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Geological Survey of Brazil Spectral Library v. 1.0: Rock reflectance signatures in the visible to shortwave infrared range

Mônica Mazzini Perrotta[1]*, Carlos Roberto Souza Filho[2], Ana Paula Justo[1], João Henrique Gonçalves(in memoriam), Leonardo Brandão Araújo[3], Juliano Alves de Senna[4], Thais Danielle Oliveira Gasparin[1], Manoel Augusto Corrêa da Costa[5], João Luís Carneiro Naleto[1]

[1]Serviço Geológico do Brasil. Rua Costa, 55, São Paulo, SP, CEP: 01304-010
[2]Instituto de Geociências – Universidade Estadual de Campinas. Rua Carlos Gomes, 250, Cidade Universitária, Campinas - SP, CEP: 13083-855
[3]Serviço Geológico do Brasil. Avenida Ulysses Guimarães, 2862, Salvador, BA, CEP: 41213-000
[4]Instituto de Ciência e Tecnologia - Universidade Federal dos Vales do Jequitinhonha e Mucuri. Rodovia MGT 367, Km 583, 5000, Campus JK, Diamantina, MG, CEP: 39100-000
[5]Avenida Engenheiro Camilo Dinucci, 989, Araraquara, SP, CEP: 14808-100

Abstract

Reflectance spectral libraries are essential reference databases for the mineralogical characterization of geological samples analyzed using visible and infrared spectroscopy. Since 2011, the Geological Survey of Brazil has been actively developing a comprehensive database of reflectance spectral signatures, based on samples collected from systematic geological mapping and mineral resource projects across the Brazilian territory. This spectral library is now available as a thematic database hosted by the geoscience system of the Geological Survey of Brazil (https://geosgb.sgb.gov.br), providing rock reflectance data for the spectral characterization of lithological types and their alteration products, whether due to weathering or hydrothermal processes.

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*Corresponding author
Mônica Mazzini Perrotta
E-mail address: monica.perrotta@sgb.gov.br

1. Introduction

Open-access reflectance spectral libraries available in public databases, such as those maintained by the United States Geological Survey (USGS) (Clark et al. 1993, Clark et al. 2003, Clark et al. 2007, Kokaly et al. 2017); the IGCP-264 project (Kruse and Hauff 1992); and the ECOSTRESS libraries - comprising datasets from the Johns Hopkins University (JHU) (Salisbury et al. 1987, Salisbury et al. 1989), NASA's Jet Propulsion Laboratory (JPL) (Grove et al. 1992), and the Advanced Spaceborne Thermal Emission Reflection Radiometer (ASTER) (Baldridge et al. 2009), serve as critical reference sources for the compositional characterization of mineral and rock samples using visible and infrared reflectance spectroscopy (Vis-IR RS). It is also important to reference the National Virtual Core Library (NVCL) (AuScope 2024), an Australian drill core mineralogical database that provides access to thousands of downloadable reflectance spectra through the AuScope Portal.

Reflectance spectroscopy measures the intensity of light reflected from a material as a function of wavelength (Clark 1999). It is based on the concept of reflectance, which is defined as the ratio between the energy reflected by a material's surface and the incident light. Typically, reflectance is measured within the wavelength range of 350 to 2500 nm, with variations arising from the molecular and ionic properties of the material.

When plotted on graphs showing the variation in reflectance intensity as a function of wavelength, the analytical results define the specific spectral signatures of different materials. For geological samples, this method is useful in identifying different mineral groups and their compositional and crystallinity variations, both in the laboratory and in spectral data acquired through remote sensing. The importance of this approach has been recognized since the first reflectance spectral studies in the 1970s (e.g., Hunt and Salisbury 1970, Hunt and Salisbury 1971, Hunt et al. 1971a, Hunt et al. 1971b, Hunt 1977, Hunt 1979, Hunt and Ashley 1979, Clark et al. 1990, Clark 1999).

