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## A reference library of thermal infrared mineral reflectance spectra for the HyLogger-3 drill core logging system

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### ABSTRACT

A new reference library of thermal infrared spectral reflectance measurements of the major rock-forming and alteration minerals has been compiled to support and enhance analysis of data acquired using the CSIRO HyLogger-3 drill-core logging system. The HyLogger-3 is a robotic system that acquires large volumes of bidirectional reflectance spectra from diamond drill core within the wavelength range of visible light, the near infrared and shortwave infrared (400–2500 nm) as well as the thermal infrared from 6000 to 14 000 nm. The library samples were selected as single pure solid mineral crystals or monomineralic hand samples judged to have a similar bidirectional spectral response to that of typical diamond drill cores. Furthermore, a large number of individual mineral samples were chosen to cover the various natural spectral variations within single mineral groups such as, for example, a range of solid solutions of plagioclase. Owing to the bidirectional measurement geometry of the HyLogger-3, spectral variations caused by crystal orientation effects are also expected. Accordingly, reflectance measurements were made for multiple surfaces/facets of each sample, and also for orthogonal orientations of the plane of incidence illumination for each facet measured. All measured spectra were compared with existing library spectra or with spectra measured from validated samples to judge whether the mineral samples could be regarded as pure and, where possible, their chemical composition and mineralogy were validated by X-ray fluorescence and X-ray diffraction. For quality control, all such relevant metadata, including macroscopic descriptions of each sample, were collated in an associated database. In total, the spectral library contains more than 2000 spectra, from 562 specimens, representing 130 mineral groups. This library focuses on the most common rock-forming minerals of relevance to metalliferous exploration and mining, with a few limitations resulting from availability of suitable samples, which will be addressed as new samples become available. Comparisons with emission spectra from existing spectral libraries show good agreement, indicating that this spectral library will also be useful in the remote sensing domain.

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### Introduction

As a major exploration and mining destination, Australia annually creates huge volumes of valuable diamond drill core, much of which is archived in state and territory geological surveys for public access. This includes reference cores from many of Australia's globally significant mining camps and represents a wide range of commodities. Industry, geological surveys and academia can benefit greatly from improved core-logging systems that can objectively extract more detailed geological, mineralogical and basin system information from this vast national resource. Such core-logging systems not only increase our national knowledge base but also capture an improved return on the considerable initial drilling investment. One way of capturing these benefits is through non-destructive spectroscopic drill-core logging systems that characterise host rock and alteration mineralogy, and record

photographic logs in ways that are both more objective and more detailed than conventional visual logging. This is not to say that experienced visual logging is not enormously valuable, but that many minerals are difficult to correctly identify in bleached, weathered and altered rocks or may be unfamiliar and unexpected in different situations. To tackle these issues, CSIRO Mineral Resources has developed a suite of tools known as HyLogging™ Systems that use reflectance spectroscopy alongside detailed imaging to extract mineralogical information from rocks.

HyLogging hardware and software systems can routinely characterise and map the relative abundance of iron oxides such as hematite and goethite (Cudahy & Ramanidou, 1997; Ramanidou & Cudahy, 1996; Ramanidou, Connor, Cornelius, & Fraser, 2002; Ramanidou, Wells, Belton, Verral, & Ryan, 2008), OH-bearing silicates such as micas, chlorites, kaolinite, smectites (Huntington & Schodlok, 2009; Huntington,

Whitbourn, Mason, Berman, & Schodlok, 2010; Quigley et al., 2009; Wells & Ramanidou, 2007; Yang, Huntington, Browne, & Ma, 2000; Yang, Lian, Huntington, Peng, & Wang, 2005), as well as sulfates and carbonates (Green & Schodlok, 2016), using the visible to near infrared and shortwave infrared (VNIR–SWIR) wavelength region (380–2500 nm). In this wavelength region these minerals show diagnostic spectral features owing to electron transition processes in the VNIR (Hunt, Salisbury, & Lenhoff, 1971; Sherman & Waite, 1985) or vibrational processes mainly of OH and functional groups such as Al–OH, K–OH or Mg–OH in the SWIR (Hunt & Salisbury, 1970, 1971, 1973). However, not all minerals show their diagnostic spectral features in the VNIR–SWIR. Anhydrous silicates such as quartz, feldspars, pyroxenes, olivines and garnets show their diagnostic features in the thermal infrared (TIR) wavelength range (>7000 nm or 7  $\mu\text{m}$ ) owing to fundamental vibrations of the  $\text{SiO}_4$  tetrahedra (Farmer, 1974; Salisbury, Walter, Vergo, & D’Aria, 1991b). Extensive work has been carried out in the TIR based on emission and reflectance spectroscopy with a focus on Lunar and planetary science and in relation to terrestrial remote sensing (Bartholomew, Kahle, & Hoover, 1989; Christensen & Harrison, 1993; Christensen et al., 2000a, 2003; Conel, 1969; Farmer, 1974; Hamilton, 2000, 2003, 2010; Hamilton & Christensen, 2000; Hecker, der Meijde, & van der Meer, 2010; Johnson, Hoerz, & Staid, 2003; Kirkland et al., 2002; Kirkland, Herr, & Salisbury, 2001; Lane & Christensen, 1997; Lane et al., 2011; Lyon, 1965; Lyon & Burns, 1963; Michalski, Kraft, Diedrich, Sharp, & Christensen, 2003; Moersch & Christensen, 1995; Nash & Salisbury, 1991; Ninomiya et al., 1997; Ruff, Christensen, Barbera, & Anderson, 1997; Sabine, Realmuto, & Taranik, 1994; Salisbury & D’Aria, 1992; Salisbury & Wald, 1992; Salisbury & Walter, 1989; Salisbury, D’Aria, & Jarosewich, 1991a; Thomson & Salisbury, 1993; Wald & Salisbury, 1995; Walter & Salisbury, 1989). In recent years, interest in the TIR wavelength region has grown steadily in the exploration and mining industries, as well as Australian state and territory geological surveys. In Australia, the National Virtual Core Library project, funded by the Federal Government of Australia and CSIRO through AuScope Pty Ltd ([www.auscope.org.au](http://www.auscope.org.au)), originally rolled out VNIR–SWIR HyLogger-2 systems during 2009–2010, and then upgraded these to TIR-capable HyLogger-3 systems (Schodlok et al., 2016) in the latter half of 2011. These systems have been in routine use since initial roll-out, and have logged approximately 1000 km of drill core so far. These HyLogger-3 systems produce large volumes of co-registered VNIR–SWIR and TIR spectroscopic drill-core data for geological/mineralogical/exploration applications. The TIR hardware development generated the requirement for improved software tools to analyse this new type of data and therefore the software package The Spectral Geologist (TSG™) ([www.thespectralgeologist.com](http://www.thespectralgeologist.com)), also developed by CSIRO, was extended to support TIR data analysis. A critical part of this software extension is its library of thermal infrared reflectance spectra of monomineralic reference samples that are used for visual reference and to drive two interpretation algorithms, the TIR version of ‘The Spectral Assistant (TSA™)’ (Berman et al. 1999, 2011) and the Constrained Least-squares

