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Towards FAIR Data Management in Heritage Science Research: Updates and Progress on the INFRA-ART Spectral Library

Ioana Maria Cortea

Department of Optoelectronic Methods and Techniques for Artwork Restoration and Conservation, National Institute of Research and Development for Optoelectronics INOE 2000, 077125 Magurele, Romania; ioana.cortea@inoe.ro

Abstract: The heritage science sector is facing a critical need for accessible and comprehensive data resources to facilitate research, preservation efforts, and interdisciplinary collaboration. The concept of FAIR data management involves embracing principles and practices that ensure that data are Findable, Accessible, Interoperable, and Reusable. This work presents an overview of the latest updates on the INFRA-ART Spectral Library, an open access spectral database of cultural-heritage-related materials that was designed as a digital support tool for heritage research specialists that work with (portable) non- or minimally invasive spectroscopic techniques such as X-ray fluorescence (XRF), attenuated total reflectance–Fourier transform infrared (ATR-FTIR) spectroscopy, or Raman spectroscopy, among others. The database is an ongoing compilation of high-quality curated data that currently incorporates primary ATR-FTIR and XRF spectra and a preliminary dataset of Raman and short-wave infrared (SWIR) reflectance spectra on over 900 different materials typically found in painted works of art. For increased and sustainable accessibility, the database follows the European Commission's recommendations on access to scientific information, as well as the FAIR guiding principles on research data that result from publicly funded research. The INFRA-ART Spectral Library is registered as a resource within the Open Science Cloud (EOSC) Portal and is among the services offered by the Romanian hub within E-RIHS (European Research Infrastructure for Heritage Science) DIGILAB.

Keywords: spectral library; heritage science; spectroscopy; pigments; art-related materials; FAIR data; data management; open science

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1. Introduction

Conservation and heritage science research play a crucial role in understanding, preserving, and managing our cultural heritage. The importance of digital technologies and the extent of data use in today's world are rapidly increasing. Like in other fields, the heritage science sector faces a critical need for accessible and comprehensive data resources to facilitate research, preservation efforts, and interdisciplinary collaboration. However, as in many other areas of research, accessibility of scientific information and tools has often been limited, hindering collaboration, knowledge exchange, inclusiveness, and research excellence of less technologically advanced organizations or research groups [1]. By eliminating financial and technical barriers, open access practices allow a wider audience to access and benefit from scientific knowledge, generating, at the same time, a more balanced and sustainable research area.

The implementation of data policies within the heritage science sector is a relatively recent development. FAIR data management refers to the adoption of principles and practices that make data Findable, Accessible, Interoperable, and Reusable [2]. This approach facilitates the discovery and utilization of data, accelerates research progress, and ensures that heritage science remains a dynamic, transparent, and collaborative field. The European Commission has been actively involved in recent years in promoting open data policies and initiatives to improve data accessibility and sharing [3–7]. Inspired by the FAIR data principles and the European Commission's recommendations on access to scientific information, several resources that facilitate online access to tools and data hubs for heritage research have been developed in recent years, such as the DIGILAB infrastructure [8] within E-RIHS (European Research Infrastructure for Heritage Science) [9].

Despite notable advancements, the shift toward open science has unfolded at a more gradual pace than anticipated, especially in terms of data sharing [10–12]. According to a study from 2018, only 12% of data coming from research studies are stored in open repositories [13]. This situation can be attributed to several factors, including data privacy and ethical concerns, data management, licensing and copyright, lack of incentives, lack of infrastructure, economic models, institutional barriers, and resistance to change [14].

In today's world, the demand for web-based open access analytical resources is huge and is even more so for niche solutions dedicated to specialized areas of research. This demand stems from the increasing reliance on digital platforms for accessing valuable tools and information in various fields. With ongoing technological advancements, the demand for web-based analytical resources is expected to grow further. In addition, as research becomes more specialized and interdisciplinary, researchers require accessible and comprehensive resources tailored to their specific needs, capable of minimizing the workload.

Material identification in artworks constitutes a significant area of research within the conservation and heritage science domain [15]. In polychrome works of art, this process involves the identification of pigments and binders, or other paint components, to better understand the composition and potential degradation mechanisms—key information for an optimal conservation strategy. Thorough characterization and diagnosis can also offer substantial evidence for dating, support provenance research, validate authenticity, or expose a forgery [16].

Thus far, a diverse array of analytical techniques has been effectively employed in the examination of cultural heritage artifacts [15–18]. Within the wide range of modern analytical instrumentation available to today's scientists, spectroscopic techniques are by far the most frequently used [18,19]. Combining elemental information from X-ray fluorescence (XRF) with molecular and structural data from vibrational spectroscopies, such as Raman and Fourier transform infrared (FTIR) spectroscopy, is a common analytical practice within the conservation and heritage science field. This complementary approach can provide a large set of significant data and overcome the intrinsic limitations of each specific method, thus achieving a high selectivity in the identification and characterization of materials [20].