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In 2011, the Geological Survey of Brazil (SGB, its acronym in Portuguese) established a partnership with the Geosciences Institute of the State University of Campinas (IG-UNICAMP, its acronym in Portuguese) to begin developing a comprehensive database of reflectance spectral signatures. This database is based on the collection of samples from systematic geological mapping projects and mineral resource investigations across the Brazilian territory. The samples were selected from the regional lithotheques of the SGB, following representativeness criteria for each mapping area: lithological variety, balanced spatial distribution, degree of weathering, and preference for samples previously analyzed by other methods, such as petrography and geochemistry.

The initial spectral measurements (2011–2012) were carried out at the Reflectance Spectroscopy Laboratory (LER, acronym in Portuguese) of IG-UNICAMP, using a portable FieldSpec 3 High-Resolution spectrometer (ASD - FieldSpec3-HiRes) manufactured by Analytical Spectral Devices (ASD). From 2012 onward, spectral measurements were conducted at the Geological Remote Sensing and Mineral Spectroscopy Laboratory of the Geological Survey of Brazil (LABSERGEM, acronym in Portuguese), utilizing the same spectrometer model (Figure 1). This activity evolved into an analytical method for the mineralogical and compositional identification of geological samples, applied to various themes in ongoing SGB projects as well as in collaborative academic research (e.g., Brumatti et al. 2015, Paes et al. 2016, Prado et al. 2016, Klein et al. 2017, Lopes et al. 2017, Costa et al. 2018, Mapa et al. 2019, Silva et al. 2019, Naleto et al. 2019, Sousa and Matos 2020, Bergmann 2021, Fernandes et al. 2022, Costa et al. 2024).

A thematic database, the Spectral Library, was developed by the SGB and is hosted within the geoscience system of the Geological Survey of Brazil (https://geosgb.sgb.gov.br). This platform, linked to the records of samples entered into the outcrop database, stores the numerical data from spectral analyses, the physical characteristics of each analyzed sample surface, illustrations of the samples, and complementary XRD analyses when available. It allows users to view and capture spectral signatures and illustrations, while automatically providing access to other descriptive and analytical data related to the samples and the outcrops where they were collected.

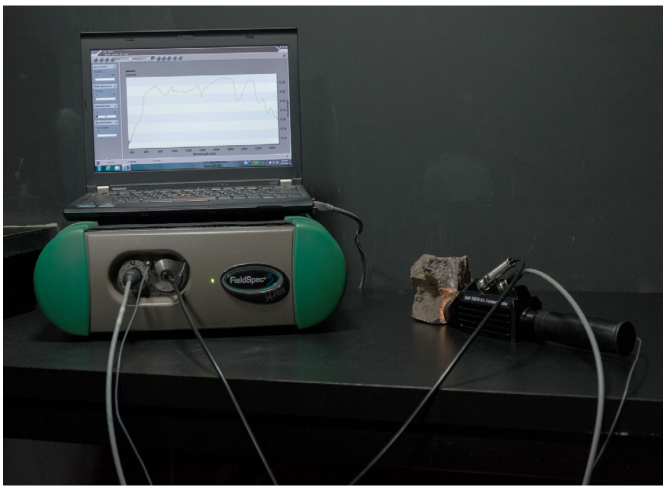

FIGURE 1. ASD FieldSpec3 Hi-Res from Geological Survey of Brazil Geological Remote Sensing and Mineral Spectroscopy Laboratory (LABSERGEM).

2. Analytical procedure

2.1. Samples Origin

The material analyzed is part of the rock sample collection gathered over the years through geological mapping and mineral resource investigation projects by the SGB. For this reason, the Spectral Library is linked to the outcrop registration and description database, where the collected samples are recorded and described based on their macroscopic, microscopic (in the case of petrographic analysis), and chemical (in the case of geochemical analysis) properties. Each sample has two codes: one assigned during field collection (and recorded in the outcrop database), and another adapted to the recent SGB coding system.

The Geological Survey of Brazil spectral library database is constantly updated with new rock reflectance data. At the time of this publication, there are 2,390 registered samples.

