**ANNEX NO. 4 OF DOCUMENTATION OF THE PROCUREMENT PROCEDURE**

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**SPECIFICATION OF THE PUBLIC CONTRACT SUBJECT**

The subject of the public contract shall meet the following requirements for technical parameters and equipment:

The Infrared Spectrometer (IS) system is planned as an extension to the existing ultra-high vacuum (UHV) system containing a combination of near-ambient pressure X-ray photoelectron spectrometer and scanning tunneling microscope (NAP-XPS/STM).

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| **Technical specification – Infrared spectrometer** | | |
| **Designation of the delivery (min. brand and type)** | |  |
| **Individual technical parameters of the performance** | | **Data about the offered performance** |
| 1 | It permits UHV and near-ambient pressure (NAP) analysis of a sample by Polarization Modulation InfraRed Reflection Absorption Spectroscopy (PM-IRRAS) |  |
| 2 | It allows the sample transfer between NAP-XPS/STM and PM-IRRAS analysis chambers without exposure to air. |  |
| 3 | It is equipped with Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) and Attenuated Total Reflection (ATR) reaction modules. |  |
| 4 | Position and size of the equipment (see **Figure 1** below) |  |
| 5 | Requirements for the controlling computer and software:   1. Desktop PC with minimum configuration:  * min. i7 processor * min. 64 GB RAM * min. 512 GB SSD * min. 1 TB HDD * min. 23.8 inch TFT display * an operating system with an active support and updates (f. e. Windows 10 or better) * min. 2x RJ-45 port  1. English manuals   The PC should contain the following software compatible with the operating system for IR spectra measurement and processing:   1. Software controlling the spectrometer enabling advanced setting of measurement parameters, measurement of spectra, their modification and evaluation including import and export of spectra, 2. ATR-FTIR spectra library, 3. Software Package for comprehensive search functionality in spectra libraries, 4. Software for quantitative spectra analysis. |  |

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| **Technical specification**­­ **­– An UHV Fourier Transform Infrared spectrometer (FTIR)** | | |
| **Designation of the delivery (min. brand and type)** | |  |
| **Individual technical parameters of the performance** | | **Data about the offered performance** |
| 1 | A spectrometer with fully evacuated optics working at a pressure of less than 0.2 hPa. |  |
| 2 | The ability to evacuate the sampling space separately from the internal optics of the spectrometer with the stored interferometer. |  |
| 3 | Automatic shutters with exchangeable KBr windows for separating the sampling space from the internal optics of the device |  |
| 4 | Spectral range of the spectrometer at least 8,000 - 350 cm-1 |  |
| 5 | Spectral resolution of at least 0.2 cm-1 |  |
| 6 | Signal-to-noise ratio at least 60,000:1 (1 min measurement, peak-to-peak) |  |
| 7 | Scanning speed of at least 110 spectra/s at a resolution of 16 cm-1 |  |
| 8 | A KBr splitter with a range of 8,000-350 cm-1 |  |
| 9 | A MIR source – globar |  |
| 10 | **Detectors with SW-controlled switching:**   * RT-DLaTGS operating in the range of min. 8,000-350 cm-1 * LN2-cooled MCT operating in the range of min. 8,000-600 cm-1 |  |
| 11 | A calibration laser: HeNe. |  |
| 12 | Communication between the spectrometer and the PC must be ensured using the TCP/IP protocol via an Ethernet network cable. The device must have a unique IP address. |  |
| 13 | **A high-pressure reaction cell for DRIFTS with the following specifications:**   * possibility of flushing the module with nitrogen or dry air, * fully embeddable in the sample space of the spectrometer for DRIFTS measurements under vacuum, * control of the internal atmosphere above the sample in the pressure range of 10-6 to 1000 mbar and temperature in the range of min. 25-900 °C, * implementation of a temperature controller in spectroscopic software to synchronise temperature ramps with measurements, * replaceable ZnSe and KBr windows, * a module including a cooling unit with a water circuit connected to the reaction chamber for better temperature control and cooling |  |
| 14 | To have the possibility of routine measurement in DRIFTS mode without the reaction cell |  |
| 15 | **An ATR module with the following specifications:**   * diamond monocrystal fixed without gluing, * measuring range min. 350 – 8,000 cm-1, * allow ATR measurements under vacuum, * pressure tip for measurement of powder samples under vacuum |  |
| 16 | **The FTIR should make possible future updates:**   * extending the step-scan mode to a time resolution of 4 ns or better, * extending the resolution to better than 0.06 cm-1, * spectral broadening in the range of min. 50,000-10 cm-1 |  |