The widespread adoption of spectroscopic techniques has been further emphasized in recent years due to advancements in portable equipment [21–27]. This trend underscores a significant shift in analytical methodologies, where researchers and practitioners are increasingly turning to portable solutions for on-site analysis and fieldwork. These portable spectroscopic devices offer unparalleled convenience and flexibility, enabling real-time data collection in diverse settings such as archaeological sites, museums, or art galleries, frequently without the need for sampling (i.e., in a nondestructive way). Moreover, their compact size and ease of operation have democratized access to analytical capabilities, empowering a broader range of users to conduct detailed spectroscopic analyses with minimal logistical constraints.

An important aspect when working with spectral data is the need for spectral libraries—a curated collection of reference spectra representing a wide range of compounds or materials, used for comparison and interpretation in spectral analysis. These reference spectra (of known materials/substances) are obtained under controlled conditions, ensuring their accuracy and reliability [28–30]. Currently, there are several commercial spectral databases that require an annual subscription for access, while, to a lesser degree, there are also several open access spectral libraries available, encompassing a diverse array of spectra sources from several different sub-disciplines. Efforts are continuously made to expand open access resources, promoting collaboration and knowledge sharing in various fields of research. However, the availability and extent of open access spectral libraries may vary depending on the specific spectral techniques and scientific disciplines involved. As highlighted in previous studies [31], there are relatively few collections of spectra dedicated for conservation and heritage science research. Furthermore, a detailed review of the existing open access resources [32] indicates a clear gap in terms of available integrated spectral libraries specialized in art-related materials.

This paper provides an overview of the latest updates on the INFRA-ART Spectral Library, a recently developed open access spectral database tailor-made to fit the necessities of heritage science specialists who work with (portable) non- and minimally invasive spectroscopic techniques and work implicitly with spectral data. Developed within the frame of the postdoctoral project INFRA-ART (grant PN-III-P1-1.1-PD-2019-1099), the INFRA-ART Spectral Library is an ongoing compilation of high-quality curated spectra, freely available online (https://infraart.inoe.ro/, accessed on 6 April 2024), that currently incorporates primary ATR-FTIR and XRF spectra and a preliminary dataset of Raman and short-wave infrared (SWIR) reflectance spectra for over 900 different reference samples.

2. The INFRA-ART Spectral Library

The main aim of the INFRA-ART project was to foster innovation and knowledge advancement in the field of heritage science, with a specific focus on the scientific examination of painted works of art. Based on the large spectral datasets obtained within the research activities employed during the framework of the INFRA-ART project, a spectral database of ATR-FTIR and XRF spectra was developed with over 500 reference samples of art-related materials. Given the clear necessities within the field (as discussed above), starting in 2021, the database was made available online as an open access digital resource tool for research specialists and other heritage-related professionals that work with spectroscopic techniques. After the completion of the project in August 2022, the database was further optimized and new datasets were uploaded on an ongoing basis, including new data types. At this moment, the INFRA-ART Spectral Library integrates four different data types—FTIR, Raman, XRF, and SWIR spectra, resulting a collection of 1843 spectral data associated with 918 known reference materials (accessed 6 April 2024).

2.1. Types of Materials Covered by the Database

Regarding the types of reference samples, the database covers a wide range of art-related materials typically found in painted artworks, which have been grouped into fourteen different classes, as follows: mineral pigments; earth pigments; inorganic pigments, synthetic; natural organic dyes and pigments; organic dyes and pigments, synthetic; special-effect pigments; mixed pigments; resins, balsams, and wax; glues, gums, and binders; artist color paints; other mixtures; metal powder; carbon-based pigments; and unclassified materials.

The exact distribution of the reference samples across the various material classes that are currently included in the INFRA-ART database can be seen in Figure 1. Compared to the initial dataset, as submitted for publication in May 2022 [31], we have significantly extended the range of artist color paints from 22 to 193 reference samples, and we have included a large set of special effect pigments (currently 93 pigments) under a new material class. Another change that occurred during the development and optimization of the database involved merging two previously separately defined material classes (synthetic dyes and organic pigments, synthetic) into one class.