spectroscopic modelling tool. The reference library (Table 1) was specifically compiled for use with the HyLogger-3 and is focused on the acquisition of spectra from solid samples, based on the assumption that these spectra would best simulate the spectra measured from diamond drill core. This approach is in contrast to several existing TIR spectral libraries. The two most cited TIR libraries are from the John Hopkins University (JHU; Salisbury et al., 1991b) and the Arizona State University (ASU; Christensen et al., 2000b). The JHU spectral library has bi-conical reflectance spectra and was developed to cover the wavelength range from 2 to 25  $\mu\text{m}$  and demonstrate spectral variation as a function of grain size—which was not covered in previous TIR work at that time. Salisbury et al. (1991b) demonstrated that bi-conical reflectance spectra in some cases show anomalous spectral features that cannot be used in a quantitative sense in comparison with emission data and recommended using directional-hemispherical reflectance if comparisons with laboratory emission data and remote sensing application data are pursued. In the ASU spectral library, emission spectra were acquired and samples were prepared with grain sizes ranging between 710 and 1000  $\mu\text{m}$  by crushing and sieving. These samples are intended to be representative of the roughness of sandy and rock surfaces. Further, the grains are randomly orientated so that any preferred crystal axis orientation effect is minimised. This is more suitable for planetary and terrestrial remote sensing research (Christensen et al., 2000b).

A factor not addressed by these libraries is that the orientation of single minerals or crystals can be of significance when analysing HyLogger-3 reflectance spectra of diamond drill cores. This paper describes the work of compiling a reference library of thermal infrared reflectance spectra for the HyLogger-3 system focusing on well-described solid, monomineralic samples of silicates, carbonates, sulfates, sulfides and oxides with an emphasis on spanning the natural spectral variability of these minerals (including varying crystal orientation). This spectral library (Table 1) thus allows instrument operators and scientists to assess and analyse their HyLogger-3 data in terms of quality and for different geological applications. It provides a diverse mineral data set for comparison with and analysis of diamond drill cores from many different geological environments and ensures relevance to a wide range of spectroscopic core data. In contrast to many of the traditional TIR studies that utilise the frequency domain (expressed in wavenumbers), this library is presented in the wavelength domain, expressed in nanometres or micrometres. This was necessary to be consistent with the earlier HyLogging systems and other commercial spectrometers that provide VNIR–SWIR data in the wavelength domain, and to make life easier for spectral geologists who are used to remote sensing applications where the wavelength domain is common.

## HyLogging system

The HyLogger-3™ is a system designed for rapid, non-destructive hyperspectral logging of diamond drill core, and

**Table 1.** Minerals, groups and subgroups represented in the new thermal infrared spectral reflectance reference library (numbers in parentheses indicate the number of individual spectra in the library).

