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**GEOLOGICAL SURVEY OF CANADA
OPEN FILE 8987**

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digital spectral (VIS-NIR-SWIR) library,
Part IV: spectral database of REE-Nb-U-Th-bearing
minerals for hyperspectral applications**

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hyperspectral applications**

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INTRODUCTION

The Geological Survey of Canada National Reference Mineral Collection (NMC) contains well over 60,000-catalogued specimens (Stirling et al., 2011). These reference specimens offer a unique opportunity to be used as standards for comparison in mineralogical research or to develop new methods in geochemistry and geochronology research. For example, tourmaline from the Collection helped establish a new geochemical method (Kelly et al., 2020; Potter et al., 2022; W.J. Davis, Pers. Comm., 2022). In 2013, about 150 specimens from the Kodama Collection of clay minerals were used to develop an in-house infrared spectral library for mineralogical research (Percival et al., 2016). Following this, the focus was on rare earth elements (REE)-, niobium (Nb), uranium (U)- and thorium (Th)-bearing minerals housed in the NMC (Percival et al., 2019). For this spectral library, over 1300 specimens were examined and spectral analyses processed for about 480 specimens. More summary information regarding these specimens are provided in Percival *et al.* (2022). This Open File is aimed at making the spectral information more accessible to the wider remote sensing community.

METHODS OF ANALYSES

Spectral Acquisition

Spectral analyses of the Kodama Collection and the REE-, Nb-, U- and Th-bearing minerals were collected using a TerraSpec Pro™ 4 VIS-NIR-SWIR portable spectroradiometer. The TerraSpec Pro™ 4 instrument was loaned to the Geological Survey of Canada by PANalytical (formerly ASD, Inc.) to ensure consistent collection with a high-resolution instrument. The TerraSpec Pro™ 4 spectral resolution ranges from 3 nm in the visible and near infrared (VNIR) range and between 8 and 10 nm in the short-wave infrared (SWIR) range, with a spectral sampling of 1 nm across the entire range.

To collect consistent, high quality data, a step-by-step approach was adopted, based on PANalytical protocols. All measurements were made in a “dark box” to reduce interference from overhead lights. Steps followed included calibration of the instrument at the beginning of each collection day, followed by optimization procedures, collection of white reference (using Spectralon® puck) and dark current. Each step is outlined in detail in Percival *et al.* (2016, 2019). The reader is encouraged to refer to the source documentation to understand the depth of information for this spectral library and its specific limitations.

Spectral Library Assembly

Two spectral libraries were created from the original OF8619 (Percival *et al.*, 2019) data (e.g., Aeschynite_NMC016485_2097.txt) in a format consistent with ENVI® software. This format is commonly used in the geological and exploration remote sensing communities and can be imported into many other spectral interpretation and processing software packages, such as The Spectral Geologist (TSG™; CSIRO) and a range of tools developed in Python. The spectral library has been load tested into a range of software packages, including ENVI®, Spectragryph, TSG™

and MS Excel™. Each software package manages data slightly differently, however, either the SLI and HDR file and/or the individual TXT files can be loaded as required.

The spectral library dataset has been produced in two manners: one to align with the original OF8619 ordering by Spectrum Index Number and one ordered by Mineral Name (Fig. 1). There are 488 individual spectra in each of the libraries, and each spectral library includes the data file (*.sli) and the header file (*.hdr). The two libraries contain the same data, but with the following structures and example:

- OF8619_SpectralLibrary_Index_NMC_Mineral
 - 2097_NMC016485_Aeschnynite
- OF8619_SpectralLibrary_Mineral_NMC_Index
 - Aeschnynite_NMC016485_2097