2.2. Sample preparation

Since the analytical tool used for the Vis-IR RS measurements of rocks and minerals is a contact probe, no specific preparation treatments are required; the samples simply need to be clean and dry. Multiple measurements are taken from each sample to account for the heterogeneities in their geological properties. The areas to be analyzed are marked with adhesive labels (Figure 2) or digitally numbered (Figure 3), depending on the sample's volume, weight, or the level of detail needed for the analyses. All samples are photographed for reference.

For each set of samples analyzed (corresponding to an SGB thematic project), a data management spreadsheet is filled out with key attributes corresponding to each spectral reading, which are restricted by a pre-established data library to ensure consistency. These attributes include: (i) type of sample (mineral/ore, rock); (ii) lithological type; (iii) type of surface (natural break, exposed, sawn, fracture/fault plane, disaggregated sample, pulverized sample); (iv) degree of weathering (non-weathered, slightly weathered, moderately weathered, weathered, highly weathered, saprolite); (v) color; (vi) orientation of the contact probe relative to the dominant planar structure (parallel, perpendicular, oblique, pocket, vein); and (vii) textural relationship (matrix, phenocryst, fragment, megacryst, matrix + phenocryst, matrix + fragment, matrix + megacryst, amygdala). For the lithological type and color attributes, predefined libraries in GeoSGB are used.

2.3. Sample analysis

The high-resolution Analytical Spectral Devices (ASD) FieldSpec3 Hi-Res spectrometer (Malvern Panalytical) used for spectral analysis operates within a spectral range of 350 to 2500 nm, covering a portion of the ultraviolet (UV) region, as well as the visible (Vis), near-infrared (NIR), and shortwave infrared (SWIR) regions. The spectral resolution is 3 nm at 700 nm (Vis/NIR), 8 nm at 1400 nm (NIR), and 6 nm at 2100 nm (SWIR). The sampling interval is 1.4 nm for the visible to near-infrared (VNIR) range (350-1050 nm) and 2.0 nm for the SWIR range (1000-2500 nm), with a total of 1251 spectral output bands. The spectrometer has three detectors: one 512-element silicon photodiode array for the VNIR, and two graded-index InGaAs photodiodes, TE-cooled, for SWIR 1 (1000-1800 nm) and SWIR 2 (1800-2500 nm). The field of view of the standard 1.5 m optic fiber is 25°.

FIGURE 2. Example of marking the analysis area on a rock sample with an adhesive label. The sample width is 5 cm.

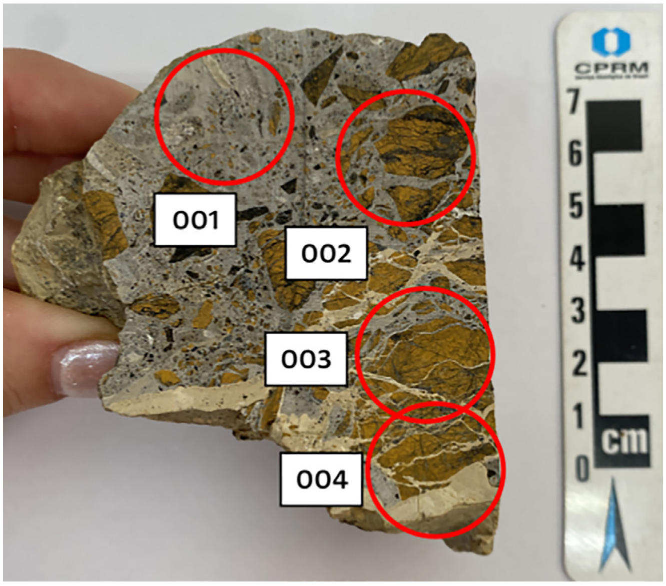

FIGURE 3. Example of marking the analysis area on a rock sample in digital file.

The contact probe, coupled to the optical fiber cable for measurements, features a built-in halogen lamp as its light source. The diameter of the measurement area is approximately 10 mm. Radiance values are calibrated to reflectance values using a calibrated Spectralon® standard. The integration time is set to 70 milliseconds.