Group	Subgroup	Mineral spectra	Group	Subgroup	Mineral spectra
Silica	Opal	Opal (2)	Kaolin	Kaolin	Kaolinite (2)
K-Feldspar	Quartz	Quartz (5)	White Mica	W-Mica	Muscovite (3)
	K-Feldspar	Anorthoclase (2)			Illite (1)
Plagioclase		Microcline (3)	Smectite	Smectite-Al	Paragonite (1)
		Orthoclase (2)			Montmorillonite (2)
	Albite	Albite (3)		Montmorillonite-Na (1)	
	Plagioclase-Ca	Bytownite (2)		Nontronite (1)	
Pyroxene		Labradorite (3)		Smectite-Fe	Smectite-Fe (1)
		Anorthite (1)	Other AIOH	Axinite	Saponite (1)
	Plagioclase-Na	Andesine (2)		Prehnite	Axinite (1)
		Oligoclase (2)		Prehnite (4)	
Pyroxene	Pyroxene-Clino	Augite (3)		Pyrophyllite	Pyrophyllite (1)
		Diopside (2)		Topaz	Topaz (1)
Olivine		Hedenbergite (2)	Chlorite	Chlorite	Chlorite (4)
	Pyroxene-Ortho	Enstatite (2)	Dark Mica	Dark mica	Biotite (1)
Garnet	Olivine	Olivine (3)	Amphibole	Amphibole-Ca	Phlogopite (1)
		Fayalite (1)			Stilpnomelane (1)
		Forsterite (1)			Actinolite (2)
Garnet	Garnet-Ca	Grossular (2)			Edenite (2)
		Andradite (1)			Hornblende (5)
Misc-Silicates		Uvarovite (1)			Ferrohornblende (1)
	Garnet-Mg-Fe-Mn	Almandine (1)			Kaersutite (1)
		Spessartine (1)			Tschermakite (1)
	Zircon	Zircon (1)		Amphibole-Mg-Fe-Mn-Li	Anthophyllite (2)
	Silicate-MetaM	Andalusite (1)			Gedrite (1)
		Cordierite (1)			Grunerite (1)
		Kyanite (2)			Holmquistite (1)
		Sillimanite (2)			Mangano-cummingtonite (1)
		Staurolite (1)			
Zeolite	Zeolite	Analcime (1)		Amphibole-Na	Riebeckite (3)
		Chabazite (1)			Arfvedsonite (1)
		Heulandite (1)			Glaucophane (1)
		Laumontite (1)	Serpentine	Serpentine	Antigorite (1)
		Mesolite (1)			Chrysotile (1)
		Natrolite (1)			Lizardite (1)
		Phillipsite (1)	Other-MgOH	Talc	Talc (2)
		Thomsonite (1)	Epidote	Epidote	Epidote (1)
Carbonate	Carbonate-Ba-Sr-Pb-Zn	Cerussite (1)			Clinozoisite (1)
		Smithsonite (1)			Zoisite (1)
		Strontianite (1)	Tourmaline	Tourmaline-Na-Fe-Mn	Tourmaline (2)
		Witherite (1)			
	Carbonate-Cu	Azurite (1)	Sulfate	Alunite	Alunite-K (1)
		Malachite (1)			Alunite-Na ((1)
		Siderite (1)		Barite	Barite (2)
	Carbonate-Fe-Mn	Ankerite (1)		Gypsum	Gypsum (1)
		Rhodochrosite (1)		Jarosite	Jarosite (1)
	Carbonate-Mg-Ca	Siderite (1)	Oxide	Oxide-Other	Cassiterite (1)
		Aragonite (1)			Ilmenite (1)
		Calcite (1)			Chromite (1)
		Dolomite (1)			Gahnite (1)
		Dolomite-Fe (1)			Psilomelane (1)
		Magnesite (1)			Pyrolusite (1)
Palygorskite-Sepiolite	Palygorskite-Sepiolite	Palygorskite (1)			Rutile (1)
Borate	Vonsenite	Vonsenite (1)		Oxide-Fe	Goethite (3)
Phosphate	Apatite	Apatite (1)			Hematite (2)
					Magnetite (1)

was developed by CSIRO Mineral Resources (Schodlok et al., 2016). It is a robotic system that scans drill core by moving the core beneath the spectrometers using a computer controlled translation stage. Its TIR capability is based on a rapid-scan Fourier transform infrared (FTIR) spectrometer from DP Instruments, Connecticut, USA. It acquires bidirectional radiance from two infrared sources reflected by the core. A liquid

nitrogen cooled MCT (mercury cadmium telluride—HgCdTe) detector captures the radiance in the wavelength range from 6  $\mu\text{m}$  ( $1666\text{ cm}^{-1}$ ) to 14.5  $\mu\text{m}$  ( $690\text{ cm}^{-1}$ ). The Fourier-transform spectrometer has an underlying spectral resolution of approximately  $6\text{ cm}^{-1}$ , which, when resampled in 25 nm steps, leads to a spectral resolution of 25 nm at 6  $\mu\text{m}$ , rising to 120 nm at 14.5  $\mu\text{m}$ . The spectrometer has a nominal field of

view (spot size) on the sample of diameter 10 mm. The wavelength calibration is based on well-known spectral features of polystyrene and quartz. Radiometric calibration is performed by two blackbody measurements of 20 and 60°C to determine the system transfer function. A detailed functional description of the HyLogger-3™ is given by Schodlok et al. (2016).

## Samples

The spectral library contains spectra from 562 individual specimens representing 130 minerals from major rock-forming mineral groups such as silicates, carbonates, oxides, hydroxides, sulfides and sulfates. All samples were single crystals or monomineralic lumps. The samples were provided by the Australian Museum in Sydney, the Victorian Museum in Melbourne, the Macquarie University and the University of New South Wales in Sydney, Australia. In addition, samples were drawn from CSIRO existing collections and others were purchased by CSIRO from various mineral suppliers worldwide. Samples were selected to cover those major minerals that are most relevant to the exploration and mining industries and driven by projects based on diamond-drill core logging. The focus, especially in the first stage of collating the library, was on anhydrous silicates. All samples underwent minor sample preparation, including dust removal to minimise spectral variation owing to volume scattering effects from clinging fines, and drying under laboratory conditions for at least 24 h in order to ensure that measurements were not affected by moisture or temperature differences. No sample crushing or grinding was performed to achieve a certain grainsize range as applied for other published spectral libraries (e.g. Christensen et al., 2000b; Salisbury et al., 1991b). This was a deliberate step based on the assumption that solid single mineral samples (either single crystals or mono-mineralic lumps) come closest to simulating the spectral response of solid diamond drill core. In addition, the solid samples were measured in different orientations to gain more knowledge of orientation effects, as varying mineral or crystal orientation in diamond drill core scanning is inevitable. Samples were identified by macroscopic description, and many were also analysed by X-ray diffraction (XRD) analysis, enabling estimation of sample purity. For samples with enough material available, bulk chemistry was also assessed by X-ray fluorescence (XRF). Museum and university samples were not assessed by XRD and XRF. Instead, careful macroscopic analysis was done using a hand lens and binocular microscope and spectra were compared with those of validated samples in order to assess purity so that only the highest quality loaned samples were selected. Finally, the purity assessments of all samples were used to produce a four-level quality classification.

