

# Spectrum 3 FT Mid-IR and Near-IR System

## Mid-IR and Near-IR Spectroscopy



Spectrum 3 NIR/MIR system NIRA II reflectance accessory

### Introduction

The PerkinElmer Spectrum 3™ IR/NIR system is a combined FT-IR spectrometer, covering the complete mid-infrared and near-infrared spectral ranges. The system combines optimum performance in both the Mid-IR and Near-IR regions with sampling versatility in a single instrument.

Fully automated switch-over between the Mid- and Near-IR spectral ranges takes a matter of seconds because key optical components do not need to be inserted by the user to change the operating range. This automated beamsplitter and detector changeover maintains the moisture-free and controlled atmosphere within the sealed optical compartment and ensures rapid and trouble-free access to either range without the need for purging.

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 to externally synchronized experiments, in Mid- and Near-IR.

PerkinElmer Spectrum 3 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		
<b>Spectral Range</b>		
Mid-IR (KBr) beamsplitter	8,300 – 350 cm <sup>-1</sup>	Other beamsplitter materials/ranges available on request.
Near-IR (CaF <sub>2</sub> )	14,700 – 2,000 cm <sup>-1</sup>	Transmission sampling (ca 680 – 4,800 nm)
<b>Spectral Resolution</b>		
Mid-IR (KBr)	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.
Near-IR (CaF <sub>2</sub> )	1-64 cm <sup>-1</sup> (0.1-6.4 nm at 1,000 nm)	As with Mid-IR above.
<b>Wavelength Repeatability</b>		
Mid-IR	±0.02 cm <sup>-1</sup> at 1,600 cm <sup>-1</sup>	±0.007 cm <sup>-1</sup> achievable
Near-IR	±0.02 cm <sup>-1</sup> at 7,200 cm <sup>-1</sup> (±0.004 nm at 1,390 nm)	
<b>Wavelength Accuracy</b>		
Mid-IR peak maximum	±0.1 cm <sup>-1</sup> at 1,600 cm <sup>-1</sup>	±0.02 cm <sup>-1</sup> achievable
Near-IR	±0.1 cm <sup>-1</sup> at 6,000 cm <sup>-1</sup> (±0.028 nm at 1,670 nm)	
<b>Signal-to-Noise</b>		
Mid-IR	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
Near-IR	<10 uAbs (10 x 10 <sup>-6</sup> Abs) RMS	1 minute, 16 cm <sup>-1</sup> , transmission measurement
<b>Available OPD Velocity Range</b>		
Range below 3,900 cm <sup>-1</sup>	0.1, 0.2, 0.5, 1, 2 and 4 cms <sup>-1</sup>	
Range below 15,000 cm <sup>-1</sup>	0.1, 0.2, 0.5, 1 and 2 cms <sup>-1</sup>	
Time resolved Spectroscopy	FastScan data acquisition	Up to ca 100 scans/sec at 16cm <sup>-1</sup> in MIR

OPTICAL SYSTEM	
General	Sealed and desiccated optical unit. Vibration isolated baseplate. All source, beamsplitter, output beam and detector switchovers performed under motorized control. No manual realignment.
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.
Sources	Combined NIR/MIR/FIR assembly incorporating proprietary Mid-Far IR long-life source with hot spot stabilization and pre-aligned tungsten-halogen NIR source. Both sources are 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 Port	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	
IR range	Proprietary optimized, multi-layer potassium bromide standard. Other beamsplitters available on request.
NIR range	Proprietary wide-range multi-layer calcium fluoride. Other beamsplitters available on request.
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.
Near-IR	Transmission: Temperature stabilized fast-recovery NIR deuterated triglycine sulphate (FR-NIR-DTGS). Reflection: Temperature stabilized indium gallium arsenide. Other options available on request.

DATA SYSTEM AND ELECTRONICS	
Signal sampling	Over-sampling delta-sigma converter.
Digital scan interface	Full-duplex TTL-compatible digital scan interface via 26-way D-connector allows synchronization with external equipment via a series of I/O logic lines.
Communication	TCP/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 trapping	Each spectrum checked for common problems. Key instrument components and functions monitored.
Automatic accessory recognition system	All 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 standardization	Unique patented instrument standardization provides accurate on-demand calibration to high resolution gas-phase spectral lines. 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 ± 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 Vapor (AVC) compensation	Minimizes the effect of atmospheric water and CO <sub>2</sub> interference without the need for purging or 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 instrument control software is fully compatible with Windows™ 10 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	
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 detector. Compatible with dedicated Frontier/Spectrum One/NTS/100/100N 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.
IR microsampling	Range of infrared microscopy options including Multiscope, Spotlight 150i and 200i available at left-hand beam port.
IR imaging and microsampling bench	Compatible with all PerkinElmer Spotlight™ 400 FT-IR imaging systems and accessories on left-hand beam port. MIR transmission, reflection, ATR and NIR imaging available on single spectrometer-microscope.
NIR Sampling	
Reflection (option)	Smart near-infrared reflection accessory available in both in-compartment and external right-hand beam versions. External version allows simultaneous installation of NIR reflection sampling with any internal MIR or NIR sampling pod, e.g. NIR reflection + MIR UATR or NIR reflection sphere + NIR fiber probe.
Transmission	Full size compartment with quick-release cover and service access. Variable beam diameter at focus (see Optical System section). Transmission configuration uses dedicated detector.
Remote liquids (option)	Allows remote transmission measurements of liquids.
Remote solids (option)	Smart high performance solids probe with LED/LCD status readout and various fiber lengths.
Tablet transmission	30-position autosampler with two dedicated detectors combine high performance tablet transmission autosampler (option) measurements with NIR diffuse reflection measurements.
NIR imaging (option)	High performance fast-imaging system in the NIR. Range of tablet autosampler and microscope productivity enhancements. Can perform NIR imaging and high resolution IR and ATR imaging on same optical bench.

SOFTWARE	
General purpose spectrum of IR/NIR software	Single software platform incorporates all functions required for IR/NIR analysis in a configurable, freeform-style 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 MIR/NIR 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 "SmartPanel" 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™ 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.
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™ software designed for FT-IR and FT-NIR materials testing and product verification. Supports Mid-IR and NIR products 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® Visual Basic and other macroprogramming environments.
Quantitative analysis	Optional software for PLS and PCR quantitative method development
Validation CD	Data validation CD contains test algorithm descriptions, test data and results for Spectrum algorithms. Comprehensive IQ/OQ documentation and services available.