On average, the instrument is recalibrated after every 15 analyses, with the Spectralon® spectrum saved as part of the analysis. This procedure helps assess the condition of the calibration plate and establishes reference points to address any inconsistencies in the analysis sequence.

2.4. Mineral interpretation of spectral signatures

Referred to in the database as "minerals identified in the sample," users can find a list of minerals recognized in the set of spectra for each sample, based on diagnostic spectral features. The evaluation of the shape and wavelength position of these features, as well as mineral identification, is conducted using the visualization and automatic mineral matching tools available in the ENVI® and TSG™ Pro software packages. The reference spectral libraries used include those from USGS (Clark et al. 1993, Kokaly et al. 2017), JPL (Salisbury et al. 1987, Salisbury et al. 1989, Grove et al. 1992, Baldridge et al. 2009), and GMEX guides (Pontual et al. 2008).

3. Database query and downloadable data

3.1. Analyzed rock data and sample images

The spectral library database system, based on the sample registry, searches the outcrop, petrography, and geochemistry databases, providing either an online view or a .pdf report of the recorded data. This includes information on the location and type of the outcrop, the macroscopic description of the rock or rocks present, and any available petrographic and geochemical analyses of the sample analyzed by reflectance spectroscopy.

At the beginning of the database compilation, it was discovered that the rock name assigned by the geologist in the field, as recorded in the outcrop database, did not always correspond to the classification determined more precisely by petrographic analysis. To address this problem, the "analyzed rock" field was created to record the correct lithological type, improving the ability to search spectral analyses by rock type.

Images of the samples, taken in a photographic studio, are available for on-screen viewing and downloading (an example is shown in Figure 4).

FIGURE 4. Example of sample image taken in the photographic studio.

3.2 Vis-IR RS data

The original reflectance spectra files (.asd, in binary format) undergo two transformation processes in the proprietary ASD-ViewSpec Pro® software to make the analytical results available. The first process is a splice correction, where displacement values for the VNIR and SWIR2 spectral regions' curves are calculated to align them with SWIR1 at the splice point, eliminating gaps between the three detectors. The second process is the exportation of the data files into ASCII text files.

The final spectra files can be viewed graphically on-screen in a .pdf pop-up report (Figure 5), and the .txt files can be individually downloaded to build the user's spectral library.

3.3 Samples Reports

Downloadable sample reports, containing outcrop information, results from additional analyses (petrography, geochemistry, and X-ray diffractometry, when available), reflectance graphical spectra, and mineralogy identified through Vis-IR RS, are interactively generated in .pdf format.

4. Database access

Open access to the Spectral Library of the Geological Survey of Brazil database is available through the online GeoSGB platform (https://geosgb.sgb.gov.br/), by selecting the Spectral Library icon (Figure 6) or directly via the Geology.GIS service, which is the data visualization module of the GeoSGB system (Figure 7). This system was developed using ESRI (ArcGIS Server) and Oracle (spatial database) technologies (Espírito Santo 2017), under license.

ArcGIS Pro® users can access the spectral library database directly through this platform by using the WMS and WFS services link and downloading the executable file via the Map Service (Figure 8).

