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D4.10.1: Implementation plan of an integrated and accessible digital platform architecture for CeTrA

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1. INTRODUCTION

The deliverable 4.10.1 is prepared in the context of the ITINERIS project, within the WP 4 that entails the integration of Research Infrastructures working in the atmospheric domain through synergistic approaches and cross boundaries developments. This is the #1 deliverable (bimester 3) produced for the activity 4.10 CeTrA harmonization and integration within the Italian Network of Environment Research Infrastructures under responsibility of the Operative Unit (OU) University Ca' Foscari (UNIVE) – Department of Environmental Sciences, Informatics and Statistics (DAIS).

The deliverable reports the implementation plan for an integrated and accessible digital platform architecture for the Research Infrastructure (RI) Centre for Trace Analysis (CeTrA), which grounds on the current state of the instrumental resources, support infrastructure and scientific-technological expertise available at the OU in the field of analytical chemistry for the study of the environmental sciences, with a particular focus on the domain Atmosphere.

The overarching objective of this deliverable is to provide a general overview of the structure and contents of the implementation plan of the CeTrA infrastructural platform, in the context of the 100% digital outcome of the ITINERIS project. Secondly, the report also provides details on the instrumental capabilities available at CeTrA, the scheduled upgrades of existing instrumental and infrastructural resources, the digital services required, and finally the activities planned to implement, operate, and monitor the CeTrA digital platform successfully.

The document is structured in 6 sections, including this introduction. An overview of CeTrA, its structure, its placement in UNIVE-DAIS, and its network at national and international level is given in section 2. Section 3 reports the current gaps and needs identified as themes of work that are instrumental to enable the digitalization of analytical and data resources. Section 4 reports the personnel procedure, with a specific focus on the organizational structure set internally to the OU UNIVE-DAIS for ITINERIS. Section 5 outlines the administrative definitions and timelines concerning the purchase procedures for the equipment. Section 6 reports the expected timeline of the implementation plan.

Annexes and references are reported at the end of the document.

2. CETRA

CeTrA is a joint infrastructure of Ca' Foscari University of Venice (DAIS and DSMN), and ISP-CNR. CeTrA develops advanced analytical methods, produces high-quality data for the identification and the quantitative determination of trace and ultra-trace chemical species in environmental matrices. The main expertise of CeTrA for environmental studies are focused on the development of innovative methods for determining anthropogenic compounds and heavy metals in different matrices, such as soil, sediment, water, snow, ice, aerosol, and biota. Special attention is paid to the atmospheric transport of micropollutants to remote areas and to the multi-proxy investigation of sedimentary and ice archives for paleo-geochemistry, climate, and fires reconstruction. The atmosphere is a priority research compartment at the OU, with particular focus on technologies for air quality monitoring, aerosols composition, dynamics of long-range atmospheric transport, and source apportionment. Within the last 20 years, the OU was involved in several air monitoring campaigns, from the area of Venice to trans-national projects on urban (harbor areas) and

remote (alpine and polar) locations. Scientific activities currently going on at CeTrA, at the service of ITINERIS through WP4, include: development of innovative analytical methodologies for the determination of chemical species in gas and atmospheric particulate phases; advanced physicochemical characterization of aerosols; study of the dispersion of emerging pollutants; study of photochemical processes, particularly at the air-snow interface; chemical tracing of general atmospheric dynamics; pollution source appointment; study of fire emissions.

The scientific-technological resources of CeTrA include a wide range of instruments dedicated to the chemical identification, bulk and spatially resolved determination of anthropogenic/natural compounds at very low levels, and the characterization of samples at the micro-to-nano scale. The major instrumentation at the OU includes: low/high resolution ICP-MS for multi-elemental and isotopic analysis; ultra-low level mercury analyzer; FTIR microspectroscopy for identification of organics (microplastics); HPIC-MS for determination of ionic and water-soluble compounds; UPLC-HRMS for wide-spectrum untargeted analysis; (Cryo/Py)GC-(MS/)MS systems for the analysis of persistent organic pollutants (POPs), (semi-)volatile species and microplastics; TEM with scanning mode and SEM for micro-to-nano compositional, structural and chemical imaging analysis of mineral and biological particles; XRD for characterization of fine-grained crystalline materials; AFM for surface physico-chemical investigations. Among the others, CeTrA also includes two clean laboratories, dedicated to the preparation of samples for inorganic and organic analysis. The full list of resources available at CeTrA is available in the ANNEX 1, including the status of the resources, a description of where data are currently stored and their availability.

CeTrA manages the GAW-WMO high-altitude observatory of Col Margherita (MRG), located in the Eastern Alps (Figure 1).

Figure 1. Location of the MRG observatory in the Eastern Alps and View of the current station.

MRG is located in within the Dolomites, a UNESCO World Heritage Site, in the southern slope of the eastern alps (46.37 N, 11.79 E), at an altitude of 2543 m a.s.l. Despite being not at a particularly high altitude, the location is considered strategic because it is representative of the synoptic condition of the southeastern slope of the Alps, where no comparable

monitoring infrastructure is present. The main characteristics of the site are: the representativeness of the synoptic conditions of the free troposphere at 700 hPa, the low influence of orographic barriers in the surrounding area, and the absence of local sources of pollution. The present station was carved out of a modified ISO 10 container (L 2.991 m; w 2.200 m; H 2.250 m) protected by a stone wall erected on three sides and the same height as the station. The instrumentation currently operated at MRG is also reported in the ANNEX 1.

As the leading Institution of the recently funded RI CeTrA, Ca' Foscari University manages the infrastructure in the framework of a strong promotion of national and international collaboration initiatives in research, technology transfer, education, and dissemination. In the research field pertinent to ITINERIS, Ca' Foscari is currently or has been recently part of broad consortia for H2020 projects, including BEYOND EPICA and DEEPICE (ice core science); EU PolarNet 2 platform; NUNATARYUH (permafrost research); EMERGE (environmental impacts of shipping emissions); ICE MEMORY (ice archives preservation). Other collaborations activated over the last years on atmosphere research include REACT (air quality for security); A-PAW (air pollution in the Arctic); POSEIDON and ECOMOBILITY (ship emissions monitoring); GMOS - Global Mercury Observation System (FP7). Ca' Foscari is also highly involved in territorial cooperation for atmosphere research, especially with the Municipality of Venice, with regional and national environmental agencies (e.g., ARPA and ISPRA, respectively). Overall, Ca' Foscari University has a long-standing tradition in research across regional, national, and international programs LIFE, FP7, Creative Europe, EuropeAid, H2020, ERC and Interreg, with a total of 282 EU projects hosted since 2014. In 1989, Ca' Foscari was the first Italian university (in parallel to the University of Bologna) to launch a Degree in Environmental Sciences. Since then, cross-cutting research and education has been carried out in the field considering all domains, with a special attention to the trans-national study of the Atmosphere, particularly related to the atmospheric dynamics and composition in coastal and transition environments; the monitoring of ship traffic emissions; the dynamics of long-range transport of atmospheric pollutants in/across remote areas such as the Eastern Alps and Polar regions (the Arctic).