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| **Technical specification**­­ **­– UHV chamber for performing PM-IRRAS in UHV conditions** | | |
| **Designation of the delivery (min. brand and type)** | |  |
| **Individual technical parameters of the performance** | | **Data about the offered performance** |
| 1 | Base pressure at least 5x10-10 mbar |  |
| 2 | Compatible with presence of gases (including O2, CO, H2) with pressure up to 1 mbar at temperatures from 150 K to 873 K (minimal range) during the acquisition of spectra |  |
| 3 | The chamber is UHV-connected to the existing NAP-XPS/STM system at the point shown in Figure 1 allowing the sample transfer by transfer rods from it without exposure to air |  |
| 4 | Equipped with a turbomolecular pump with a pumping speed of at least 60 l/s (N2), connected to an oil-free roughing vacuum system |  |
| 5 | Equipped with a pneumatic gate valve in front of the turbomolecular pump |  |
| 6 | Equipped with a full range pressure gauge, range min.  1x10-10 to 1000 mbar |  |
| 7 | Equipped with a motorized min. a 4-axes sample manipulator (XYZP) that allows sample cooling to 150 K and heating up to 873 K while exposed to 1 mbar of gas (minimal range) |  |
| 8 | Made from NAP-compatible materials |  |
| 9 | Allowing application of the sample bias |  |
| 10 | Allowing measurement of the manipulator temperature and the sample temperature via K-type thermocouples |  |
| 11 | Compatible with the sample holders used in NAP-XPS/STM measurements (see its drawing in Figure 2) |  |
| 12 | Equipped with an appropriate power supply unit containing an integrated PID temperature controller |  |
| 13 | A high precision UHV gas inlet leak-valve |  |

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| **Technical specification**­­ **­– Parts for the adaptation of the FTIR with the UHV chamber** | | |
| **Designation of the delivery (min. brand and type)** | |  |
| **Individual technical parameters of the performance** | | **Data about the offered performance** |
| 1 | Adaptation of the spectrometer is realized outside the main sampling compartment (from the instrument side) |  |
| 2 | It contains a transfer chamber equipped with a turbomolecular pump connected to a roughing pump system and allowing chamber evacuation to 5x10-10 mbar |  |
| 3 | It contains a full range pressure gauge, min. range 1x10-10 to 1000 mbar |  |
| 4 | It contains a pneumatic gate valve in front of the turbomolecular pump |  |
| 5 | It contains sample transfer rods to transfer samples from NAP-XPS/STM to PM-IRRAS chambers |  |
| 6 | SW controlled switching between measurements in the sample compartment and in the UHV chamber |  |
| 7 | The adaptation must allow IRRAS and PM-IRRAS measurements of samples placed in the UHV chamber |  |
| 8 | Highly sensitive LN2-cooled MCT detector working in the range min. 8,000-850 cm-1 |  |

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| 9 | Parts for measurements in PM-IRRAS mode that include   * a photo-elastic PEM modulator, operating at a frequency of at least 42kHz, * A polarizer for measurements in the MIR region * Apertures: adjustable in the range of min. 0.25 – 8 mm, at least 12 different apertures |  |

A blue drawing of a square with measurements

Description automatically generatedA yellow machine with blue lines and arrows

Description automatically generated with medium confidence

Figure 2: Drawing of the sample holder used in the NAP-XPS/STM system. The thickness of the sample holder is 1 mm

Figure 2: Drawing of the existing NAP-XPS/STM system (in yellow) and the expected position and space limitations for the in-situ IS system. Also, the point for connecting IS to the NAP-XPS/STM system is shown