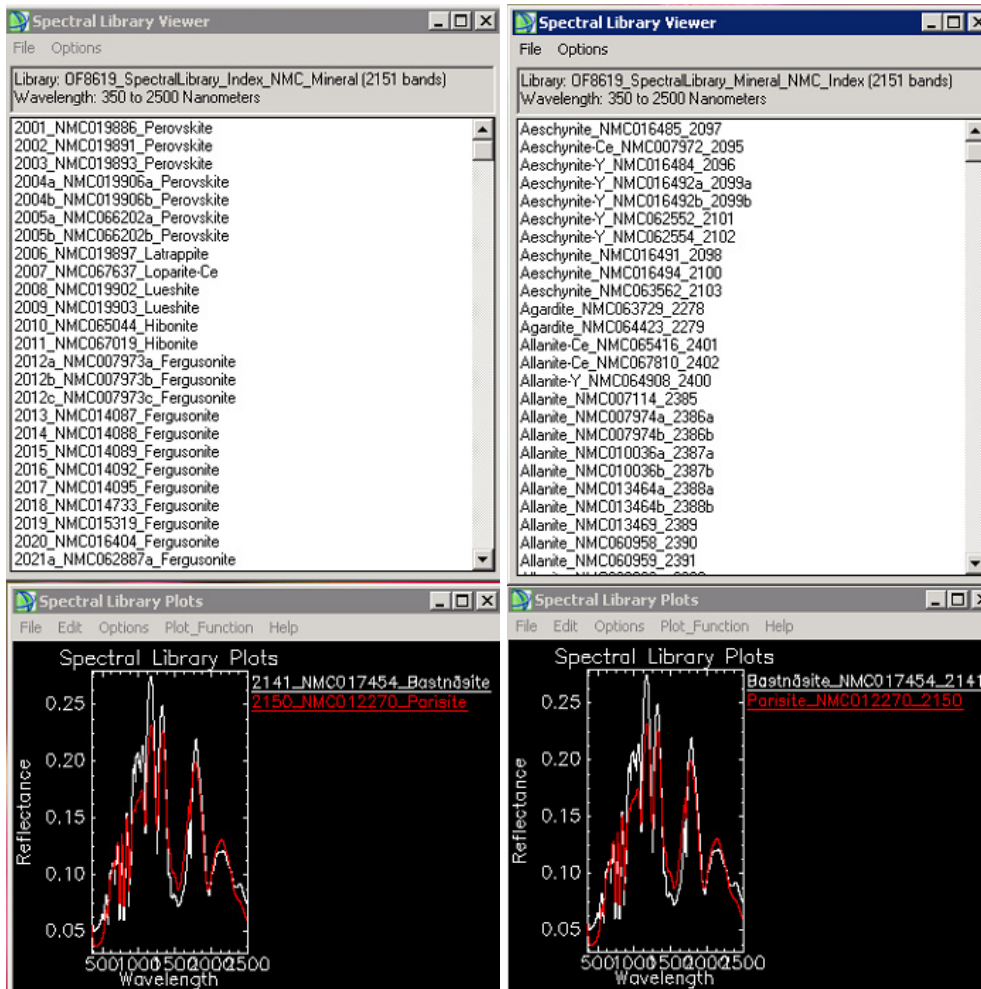


Figure 1. Screenshots of the assembled spectral libraries showing the structure of the data. Left is “OF8619_SpectralLibrary_Index_NMC_Mineral” and right is “OF8619_SpectralLibrary_Mineral_NMC_Index”.

NEXT STEPS

As part of this ongoing TGI project, each spectrum is being vetted for quality and relevance for exploration. Table 1 shows the commonly mentioned REE-bearing minerals (Main Suite), followed by four more commonly referenced REE-bearing minerals (Secondary), which have been prioritized for further study. The exclusion of minerals does not indicate that they are not amenable to being a dominant or important ore mineral, such as in the cases of mosandrite at Kipawa (Edhabi *et al.* 2018) or steenstrupine at Kvanefjeld (Yun *et al.* 2020). Articles being used in this review include Booyesen *et al.* (2020), Chakhmouradian and Wall (2012), Goodenough *et al.* (2016, 2018), Hoefen *et al.* (2015), Kynicky *et al.* (2012), Liu and Hou (2017), Long *et al.* (2010, 2012), Mariano and Mariano (2012), Schulz *et al.* (2018), Turner (2015, and references therein), and Xu *et al.* (2008). Additional research will refine and expand this list and may result in shuffling of the order, especially if newly identified resources are discovered or there are other breakthrough metallurgical advances. Notably, apatite and zircon were listed as the only minerals that can contain appreciable amounts of REE as nonessential elements, but others do exist (e.g., fluorite) and would be worthwhile future additions.

