



TENNESSEE BUREAU OF INVESTIGATION

Forensic Services Division

Forensic Chemistry Standard Operating Procedure Manual

Fourier Transform Infrared Spectroscopy

20.0 FOURIER TRANSFORM INFRARED SPECTROSCOPY (FTIR)

20.1 Application

Fourier Transform Infrared Spectroscopy (FTIR) is a confirmatory test used in the analysis of legally significant substances. FTIR will generate a unique spectrum in the infrared region of 400-4000 wave numbers for liquid, solid, or vapor samples. The samples must be relatively pure to obtain the best results.

20.2 Equipment

The TBI FCU currently utilizes FTIR instruments manufactured by Thermo Fisher Scientific for the qualitative analysis of legally significant substances. The hardware systems are controlled by proprietary Thermo OMNIC software packages. While versions of this software vary on each instrument, they all have the ability to search library databases for spectral comparisons.

Attenuated Total Reflectance (ATR) sampling accessories are used within the TBI FCU for FTIR analysis.

20.3 Standards

Traceable polystyrene and/or glass standards provided by the manufacturer will be used for performance verification.

20.4 Method

Samples can be extracted to remove any potential extraneous compounds before any FTIR analysis method is performed.

Attenuated Total Reflectance (ATR) requires very little sample preparation. The instrument window should be completely covered with the sample and properly compressed. Liquid samples can be analyzed by placing them directly on the ATR window. An accessory cap is available to cover the liquid to prevent or reduce evaporation for volatile compounds. Extremely corrosive liquids **should not** be placed on the ATR accessory.



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Please refer to the FTIR, iS10 FTIR with Smart iTR Accessory, iS20 FTIR with Smart iTX Accessory, and FTIR iS10 with Golden Gate Accessory Operating Instructions found in the Lab Documentation folder in Ensur.

20.5 Quality Assurance

Running daily primary standards for making spectral comparisons to unknown samples is not required since all primary standards and samples are run using the same instrument spectral parameters.

The IR source can deteriorate over time and will eventually need replacement, but the spectra generated from a new source will not differ from the previously collected spectra.

The ATR window will be cleaned and examined before a new sample is placed on it. A background spectrum will be collected prior to each sample analysis.

20.6 Performance Verification and Acceptance Criteria

20.6.1 Performance Verification

Monthly instrument performance verification will be conducted using the OMNIC validation program. Other internal diagnostic software will be used to monitor the source and detector if available.

Wavelength placement, noise level, and energy (energy ratio or peak-to-peak) must be monitored. The TBI FCU may choose to monitor additional parameters for diagnostic purposes.

Results will be compared to manufacturer specifications or to previous results from that instrument. Tolerances for each piece of equipment will be specified in the instrument's maintenance and verification notebook according to the manufacturer.

The diagnostic software will generate an alignment value for the instrument. This value should be higher than three (3) at a max gain of one (1). Any values less than three (3) may indicate that the source should be replaced.

Instead of a traditional He/Ne laser, the iS20 model is equipped with a solid-state diode laser that can experience a drift in laser values over time. While Thermo recommends adjustment approximately every two months, the alignment and drift of this laser will be monitored and adjusted as part of the required monthly maintenance.

The detector signal should be checked on a regular basis to ensure that the interferogram is producing an adequate signal. The system software will show the acceptable range for signal strength.

20.6.2 Acceptance Criteria

The spectrometer's proprietary software will generate pass/fail results for the following tests:

- Signal to Noise (if applicable)
- Noise Performance
- Val-Pro or Val-Q qualification



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If any of these tests produce failed results, the internal diagnostics will be repeated. The instrument will be removed from service if it fails the repeated diagnostic, and the unit supervisor will be notified.

Refer to Appendix F for maintenance requirements and intervals.

20.7 Criteria for Initial Evaluation

Any peaks generated that are below 100% reflectance will be considered valid for further comparison.

20.8 Interpretation

Direct peak-to-peak comparison between the primary reference standard and the sample must be made for confirmation. Spectral data must be compared to a primary reference standard that has been analyzed using the same spectral parameters.

Spectral differences between samples and standards are usually due to the presence of additional compounds in the sample.

A spectrum that may not have sufficient data for compound identification may be used to determine the salt form. Adequate salt form data must be present to justify the determination. Another confirmatory test must be performed in these instances.