3. IDENTIFIED GAPS AND NEEDS FOR THE ENHANCEMENT AND DIGITALIZATION OF CETRA RESOURCES

The formal constitution of CeTrA has been a critical step forward in the structuring of historical research expertise and technical/scientific resources at the UO UNIVE-DAIS and ISP-CNR, oriented towards a full sustainability and a strategic opening to the territory and the national-to-international research community. Still, the full transformation of CeTrA from the original essence of a core facility (an ensemble of technical capabilities oriented towards internal demand) into a center of excellence opened to the international dimension, requires critical improvements in digitalization and digital networking, which are also instrumental to cover the gaps with other, more developed RIs, i.e., to achieve harmonization. In this framework, CeTrA's involvement in ITINERIS pursues specific objectives formally integrated in the WP4 – Atmosphere, specifically through the single Activity 4.10, but also informally organic with transversal WPs: access, FAIR data, training. The specific objectives include:

- Expansion of advanced observational capability

- Digitization of instrumental resources
- Opening of instrumental/infrastructural resources
- Opening of advanced non-routinary data, user-oriented streaming
- User-driven development of innovative methodologies
- Early and systematic standardization of innovative methodologies (from research to monitoring)
- Integrated cross-training, education, information, public awareness on environmental topics.

The hardware/software upgrade and integration of existing instrumentation is a critical background requirement to allow 1st stage internal cross-connectivity and integrated management; followed by 2nd stage inter-institutional integration trough the ITINERIS digital platform. In addition, instrumental upgrades are critical to enhance the throughput of data generation processes within CeTrA, which are key requisites to make the datasets streamable into a trans-institutional elaboration and fruition platform (particularly considering near-real time sensing technologies). On top of this, connectivity and remote control of existing and new instruments must be implemented efficiently to achieve the 100% digital outcome of the ITINERIS project. For example, despite most of the instrumentation at CeTrA being configured for remote control, the latter relies on a panorama of heterogeneous licensed or open-source software, independently managed by the reference personnel. Similarly, the data (both raw and processed) and metadata generated throughout research activities at CeTrA, are lacking a top-down supervised repository or database system, which is pivotal for effective implementation of FAIR principles.

In this section, the specific gaps end corresponding needs concerning the implementation integrated and accessible digital platform architecture for CeTrA are discussed in two main directions: A) enhancement and upgrade of CeTrA scientific resources; and B) development of the CeTrA digital platform.

A) Specific needs for the enhancement and upgrade of CeTrA scientific resources.

A list of activities and instruments required to improve CeTrA resources is reported hereafter. The list results from an in-depth survey and analysis of the current availability and status of instrumentation, ancillary equipment and infrastructural integration at CeTrA, with a particular focus on the network connectivity status. More technical details can be found in the instrument-by-instrument description reported as Annex 1 of this deliverable. All the items of the following list apply to the CeTrA budget within the ITINERIS project, and their definition is a result of the planning activities that took place in the first semester of ITINERIS. All items are individually and correspondingly reported in the section 5 of this deliverable for what concern the acquisition timeline and the administrative specifications.

A.1. **Improvement of the IT infrastructure of MRG observatory**, including dedicated server, and new network/radio/Wi-Fi/fiber optics equipment. At MRG observatory, the main critical issues encountered concern the power supply system. At the moment, the station is highly dependent on the grid provided by the nearby San Pellegrino cable car. The current configuration, although buffered using a battery pack, is unable to cope with the continuous energy needs of the instrumentation. This deficit is the main cause of frequent interruptions in the acquisition of meteorological and environmental parameters.

A.2. **Update of the Automatic Weather Station at MRG**. The quality of the meteorological data is currently affected by the position of the station close to the weather pole, which causes a considerable disturbance, especially for wind speed and direction data. The station and the additional boulder cover, erected for protective purposes, cause a shaded area that shields the sensors from air masses coming from the western and northern quadrants affecting both wind and precipitation data. Still, it cannot be ruled out that the proximity of the station also affects the measurement of air temperature and humidity due to the strong radiation emanating in the summer months. In order to ensure the best possible quality of weather data according to WMO international guidelines, a new installation site and configuration for the weather station needs to be identified.

A.3. **Enhancement of the analytical capabilities at MRG**. Beside meteorological data, a very limited range of atmospheric chemical parameters are currently measured at MRG, making the station strongly underused considering the high scientific potential of the site, at the cost of a still significant running effort. A substantial enhancement of data production through new instruments is needed at MRG, to provide a comprehensive and cross-institutionally mergeable pool of atmospheric data. A deep technical-scientific analysis has been carried out to identify the most useful enhancements, synthetically outlined in the following.

A.3.1. **O_3, CO and NO_x analyzers**. These instruments, currently unavailable at MRG, are the basis to generate a sharable and mergeable set of atmospheric data.

A.3.2. **Automatic continuous analyzer, optical particle counter**: the determination of aerosol particle size distribution at high temporal frequency will allow to estimate the impact of aerosols on climate, understand their fate, and investigate their natural and anthropogenic sources in the mountain regions.

A.3.3. **Aethalometer for black carbon online measurement**: the instrument will increase the aerosol data throughput, providing the real-time measurement of the optical properties of aerosol in the atmosphere. By measuring the absorption of visible light produced by aerosol particles, this instrument allows the quantification of the aerosol climate's direct effect, i.e., the ability of particles to warm up the atmosphere by absorbing incoming solar radiation.

A.3.4. **Mercury analyzer**: with the purpose of increasing open data quality and consistency, the atmospheric a mercury analyzer designed for fully automated unattended operation and remote data transfer is of high scientific value. The currently available instrument (Tekran 2537B) is obsolete; thus, a replacing updated model is necessary for cross-connectivity.

A.4. **Enhancement of the analytical capabilities at CeTrA** (both on-site and deployable in the field). New instrumentation to be used on-site at CeTrA and/or deployed in the field are necessary to provide integrative/mobile support to the monitoring activities at MRG, and to expand them well beyond the nearby territory, i.e., to implement inter-institutional data production campaigns within the ITINERIS network. A deep technical-scientific analysis has been carried out to identify the most useful enhancements, synthetically outlined in the following.

A.4.1. **Sequential high-volume sampler of atmospheric aerosols**: collecting high volumes of aerosols into filters for subsequent laboratory analysis will provide a sufficient amount of aerosol for the comprehensive determination of chemical

species at trace and ultra-trace levels, an activity which cannot be performed remotely with comparatively adequate analytical performances.

A.4.2. **Ion chromatography dual pump system with thermostatic autosampler coupled to mass spectrometry detector.** This hyphenated technique will allow to investigate several environmental samples to determine ionic species. In particular, this system will be used to analyze the aerosol samples collected at the MRG observatory, determining in these samples ionic species, carboxylic acids, organic acids, sugars, anionic pesticides, etc. This instrumentation will allow an online connection to manage the instrumentation and the analysis, extract dataset and to download environmental data.

A.4.3. **Mobile remote air monitoring sensing station** consisting in a structurally modified vehicle equipped with low-cost sensors (PM, O_3, CO, NO_x, methane) and technical components (weather station, LoRa and computer). The mobile station will be used for monitoring in real-time, key air parameters in different remote mountain areas. These data will be compared with the dataset from MRG remote station for modeling purposes. Possibly the mobile lab could be equipped with additional sensors and instruments to increase the environmental and meteo parameters to improve temporal and geo-spatial visualization of air quality data.

A.4.4. **Low-cost (multi)sensors monitoring station for air quality** (PM-SO_2-NO_2-meteo-T-RH-noise). The acquisition of this bench of sensors will permit the enlargement of the atmospheric open data throughput, more specifically by providing new quickly-deployable and sharable resources to perform validation and monitoring campaigns focused on the emerging field of low-cost atmospheric monitoring, which might have important implications for citizens science.