Table 1. Prioritized REE-bearing minerals for exploration.

	Mineral (Selected)	Grouping	Formulae (without consideration for $-(Ln)$)
Main Suite	Monazite	Phosphates	Ce(PO ₄)
	Bastnaesite	Carbonates	Ce(CO ₃)F
	Xenotime	Phosphates	Y(PO ₄)
	Parisite	Carbonates	CaCe ₂ (CO ₃) ₃ F ₂
	Synchysite	Carbonates	CaCe(CO ₃) ₂ F
	Apatite	Phosphates	Ca ₂ Ca ₃ (PO ₄) ₃ F
	Allanite	Silicates	(CaCe)(Al ₂ Fe ²⁺)(Si ₂ O ₇)(SiO ₄)O(OH)
	Ba/Sr Carbonates	Carbonates	e.g., ancylite: SrCe(CO ₃) ₂ (OH) · H ₂ O
	Fergusonite	Oxides	YNbO ₄
	Eudialyte	Silicates	Na ₁₅ Ca ₆ (Fe ²⁺ , Mn ²⁺) ₃ Zr ₃ [Si ₂₅ O ₇₃](O,OH,H ₂ O) ₃ (OH,Cl) ₂
Secondary	Loparite	Oxides	(Na,Ce,Ca,Sr,Th)(Ti,Nb,Fe)O ₃
	Zircon	Silicates	ZrSiO ₄
	Britholite	Silicates / Phosphates	(Ce,Ca) ₅ (PO ₄ ,SiO ₄) ₃ OH
	Kainosite	Silicates	Ca ₂ (Y,Ce) ₂ (Si ₄ O ₁₂)(CO ₃) · H ₂ O

Colour Key: Phosphates Silicates Carbonates Oxides

Examples of each of the different mineral groups are provided in Figs. 2-5 showing the reflectance spectra of select minerals and with their continuum removed, as processed by the standard ENVI® tools. For these specimens, the absorption features in the NIR region clearly indicate the presence of REE. All specimens will be classified and the best are being characterized by additional reflectance spectroscopy, X-ray diffraction, X-ray fluorescence and micro-probe analyses, providing the foundation for a comprehensive field guide.