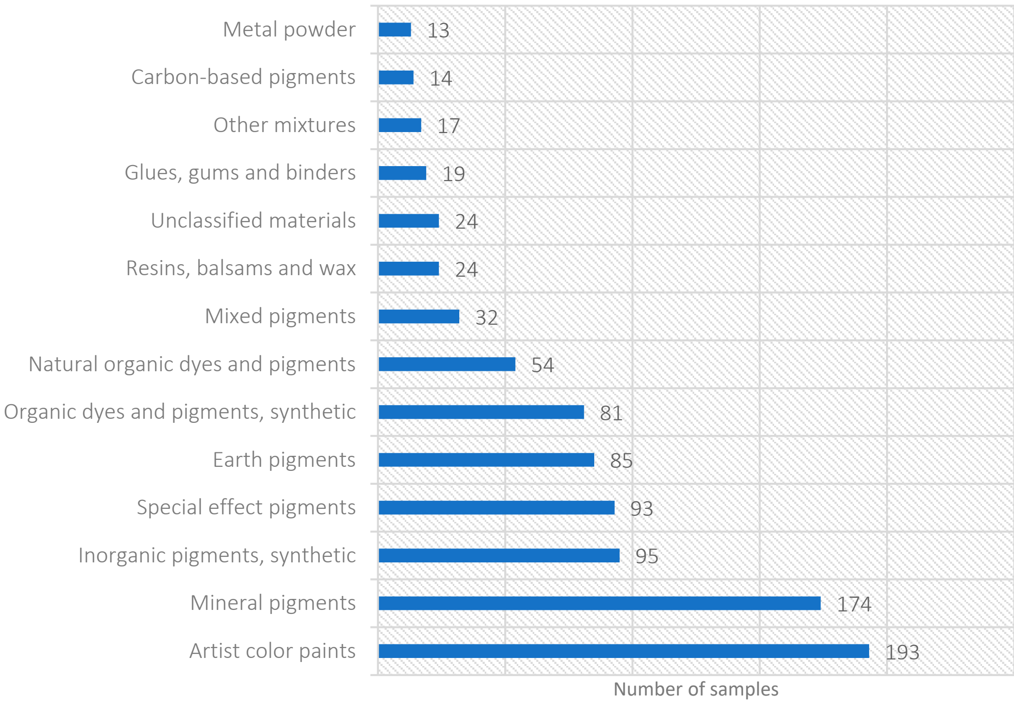


Figure 1. The distribution of the reference samples across the fourteen different material classes that are currently included in the INFRA-ART database (accessed 6 April 2024).

The current range of artist paints included in the database covers an impressive collection, from traditional painting techniques, such as oil, egg tempera, gum Arabic gouache, or watercolor, to modern paint media based on synthetic resins: acrylic, alkyd, and vinyl paints and modified alkyd resin spray paints. While, currently, all the traditional painting medium reference samples are based on commercially manufactured tube paints, the selected materials are high-quality, professional artist colors, formulated according to traditional methods without the addition of additives. In contrast, most modern paints are complex mixtures of various major and minor components: one or more binder, pigment(s)/dye(s), along with several additives, such as emulsifiers, light stabilizers, antioxidants, plasticizers, etc. [33]. For some of the reference materials included (e.g., the current selection of spray paints), no specific composition is declared by the manufacturer, as proprietary rights apply. However, we decided to include these samples in the database as well, as the spectral data acquired can nevertheless be valuable to researchers who study similar materials and need access to chemical/structural information or spectral fingerprints [34].

The so-called special-effect pigments, an important group of materials covered by the database, provide unusual optical effects like angle-dependent color or decorative texture and are nowadays used for a variety of applications including industrial design, architecture, or contemporary art. Effect pigments are generally classified as metal-effect pigments or pearlescent pigments, but a wide range of new effect pigments consisting of platelets/flakes of transparent materials have also been developed in recent years [35]. Historically, the first transparent luster pigment was developed in 1656 in Paris, a pearl luster suspension made from the inside of fish scales called "Essence d'Orient". Around 1960, pigments based on mica platelets were introduced to the market and, from that point onward, continuous development has been taking place in the field [36]. Around the same period (starting with the 1960s), special-effect pigments like UV- and daylight fluorescent pigments were adopted by pop artists such as Andy Warhol [37]. Special-effect pigments are often made up of multiple layers of different materials that work together to create their unique optical properties. The investigation of such materials can be challenging, and a full characterization often requires a combination of specialized analytical techniques.

The INFRA-ART database includes a wide range of effect pigments, from pearlescent and holographic glitter pigments to glimmer, fluorescent, and phosphorescent pigments.

Based on our review of exiting web-based spectral databases relevant to conservation and heritage science [32], the INFRA-ART Spectral Library is currently the only resource that covers special-effect pigments alongside other rare or hard-to-find materials such as traditional Japanese iwa-enogu mineral pigments (made in exactly specified particle sizes) for watercolor painting and woodblock printing [38].

Natural earth pigments are also strongly represented within the database, with approximatively 85 different earth pigments of various geological origin currently included. Due to their abundance, high coloring capacity, and stability, natural earths have been extensively employed as pigments since ancient times, and are ubiquitous in most archaeological contexts. Depending on the environment that led to their formation, earth pigments are characterized by a complex chemistry, being mixtures of possibly several chromophore minerals (iron and manganese oxides and hydroxides) plus several accessory phases [39]. Found in a variety of geological contexts, earth colors have geochemical fingerprints (e.g., unusual element concentrations or specific trace elements that form chemical patterns that are specific to the particular geological source from which the pigment was extracted) that can aid in provenance studies and in determining patterns of resource use, trade, and exchange [40–42].

The INFRA-ART database covers natural earth pigments from different geographical areas, including important ancient centers of pigment extraction and production located in Spain, France, Germany, Italy, and Cyprus [43]. Unique earth colors originating in Morocco (around Midelt) or Iceland (around the Snaefellsjoekull volcano area) are also included.

The number of samples in each of the other groups of materials has been expanded in the last two years on an ongoing basis as new reference samples have become available. Besides the above-mentioned material classes, currently, the largest groups are represented by mineral pigments (174 samples), synthetic inorganic pigments (95 samples), and synthetic organic dyes and pigments (81 samples), respectively. The material classes were established using criteria based on shared characteristics, properties, or composition. However, we also took into account some classification criteria that can help the end user to navigate within the database more effectively.