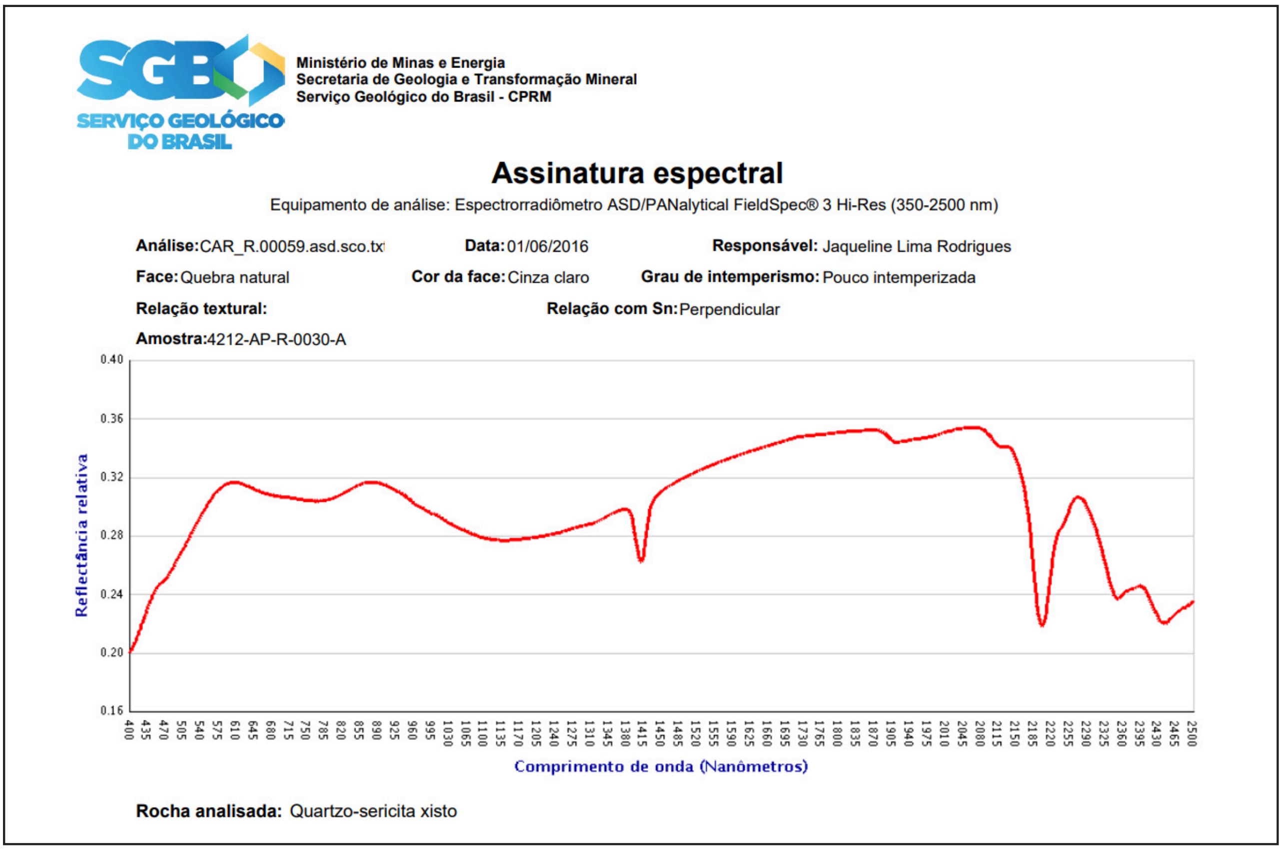

FIGURE 5. Example of graphical spectra file generated as a pop-up report, output in Portuguese. *Assinatura espectral*: Spectral signature, *Equipamento de análise*: Analysis equipment, *Espectrorradiômetro*: Spectroradiometer, *Análise*: Analysis code, *Data*: Date, *Responsável*: Responsible for analysis, *Face*: type of surface (natural break in this case), *Cor da face*: Surface color (light gray in this case), *Grau de intemperismo*: Degree of weathering (slightly weathered in this case), *Relação textural*: Textural relationship (no data in this case), *Relação com Sn*: orientation of the contact probe relative to the dominant planar structure (perpendicular in this case), *Amostra*: Sample code or number, *Reflectância relativa*: Relative reflectance, *Comprimento de onda (Nanômetros)*: Wavelength (Nanometers), *Rocha analisada*: Analyzed rock (quartz-sericite schist in this case).

FIGURE 6. GeoSGB platform (https://geosgb.sgb.gov.br/), Geology.GIS service and Spectral Library icon.