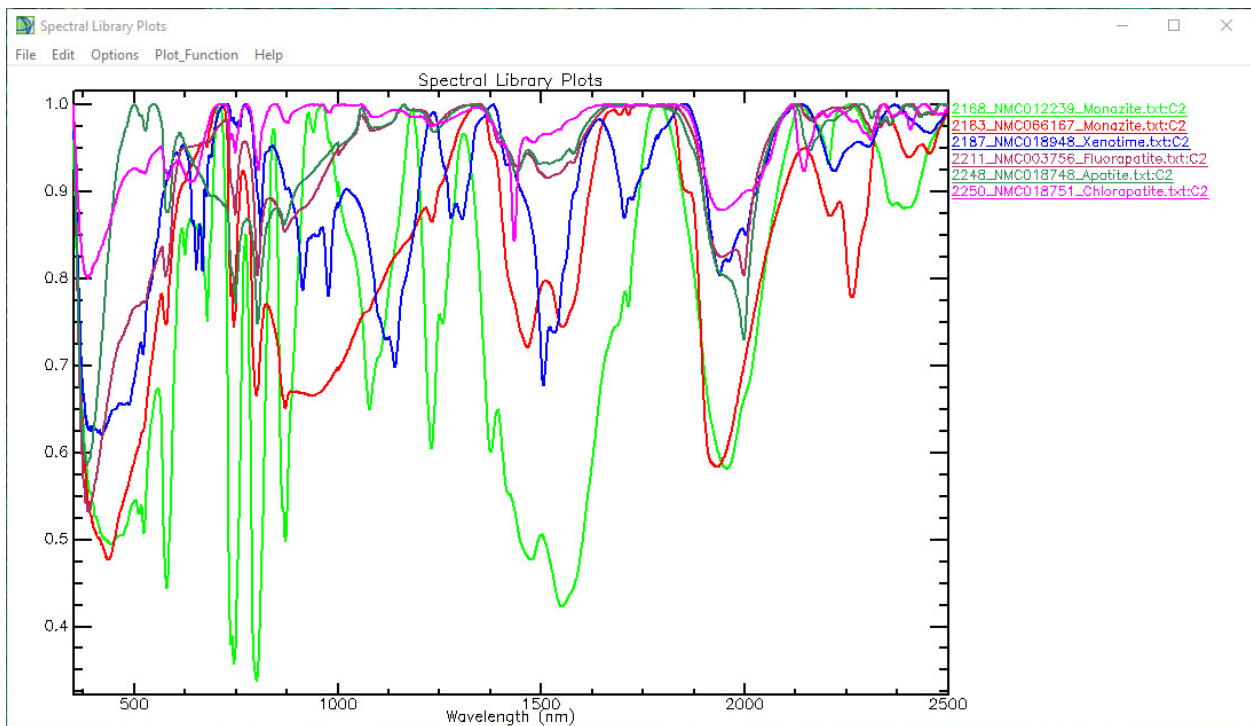
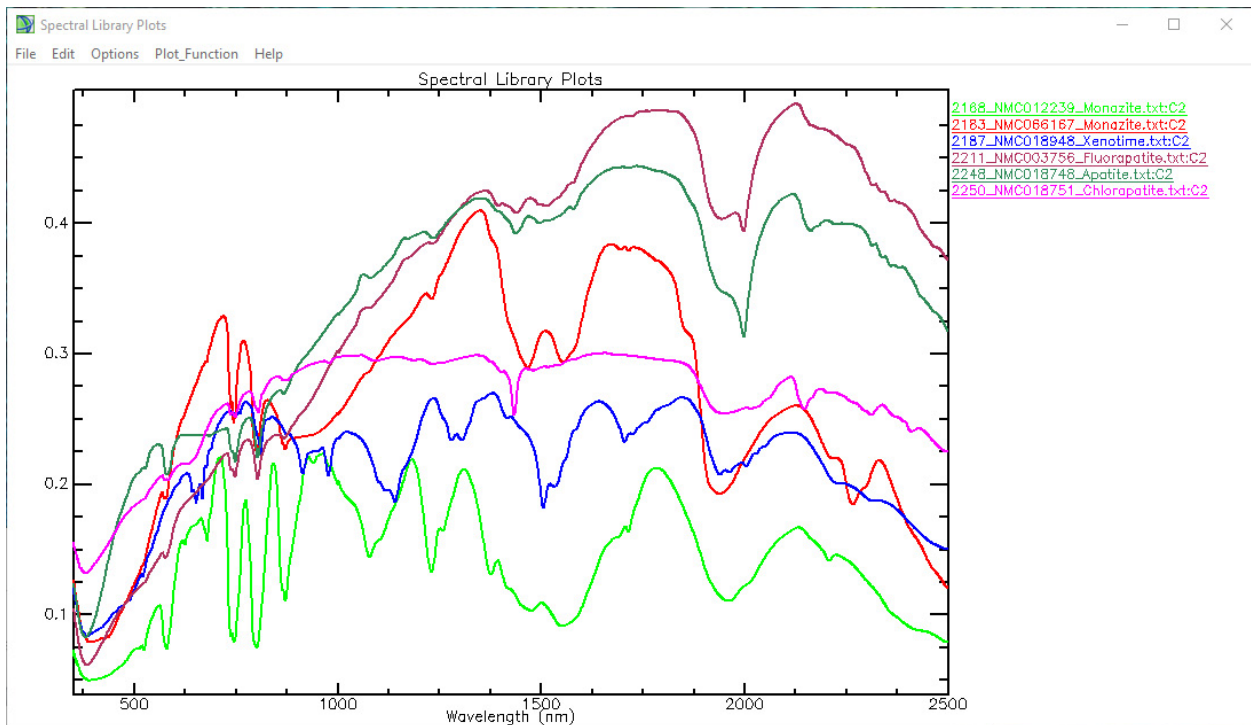