A.5. **Software, libraries and hardware/software update of current instruments for data elaboration and connectivity**. Each one of these components were identified as being critical to achieve the alignment of connectivity level amongst all instrumental resources currently available at CeTrA, together with an improvement of their data production capability in view of the state-of-the art, which is pivotal for harmonization and integration of the CeTrA local platform in ITINERIS. A detailed survey of the current state of instrumentation and a deep technical-scientific analysis have been carried out to identify the most useful enhancements, synthetically outlined in the following.

A.5.1. **Software license for laboratory automation** (LabView): a graphical programming environment is required to develop automated research, validation, and production test systems to be implemented for the management of the internal (custom) network of instruments at CeTrA.

A.5.2. **Upgrade and digitalization of temperature/pressure control system for clean room laboratories.** The clean rooms currently available at CeTrA are equipped with a local control system that manages the internal infrastructure, particularly for what concerns the air filtering/pressure and temperature conditions in all the internal rooms. Still, the control system allows only limited parametrization of the infrastructure and can be monitored/operated only locally on touchscreens. An upgrade of the electronic/software system will allow to

integrate the clean rooms in to the CeTrA digital platform, particularly to achieve remote control and to implement automatic routines.

A.5.3. **Instrument-specific big data elaboration package for UPLC-HRMS (Thermo Orbitrap) and database access license**: (UPLC-) HRMS fragmentation spectra library METLIN Gen2 multiuser. These software and library are fundamental for the improvement of the local identification power of unknown chemical species in complex mixtures (big data from untargeted analysis by UPLC-HRMS) for aerosols characterization studies.

A.5.4. **General application software for data elaboration** (OriginPro): 16 licenses. Data elaboration software permits the upgrade of the local and remote power of the entire RI to elaborate raw physicochemical atmospheric data into significant open and re-usable information. All licenses will be installed in remotely accessible and dedicated virtual machines (VM).

A.5.5. **Instrument-specific software:** Chromeleon 7.3 for control ICS5000 IC and ALTIS MS. This new software, together with the new workstation provided by Thermo Scientific, will make the remote connection easier and will simplify the interface with other instrumentation, aiming a network infrastructure for instrument management, and will permit the handling more than one instrument simultaneously. Moreover, the technical support will account for the full installation of the workstation and software and will set up the connection with the ALTIS MS system. The computer will be equipped with a solid disk drive that will speed up instrument method development operations.

A.5.6. **Instrument-specific control/elaboration software upgrade for 2 GC-MS Agilent instruments**; 150 positions autosampler and automatic injector for one GC-MS. This full upgrade is pursued to improve the local robustness of the quality assurance (QA) system and identification power of unknown (semi)volatile compounds in atmospheric aerosols and related matrices by GC-MS analysis; the software upgrade and OS update are also essential to connect the instruments to the digital platform; hardware upgrade will dramatically improve the throughput and automatization/standardization level of analyses.

A.5.7. **Instrument-specific elaboration software F-search system (FrontierLab) for PyGC-MS Agilent instrument**. The software will improve automatic library-based search and identification of polymers and additives based on EGA thermograms and pyrograms. The software upgrade and OS update are essential to connect the instruments to the digital platform.

A.5.8. **Instrument-specific control/elaboration package for FTIR microscope (Thermo Nicolet).** The required upgrade improves the implementation and automatization of the local identification power of unknown chemical species in complex mixtures by FTIR microscopy for aerosols characterization studies.

A.5.9. **Databases access license**: ICSD, PDF-4+ and PDF-4/organics for XRD station Empyrean Series 3 Malvern Panalytical. This database is necessary to improve the speed of analysis and the automatization of the crystalline phases assignments, integrating and improving the XRD data.

A.5.10. **Instrument-specific control/elaboration software** (Zeiss ZEN Core) for FE-SEM Zeiss Σigma VP machine and control/elaboration software (JEMS) for

(S)TEM machine JEM-F200 JEOL. These two upgrades are required for the automatization of microscopic image analysis.

B) Specific needs for the digitalization of CeTrA resources

From the point of view of ICT development, ITINERIS consists in designing and developing a network infrastructure to extend the CeTrA digital research tools capabilities. CeTrA's scientific instrumentation, operating in the laboratories of Ca' Foscari University (Scientific Campus), must be fully and efficiently reachable and controllable remotely through the Internet as a requisite to achieve the digital integration of the RI within the national network of ITINERIS. Both internal and external researchers interested in using the instruments of CeTrA need an efficient digital platform for entering in contact with the internal personnel (technicians and reference researchers), booking instrumental resources and work sessions, following or even performing (whenever technically possible) their experiments remotely, and having access to the data processing operations through a secure system. The platform must be complemented by an Electronic Lab Notebook (ELN) to allow researchers to record the salient phases of the experiments, and by an open-source repository to share, store, cite, explore and analyse research data. To achieve a better management of the maintenance of instruments, and to have constant monitoring of their usage, the digital platform of CeTrA must also be supported by a Laboratory Management System (LMS). The entire digital platform of CeTrA will be developed and harmonized within ITINERIS thanks to the dedicated budget resources. Overall, the platform will consist of the following modules:

B.1. Remote access system and network connection
B.2. Data Repository
B.3. Booking application
B.4. ELN
B.5. LMS

During the first three bimesters of the ITINERIS project, the team of the OU, coordinated by the Computer Services and Telecommunications Area (ASIT), carried out a detailed survey and analysis of internal requirements, designed the structure of the platform and started the market analysis needed for the acquisition of software tools. Details on the software tools and the analysis process are reported below.

B.1. **Remote access system and network connection.** This module consists in a tool for remote access to the instrumentation, ruling out the need for specific remote-control software which have been installed by the users on specific machines. The main benefit of using a single tool (or a harmonised set of tools, depending on the type of instrument) is to enable users for connecting to multiple instruments from the same client. Currently, 11 instruments at CeTrA are connected to control PCs. The systems are very different from an IT point of view, and can classified into 3 groups:

- Group 1: instruments connected via ethernet to a PC with virtualizable software (open source or with the possibility of moving the license).
- Group 2: USB connected instruments or proprietary connections to a console machine.
- Group 3: Instruments connected to a non-replaceable console machine (e.g., license locked on specific machine; machine with particular sw/s requirements that cannot be upgraded).

Group 1 instruments - the physical consoles - will be replaced by VM connected via LAN directly to the instrument. VM client will be installed in the physical machines located in the laboratories to allow convenient local access to the system but keeping the instruments operation independent by the local physical machines. The consoles of Group 2 and 3 instruments cannot be virtualized, thus a VM will be created as a bridge, to host an access system to the local physical machine. In this way the physical machine (e.g. obsolete but still necessary XP OS) will not be directly exposed to the internet. Access to the instruments for external users will be pre-authorized and then allowed using a VPN and ad hoc credentials. Integration details and requirements will be defined for all the connection tools during the next months of the project, complementally to the acquisition of the hardware infrastructure allocated in the budget.