## Documentation

The spectral library uses the Environment for Visualising Images (ENVI; <http://www.harrisgeospatial.com/>) Spectral Library format, which is supported by software packages

TSG and ENVI. Spectral data as well as their metadata are stored in a Microsoft SQL Server database and managed by a Microsoft Visual Studio Lightswitch application. The database stores the common critical and important information related directly to a sample and its spectra such as sample name, sample ID, source or locality, etc. Since cases occurred where samples had to be renamed after validation analyses, the database includes a field to keep the original sample name and allow tracking of the sample should further information be available under the original name, e.g. in earlier papers and reports. The database also includes all independent validation data when available, e.g. XRD, XRF and/or solid solution data. All information is stored in specific fields in order to allow access to the validation data itself and/or to reports in which samples have been described. Another important area within the database has information about the data acquisition. This includes, for example, instrument used, date of acquisition, name and contact details of the operator and a comment. The latter is a very important field as it provides additional valuable information about sample and spectra delivered by the operator during both data acquisition and quality assessment. It includes information such as specific sample and measurement conditions or describes possible discrepancies between sample and spectrum. All this information serves to track samples and their spectra to provide transparency of data quality. Finally, there is the quality assessment that classifies spectra/samples into four spectral quality levels similar to those described by Christensen et al. (2000b):

- L1—impure with uncertainties, spectra showing multiple spectral features of different minerals and at least one unidentified mineral. Impurities considerably affect the spectra.
- L2—impure, spectra showing minor impurities but still having reasonable spectral characteristics that can be used to identify the mineral components of the sample, or the impurities have been identified by XRD.
- L3—pure, sample is not validated but shows the spectral characteristic of a pure mineral sample.
- L4—pure and validated, sample and spectra are pure and the mineral was validated confirming the pureness.

## Data acquisition and processing

The library spectra were acquired in 'library mode' of the HyLogger-3 system. This is a static measurement where the X–Y translation table moves the sample beneath the spectrometer, remains stationary for 8 s while the sample is measured, and finally moves the sample back to the loading position. The spectral data acquisition follows a consistent acquisition protocol.

All samples are stored in the laboratory for at least 24 h to ensure that samples and system are temperature equilibrated. With the aid of a fixed laser pointer, the selected area of interest of the sample is mounted at a defined position on the X–Y

table, which then moves it precisely to the centre of the field of view of the instrument during the measurement cycle. This procedure gives the operator full control over selecting the area of interest on a sample. The surface to be measured is orientated horizontally to avoid specular reflectance effects, and mounted as accurately as possible at the same height as the gold reflectance transfer standard to minimise reflectance errors owing to path differences between the reference and the sample. The library spectral measurement is as follows. First, the laboratory background radiance is sampled via the background mirror (producing a system response  $V_b$ ), then the diffuse reflectance transfer standard is measured ( $V_t$ ), and finally 100 individual spectra of the mineral sample are measured ( $V$ ) and recorded in one file. The base reflectance  $\hat{\rho}$  is then calculated for each of the 100 sample spectra as follows:

$$\hat{\rho} = \rho_t \frac{V - V_b}{V_t - V_b}$$

where  $\rho_t$  is the NIST-traceable directional-hemispherical reflectance of the transfer target as described in Schodlok et al. (2016).

After a cooling down period that allows the sample to re-equilibrate with the laboratory room temperature, a second measurement of the same surface is taken with the sample rotated 90 degrees in azimuth direction. The procedure of running two measurements per surface is done to assess the maximum possible wavelength shifts of feature positions owing to a rotation of a surface (Schodlok, Green, Huntington, & Whitbourn, 2009). Thus, for each measured sample surface, a minimum of two spectra were acquired. Depending on the quality of the samples and availability of suitable surfaces, up to 10 spectra were acquired for each sample.

The library measurements are carried out in batches of about 10 samples to decrease measurement time. A digital picture is taken of each measured surface to document the position of the spectrum on the sample, as indicated by the laser pointer.

The sample temperature rises by up to 6°C during the 8 s measurement time, and it is necessary to correct the base reflectances for that. Once or twice a day, a pair of hot and cold black bodies are measured in a similar manner to the sample measurement procedure described above. A linear transfer function between system response and radiance is assumed. The validity of the linearity assumption was tested using blackbodies at multiple temperatures and was found to be satisfactory to within 2 percent. The observed effect of sample heating during the measurement of 100 spectra, is a small and systematic 'drift' difference between each of the 100 individual reflectance spectra. This drift contribution is the result of additional blackbody emission by the sample as its temperature rises. For an increase in temperature of 1°C it is an approximately linear function of wavelength that rises from almost zero at 6  $\mu\text{m}$  to an apparent 'reflectance' of 1% at 14  $\mu\text{m}$ . A detailed model of the sample heating process was developed using classical heat conduction theory (Carslaw & Jaeger, 1959) but it was decided that it was simpler and just

as effective to model the change in each channel of the Standard Reflectance over the 100 spectra as a quadratic function of time. Under this model, assuming that the first sample spectrum of the 100 is in thermal equilibrium with the laboratory, the constant term in the quadratic fit at each channel becomes the best estimate of the final reflectance at that channel.

