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Technical Specifications for ATR-FTIR Spectrophotometer

ATR- FTIR Instrument with choice of accessories, wide range sampling modules and software for quick, easy and reliable IR-analysis of solids, liquids, gaseous and gel like samples.

Powerful but easy to use functions for verifying and identifying IR-spectra and performing quantitative analysis should be part of the software.

General Specifications:

1. Wave number range: preferably between 8000 to 340 cm^{-1} .
2. Wave number accuracy: Should be better than 0.01 cm^{-1}
3. Spectral resolution: Should be better than 0.75 cm^{-1}
4. Preferable S/N Ratio: 1 Min: >45,000:1 (= <9.7 x 10⁻⁶ AU noise) peak-to-peak, 4 cm^{-1} resolution
5. Interferometer: We prefer permanently aligned mirrors with high stability cube corner mirror design. Interferometer should be capable of acquiring data in both scanning directions to ensure the maximum signal-to-noise ratio in the shortest possible time.
6. IR-Source with Optimized light flux, long life-time > 5 years. Diode laser, high wave number accuracy and precision
7. Detector: High sensitivity, Temperature-controlled detector. Please mention detector sensitivity, wavelength range. Detector must be easily replaceable and auto align with security lock. Detector must have 24-bit A/D converter for fast response.
8. Sealed and desiccated optics
9. Internal validation unit with reference standards for automated instrument tests of every setup and every measurement mode
10. Automated instrument tests for operational and performance qualification
11. Easy exchange of different sampling modules
12. Standard compartment FTIR base plates should preferably have suitable slide mount holderto accept 2 x 3-inch cards/slide (standard in the industry) and thus should be compatible with various slide- in sampling accessories (optional).
13. Automatic recognition and individual calibration of modules and ATR-crystal plates, automatic performance test and load of appropriate measurement parameters when changing the configuration.
14. The modules should be easily interchangeable. Suitable measurement settings for the used configuration are automatically loaded.
15. Possibility of extension of spectrometer for operation in regions with high humidity (use of ZnSe for all IR light-transmissive optical components including the moisture resistant beam splitter)
16. ATR-sampling module, with diamond crystal for enabling a fast and reliable FT-IR-analysis of solids and liquids
17. Diamond crystal single reflection, monolithic providing long life-time >10years. (Please provide

list of all compatible accessories: single reflection vs multi-reflection, and choice of crystal)

18. Working plate: trough-like stainless steel plate; Spectral range:350-8,000cm⁻¹
19. Pressure controlled clamp
20. Working distance (max. sample height)20mm
21. Easy cleaning of the ATR applicator. 360-degree rotation possible of the pressure rotor.
22. Temperature: room temperature up to120°C.
23. Desiccant and set of tools
24. Suitable PC should be provided along with the instrument.
25. Warranty: 5 yr. comprehensive warranty with spare parts and consumables if any.

Software Preferred Requirements:

Easy to use and powerful for routine and research experiments. The software should provide customizable work spaces.

1. The spectrometer software should provide wizards for routine applications (baseline correction, zapping, subtraction,curvefitting,normalization,FSDetc).Thiswizards should guide the user through the full measurement and evaluation process and should change its appearance at each step for highest convenience in real-time.
2. All spectral data resulting from one measurement must be stored within one single file. Additionally the results of manipulations (e.g. calculation of derivatives, FSD) and evaluations (e.g. peak picking, quantification) performed on this data shall be stored in the same spectrum file for easy data handling and well-arranged filing.
3. Software must have real time diagnostic features of critical components of FTIR like laser, source, detector and interferometer, and alignment. The software must offer detailed information about the nature of the failure and suggest possible remedy and be capable of sending real time error reports.
4. Continuous monitoring of all the spectrometer components, performance and environmental factors like humidity.
5. Software fully compliant to GLP and GMP regulations.
6. Instrument/software equipped with spectra library of common small molecules/polymers etc.
7. An advanced ATR correction that includes the compensation of the anomalous dispersion effects must be available.
8. Functions for the removal of different shaped base lines should also be included.
9. The software should have provision for analyzing multiple files at the same time, i.e. should include macro wizard.
10. The software should preferably have 3-D data representation /view, and should be able to show real-time time-course data collection and viewing for time-dependent experiments (Preferably at a single wave number unit)
11. The spectral collection software should be compatible (i.e. direct command) with the external water recirculation unit for temperature ramp measurements with heating and cooling functions without any manual intervention.
12. Demountable transmission cell. The cell should include circular CaF₂ windows 32x3mm, suitable mount and 50µm mylar spacers – 12 nos, and suitable syringes for injection.
13. Flow-through Cell is optional but not mandatory: Stainless steel body with 100 micrometers thickness or better, with ZnSe windows, operating pressure: 30psi-60psi, windows with clear aperture with channels to improve cross-flow characteristics.
14. Multi-bounce flow through ATR sampling accessories with heating facility is optional. ATR must be heated up to 120 °C. Temp Accuracy: ±0.5 °C, Temp. Sensor: 3 wire Pt RTD (low drift, high stability)
15. High humidity ZnSe windows and Beam splitter as optional items for consideration. The given beam splitter should be moisture resistant.