Figure 2. Spectra of Phosphate Minerals. Upper-reflectance; lower-continuum removed. The apatite samples exemplify how REE can be hosted as trace elements in another mineral, and xenotime vs. monazite exemplify how differences in crystal structure and REE distribution are important parameters that control the final spectral shapes.

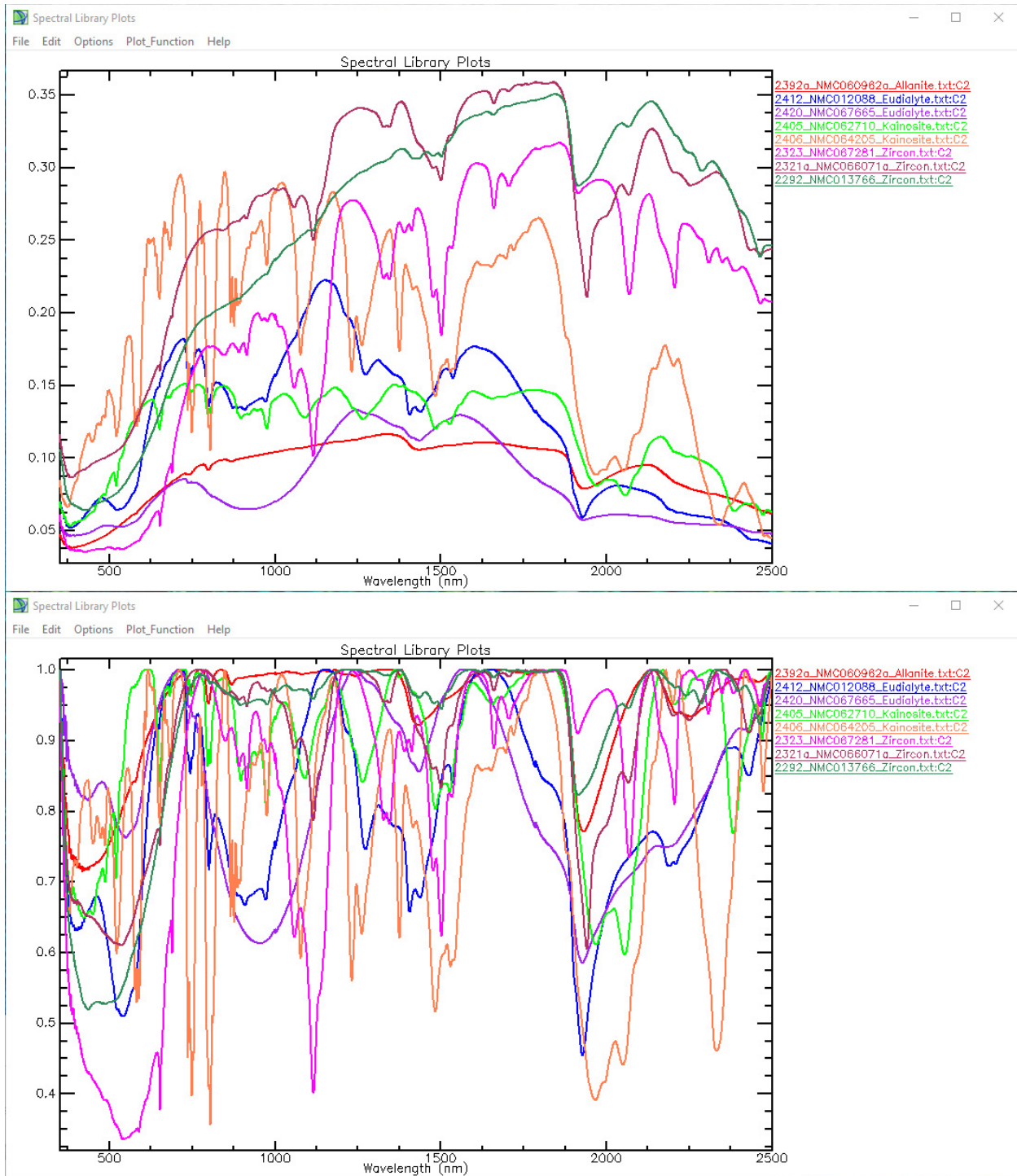


Figure 3. Spectra of Silicate Minerals. Upper-reflectance; lower-continuum removed. Although busy, this plot shows the consistent sharp features related to REE in a range of mineral species, but also how specific patterns allow for distinction between them.