The reflectance transfer standard is also checked against a well-calibrated primary reflectance standard once or twice per day, in order to correct for any change in reflectance of the transfer standard or changes in overall system response.

## Spectral data

Figure 1 shows example spectra representative of different mineral classes of silicates, carbonates, hydroxides, oxides, sulfates and sulfides. These groups are clearly separated by their major reflectance features (peaks and troughs) in different wavelength positions. Examination of subgroups within a mineral class, for example for silicates, reveals that the crystal structure has a significant impact on the spectral characteristics (Salisbury et al., 1991b). This is demonstrated in Figure 2, which shows the spectral variation of silicates from tectosilicates at the top to the nesosilicates at the bottom. The general wavelength positions of the spectral features are driven by the degree of polymerisation of the  $\text{SiO}_4$  tetrahedron (Salisbury et al., 1991b). Fine compositional (e.g. solid-solution) and structural differences result in distinctive variations in spectral characteristics within a mineral subgroup, e.g. plagioclase feldspars as demonstrated by Christensen et al. (2000b).

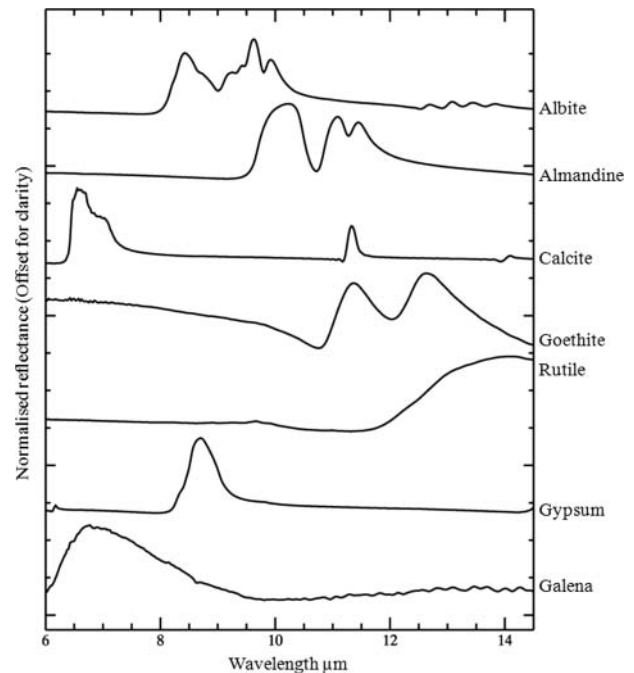


Figure 1. Example mineral reflectance spectra of different mineral groups representing silicates, carbonates, hydroxides, sulfates and sulfides acquired with the HyLogger 3. From top to bottom: albite, almandine, calcite, goethite, rutile, gypsum, galena.

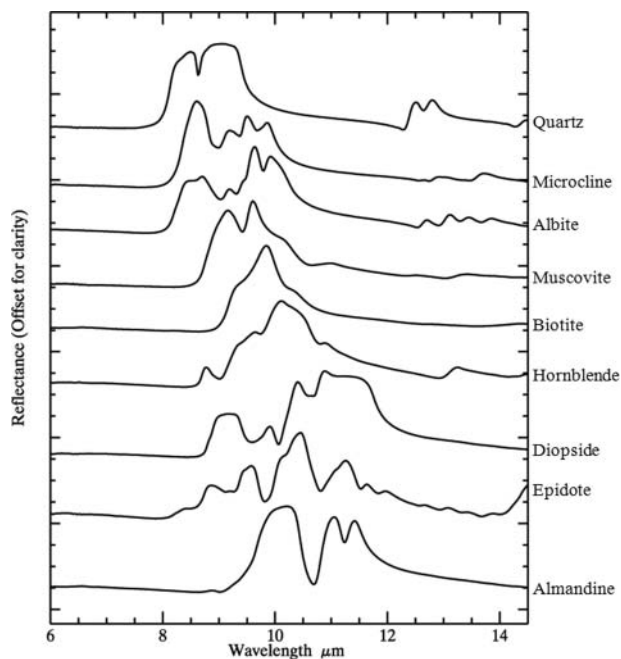


Figure 2. Example reflectance spectra of different silicate minerals from tectosilicates to neosilicates. These spectra demonstrate the significant and well documented shift of spectral features from the shorter towards the longer wavelengths owing to the depolymerisation of the  $\text{SiO}_4$  ion (Salisbury et al., 1991b).

These systematic changes in spectral features can be used to map mineral distributions in drill core and support the characterisation of mineral systems in exploration and mining.

As the HyLogger-3 system acquires bidirectional reflectance data of whole or half diamond drill core, orientation effects can be seen in the spectral characteristics of a single mineral when different facets are in view, or the geometry between the spectrometer and crystal lattice varies. Figure 3 shows significant spectral differences for: (a) a microcline crystal measured parallel to the c-axis and the a-axis, and (b) muscovite measured parallel to and perpendicular to the layer structure. In both cases, prominent spectral peak features increase/decrease in intensity and change in shape for different orientations, or disappear altogether. Therefore, it is very important to appreciate and document such spectral variability, especially when comparing samples with known mineralogy but unknown crystal orientations (e.g. granites) and dealing with foliated rocks. Analytical and classification methods such as spectral unmixing have to address these complexities by having available a spectral library that includes information about orientation-dependent spectral variations within single minerals.

