Technical Specification: Infrared High Resolution Spectrometer

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1.0 Technical Specifications

The CLS approved the Preliminary Design Report for the Canadian Far Infrared Facility 01B1-01 beamline. The main scientific application performed at this beamline will be Far Infrared gas phase molecular absorption experiments and collecting high-spectral-resolution data. A bending magnet will illuminate the beamline. The design of the beamline is characterized by main components such as a custom wide-angle aperture front end and focusing optics to transfer the beam via a vacuum beamline to the spectrometer experimental station. The overall design of the 01B1-01 beamline is described in the CLS Preliminary Design Report 6.2.72.2.

1.1 Introduction

Fourier transform spectrometers (FTS) based on the Michelson interferometer principle remain the instruments of choice for medium and high resolution Infrared (IR) spectroscopy, because of their advantages of high optical throughput and multiplex signal acquisition compared to dispersive (prism or grating) spectrometers. All the planned CLS IR beamlines will therefore be equipped with FTS instruments. For the Far Infrared (FIR) beamline, a primary requirement is very high spectral resolution in order to exploit the synchrotron brightness advantage as well as the very narrow intrinsic Doppler widths of FIR molecular absorption lines. This and other requirements are described in the following sections. The purchase shall be made as part of the CLS tendering and procurement procedure.

1.2 Performance Requirements

Equipment requested is a Fourier Transform Infrared spectrometer (FTIR) that meets certain spectroscopy related specifications.

1.2.1 Spectral resolution

The spectrometer shall have a maximum optical path difference (MOPD) of 9.0 meters or greater, corresponding to a spectral resolution limit of 0.00067 cm^{-1} or better (cm^{-1} is wavenumbers). This is given by the full width at half maximum (FWHM) of the unapodized instrumental line shape, namely

$$\mathrm{FWHM} = \frac{0.60}{\mathrm{MOPD}} \qquad \text{(MOPD in cm)}$$

This ultra-high-resolution (< 0.001 cm^{-1}) is required to approach the intrinsic Doppler widths of gas-phase molecules in the FIR region.

Spectrometer shall operate at low (> 1 cm^{-1}) and medium (0.1 - 1 cm^{-1}) spectral resolution, as well as at higher resolution (< 0.1 cm^{-1}). This is required so that the

instrument can be used effectively both for high spectral resolution (gas phase) studies and for lower spectral resolution, high spatial resolution (condensed phase) studies.

The ultra-high-resolution (< 0.001 cm^{-1}) requirement, which is crucial to the choice of spectrometer, may seem extreme to the uninitiated. We note the following:

1) Molecular absorption lines have very narrow Doppler widths in the FIR (e.g. 0.0004 cm^{-1} for CH3OH at 200 cm^{-1} and room temperature).
2) The high brightness of the synchrotron IR beam makes it practical to achieve such ultra-high-resolutions with an FTS.
3) Ultra-high resolution allows spectra to be obtained at the intrinsic limit (Doppler broadening), which is natural for gases in the FIR region, thereby maximizing the information gained from the experiment. Moreover, if signal-to-noise ratio can be maintained, then high resolution leads to high sensitivity, since the peak height of an under-resolved absorption line increases in proportion to the resolution.

1.2.2 Wavenumber range

Spectrometer shall provide spectral coverage from < 50 cm^{-1} to > 10,000 cm^{-1}. The primary range for the CLS FIR beamline is 50 – 1000 cm^{-1}. However, coverage to higher wavenumbers is required to allow for complementary FIR / mid-IR / near-IR studies on the same samples, and to be able to optimize the production of unstable molecules using known bands in the mid- and near-infrared regions. This is attainable through a combination of beamsplitters that are interchangeable, with an automatic alignment process provided. This will also require a combination of detectors that are also provided, either switchable through mirror path selection or attachable on pre-aligned mountings. This will also require a combination of light sources and filters, either switchable through mirror path selection or attachable on pre-aligned mountings.

1.2.3 Detectors

System shall include several detectors for various diagnostic and experimental purposes. To be included:

Far Infrared detector of liquid nitrogen cooled MCT and liquid Helium cooled Si type. These shall be aligned to the bench optics and software selectable. The detectors shall be supplied with internal and external filters, transfer optics, cooling transfer lines and pumpout ports, seals, gaskets, funnels as required.

Si bolometer for 10 – 600 cm^{-1} range. Operation at 4.2 ºK.

(see section 1.4 Accessories for optional Si bolometer for < 5 cm^{-1} range)

The following Mercury Cadmium Telluride (MCT) types are optimized for narrow or wide band operation; either one or both may be ordered:

MCT-A type detector for 750 – 4000 cm^{-1} range

MCT-B type detector for 400 – 4000 cm^{-1} range

Mid and near Infrared detectors shall also be included of these types:

DTGS detector with KBr window covering 350 cm^{-1} – 7400 cm^{-1} bandwidth.

InSb detector for 1850 – 10,000 cm^{-1} range.

1.2.4 Beamsplitters

The system shall include the following beamsplitters. Preferably the operation of changing the beamsplitter may be carried out with computer-controlled realignment being the only adjustment; performing mechanical alignment and adjustments shall be kept to a minimum.

1.) Set of Mylar beamsplitters (or equivalent) for the 30 – 500 cm^{-1} region

2.) Ge on KBr beamsplitter (or equivalent) for the 400 – 4000 cm^{-1} region

3.) CaF2 beamsplitter (or equivalent) for the 1700 – 10,000 cm^{-1} region.