Currently, the database covers only reference materials (single-type materials, pigment mixtures, pigment–binder mixtures, etc.), but we plan to integrate data associated with mock-up paint samples, as well as with historical and archaeological samples, in the next years. Regarding the source of the existing reference samples, the vast majority of these materials were purchased from well-known professional art material manufacturers and suppliers like Kremer, Maimeri, Winsor & Newton, Lefranc Bourgeois, Sennelier, Schmincke, Liquitex, Montana Cans, Divolo, and Ferrario and Lukas, among others. Materials sourced from contemporary artists and pigment makers, such as London Pigments, have also recently been included. A complete list of the art supply manufacturers covered by the database can be found on the INFRA-ART Spectral Library webpage, under "Sample details".

2.2. Spectral Data and Experimental Design

As already mentioned, the INFRA-ART Spectral Library covers spectral data associated with several (portable) non- and micro-invasive spectroscopic techniques frequently used within the conservation and cultural heritage field. More precisely, currently, the database incorporates four different data types: ATR-FTIR, Raman, XRF, and SWIR spectra.

The INFRA-ART Spectral Library stands out from other available spectral databases by integrating multi-analytical data (elemental and molecular data obtained from the same sample through complementary spectroscopic techniques) and by incorporating a rich set of metadata. Most of the existing spectral databases and/or spectral collections relevant to conservation and heritage science primarily focus on a single type of spectral data, thereby providing only a limited level of characterization for a given material [32].

Additionally, with few exceptions, the spectral databases available typically provide spectra as image files, and the accompanying information about the materials is often not sufficiently detailed, thus offering limited potential for reuse. By incorporating several types of data, the INFRA-ART database offers, for each sample, several levels of characterization, enabling end users to cross-validate their findings and mitigate potential ambiguities. Accessing integrated elemental and molecular data streamlines the identification process, enabling researchers to perform the characterization of unknown samples with greater reliability and efficiency. Moreover, researchers can quickly assess similarities and differences between samples, accelerating decision-making and facilitating more informed conclusions.

The choice of employing the aforementioned techniques was not arbitrary. Currently, FTIR and Raman spectroscopy are probably the most frequently used molecular techniques in the study of cultural heritage objects. Since the mid-1960s, when the first applications of infrared spectroscopy on cultural heritage artifacts were published [44], followed by the first Raman applications in the 1980s [45], there has been a remarkable surge in the utilization of both these techniques. Besides their clear analytical advantages (the characterization of a wide range of organic and inorganic compounds, alone or in mixtures, with little or no sample preparation), this growth has been propelled significantly by advancements in instrumentation, which have facilitated more refined and comprehensive analyses, including those in situ [21,23,46–49].

In terms of elemental characterization, portable, handheld XRF spectrometers are currently the first-choice tools in conservation and heritage science. Over the last decade, these devices have witnessed exponential technological advancements and are currently among the most accessible analytical instruments available on the market [21,22,50].

In 2023, we decided to extend the database, with SWIR reflectance spectra recorded by a hyperspectral camera. Originally developed for remote sensing and astronomical applications, hyperspectral imaging has been successfully applied in the last decade for the non-invasive chemical identification of historical materials including pigments, colorants, inks, and substrates [51–55]. As highlighted within the literature, reflectance spectroscopy in the near-infrared (NIR, 750–1000 nm) and short-wave-infrared (SWIR, 1000–2500 nm) ranges provides information on vibrational transitions (mostly overtones and combinations bands whose fundamental transitions occur in the mid-IR range), often related to functional groups like hydroxyls and carbonates [56,57].

The choice to integrate SWIR reflectance spectra into the INFRA-ART database was supported by the increased use of hyperspectral imaging within the heritage science field in recent years, as well as by the lack of open access spectral libraries suitable for the spectral identification of SWIR spectral profiles. Furthermore, the inclusion of SWIR reflectance data enhances the database's analytical capabilities and facilitates cross-referencing for improved discrimination and sensitivity.

Currently, the INFRA-ART Spectral Library incorporates over 1840 different spectra. The largest spectral collections are currently represented by ATR-FTIR (over 850 spectra) and XRF data (over 800 spectra), respectively. The Raman dataset is significant lower, as well as the SWIR reflectance spectra dataset, slightly below 200 spectra altogether (see Figure 2). This discrepancy regarding the volume variation in the different spectral data types is due to the fact that both Raman and SWIR data began to be integrated after the initial development of the INFRA-ART database. We intend to balance this distribution by expanding the Raman and SWIR datasets this year.

In order to obtain a strong and robust library, all the spectra incorporated into the database were obtained using the same instrumental configurations and acquisition conditions (for Raman measurements, the laser power and the integration time varied depending on the sample). Exact details on the equipment employed and on the experimental parameters used for data acquisition can be found in Table 1.

