows.
Desiccant	Accepts disposable or rechargeable desiccant packs. Visible desiccant status indicator.
IR beam at sample position	User variable beam ca. 2-11 mm diameter. f/4 vertical plane, f/6 horizontal plane.
External Beam Ports	An optional external beam pack providing 2 additional output and one additional input beam is available.
General Purpose Optical Bench (GPOB)	Optional optical bench available for custom accessories and detectors.
Beamsplitters	
Mid-IR range	Proprietary optimized, multi-layer potassium bromide standard. Other beamsplitters available on request.
Far-IR range	Proprietary optimized, polypropylene/wire grid
Detectors Capabilities for multiple permanently installed detectors:	
Mid-IR	Temperature stabilized fast-recovery deuterated triglycine sulphate (FR-DTGS). Optional liquid nitrogen cooled mercury cadmium telluride (MCT). Other detectors available on request.
Far-IR	Temperature stabilized fast-recovery deuterated triglycine sulphate (FR-DTGS) with polymer window.

Signal samplingOver-sampling delta-sigma converter.Digital scan interfaceFull-duplex TTL-compatible digital scan interface via 26-way D-connector allows synchronization with external equipment via a series of I/O logic lines.CommunicationTCP/IP interface allows direct connection with LAN. Instruments can be configured with their own IP address allowing control via the internet.Internal system monitoring and error trappingEach spectrum checked for common problems. Key instrument components and functions monitored.Automatic accessory recognition system Instrument standardizationAll key sampling systems, including individual ATR top-plate types are automatically detected and instrument parameters are set up accordingly. Custom accessories may be programmed to be automatically recognized and instrument settings configured.Instrument standardizationUnique patented instrument standardization provides accurate on-demand calibration to high resolution gas- phase spectral lines.
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Standardization on both wavelength calibration and instrument line-shape.
Inter-instrument calibration transfer Instruments will reproduce the absorbance spectra of toluene (4800-4200 cm <sup>-1</sup> ) in a 0.5 mm transmission cell at 28 °C $\pm$ 0.5 °C to within 0.002 A.
J-stop wavenumber correction Removes expected frequency shifts of sharp bands that occur due to changing beam divergence with optical resolution (J-stop) setting.
Automatic Atmospheric (AVC) compensation Minimizes the effect of atmospheric water and CO <sub>2</sub> interference without the need for purging or Vapor reference spectra.
Extra-productivity switch "Look-ahead" function detects when sample is placed in position and initiates scanning, enabling data to be collected while the operator is entering sample information.
General Spectrum 10 control software is fully compatible with Windows <sup>™</sup> XP, Vista and Windows <sup>™</sup> 7 operating systems

BENCH DETAILS	
Size	520 mm x 600 mm x 300 mm (W x D x H). Additional bench space for power supply not required.
Weight	34 kg (74.8 lbs).
Sample compartment	Full size sample cover with quick-release cover with service access.
External accessory provision	Left and right side external beam provision via internal motorized mirrors and user-replaceable windows. Auxiliary detector input switching for custom accessories and detectors. External source option to rear. General Purpose Optical Bench (GPOB) option to right-hand side.

SAMPLING	
Mid-IR Sampling	
Internal sample compartment (standard) configured for transmission	Full size compartment with quick-release cover and service access. Variable beam diameter at focus (see Optical System section). Transmission configuration uses dedicated MIR DTGS detector. Compatible with dedicated Spectrum One/Spectrum 100 sampling pods and a wide range of third party accessories.
HATR sampling (option)	Smart horizontal attenuated total reflection pod with a wide range of crystal options.
UATR sampling (option)	Smart universal diamond ATR pod with a range of crystal options.
Diffuse reflection (option)	Smart diffuse reflection pod with a range of sampling options.
Liquids sipper (option)	Smart sipper pod fully controllable pump operation with Spectrum 6.
IR microsampling	Range of infrared microscopy options including Multiscope, Spotlight 150 and 200 available at left-hand beam port.
IR imaging port and microsampling	Compatible with all PerkinElmer Spotlight <sup>™</sup> 400 FT-IR imaging systems and accessories on left-hand beam MIR transmission, reflection and ATR available on single spectrometer-microscope bench.
Far-IR Sampling	
Internal sample compartment (standard) configured for transmission	Full size compartment with quick-release cover and service access. Variable beam diameter at focus (see Optical System section). Transmission configuration uses dedicated Far-IR DTGS detector. Compatible with dedicated Spectrum One/Spectrum 100 sampling pods and a wide range of third party sampling accessories.

SOFTWARE	
General purpose spectrum Mid- / Far-IR software	Single software platform incorporates all functions required for IR analysis in a configurable, freeform-style of interaction; instrument control, data manipulation and flexible report utilities. A suite of optional software packages provides advanced capabilities or functions designed for specific application areas.
Instrument control	Comprehensive suite of control functions with multi-level user interface, graphical display of optical element ranges for optimized operation, automatic instrument setup with smart sample accessories. Rapid Mid- / Far-IR range changing with automatic system optimization. Range of productivity features including Sample Table allowing multiple sample data entry, Look-Ahead for faster data collection with multiple samples and instrument "Go" button for remote operation.
Access control	Password-protected user login with local domain or Windows® system passwords. Access to methods and functions, toolbar and toolbox functions can be controlled by supervisor.
Reports	Quick-print facilities plus user-definable templates for customized reports.
Spectral processing	Extensive range of derivative, smooth, subtraction, normalization and other spectral data transforms available. Spectra calculator for custom operations.
Materials testing	Patented COMPARE <sup>™</sup> spectral comparison algorithm and Euclidean searching. Spectral searching against commercially available or customer-developed libraries.
Quantitative analysis	Single frequency method development software can run single frequency, PLS or PCR quantitative predictions.
Validation	Instrument performance and user configurable system suitability routines available as standard.
Macros	Built-in macro editor and equations editor for defining customised data collection and spectral manipulation sequences.
User training	HTML tutorials provide on-line training for common operations and maintenance. Context-sensitive help provides assistance throughout the software. Instrument performance and user-configurable system suitability routines available as standard.
Optional Software Packages	
21 CFR Part 11	Spectrum Enhanced Security (ES) software meets the technical requirements for the FDA's 21 CFR Part 11.
Sample analysis workflows	AssureID <sup>™</sup> software designed for FT-IR (Mid-IR) materials testing and product verification. Supports testing through a customizable wizard-style interface. Simple turnkey COMPARE, SIMCA, quantitative analyses with user defined instructions and reports can be readily configured. OLE-DB compliant data storage with ES and non-ES versions available.
Custom applications	Direct access to instrument scan functionality via Microsoft <sup>®</sup> Visual Basic and other macroprogramming environments.
Quantitative analysis	Optional Software for PLS and PCR quantitative method development, including Expert Assist for method troubleshooting.
Validation CD	Data validation CD contains test algorithm descriptions, test data and results for Spectrum algorithms. Comprehensive IQ/OQ documentation and services available.

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