1.2.5 Evacuation

The spectrometer shall be fully evacuable to a pressure of less than 0.10 Torr. This is an essential requirement in order to minimize the strong absorption due to atmospheric H_2O and CO_2 in the FIR region. Pumping, gauging, venting, and control shall be provided. When not evacuated the spectrometer enclosure shall allow purging with Nitrogen or other dry gas.

1.2.6 Internal Infrared Source

The system shall include mid- infrared source (glower type or equivalent) with 6000 – 400 cm^{-1} spectral range. System shall include far- infrared source (quartz envelope, Mercury arc type or equivalent) with 600 – 20 cm^{-1} spectral range. System shall include near (tungsten lamp or equivalent) infrared source with 10,000 – 1850 cm^{-1} range. Sources may be water or air-cooled and shall be user replaceable. Appropriate filters supplied as needed. Sources shall have separate price listed for ordering spares.

1.2.7 External Source Port

System shall allow an external light source to enter the interferometer via an external port without need of intermediate optics. This port shall allow mechanical attachment of an external O-ring sealed flange with mechanical layout information provided, and selection of this source port shall be software controlled. Due to the nature of the beam CLS will provide, interfacing optics may be required and vendor shall state availability of collimating or F/number requirements of their port. The port shall be sealable, when not in use, with a suitable Infrared transparent material for either the Mid- or Far- Infrared regions.

1.2.8 Output Beam

The system shall provide a collimated, modulated infrared beam that can exit the bench from a windowed port. The selection of external beam shall be computer controlled. The major use of the spectrometer is to feed light to a custom designed gas cell, and provision shall be made for optical interfacing to various F/number light beams from either this external port or the standard sample compartment. The spectrometer system shall have a full one (1) year warranty including the optical bench, accessories, and computer. A standard sample compartment shall be provided. Access to drawings for optical layout and dimensions shall be provided.

1.2.9 Operational considerations

The spectrometer shall be a standard production item, not a 'one-off' or prototype instrument. This requirement is dictated by the fact that the CLS is a user facility with short-term users and a limited resident support staff. The instrument shall be fully supported by the manufacturer now and in the future, and this is best assured by having a standard production spectrometer, which is used in many other labs. The spectrometer shall be mounted on it's own floor mounted framework with stable vibration isolation. The spectrometer shall be interfaced to a desktop type computer that is compatible with the operating system specified in Section 1.3.1 Software Components. All normally required components and tools shall be provided.

1.3 Data Acquisition Requirements

Spectrometer shall be provided with a data collection and manipulation system consisting of a computer and software package, the components are described in the following sections.

1.3.1 Software Components

The spectrometer shall utilize a well-supported standard software package for instrument operation, data collection, and data manipulation. The software shall operate with an industry standard operating system. It shall support very high-resolution data sets (i.e. precision <0.0001 cm^{-1} for peak finding, interpolation, transmittance, etc.; interferogram sizes > 500,000 points). The manufacturer shall actively support the software and files generated compatible with industry standards, JCAMP or other Infrared file types. The software license shall allow for several viewing/spectral manipulation copies to be operated simultaneously by users off-site after they have collected data.

A second software package shall be provided that allows full data manipulation without data acquisition capability. This will allow users to work on data sets on a separate data station without disturbing the spectrometer during data collection. Applications software shall be fully Microsoft Windows 2000 compatible. It shall allow true multi-tasking, performing searching, plotting, word processing, and

data collection simultaneously. Provide a macro-programming package to automate routine operations in the application software with Windows 2000 as standard. Standard Spectral manipulation features shall include: baseline correction, straight line generation, blank region, smoothing, derivatives, multiplication, addition, peak finding, peak annotation, noise computation (RMS and PP), searching against libraries, interactive spectral subtraction, interactive Fourier self-deconvolution, peak height and area, Kramers-Kronig function. Data file storage and retrieval in JCAMP data exchange format, XY pair and ASCII text file format. Software shall be available and quoted for library searching with libraries available by vendor, third party, and user definition.

1.3.2 Hardware Components

System hardware shall perform at the level of a 2 GHz Pentium or equivalent processor chip. Shall include: minimum 512 Mbytes of RAM memory; a removable storage media consisting of at least one (1) 3.5" 1.44 Mbytes floppy disk drive; 100 Mbytes Zip drive; a CD-ROM drive with DVD+RW/+R, 24X-48X capabilities; a sealed internal hard disk drive of at least 120 GBytes storage; a color monitor with 0.28 mm dot pitch, 17 inch diagonal display with built in bus graphics and 64MB video RAM, an Ethernet interface capable of 100 Mbps operation, and 2 USB ports. A color printer shall be included that allows both black-and -white and color output.

1.4 Accessories

Calibration material, performance test spectral files, port seals and windows, pump maintenance kits, valve maintenance kits, shall be provided. A list of available accessories for: Photo-acoustic Cell, Sample Compression cell, and their pricing shall be included. Option to provide a second Si bolometer for < 5 – 40 cm^{-1} range. Operates at <1.7 ºK (which requires pumping the liquid Helium), pump included.

1.5 Training Requirements

User training on the hardware and software operation of the spectrometer shall be available either on-site or at the vendor's offices.

1.6 Spare Parts Requirements

An inventory of consumable parts shall be maintained at CLS. These shall be available from the vendor for a period of years. The spectrometer shall be covered under a warranty of 1 year and for the interferometer component for 2 years minimum. There shall be service contracts available and a 24-hour service program available to the CLS site.