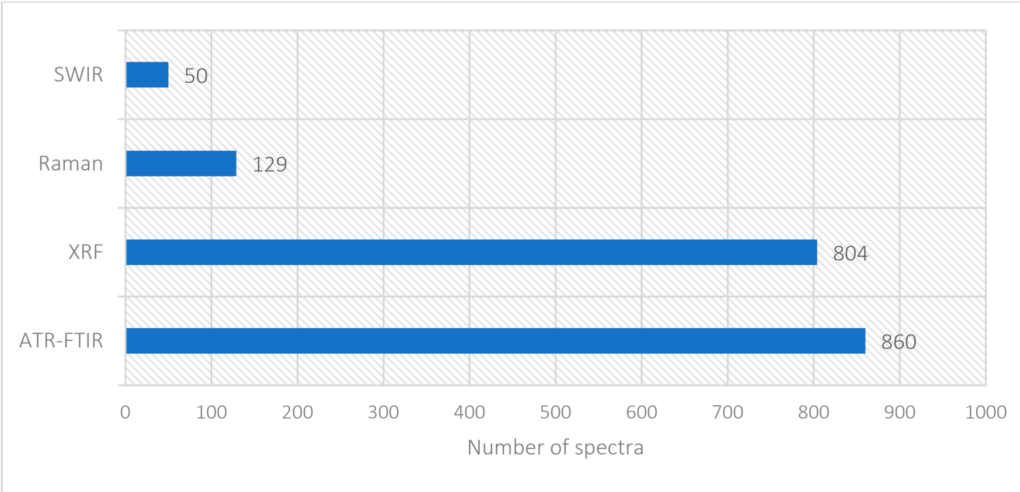
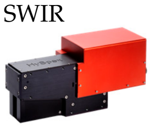


Figure 2. The distribution of the spectral data types across the INFRA-ART database (accessed 6 April 2024).

Table 1. Equipment and experimental conditions used for data acquisition.

Technique	Equipment and Main Characteristics	Experimental Conditions
FTIR 	Perkin Elmer SpectrumTwo FTIR spectrometer equipped with a GladiATR Single Reflection ATR accessory (monolithic diamond crystal, 3.0 mm diameter, 45° angle of incidence) from Pike Technologies.	Acquisition mode: ATR (attenuated total reflectance) Resolution: 4 cm^{-1} Scans: 128 Spectral range: 4000–380 cm^{-1}
XRF 	TRACER III-SD portable energy-dispersive instrument from Bruker, equipped with a Rh anode X-ray tube and a 10 mm^2 X-Flash SDD, with a typical resolution of approx. 145 eV for the Mn Kα line at 100,000 cps.	Current intensity: 10.60 µA Tube voltage: 40 kV Analysis time: 300 s Atmosphere: air Filters: -
Raman 	WP 785 ER Raman spectroscopy system from Wasatch Photonics equipped with a f/1.3 Raman spectrometer, a 785 nm integrated laser with power up to 450 mW, and a standard fiber-optic probe (collection area of 1 mm diameter at an 11 mm working distance).	Laser spot size: 170 µm Laser power: between 1 and 11 mW Acquisition time: between 2 and 10 s Resolution: 7 cm^{-1} Raman range: 3600–100 cm^{-1}
SWIR 	HySpex SWIR-384 hyperspectral camera from NEO equipped with a state-of-the-art mercury cadmium telluride (MCT) detector and a 30 cm working distance close-up lens.	Spectral range: 954–2514 nm Spatial pixels: 384 Spectral channels: 288 Spectral sampling: 5.45 nm Integration time: 7 ms

When determining the appropriate experimental conditions, we considered the importance of obtaining robust, high-quality spectra with minimal noise suitable for databases. Both sample-specific factors and environmental conditions were taken into account [29]. All measurements were carried out in a constant laboratory environment to minimize the impact on the signal-to-noise ratio (SNR) for a given exposure time. Rigorous cleaning procedures were followed for all analytical measurements to ensure that no contamination from previous samples was present, knowing that this could cause extra peaks or noise in the baseline.

For situations where we had access to reference materials with different crystalline structures and/or different particle sizes, multiple records of the same reference material type were registered and included in the database. It is well known that gross differences in particle size and crystallinity can alter the shape of the peaks or induce small shifts in the peak positions, situations that could affect the end-user experience when looking for a representative spectrum of a given material. Before entering the database, all data undergo curation to ensure their accuracy, relevance, and reliability for the intended research purposes.

FTIR spectra were registered in attenuated total reflectance (ATR) mode using a Perkin Elmer SpectrumTwo FTIR spectrometer equipped with a GladiATR Single Reflection ATR accessory (monolithic diamond ATR crystal, 3.0 mm diameter, 45° angle of incidence) from Pike Technologies. During the measurements, we ensured that the ATR crystal was perfectly clean and that appropriate pressure was applied on the crystal when collecting the spectra. For an optimal signature, 128 scans were used. Increasing the number of scans in FTIR measurements enhances the sensitivity, enabling the detection and quantification of chemical constituents present in lower concentrations, while also mitigating the effects of sample heterogeneity by providing a more comprehensive representation of the sample's average spectral characteristics. All FTIR spectra included in the database were baseline-corrected; automatic baseline correction was carried out in Spectrum 10 (Perkin Elmer).

Raman measurements were carried out using a compact WP 785 ER Raman spectroscopy system from Wasatch Photonics equipped with a f/1.3 Raman spectrometer, a 785 nm integrated laser with power up to 450 mW, and a standard fiber-optic probe (with a collection area of 1 mm diameter at an 11 mm working distance). With a comprehensive measurement range of 100 to 3600 cm^{-1}, the system provides a spatial resolution of 7 cm^{-1}. The power ranged from 1 to 11 mW and the collection time varied between 2 and 10 s, depending on each sample. All the spectra were acquired in the absence of room lights to avoid any interference. Data collection was carried out in ENLIGHTEN Raman spectroscopy software version 2.2.7 (Wasatch Photonics). No baseline correction has been applied.