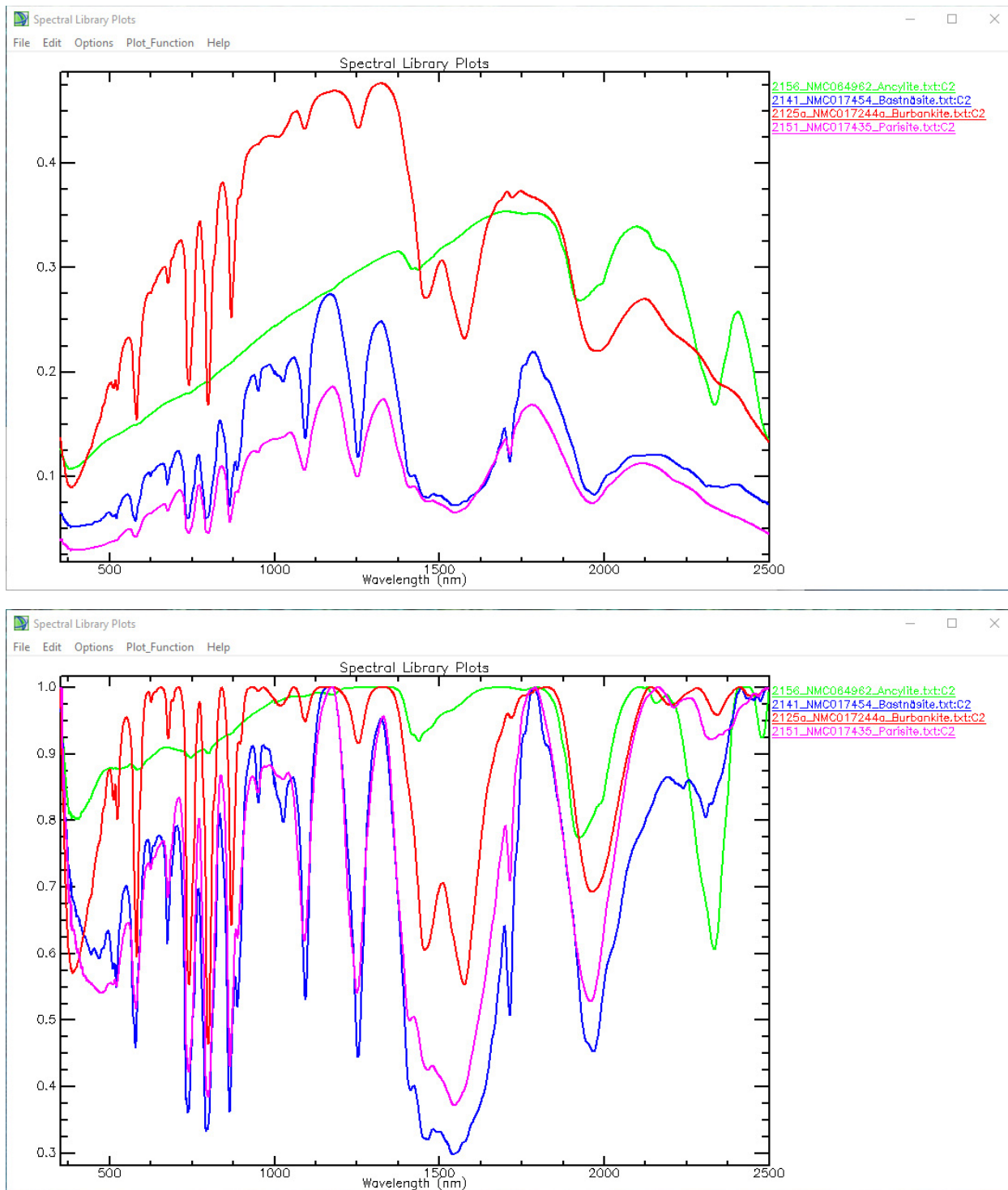


Figure 4. Spectra of Carbonate Minerals. Upper-reflectance; lower-continuum removed. These samples exemplify the sharp features typical of REE-bearing carbonate minerals. Sample spectrum 2156 of ancyrite displays well a challenge seen when collecting spectra from rock samples for spectral libraries, in that while the sample has been properly identified as having ancyrite, it is instead a mixture of minerals that comprise the rock specimen.