It is interesting to compare our results with spectra from two well-known infrared spectral libraries, ASU and JHU. The ASU library (Christensen et al., 2000b; Salisbury et al., 1991b) was measured in emission, and here we have transformed to reflectance by Kirchhoff's law assuming Lambertian scattering (Nicodemus, 1965). The JHU library (Salisbury et al., 1991b) was mostly measured with a bi-conical reflectance attachment, which caused a significant part of the illuminating

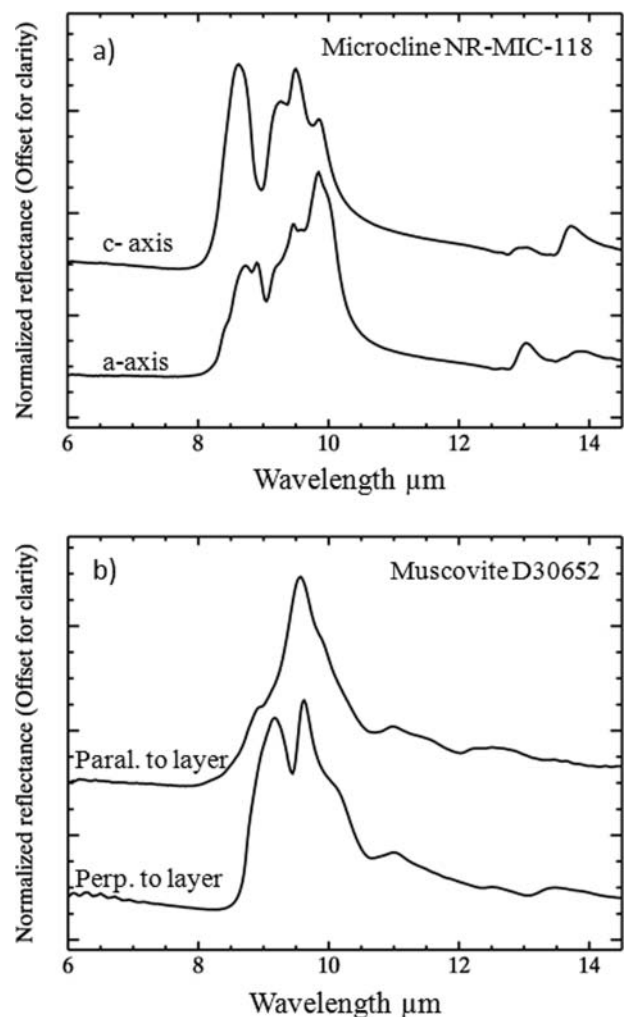


Figure 3. Demonstration of spectral variations owing to mineral crystal orientation during measurement showing reflectance spectra of two different facets (measured in c- and a-axis directions) of (a) microcline sample, and (b) muscovite sample (measured parallel and perpendicular to its layer structure). In both cases it is obvious that depending on which orientation was measured certain spectral features can disappear and/or change intensity, shape or position.

radiation to have a grazing or near grazing incidence angle (Salisbury, 1993).

Figure 4 (top) shows the spectra of crystalline quartz from the ASU, JHU and CSIRO libraries. The difference between absolute values arises quite naturally from differences between angle-of-incidence and bidirectional reflectance distribution function (BRDF) effects in directional-hemispherical vs bi-directional measurement configurations. Figure 4 (bottom) shows the same spectra with range normalisation to illustrate similarities and differences. It is notable that, relative to the other two, the JHU spectrum shows markedly higher reflectance just short of 8  $\mu\text{m}$ . Salisbury (1993) showed that preventing low angle illumination in his measurement geometry resulted in spectra identical in shape to hemispherical measurements. In support of this observation we have used standard Fresnel equations (Hapke, 2012) and the complex refractive index for quartz (Spitzer & Kleinman, 1961) to show that specular reflectance increases in the same way just short

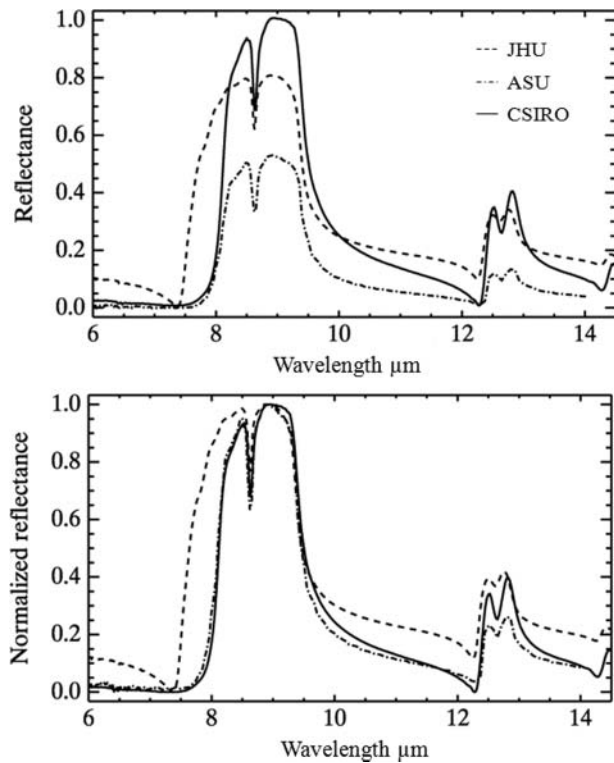


Figure 4. Top: Comparison of a CSIRO HyLogger 3 reflectance spectrum of quartz (ID: UNSW-QTZ01) with quartz spectra from the JHU (ID: Quartz.1) and ASU (ID: BUR-4120 55) spectral libraries. The JHU spectra were measured in bi-conical reflectance mode, the ASU spectra in emission mode (transformed to reflectance) and the CSIRO spectrum in double bidirectional reflectance mode. There is a good agreement of the ASU and CSIRO spectra whereas discrepancies against the JHU spectrum occur at the shorter wavelengths as discussed. The spectra from the ASU and CSIRO libraries are comparable, except for quite minor differences. Bottom: same spectra as above but normalised to allow a more detailed comparison.