B.2. **Data repository**. The activation of a data repository within CeTrA is pivotal to achieve harmonization and integration of the RI in the ITINERIS network and platform, particularly to share, store, cite, explore, and analyse research data. The system must be complementary to ARCA (system used for the publication of research results used at Ca' Foscari University) and compliant with the H2020 requirements for Open Data, particularly with re3data. The main features provided are:

- Permanent data citation
- Metatagging (citation-related, domain-related, file-related)
- Faceted search
- Access control
- CC0 licenses/terms of use/restrictions/guestbook
- Management of roles and permissions
- Versioning of published data
- Reformatting tabular data
- Metadata separated from data
- API for integrating with magazines
- Data visualizations and analysis

With the support of personnel from different university areas (Research, Digital library, IT), an in-depth analysis has been performed, converging to the adoption of Dataverse, a tool developed by the Institute for Quantitative Social Science of Harvard University (https://dataverse.org/). The choice was driven by the following reasons:

- Dataverse is a software specifically developed for research data management. It differs from other repositories born to manage academic publications (e.g., DSPace) or to respond to needs not directly related to the academic research, such as CKAN, which is used for the exhibition of open data to local authorities or more generically to government realities.
- It is an open-source software that can rely on a large community of developers and a very large number of users all over the world. Unlike proprietary software such as, for example, Elsevier's Data Monitor or Clarin's ERIC, it offers more guarantees of long-term continuity because the availability of data infrastructure is not tied to a publisher. Similar cons. might be raised for Figshare, produced by Digital Science part of Holtzbinck Publishing Group.
- It is capable to meet the needs of a multidisciplinary structure such as both CeTrA and the ITINERIS network, thanks to its modular organization and the ability to manage metadata files and schemes produced by different disciplines. These features

differentiate Dataverse from other open-source repositories for the management of research data, such as Dryad and Open Science Framework, which focused on specific disciplines such as evolutionary, genetic and ecological biology; and the medical-psychological area, respectively.

- It is customizable to respond to the needs of the various research communities unlike Zenodo, which, despite being a multidisciplinary repository, does not allow for extreme customizations of the organizational structure of data and user interface.
- It allows for integration with other open science tools (DOI, versioning tracking, access management and usage licenses, ORCiD) and OAI-PMH protocol support. Taking advantage of the latter technology, Dataverse has implemented the possibility of viewing the descriptive metadata of datasets stored in other archives, to avoid costly duplications of large amounts of data.

All technical documents required to acquire hosting and management for Dataverse have been prepared, and the deployment of the system is foreseen by the end of July 2023.

B.3. **Booking system**. A booking system which allows pre-authorized users to book instrument-time, and enable an efficient planning of the instrumental resources, will be another key element of the CeTrA digital platform. The access to CeTrA instruments and laboratories will be regulated by an online booking system. The system will provide a simple way to manage the lab instrument scheduling and get all team members' schedules aligned. Lab managers will individually include their respective instrument into the system, and will define customized booking rules, allowing all users to access the booking system through a simple interface. The system will be complemented by reporting and analysis tools, that will allow the lab managers to verify booking data vs actual usage data. Overview of the time booked, and downtime will help to forecast the infrastructural capacity, to achieve sustainability of the infrastructure, and support strategic planning. Market analysis is currently in progress to identify the most suited software given the requirements of CeTrA platform and its harmonization within ITINERIS. This analysis must be integrated with the ones for the LMS and the ELN because a number of commercial products incorporate multiple of such functionalities, but in different combinations. The definition of software main functionalities will be completed by June 2023 in order to acquire the software by the end of August 2023.

B.4. **ELN**. A laboratory notebook system is intended to replace physical laboratory notebooks, and is conceived to maximize the standardization, automatization, routinization and sharing of operating conditions, procedures, notes and other data concerning the experimental sessions. ELNs offer several advantages over traditional paper notebooks: they facilitate good data management practices, providing data security, control and collaboration. ELNs support the FAIR principles, which are recognized by the research community and pivotal within ITINERIS. They allow supervision by the PIs, allow the simple sharing of data and documentation with collaborators, and eliminate text readability problems and reduce the likelihood of data loss. The definition of software main functionalities will be completed by June 2023 to acquire the software by the end of August 2023 (see above, booking system).

B.5. **LMS**. The implementation of a laboratory management system aims to optimize the management of equipment and consumables necessary to carry on the experimental activities. The integration of a LMS in the platform of CeTrA will allow the technicians and reference researchers to improve and standardize the management of

instrumentation, ancillary laboratory equipment and consumables, resulting in a significant upgrade towards sustainability. Trough integration in the CeTrA platform, the LMS will be remotely accessible, thus enabling to monitor continuously the maintenance status of the instruments and to produce reports on their use. Furthermore, the individual technician/researcher will be able to check whether the stocks of materials and consumables necessary for the experiments are sufficient well in advance. The definition of software main functionalities will be completed by June 2023 in order to acquire the software by the end of August 2023 (see above, booking system and ELN).

Overall, all modules of the CeTrA digital platform are expected to be activated as a beta-version by the bimester 10 (correspondingly to the deliverable D4.10.2 - catalogue of digital services) and fully validated by the bimester 14, as originally foreseen in the ITINERIS timeline (see also section 5)

4. PROCEDURES FOR THE PERSONNEL

A graphical overview of the OU's organizational structure for CeTrA activities in the context of the ITINERIS project is reported in Figure 2. Briefly:

- The **Coordination Board** is responsible for the management and for the scientific advisory of all the CeTrA activities within ITINERIS and acts as a direct link to the top-level coordination of WP4 and of the ITINERIS project. The Board is leaded by the Scientific Responsible, the Administrative Responsible and the Project Manager (PM) of the Co-Proponent UNIVE, coincident with the UO DAIS. The PM is also formally the task leader of the OU, in this specific case being the OU responsible for the only 4.10 activity, coincident with a single task.
- The **Executive Board** includes internal representatives in charge of the management of specific infrastructural components of CeTrA (DAIS, DSMN, ASIT and ISP-CNR, each represented by one person). The Executive Board coordinates the scientific operation at CeTrA premises with feedback and support from the main coordination block. The Board is comprised of the Scientific Responsible of the OU as responsible for DAIS instrumentation; a representative of DSMN as responsible for corresponding instrumentation; a representative of ISP-CNR as responsible for the instrumentation and infrastructural implementation at MRG; a representative of ASIT as responsible for the ICT activities and contact point for transversal Access WPs.
- The **scientific operation** group is responsible for technical implementation (and management) of instrumental resources upgraded and deployed at CeTrA, as well as the operational implementation, testing and running of the CeTrA digital platform, particularly for what concerns the physical, remote and virtual access to the RI laboratories, data and services overall, including ICT support and data management under FAIR principles (in coordination to the transversal Access and FAIR WPs), and interaction with the users.
- The **administrative activities**, managed by the Administrative Representative of the Coordination Board, are operatively implemented by a dedicated team (two personnel units) for what concerns purchase procedures and financial reporting.

Three new personnel units are specifically hired by/for the project ITINERIS, namely:

- 1 specialized local project (and RI) manager (fix-term position 30 months, Technologist level D3), member of the Coordination Board. The new staff member took up his duties on Feb. 2023.
- 1 specialized laboratory technician (fix-term position 30 months, Technician level D1), member of the Scientific Operation group. The new staff member took up her duties in Nov. 2023.
- 1 specialized ICT technician (fix-term position 30 months, Technician level D1), member of the Scientific Operation group. The new staff member recruitment is currently in progress, advanced stage, with the interview that took place on Mar. 2023 the new contract will likely be activated shortly.