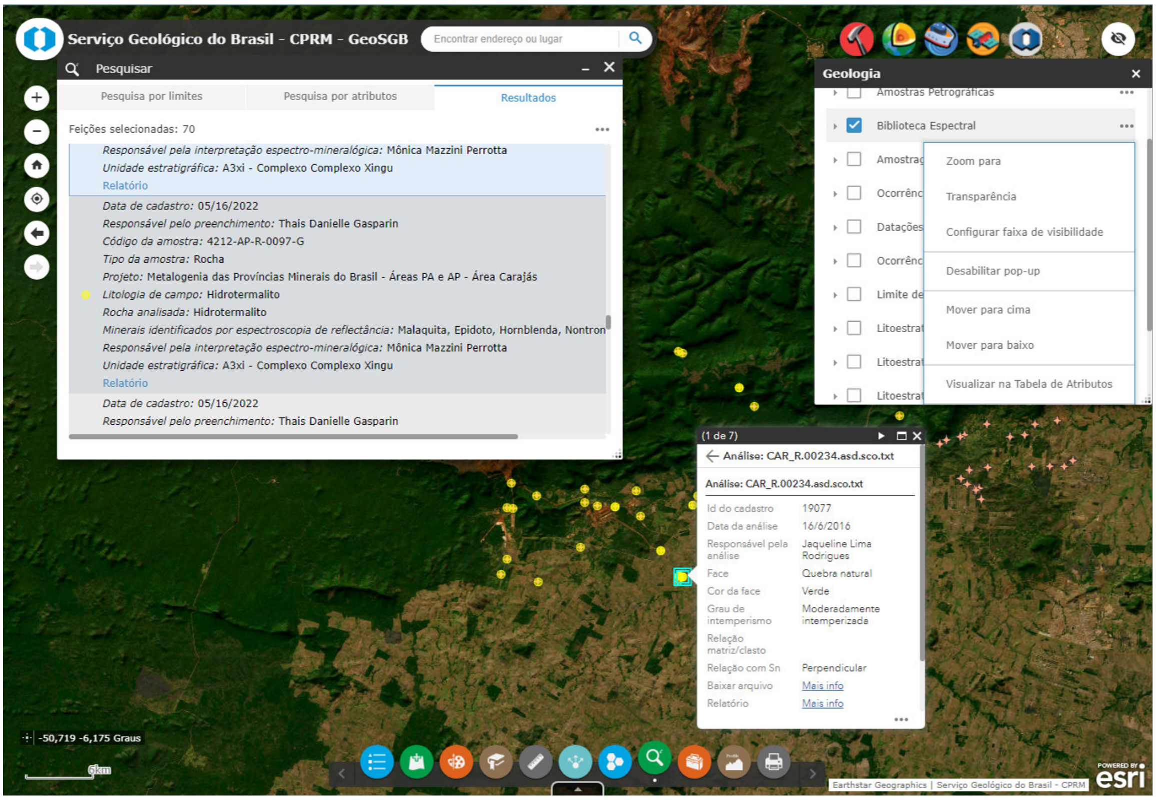

FIGURE 7. GeoSGB interactive platform screen showing an example of the result of a query.

Figure 8. GeoSGB Spectral Library Map Service through WMS and WFS services link.

5. Conclusions

As artificial intelligence technologies rapidly advance and data storage capacity expands within the big data context, the production and provision of numerical geoscientific data by public institutions—responsible for a significant portion of this information—are crucial to ensuring the availability of consistent content for training increasingly efficient machine learning algorithms.

In this regard, the Spectral Library of the Geological Survey of Brazil v.1, which offers abundant rock reflectance data for geological applications, represents a significant effort to provide quantitative data for the numerical characterization of lithological types and their alteration products, whether due to weathering or hydrothermalism.

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Authorship credits

Author	A	B	C	D	E	F
MMP	■	■	■	■	■	■
CRSF	■	■	■		■	■
APJ	■	■	■			
JHG	■					
LBA	■					
JAS	■	■	■			
TDOG	■	■				
MACC	■	■	■			
JLCN	■	■	■		■	

A - Study design/ Conceptualization **B** - Investigation/ Data acquisition
C - Data Interpretation/ Validation **D** - Writing
E - Review/Editing **F** - Supervision/Project administration

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