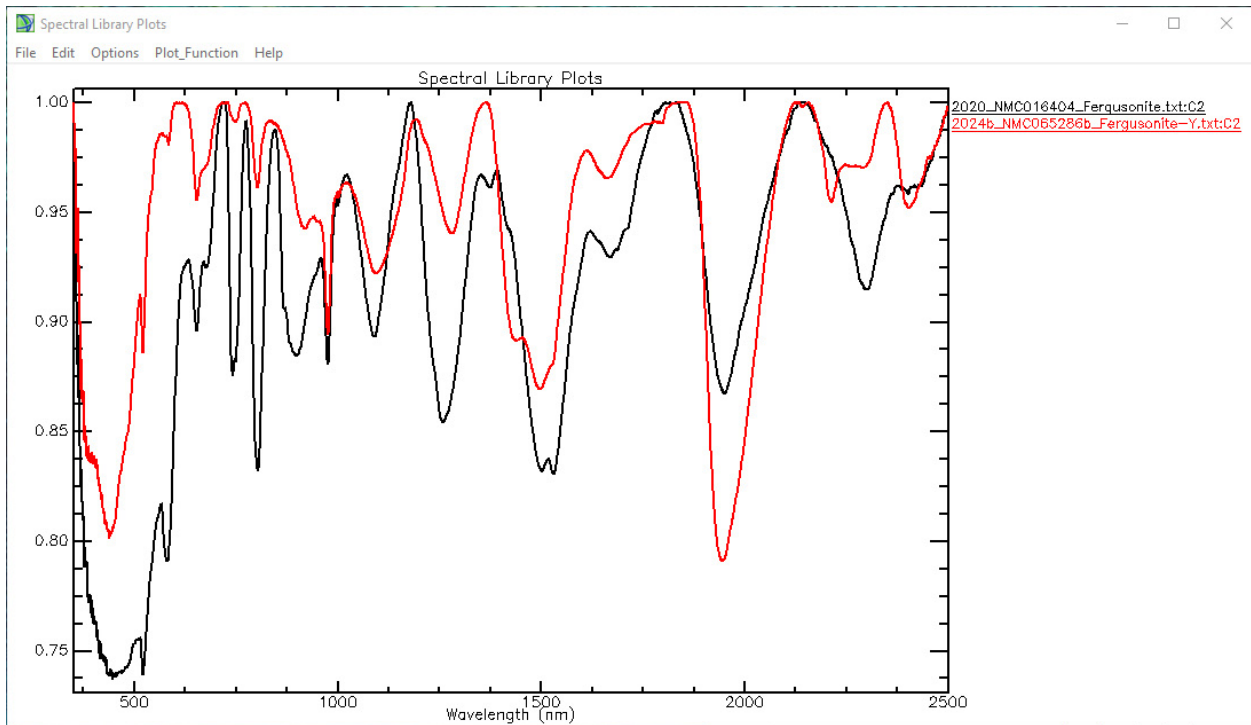
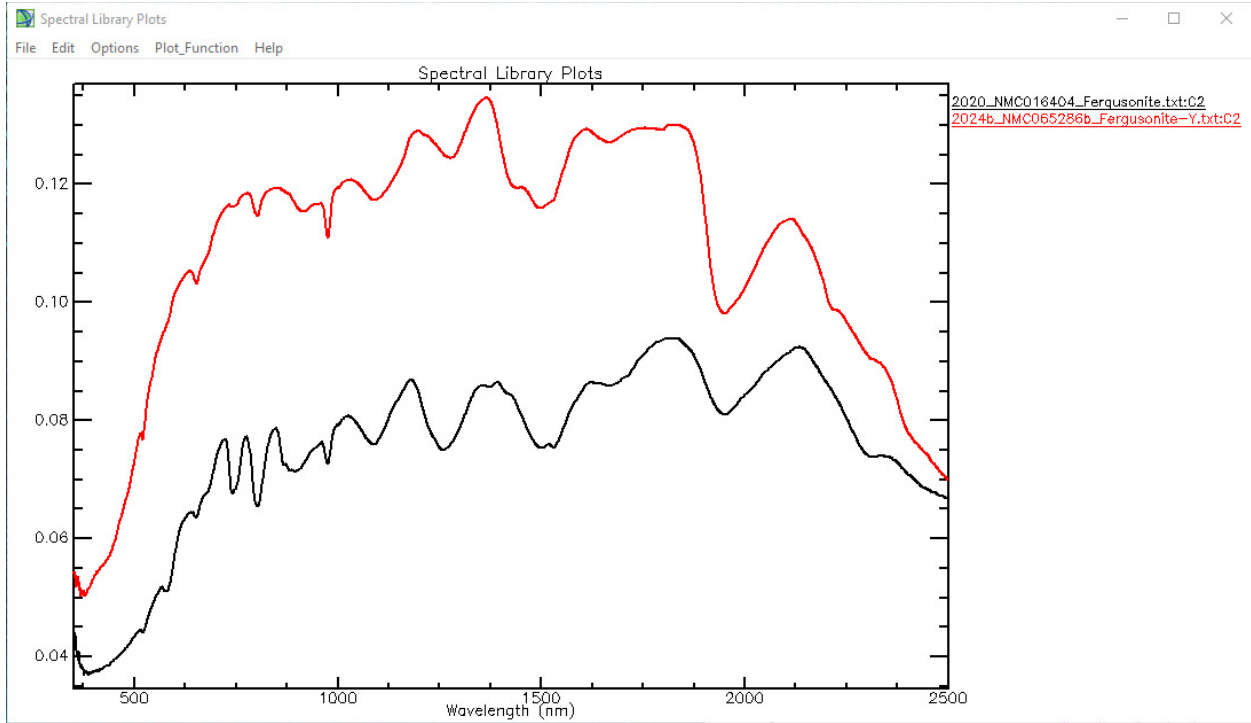


Figure 5. Spectra of Oxide Minerals. Upper-reflectance; lower-continuum removed. Many REE oxide minerals also contain U and Th, leading to crystal structure damage and samples becoming metamict, as well as Fe that leads to dampening of signals. These two spectra of fergusonite are distinct in that they have retained their sharp REE related features despite being dark samples (average reflectance of ~ 0.1).

SUMMARY

This Open File report provides an alternate form for using the Spectral Library database published by Percival et al. (2019). The files were converted using ENVI® software and make them more amenable for use in third party software (e.g., ENVI®, Spectragryph and TSG™) for hyperspectral analyses, aimed at the remote sensing community.

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