In summary, 2 of the 3 budget-allocated personnel units already on duty, whereas the third is about to be hired. The (minor) delays in the starting dated of the 3 contracts with respect to that originally planned (the starting date of the project), inevitably originated from administrative times, will be covered by the overheads of the Co-Proponent UNIVE.
In addition, 1 extra personnel unit has been hired through funding by UNIVE, external to the ITINERIS budget, to be specifically dedicated to the administrative operation of the project (member of the administrative operation group).

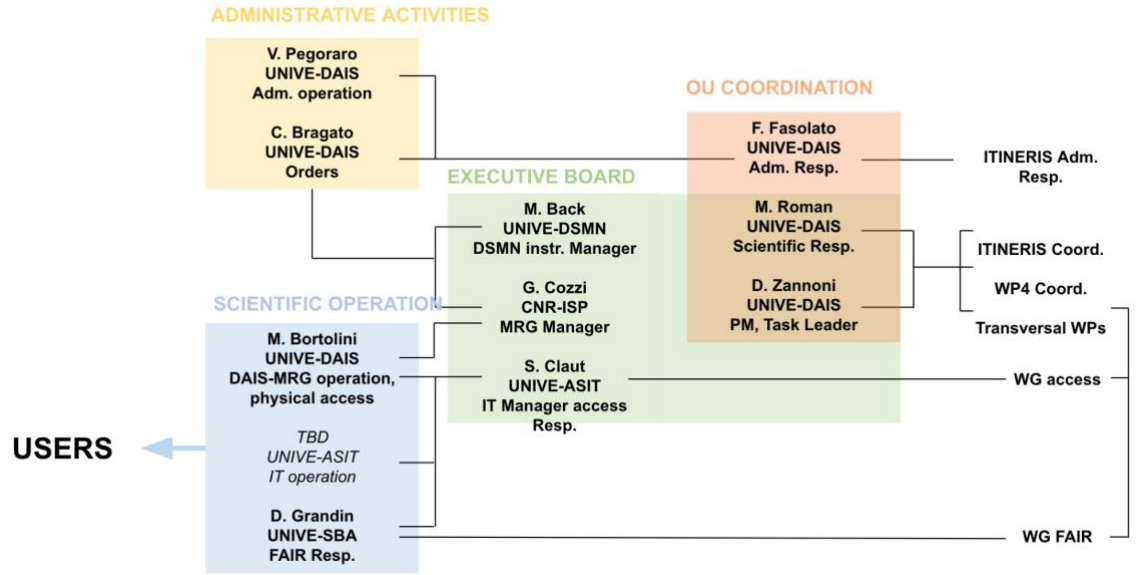

Figure 2. Organization Breakdown Structure of the UO UNIVE-DAIS working on the development and harmonization of the RI CeTrA in ITINERIS.

5. EQUIPMENT PROCEDURES

All of the needs described in the section 3 as the identified responses to fill the current gaps in the framework of harmonization of the RI CeTrA within the ITINERIS network are reported in this section as individual budget entries with encoded names (#item) listed in Table 1, and specification of their planned acquisition timeline, administrative details and setting with respect to the intermediate objectives (IO) of ITINERIS listed in Table 2. The following timeline is an updated version (at the time of this deliverable – B3) compared to the original timeline approved with the project proposal (post-negotiation). Minor changes are reported anyhow, resulting in negligible shifts/exchanges of temporal frames and with

no impact on the overall budget, nor the partitioning of budget items into cost categories (as all items were and still are identified as instrumentation). A few shifts forward for the completion of purchase procedures implied translation of corresponding items from the financial temporal term of IO4.2 to that of IO4.5, but without impact on the achievement of corresponding scientific activities, as demonstrated by this deliverable (the development/implementation plan for the CeTrA digital platform has been completed as reported herein).

A brief description of the purchase procedures for instrumentation follows Table 2.

Table 1 List of encoded instruments to be acquired for CeTrA trough/for ITINERIS.

Item #	Description
1	Server infrastructure with adequate redundant storage and component dedicated to Col Margherita Observatory
2	Network apparatus for equipment and systems connectivity
3	Scientific instrumentation update for connectivity
4	Laboratory management system license
5	Data repository licence
6	Booking and access system and remote connection system license
7	Backup system
8	Instrument: Optical Particle Counter (EDM 264 Eco. automatic continuous analyzer)
9	Instrument: Aethalometer (AE33 for black carbon online measurement)
10	Instrument: Ion Chromatography ICS-6000 Dual Pump with AS-AP thermostatic autosampler and Mass Spectrometer ISQ-EC
11	Instrument: high volume sequential sampler of atmospheric aerosols (digitel DH77)
12	Instrument: mercury analyzer
13	Instrument: Automatic Weather Station (AWS) for Col Margherita Observatory
14	Instrument: O_3, CO and NO_x online analyzers for Col Margherita Observatory
15	Infrastructure: radio/Wi-Fi communication module + router + Switch Ethernet + Touchscreen 17" (5:4)
16	Observatory-dedicated data transfer-storage platform (harmonized with CeTrA platform)
17	Software: LabView 2 licences + training
18	Instrument: mobile remote air monitoring sensing station consisting of (PM, O_3, CO, NO_x, methane, meteo, solar panel, LoRA, battery, CPU) + pc
19	Infrastructure: upgrade and digitalization of temperature/pressure control system for clean room laboratories
20	Instrument-specific big data elaboration package for UPLC-HRMS and dedicated PC
21	Database access license: (UPLC-) HRMS fragmentation spectra library
22	General application software for data elaboration (Origin Pro): 16 group licenses
23	Instrument-specific software: Chromeleon 7.3 for control ICS5000 IC and ALTIS MS
24	Instrument-specific control/elaboration software upgrade, software training for 2 GC-MS Agilent instruments, 150 positions autosampler
25	Instrument-specific elaboration software for PyGC-MS Agilent instrument
26	Instrument-specific control/elaboration package for FTIR microscope, dedicated PC
27	Databases access license: ICSD, PDF-4+ and PDF-4/organics for XRD station
28	Instrument-specific control/elaboration software for FE-SEM Zeiss Σigma
29	Instrument-specific control/elaboration software for (S)TEM machine
30	Instrument: low-cost (multi)sensors monitoring station for air quality (PM-SO_2-NO_2-meteo-T-RH-noise), cloud storage and open data visualization platform

Table 2 Timeline, status and administrative specifications of encoded instruments to be acquired for CeTrA trough/for ITINERIS

	Purchase timeline (by bimesters – B)															Status at B3		
Item #	**B 1**	**B 2**	**B 3**	**B 4**	**B 5**	**B 6**	**B 7**	**B 8**	**B 9**	**B 10**	**B 11**	**B 12**	**B 13**	**B 14**	**B 15**	n – Not started **S – Started** **C – completed**	**IO**	**Type of procedure**
1																**S**	4.5	RdO Mepa n.1
2																n	4.5	Exclusivity n.1
3																n	4.5	RdO Mepa n.2
4																**S**	4.5	Exclusivity n.2
5																**S**	4.5	Exclusivity n.3
6																**S**	4.5	Exclusivity n.4
7																**S**	4.5	Exclusivity n.5
8																**C**	4.2	Exclusivity n.6
9																n	4.5	Exclusivity n.7
10																n	4.5	EU n.1
11																n	4.5	RdO Mepa n.3
12																n	4.5	RdO Mepa n.4
13																**C**	4.5	RdO Mepa n.5
14																**S**	4.5	RdO Mepa n.6
15																n	4.5	RdO Mepa n.7
16																n	4.5	RdO Mepa n.8
17																n	4.5	Exclusivity n.8
18																**S**	4.5	RdO Mepa n.9
19																n	4.7	Exclusivity n.9
20																**S**	4.5	Exclusivity n.10/batch 1
21																**S**	4.5	Exclusivity n.11
22																**S**	4.5	Exclusivity n.12
23																**C**	4.2	Exclusivity n.10/batch 2
24																n	4.5	Exclusivity n.13
25																**S**	4.5	Exclusivity n.14
26																**S**	4.5	Exclusivity n.10/batch 3
27																n	4.5	Exclusivity n.15
28																n	4.5	Exclusivity n.16
29																n	4.5	Exclusivity n.17
30																n	4.5	RdO Mepa n.10
				IO4.2/D4.10.1							IO4.5/D4.10.2							