XRF data were recorded using a handheld TRACER III-SD energy-dispersive instrument from Bruker, provided with a Rh anode X-ray tube and a 10 mm^2 X-Flash Silicon Drift Detector (SDD), with an energy resolution of approximately 145 eV at 100,000 cps (Mn K_α line). Each sample was placed onto a Mylar thin film in order to avoid contamination in the examination window and instrument nosepiece. The detection mode was universal, optimized for the mid-energy range (0–40 keV domain). The exact experimental parameters employed can be seen in Table 1. Data collection was carried out with the S1PXRF (v.3.8.30) software from Bruker.

The hyperspectral data acquisition was performed using a HySpex SWIR-384 hyperspectral camera system developed by NEO (Norsk Elektro Optikk, Oslo, Norway). The camera features a state-of-the-art mercury cadmium telluride (MCT) detector and is equipped with a cryogenic cooling system, which ensures a constant temperature at 147 K. These characteristics enables low background noise, a high dynamic range, and an optimal signal-to-noise level at a maximum speed of 450 fps. The system, which operates between 950 and 2500 nm, covers parts of the near-infrared (NIR) and short-wave-infrared (SWIR) spectral region and it records simultaneously 288 different spectral bands, with a spectral sampling of 5.45 nm. For data acquisition, a 30 cm working distance close-up lens was used in order to provide the best available resolution. Diffuse illumination was provided by two custom-made lamps. Focusing the illumination on a line overlapping the camera FOV (16°), the lamps, equipped with T3 halogen incandescent light bulbs R7S, provided a light output of 2500 lumens and a proper excitation source in the range covered by the hyperspectral camera detector. The radiometric calibration of the SWIR data was carried out using Hyspex RAD software (v.3.1.), which converted the digital number (DN) to at-sensor absolute radiance values ($W/sr \cdot nm \cdot m^2$) by using a scaling factor included in the header file. The conversion of the radiance to apparent reflectance was performed using the QUAC (Quick Atmospheric Correction) module in ENVI (v.5.3.).

The database was developed with a flexible structure (bottom–up architecture) to allow for the easy integration of new types of data or additional features over time. Information related to the development of the database system can be found in a previous publication [31].

As already mentioned, FTIR, XRF, Raman, and SWIR datasets will be expanded on an ongoing basis as new reference samples are acquired. In addition, FORS (fiber-optic reflectance spectroscopy), as well as LIF (laser-induced fluorescence) spectra stand among the new data types that we plan to incorporate into the database in the future.

With applications dated back to the 1930s, reflectance spectroscopy (or spectrophotometry) is nowadays a routine analytical tool used for the characterization of a wide range of natural and synthetic organic and inorganic compounds [58–61]. Over the last several decades, LIF spectroscopy has also been successfully applied to the study of a wide range of materials associated with works of art, including minerals, pigments, colorants, and organic binding media [62–67]. Both these techniques have several advantages that render them suitable for heritage science studies: their non-invasiveness, the lack of sampling requirements; and their portability, in situ operability, ability to work in scanning/imaging mode, and high spatial resolution.

Compared to the other data types already included in the INFRA-ART database, FORS and LIF data can add complementary molecular and structural information. In FORS, the processes most likely to produce absorption bands observable in the reflectance spectra of the investigated materials are electronic transitions (crystal field effects, charge transfer absorptions, color centers, etc., typically observed between 400 and 1000 nm) and vibrational features (such as hydroxyl and carbonate bands, generally observed at wavelengths above 1000 nm). In LIF, the characteristic fluorescence emissions (as a function of the laser excitation wavelength) are linked with the optical properties of intrinsic fluorophores present in the investigated materials.

The integration of FORS and LIF data will add complementary analytical information, yielding improved analysis accuracy, enhanced identification capabilities, and allowing a more comprehensive understanding of the physico-chemical characteristic of the diverse materials included within the database. Moreover, integrating data acquired using a wide range of analytical techniques fosters equity by ensuring that researchers with limited access to specific equipment can still benefit from a broad spectrum of analytical information.

2.3. Metadata

For each reference material that has been analyzed and introduced within the database, a series of metadata descriptors are also included. An exact list of the currently implemented metadata descriptors within the INFRA-ART database can be seen in Table 2. Metadata (defined as data affixed to other data) play an essential role in data science and data analytics, as they describe data and provide more context. Among others functions, a rich set of metadata can support and enhance data discovery, access, (re)use, and provenance tracking [68]. Additionally, metadata descriptors facilitate effective data management and organization [69].

In the case of the INFRA-ART database, the metadata descriptors were formulated to answer basic inquiries that might arise when working with a specific dataset and can be grouped into four different groups: dataset descriptors, data structural descriptors, supplementary descriptors, and research origin descriptors. These detailed metadata descriptors provide crucial context for interpreting spectral information; they offer insights into sample characteristics, such as composition, state, and purity, which are essential for accurate spectral analysis and comparison. Furthermore, information about experimental conditions helps researchers understand potential sources of variability or artifacts in the data.