of 8  $\mu\text{m}$  as the incidence angle is increased. Thus, although our measurements and the JHU measurements are both bidirectional, it appears that the HyLogger spectra are more similar to the ASU emission spectra because the HyLogger spectra involve measurement at a small angle of incidence ( $20^\circ$ ).

This leads to the conclusion that the measurement geometry of the HyLogger-3 system, with its two IR sources, generates spectra that are comparable with emission spectra transformed to reflectance. We call the configuration 'double-bidirectional reflectance.' Apart from the short-wavelength differences in the ASU spectra discussed above, the residual differences between these normalised double bidirectional reflectance and emission spectra are quite typical of all our measurements, and are discussed further in relation to Figure 5 below. In relation to the comparison between directional reflectance and directional hemispherical reflectance, double bidirectional reflectance has two advantages over single bidirectional reflectance. First, when irradiating round core that is not well centred in the core tray section, the Lambertian reduction in signal from one side is compensated by a corresponding enhancement on the other side. Second, it reduces susceptibility to very low return signal into the receiving telescope from flat facets in broken core that are

orientated towards a source. In effect, it makes the measurement closer to what one would get with a directional-hemispherical reflectance (DHR) configuration (and by inference, with hemispherical emission results).

To test this conclusion, a large number of samples from the mineral collection of this spectral library have been measured in DHR using a 10.5 mm, gold coated integrating sphere attached to a Perkin Elmer FTIR spectrometer (Schodlok, 2004). Figure 5 shows the comparison of DHR and our double bidirectional reflectance spectra for six typical samples, where again the spectra have been normalised in order to facilitate comparison. It demonstrates that ankerite, albite, kaolinite, oligoclase, riebeckite and quartz show very similar spectral characteristics. Similar findings have been given in Cudahy et al. (2009) comparing HyLogger data with emissivity data, in agreement with this study. Only minor shape differences appear between the two data-acquisition methods for these six samples, and this is generally the case for all the samples that we measured, including clay minerals. For example, minor differences in intensity are visible for albite at around 9  $\mu\text{m}$  and for kaolinite at around 6–9  $\mu\text{m}$ . This might be explained by the inability of the two systems to measure exactly the same spot on a sample owing to differences in their spatial resolution. The spot size of the HyLogger-3 in library mode is nominally 10 mm diameter whereas the viewing port of the integrating sphere is 18 mm in diameter. The slight differences in spectral shape in the quartz are possibly explained by subtle variability in the BRDF of the sample. This comparison indicates that the library spectra are of high

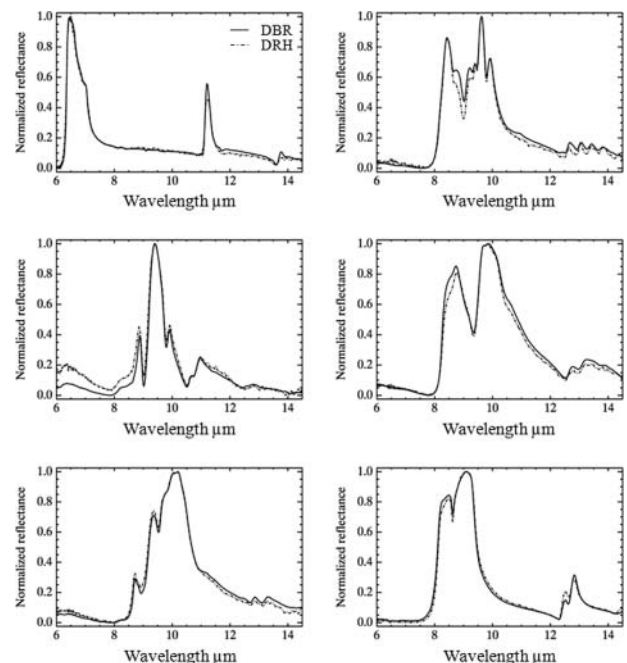


Figure 5. Comparison of normalised directional-hemispherical (DHR) reflectance spectra with normalised double bidirectional reflectance spectra of left–right, top–bottom, ankerite, albite, kaolinite, oligoclase, riebeckite and quartz, respectively. This plot demonstrates that the HyLogger 3 spectra are very similar to DHR spectra, which are widely used as reference spectra in remote sensing applications, and thus can be used for quantitative analyses if needed.



quality. They should be useful for remote and proximal sensing applications, and for quantitative unmixing if needed. While the difference between hemispherical and bidirectional measurements should not be neglected, these results show that BRDF-related variability is much less than we find from other sources such as surface condition (Salisbury & Wald, 1992) or sample orientation.