Deliverables associated to the activity 4.10 (UNIVE-DAIS, CeTrA)

- D4.10.1 Implementation plan of an integrated and accessible digital platform architecture for CeTrA
- D4.10.2 Documentation of the platform catalogue of services giving access to all modules of the CeTrA platform in its beta-version
- D4.10.3 Report on CeTrA digital platform performances

Items from #1 to #7 are purchased with the aim of the full implementation of the comprehensive digital platform for CeTrA harmonized with Ca' Foscari University research products management system, ITINERIS network and EU standards. The platform will provide a core management system for CeTrA instrumentation, a resources catalogue and access portal (physical, remote, VM), and research product (metadata, data, methods) repository. Items #1 and #3 will be purchased through RdO procedure in MePA platform. Items #2, #4, #5, #6, and #7 will be acquired following an exclusivity purchase procedure.

Items #8, #9 and from #11 to #14 are instruments and sensors that will be deployed at the MRG Observatory to increase open data range and throughput. Instruments #8 and #9 will be acquired through an exclusivity purchase procedure. Sensors and analysers from item #11 to #14 purchasing procedure will be through RdO in MePA and will be all installed at MRG.

Items #15 and #16 will be acquired through MePA RdO procedure and exclusivity purchasing procedure, respectively, and will improve the data storage, transfer, and connectivity through the infrastructure. These products will be deployed at MRG and will guarantee the harmonization of data management system. Item #17 is required for the software upgrade, the purchasing procedure will be done through an exclusivity procedure (unique supplier). Item #18 will integrate the atmospheric data from MRG with the data from other remote sites, MePA RdO as buying procedure. Item #19 will also be acquired through exclusive purchase procedure being a straight upgrade of currently available infrastructural and maintenance systems, subjected to exclusive supply.

Items from #20 to #29 are software and hardware upgrades acquired with the purpose of increase and automatize open data throughput, quality and (re)usability (FAIR) on instruments currently present in CeTrA. Items from #20 to #29 will be acquired with exclusivity purchasing procedure as the upgrades are solely supplied by the instruments' manufacturer. Briefly, items #20 and #21 will permit the improvement of the identification power of unknown chemical species from untargeted analysis by UPLC-HRMS. Item #22 will permit the upgrade of the local and remote power of the entire RI to elaborate raw physicochemical atmospheric data into significant open and re-usable information; this item will be configured in order to be remotely accessible for internal users through installation on virtual machines. Items #23, #24, #25, and #26 guarantee the improvement of local robustness of QA system and identification power of compounds in atmospheric aerosols and related matrices by GC-MS, IC-MS, ALTIS-MS, Py-GC-MS, and FTIR analysis, respectively. The related software upgrade and OS update are also essential to connect the instruments to the digital platform; hardware upgrade will dramatically improve the throughput and automatization/standardization level of analyses. Item #27 regards the digital crystalline structure databases for XRD and (S)TEM instruments aimed to improve the speed of analysis and the automatization of the crystalline phases assignments. Items #28 and #29 are required for the automatization of image analysis for FE-SEM, (JEMS), and (S)TEM machine. The software upgrade and OS update are also essential to connect the instruments to the digital platform. Item #30 will be acquired with a MePA RdO procedure; this item will enlarge the number of low-cost instruments for atmospheric parameters monitoring and open data throughput.

ANNEX 1 – INSTRUMENTATION CURRENTLY AVAILABLE AT CETRA

The following list reports the technical information of the CeTrA instruments target of software and hardware upgrades. Specific information of the current status of the connection between instruments and workstations and the data storage are reported.

- Gas chromatograph (GC) HP6890 – mass spectrometer (MS) 5973N (Agilent Technologies) equipped with a CDS 5150 pyrolizer (CDS Analytical) (Py-GC/MS): The GC-MS is connected to a PC via LAN cables on a network switch. The pyrolizer is connected to the GC-MS and separately to the PC via serial connections. The currently available software for data elaboration is MDSChem (revision E.02.00, release October 2008) licensed software for elaborating chromatograms and mass spectra, permitting qualitative and quantitative chemical analysis, implemented in a Windows XP operative system. PC and instruments are not connected to the network and cannot be accessed remotely. There is no automatic backup system: once generated, data files are manually transferred to web storage. The required upgrade for this instrument is the software F-search 3.6 (Frontiers Lab). It is the only software specifically dedicated to the interpretation of pyrograms for the analysis of polymers and additives. For this purpose, extensive libraries of polymers and additives are provided with the software.
- Gas chromatograph (GC) 7890A - mass spectrometer (MS) 5975C (Agilen Technologies) (GC/MS): The two instruments have a similar hardware configuration and are currently used. In detail there is a single quadrupole 7890A-5975C GC-MS instrument (Agilent Technologies), equipped with a 16 slots autosampler (G4513A, Agilent Technologies) and electron ionization source operated in positive mode. The instrument allows qualitative screening and quantitative determination of pesticides, lipids, persistent organic pollutants in environmental and biological matrices (aerosol, water, soil, sediment, biota). The second instrument is single quadrupole 7890A-5975C Cryo-GC-MS instrument (Agilent Technologies), equipped with a Unity2 (Markes International) thermal desorption system. The instrument is suited for the analysis of volatile and semi-volatile organic compounds (VOCs and SVOCs) in environmental matrices (indoor and outdoor air quality), food, forensics, consumer, and other application fields (flavors and fragrances). This instrument does not provide an autosampler. The instruments are connected to the PC with ethernet cables and two dedicated LAN. The two workstations are not online and cannot be reached working remotely. There is not a dedicated backup system, and the transfer of the data is based on USB pens. The control software is Agilent G1701EA MSD Productivity ChemStation Software E02.00 (Agilent, release March 2008). The operative system required by the software is Windows XP which is installed on both the workstations. The use of the software is allowed by a single-user license. The necessary upgrade mainly focuses on the software part with the acquisition of two dedicated new PCs and the OpenLab ChemStation Data Analysis software integrated with MassHunter. The operative system will be thus updated to a more recent version of Windows. MassHunter software will improve the efficiency to determine and identify unknown molecules. Secondly, the instrument which is not equipped with an autosampler will be improved, adding a new 150 positions autosampler. This requirement is aligned with the project of the infrastructure, the new autosampler will provide a longer time of autonomy of the instrument that will be background controllable.