Table 2. Metadata descriptors currently implemented within the database.

Metadata Descriptor	**Type of Descriptor**	**Related Information**
Sample ID	Dataset descriptor	Unique alphanumeric code established according to internal criteria.
Sample type	Dataset descriptor	Distinct (predefined) category that refers to the type of the investigated material (e.g., reference material, mock-up painting sample, historical sample).
Sample source	Dataset descriptor	Information related to the source from which the sample comes; in most cases, this is the name of the professional art material manufacturer/supplier.
Material class	Dataset descriptor	Distinct (predefined) category that refers to a grouping of materials based on shared characteristics, properties, or composition.
Description	Data structural descriptor	Physical description of the investigated sample (e.g., powder, flakes, grains, bulk sample, dry paint layer, etc.).
Chemical information	Data structural descriptor	The chemical information and/or chemical formula of the investigated sample.
Origin	Supplementary descriptor	The nature of the investigated sample (e.g., mineral, vegetal, synthetic/artificially produced). For naturally occurring materials, the provenance was also specified whenever this information was available.
Alternative names	Supplementary descriptor	A list of alternative names (including historical non-English names or nomenclature variations) for each specific material, where documented. For pigments and dyes, the Color Index code is also specified.
History of use	Supplementary descriptor	Time when the material was used and/or introduced into artistic practice.
Acquisition conditions	Research origin descriptor	Information on experimental parameters employed for the data acquisition.
Type of equipment	Research origin descriptor	Information on the equipment used for the data acquisition model and the manufacturer.

The structural and supplementary information provided for each reference sample, such as the chemical information, provenance, additional historical names and color index code, or information on the time when the material was used and/or introduced into artistic practice, adds further details that can be used by external users when navigating within the database. For an enhanced user experience, all metadata fields are keyword-searchable.

An example of a library entry showcasing the pigment Bohemian Green Earth (Figure 3) exemplifies all of the characteristics and features discussed above: sample metadata, experimental metadata, data type buttons (active spectra in blue box), and the interactive spectra-viewer that shows the FTIR spectra registered for this sample.

Figure 3. Example of a database entry for the pigment Bohemian Green Earth, sample ID: PSC18519 (accessed 6 April 2024). The main characteristics and features of the database display area are highlighted.

2.4. FAIR Data Management

To enhance and maintain accessibility over the long term, the INFRA-ART Spectral Library aligns with both the European Commission's guidelines [3,4] concerning research data arising from publicly funded research and the FAIR data principles regarding access to scientific information [5,70]. The FAIR guiding principles for scientific data management and stewardship, established by the international research community in 2016 [2], serve as a cornerstone for advancing knowledge discovery and innovation. These principles ensure that information is readily available and that data are Findable, Accessible, Interoperable, and Reusable (FAIR), promoting transparency and maximizing the utility of research outputs including the (re)use of scholarly data.

The original publication by Wilkinson et al. [2] underscores the importance of certain factors for achieving FAIR data, including thorough metadata and documentation, the utilization of open or universal/standardized file formats, the incorporation of persistent unique identifiers for data objects, and the explicit application of data licenses to govern access and (re)use. As already highlighted in this paper, the INFRA-ART database includes a rich set of metadata descriptors that offer context and basic information on each investigated sample, including on the experimental conditions employed for data acquisition. Each sample has a unique persistent identifier that facilities data management and ensures the accuracy, integrity, and traceability of data within the database.

In terms of data licensing, initially, the database was released under a CC BY-NC-SA 4.0 (Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International) license. However, due to legal and community considerations, we recently decided to change to a CC BY-NC 4.0 (Attribution-NonCommercial 4.0 International) license. This offers greater flexibility on how the database content may be transferred and utilized by different stakeholders, potentially expanding reuse opportunities, simplifying compliance, providing a clearer legal framework, and influencing collaborative dynamics [12].

An overview of the FAIR principles adopted by the INFRA-ART Spectral Library can be found in Table 3, along with further details.

For increased accessibility and visibility, starting in 2022, the INFRA-ART Spectral Library is registered as a resource within the Open Science Cloud (EOSC) Portal (currently under transition to the EOSC EU Node), an open multi-disciplinary environment that serves as a centralized gateway for hosting research data, research tools, and cloud-based services that support EU science [6,71]. Furthermore, starting in 2023, the INFRA-ART database is part of the services offered by the Romanian hub within E-RIHS DIGILAB, a platform that provides remote services to the heritage science research community [8].

Table 3. FAIR principles adopted by the INFRA-ART Spectral Library.

