# INDIAN INSTITUTE OF TECHNOLOGY BOMBAY

**MATERIALS MANAGEMENT DIVISION**

**Powai, Mumbai 400076**

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**Detailed Technical Specifications for React IR In situ FT-IR Spectroscopy**

A real-time, in situ mid-FTIR reaction analysis system equipped with a multi-reflection ATR (Attenuated Total Reflectance) probe & can also be utilized as a general purpose mid-FTIR for the off-line analysis of liquid samples.

**General Requirements:**

1. One vendor should manufacture, sell, service and provide technical support for the entire reaction analysis system including spectrometer, probe technology, sampling interfaces and software.
2. Instrument should have facility to use it in batch mode (with the help of probe) as well as in flow mode (with the help of flow cell) in real time.

**Hardware and Sampling Technology Requirements:**

1. Diamond must be available as ATR sensor materials
2. Optical Range: 3500 $cm^{-1}$ to 800 $cm^{-1}$ or better
3. All probe wetted parts should be compatible with typical organic reagents and solvents using no O-ring or brazed seals of any kind, and materials of probe construction must be chemically and physically inert consisting only of Hastelloy C-22 and gold.
4. The ATR sensor must have than 6 reflections or more for the best sensitivity.
5. An RTD (resistance temperature detector) must be integrated into the probe tip to automatically capture temperature of the reaction mass with each spectrum collected.
6. The ATR sensor should not protrude outside the probe body eliminating the possibility of damaging the sensor
7. A wide variety of sampling technology must be currently available for purchase fulfilling the requirements to monitor a wide variety of chemistry
    a. Pressure range: vacuum to 65 bar or better
    b. Temperature range:**-80 ºC to 180 ºC or better**
    c. pH range from 1 to 14
8. The fibers should be housed in a single protective conduit to minimize possibility of damage

9. The fiber and probe assembly should be designed to be serviceable so that any individual component can be replaced by the system vendor.

10. A sensitive MCT detector should be included. Advanced cooling and heating facility should be included.

11. **Purge:** No purge required

**Software Requirements:**

1. Software should be designed specifically for reaction analysis
2. All data analysis functionality should be available in real-time as well as in post reaction mode
3. Integrated quantitative analysis software available with capability to predict absolute concentration in real-time

4. Temporal resolution (time between spectra) should be changeable in real-time while acquiring experimental data so that the sensitivity can be optimized based on reaction kinetics

5. An algorithm should be provided at no additional cost that will automatically deconvolve the three dimensional data sets providing concentration profiling of reaction species along with their calculated infrared component spectra

6. An algorithm should be included that automates the picking of peak height or peak area to zero or baseline points to find the best fit to the multivariate deconvolved trend, and the functional groups that correlate to each of those peaks (and trends) should be provided

7. Real-time data treatments to aid in the interpretation of the data (including at a minimum: baseline correction, solvent subtraction, normalization and $1^{st}$, $2^{nd}$ and $3^{rd}$ derivatives)

8. User defined trends for advanced math functions applied to relative concentration values

9. Dynamic and automatic real-time solvent subtraction to effectively remove solvent characteristics from the data making it easier to interpret the data

10. Automated and real-time export of spectral and profile (concentration) data to specified location on local workstation or to intranet

11. Backwards compatibility to analyze data collected with older software versions from the same manufacturer

12. Capable to import off-line analytical data to scale and quantify Infrared peak profiles

13. The software should run under Windows 7, 8 and 10 operating systems with all service pack versions, and should be touch screen enabled

**14. Warranty : Instrument should be supplied with 3 years Comprehensive Warranty**