- µ-FT-IR Nicolet iN10 (Thermo Fisher): The instrument is an infrared microscope Nicolet iN10 (Thermo Scientific) integrating a high-resolution CCD optical camera and a FT-IR spectrometer and is designed to perform microanalysis with lateral resolution down to a 50-microns at room temperature or a few microns with liquid nitrogen cooling. The instrument is equipped with motorized stage, MicroTip ATR device for direct contact sampling and analysis of fine structures (down to 3 microns), motorized visible polarizer for visual inspection, MTC-A detector with spectral range 7800–650 cm-1 and the dedicated software package OMNIC Picta for spectral identification of pure compounds and mixtures. Acquisition can be performed in transmission, reflection, or ATR modes. Particles analysis can also be performed to extract species-specific distributions of morphological parameters (size, shape). The instrument is connected to the workstation via USB wire. The software is Omnic Picta is licensed. The operative system is Windows 7. The actual (non-working) PC was web connected. An automatic data backup has never been improved, the remote control of the PC is possible, but it is impossible to connect to the PC while the instrument is acquiring analysis. In order to operate the actual hardware configuration it is necessary to upgrade the workstation with a new dedicated PC with upgraded operative system (windows 10) and the new version of the software. The software upgrade required is OMNIC 9. Moreover, the hardware upgrade consists of iN10 Visual kit: OMNIC Picta update, flat-field correction software, increased safety margin when working with ATR, lenses and mount for visual improvements, LEDs for illumination, brighter illumination, more even lighting.
- Ultra-Performance Liquid Chromatography (UPLC) Ultimate 3000 – Orbitrap XL High Resolution Mass Spectroscopy (HRMS) (Thermo Fisher Scientific) (UPLC-HRMS): The ionization is obtained using a Nanospray Flex ion source (Thermo Scientific) equipped with a Picotip silica emitter. The MS/MS acquisition is downstream to a collision induced dissociation (CID) fragmentation and provides accurate mass measurement (<10 ppm) with high mass resolution (600,000) and sensitivity (low femtomole to high attomole). This instrument can carry out quantitative proteomics and metabolomics analyses over a wide dynamic range, including low-abundance peptides, and untargeted analysis of environmental and clinical samples with accurate identification of unexpected compounds. At the moment the hardware and his dedicated software manager will not be interested by any upload. The instrument is connected to the workstation by a dedicated LAN with ethernet ports for the HRMS part, whereas the UPLC instrument is connected to the workstation via USB cable. The workstation is not controllable remotely and has a Windows 7 professional as operating system. Dedicated and automated backup system is not developed. The bigger limitation is the data processing software. The software Sieve 2.0 (Thermo Fisher Scientific, release June 2011) supplied with instrumentation at the time of purchase, is obsolete and unusable: it is very limited regarding the statistical tools available for data processing, and it is not connected to database useful for compound identification. Data elaboration is complex and very time consuming: this limit seriously the productivity of this analytical instrumentation. Sieve 2.0 software is covered by a single user license. The instrument and workstation interface is currently via USB port. The workstation has a dedicated LAN network and it is remotely controllable using the Teamviewer software (free license). The workstation does not currently have a local and dedicated

data backup system. The operating system of the workstation is Windows 10. The current version of the instrument software is Xcalibur 4.3 (Thermo Scientific, release June 2019) with a single user license. The current software (Xcalibur 4.3) is obsolete for the chemical determinations that is one of the aims of ITINERIS project.

- IC-ALTIS-MS: The instrumentation consists of a high performance ion chromatograph ICS-5000 Standard Bore and Microbore System (Dionex, Thermo Scientific) coupled to a single quadrupole mass spectrometer MSQ Plus (Thermo Scientific) and is dedicated to the quantitative determination of and water-soluble and ionic organic/inorganic compounds in liquid media. The chromatograph can operate up to 5000 psi to achieve high performance separation and is equipped with an eluent generator ICS 5000EG (Dionex, Thermo Scientific) configured with carbonate or hydroxide eluents for anions and metanesulfonic acid (MSA) for cations determination, suppressors ASRS 500 or CCES 300 (Thermo Scientific) to remove the salts form mobile phase before entering the MS source, and CD conductivity detector. The mass spectrometer is equipped with an electrospray source (ESI). The upgrade of the current state of the ALTIS MS instrument (Thermo Scientific) is essential because the Chromeleon 7.3 (Thermo Scientific, release February 2020) software will enable the instrument to be operated with greater rapidity and efficiency. The new software, together with the new workstation provided by Thermo Scientific, will make the remote connection easier and will simplify the interface with other instrumentation, aiming a network infrastructure for instrument management. The technical support will account for the full installation of the workstation and software and will set up the connection with the ALTIS MS system.
- Transmission electron microscope with scanning mode (S/TEM) (JEOL): the instrument JEOL JEM-F200 is a 200 kV TEM with scanning capabilities (S/TEM) equipped with a range of imaging detectors including: bright-field (BF); high-angle annular dark-field (HAADF); secondary electrons (SE); back-scattered electrons (BSE). The electron source is a Cold Filed Emission Gun (CFEG) which provides:
    - an electron beam energy spread ≤ 0.3 eV (FWHM) @ 200 kV;
    - a brightness ≥ 8e8 A/cm2sr @ spot size = 0.7 nm;
    - a probe current ≥ 2.5 nA @ spot size = 0.7 nm, in conjunction with the 4-lense illumination system.

  The point resolution is ≤0.23 nm in conventional TEM mode and ≤0.16 nm in STEM mode, using the HAADF detector, with still the capability to tilt the sample up to angles ≥ 80°, which will allow the implementation of tomographic techniques in future.

  The microscope is equipped with an energy dispersive X-ray spectrometry (EDS) detector with analytical resolution ≤ 133 eV @ 5.6 keV. The 100 mm2 active area assures a collection angle ≥ 1 sr, which, also given the probe current values, allows fast acquisition of EDS spectra and X maps even at the high spatial resolution corresponding to small probe sizes. This instrument enables extended experiments for a wide variety of applications allowing morphological, structural, and chemical nanoscale investigations.

- Scanning electron microscope (SEM) (Zeiss): the field emission (FE) SEM Zeiss Σigma|VP is equipped with a thermal field emission gun (Schottky emitter) source.

The electron-optical column is a GEMINI design, and the instrument can work in variable-pressure (VP) mode, with pressures adjustable from 1 to 133 Pa, avoiding the need to coat non-conductive samples. The instrument is provided with a range of imaging detectors:

- conventional Everhart-Thornley detector for secondary electrons (SE), with high collection efficiency;
- 4-sector semiconductor detector for back-scattered electrons (BSE);
- high-resolution in lens detector for SE, which (together with the electron source and the column design) allows a nominal resolution down to 1.5 nm @ 15 kV.

The machine is also equipped with a Bruker Quantax 200, an energy dispersive X-ray spectrometry (EDS) system of the SDD type, with a 30 mm2 window which allows fast spectra and X maps acquisition; analytical resolution ≤127 eV @ 5.6 keV.

- Atomic force microscope (AFM) (Bruker): dimension Icon (Bruker) is a tip-scanning AFM platform allowing nanoscale imaging. The analysis can be conducted in ambient and liquid environments. Depending on the requirements, three main modes with suitable probes are available: (i) contact mode, (ii) tapping mode and (iii) non-contact mode. In addition to the morphology of the samples, a wide variety of properties can be investigated. Nano-electrical properties of the materials with a spatial resolution of the order of 10 nm or less (depending on the AFM probe) can be investigated by means of conductive AFM (c-AFM) and Kelvin probe force microscopy (KPFM). The c-AFM allows to obtain topography and electrical conductivity maps of the samples by using a conductive tip. Nanomechanical analysis is also available (PeakForce-QNM®) by means of PeakForce Tapping® technology.