FAIR Principles *	Compliance
Findability F1. (Meta)data are assigned a globally unique and persistent identifier. F2. Data are described with rich metadata. F3. Metadata clearly and explicitly include the identifier of the data that they describe. F4. (Meta)data are registered or indexed in a searchable resource.	F1. Datasets are uploaded to a public open access institutional repository (URL link: https://infraart.inoe.ro/, accessed on 6 April 2024). F2. Data are assigned a rich set of metadata (dataset descriptors, data structural descriptors, research origin descriptors, etc.). F3. The metadata and the datasets that they describe are separate files. Each dataset record has a unique URL link. F4. Meta(data) are keyword-searchable.
Accessibility A1. (Meta)data are retrievable by their identifier using a standardized protocol. A1.1 The protocol is open, free, and universal. A1.2 The protocol allows for authentication and authorization, as needed. A2. Metadata are accessible, even when the data are no longer available.	A1.1. All dataset records are freely accessible to view and explore via an interactive spectra-viewer. The spectra can be downloaded as image files (and raw data files = upcoming update). A1.2. The database is accessible to anyone with a computer and an internet connection; no user account is required. A2. Comprehensive data indexes are updated periodically, and backup files are stored on external hard disks.
Interoperability I1. (Meta)data use a formal, accessible, shared, and broadly applicable language. I2. (Meta)data use vocabularies that follow FAIR principles. I3. (Meta)data include qualified references to other (meta)data.	I1. The spectral data files are uploaded within the database using common, universal formats (.ASC, .CSV), making the data interoperable with various spectrum-processing software. I2. The vocabulary used to describe the datasets is clear and easy to understand. I3. Each database record's dataset descriptors are linked with the research origin descriptors associated with each type of spectral data.

Table 3. *Cont.*

FAIR Principles *	Compliance
Reusability R1. Meta(data) are richly described with a plurality of accurate and relevant attributes. R1.1. (Meta)data are released with a clear and accessible data usage license. R1.2. (Meta)data are associated with detailed provenance. R1.3. (Meta)data meet domain-relevant community standards.	R1.1. Data are released under a CC BY-NC 4.0 international license. R1.2. Metadata concerning data and dataset records are richly described with a plurality of accurate and relevant attributes. R1.3. Data are organized in a standardized way, and the datasets follow well-established and sustainable file formats.

* According to Wilkinson et al. [2].

3. Conclusions

The integrated use of multi-analytical data is nowadays a recognized trend in conservation and heritage science research. Among the wide array of modern analytical instrumentation, spectroscopic techniques stand out as the most prevalent and frequently employed tools for material characterization. The widespread use of spectroscopic methods such as FTIR, Raman, FORS, and XRF is mainly due to their analytical sensitivity and specificity, along several other advantages, like their non- or micro-invasiveness, minimal or no sampling preparation being required, and their ability to provide complementary information. Moreover, recent advancements in portable equipment have led to an exponential expansion in the application of these techniques, rendering them increasingly indispensable/first-choice tools in the study of cultural heritage objects.

Reference spectra are crucial components of spectral analysis, providing a foundation for identification, validation, and interpretation of spectral data. As highlighted in the introduction of this manuscript, although, currently, there is a vast amount of reference spectral data accessible to the wider scientific community, there are inherent limitations to the applicability and (re)use of these data. Furthermore, traditional spectral databases, including both commercial and open access resources, often provide limited information, focusing solely on one spectral data type. With the aim of overcoming these limitations, and therefore improving data accessibility in conservation and heritage science research, an open access spectral library that integrates multi-technique analyses has been developed.

The INFRA-ART Spectral Library has been designed, implemented, and optimized over several years, and it currently integrates ATR-FTIR, Raman, XRF, and SWIR reflectance spectra for over 900 different reference samples. This integrated approach offers a comprehensive understanding of the sample composition and structure, providing end users with access to a more complex dataset that can facilitate the more accurate identification and characterization of unknown materials. Throughout the database development process, several functionalities have been integrated to assist end users in navigating it more effectively. These include implementing a rich set of metadata descriptors, integrating keyword search and filtering options, and incorporating data visualization tools.

Currently, the database encompasses an extensive array of materials typically found in painted works of art, grouped into several classes. The content is updated quarterly as new reference materials become available. Recent updates include the integration of a significant number of special-effect pigments and the expansion of artist paint samples, further enriching the range of reference samples offered.

Compared to the initial dataset, as submitted for publication in 2022, other important updates are the extension of the Raman dataset and the recent integration of SWIR reflectance spectra. The decision to incorporate SWIR data into the INFRA-ART database was driven by a desire to enhance the database's analytical capabilities, based on the potential of hyperspectral imaging in the near-infrared and short-wave-infrared ranges to discriminate between art-related materials. In terms of data distribution within the database, the FTIR and XRF datasets currently hold the largest share, followed by the Raman and SWIR datasets. We plan to balance this distribution in the future by substantially expanding both the Raman and SWIR datasets. Future updates to the INFRA-ART Spectral Library will also introduce new data types (such as FORS and LIF spectra), as well as a range of analytical tools aimed at building up the database's analytical capabilities and functionalities.

The INFRA-ART Spectral Library represents a commitment to accessibility, transparency, and collaboration in heritage science research, underscored by its integration into platforms like the EOSC Portal. By aligning with the FAIR data principles and European Commission guidelines, the database ensures that valuable research outputs are readily available and easily reusable. The recent transition to a more flexible license further enhances its usability and expands its potential impact. Originally released under a CC BY-NC-SA 4.0 license, the database recently transitioned to CC BY-NC 4.0 for increased flexibility and ease of use, aiming to expand reuse opportunities and simplify compliance.

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