The following list reports the instruments part of the CeTrA platform with the main technical information.

- The facility includes two Clean Laboratories dedicated to the ultra-clean manipulation/preparation of samples for inorganic and organic analysis, respectively. The inorganic clean laboratory is entirely made of plastic-coated materials designed for the low release of airborne particles, while the organic clean laboratory is entirely made of steel materials and components designed to minimize the release of organic substances and maximize the effectiveness of decontamination procedures. The inorganic clean laboratory consists of 4 rooms ISO 6 equipped with laminar flow benches (one is additionally equipped with an extractor hood and glove box for the preparation of atmospheric aerosols filters), 1 room ISO 5 equipped with laminar flow bench and 1 room ISO 4. The organic clean laboratory consists of 1 room ISO 7 for intermediate sample preparation, 2 rooms ISO 6 equipped with laminar flow benches, 1 room ISO 5 equipped with laminar flow bench and 1 room ISO 4. All the clean rooms are at overpressure increasing as function of their class, equipped with ceiling installed HEPA filters for continuous filtering of the internal air and dedicated internal production systems of Milli-Q water (Elga LabWater).
- Inductively coupled plasma (ICP) high-resolution mass spectrometer Element XR (SFMS) (Thermo Scientific) (ICP-SFMS): the high-resolution mass spectrometer

Element XR (Thermo Scientific) allows performing interference-free high-precision quantitative determination of elements and isotopic/elemental ratios in liquid samples down to the ultra-trace level. Thanks to a combination of high-resolution mass filter and counting, analog and Faraday detection modes, the linear dynamic range of the detector extends from sub fg/g (ppq) to over 12 orders of magnitude in solution mode. The instrument is equipped with a SC-4 autosampler (ESI) for continuous data acquisition and can be equipped with ARIS (ESI) or ARIDUS (Cetac) desolvating nebulizer systems for further reduction of solvent-based interferences such as oxides and hydrides. The instrument is connected to the workstation with a USB and Ethernet cable. The dedicated PC's operative system is Windows 10. The PC is on a LAN network system abs it is possible to connect remotely to the PC using Anydesk (free software), there is no backup system dedicated to the data management. The software that controls the instrument is licensed.

- Inductively coupled plasma - quadrupole mass spectrometer (ICP-QMS) (Thermo Scientific): the instrument iCAP-RQ (Thermo Scientific) is dedicated to the quantitative determination of trace elements and elemental ratios in liquid samples. The system is equipped with a Qcell technology assembly which can be run using He as collision gas and/or H2 as reaction gas to achieve reduction of spectral interferences. Additional accessories include an autosampler ASX-560 (Cetac) for high-throughput analysis, sample introduction kit for the analysis of HF mineralized samples and cone inserts for high sensitivity/robust/high matrix analysis. The instrument allows performing highly reproducible quantitative multi-elemental determinations over 9 orders of magnitude in concentration in a variety of sample matrices across the entire mass range. The instrument and workstation are connected via USB cable, the PC is on the LAN university network, and it is remotely accessible using Team Viewer. Data backup is manually operated using external disks. The OS of the PC is Windows 7 and the software is single licensed with USB key authentication.
- Inductively coupled plasma - optical emission spectrometer (ICP-OES): The instrument iCAP 7400 (Thermo Scientific) is dedicated to the quantitative determination of major-to-trace elements and elemental ratios in liquid or (appropriately) dissolved samples. The system is equipped with high-efficiency light transmission system, radial or duo (radial + axial) plasma view configurations to suit a wide variety of sample types and elements of interest and a simultaneous wavelength acquisition system. Elemental concentrations can be determined with detection limits in the ppb or sub-ppb level with high instrumental precision and long-term signal stability even in complex matrices or at consistently high levels with minimized memory effects. Additional accessories include an autosampler ASX-560 (Cetac) for high-throughput analysis. The instrument and workstation are connected via USB cable, the PC is on the LAN university network, and it is remotely accessible using Team Viewer. Data backup is manually operated using external disks. The OS of the PC is Windows 7 and the software is single licensed.
- Mercury analyzer: the Mercur DUO plus (Analytik Jena) is an atomic absorption (AAS) and atomic fluorescence (AFS) spectrometer specifically designed and dedicated to the analysis of mercury in compliance with the standards EPA, EN and ISO. An integrated module with two gold collectors allows simple or cascade

enrichment of mercury (according to EPA method 1631) to achieve determination limits from the low ppt to the ppq range with high method robustness, depending on the type of sample and configuration. Additional accessories include an autosampler AS-FD for high-throughput analysis. The instrument and workstation are connected via USB cable, the PC is not online, and it is not remotely accessible. Data backup is manually operated using external disks. The OS of the PC is Windows 7 and the software is single licensed.

- Gas chromatograph - tandem mass spectrometer (GC-MS/MS) (Agilent Technologies): the instrument consists of a GC Trace 1310 (Thermo Scientific) equipped with user-exchangeable instant connect injector and detector modules, coupled to a TSQ 9000 triple quadrupole MS/MS detection system. The ExtractraBrite ion source is fully removable without breaking the vacuum probe interlock (VPI) to achieve fast operationality and switching from electron ionization (EI) to chemical ionization (CI). For the highest level of sensitivity, the Advanced Electron Ionization (AEI) source can be configured to reach instrument detection limits into the attogram range. The instrument is suited for quantitative targeted and untargeted analysis of volatile/semi-volatile compounds. The connection between the instrument and the workstation is provided directly with an ethernet cable. The workstation has internet access, and it is remotely accessible using VNC viewer. There is no backup system dedicated to the whole workstation or data. The workstation operating system is Windows 10 and the instrument has a single user license.

The following list represents the instruments currently available in the MRG observatory:

- Bulk deposimeter for Hg in atmospheric deposition (MercuryBulk, Bus100, Eigenbrodt);
- Weather sensors (temperature and relative humidity of air, atmospheric pressure, wind direction and speed, snow height and soil temperature):
  - Plate Naturally – Aspirated Solar Radiation Shield 41003-5 | 10 – Campbell Scientific;
  - Sensor for Temperature and Relative Humidity: CS215 – Campbell Scientific;
  - Sonic Ranging Sensor SR50A - Campbell Scientific;
  - Sensor for Temperature: model 109 (internal temperature of the Shelter) – Campbell Scientific;
  - PTB110 barometer – Vaisala;
  - Wind monitor – hd alpine model 05108-45 – Young;
  - Infrared radiometer model SI-111 – Apogee instrument;
- PM10 sequential low volume particulate autosampler (Skypost, Tecora);
- Internal shelter temperature probe;
- Internal and external webcam (IP camera Foscam FI9901EP);
- Hard disk data backup system;
- Data transmission system via GSM on remote call;
- Online data visualization system on the terminal located in the cable car arrival station;
- Solar electric supply – 10W photovoltaic module 410M;
- Power Supply: PS200 12V–Campbell Scientific;
- Datalogger: CR800 – Series - Campbell Scientific;
- Aluminum Tower (3m): ATW3 - Campbell Scientific;
- Server NI – CRIO;

- Router Teltonika RUT955;
- Switch Netgear FS108P;
- µ-controllers Raspberry Pi