## Conclusion

This paper has presented the methodology and given typical examples of high-quality, high-resolution, traceable thermal infrared reflectance spectra of a wide range of minerals, and their natural variations, in support of voluminous spectroscopic analysis of HyLogger-3 drill core data. Detailed spectroscopic data of 562 specimens covering more than 130 minerals, as listed in Table 1, have been assembled in the current thermal infrared spectral reflectance reference library, useful for HyLogging and related applications, a work which continues to be upgraded. This library is used in the publicly available Core version of the TSG software package. It will also find wide application outside the HyLogging domain for anyone interested in the thermal infrared characteristics of minerals. The library does not cover all mineral classes, since its development was focused on the most common rock-forming and alteration minerals encountered in minerals exploration and mining projects. Mineral selection was also influenced by the availability of samples and by applications demand from research and industry. So far, this includes minerals of the silicate, carbonate, sulfide, sulfate, oxide and hydroxide groups. Given the close comparison with emission data of Christensen et al. (2000b) and the good agreement in spectral characteristics with our spectra, this spectral reflectance library should also be useful for comparison with airborne and satellite-borne remotely sensed data.

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## Disclosure statement

No potential conflict of interest was reported by the authors.

## References

Bartholomew, M. J., Kahle, A. B., & Hoover, G. (1989). Infrared spectroscopy (2.3–20  $\mu\text{m}$ ) for the geological interpretation of remotely-sensed multispectral thermal infrared data. *International Journal of Remote Sensing*, 10, 529–544.

- Berman, M., Bischof, L., & Huntington, J. (1999). Algorithms and software for the automated identification of minerals using field spectra or hyperspectral imagery: In Proceedings of the 13th International Conference on Applied Geologic Remote Sensing, Vancouver. Volume 1, 222–232.
- Berman, M., Bischof, L., Lagerstrom, R., Guo, Y., Huntington, J., & Mason, P. (2011). An unmixing algorithm based on a large library of shortwave infrared spectra. North Ryde NSW: CSIRO Report EP117468.
- Carlsaw, H. S., & Jaeger, J. C. (1959). *Conduction of heat in solids*. New York, NY: Oxford University Press.
- Christensen, P. R., & Harrison, S. T. (1993). Thermal infrared emission spectroscopy of natural surfaces: Application to desert varnish coatings on rocks. *Journal of Geophysical Research–Solid Earth*, 98, 19 819–819 834.
- Christensen, P. R., Bandfield, J. L., Clark, R. N., Edgett, K. S., Hamilton, V. E., Hoefen, T., ... Smith, M. D. (2000a). Detection of crystalline hematite mineralization on Mars by the Thermal Emission Spectrometer: Evidence for near-surface water. *Journal of Geophysical Research-Planets*, 105, 9623–9642.
- Christensen, P. R., Bandfield, J. L., Hamilton, V. E., Howard, D. A., Lane, M. D., Piatek, J. L., ... Stefanov, W. L. (2000b). A thermal emission spectral library of rock-forming minerals. *Journal of Geophysical Research*, 105, 9735–9739.
- Christensen, P. R., Mehall, G. L., Silverman, S. H., Anwar, S., Cannon, G., Goriell, N., ... Squyres, S. (2003). Miniature thermal emission spectrometer for the Mars Exploration Rovers. *Journal of Geophysical Research – Planets*, 108, 8064. doi:10.1029/2003JE00211, p.23
- Conel, J. E. (1969). Infrared emissivities of silicates: Experimental results and a cloudy atmosphere model of spectral emission from condensed particulate mediums. *Journal of Geophysical Research*, 74, 1614–1634.
- Cudahy, T. J., & Ramanaidou, E. R. (1997). Measurement of the hematite: goethite ratio using field visible and near-infrared reflectance spectrometry in channel iron deposits, western Australia. *Australian Journal of Earth Sciences*, 44, 411–420.
- Cudahy, T., Hewson, R., Caccetta, M., Roache, A., Whitbourn, L., Connor, P., ... Quigley, M. (2009). Drill core logging of plagioclase feldspar composition and other minerals associated with Archean gold mineralization at Kambalda, Western Australia, using a bidirectional thermal infrared reflectance system. *Reviews in Economic Geology*, 16, 223–235.
- Farmer, V. C. (1974). *The infrared spectra of minerals*. London: Mineralogical Society Monograph 4.
- Green, D., & Schodlok, M. C. (2016). Characterisation of carbonate minerals from hyperspectral TIR scanning using features at 14 000 and 11 300 nm. *Australian Journal of Earth Sciences*, 63, <http://dx.doi.org/10.1080/08120099.2016.1225601>
- Hamilton, V. (2003). Thermal infrared emission spectroscopy of titanium-enriched pyroxenes. *Journal of Geophysical Research*, 108, 5095–5102.
- Hamilton, V., & Christensen, P. R. (2000). Determining the modal mineralogy of mafic and ultramafic igneous rocks using thermal emission spectroscopy. *Journal of Geophysical Research*, 105, 9717–9733.
- Hamilton, V. E. (2000). Thermal infrared emission spectroscopy of the pyroxene mineral series. *Journal of Geophysical Research-Planets*, 105, 9701–9716.
- Hamilton, V. E. (2010). Thermal infrared (vibrational) spectroscopy of Mg–Fe olivines: A review and applications to determining the composition of planetary surfaces. *Chemie Der Erde–Geochemistry*, 70, 7–33.
- Hapke, B. (2012). *Theory of reflectance and emittance spectroscopy* (2nd ed.). Cambridge: Cambridge University Press; p. 531. doi: 10.1017/CBO9781139025683
- Hecker, C., der Meijde, M. V., & van der Meer, F. D. (2010). Thermal infrared spectroscopy on feldspars – Successes, limitations and their implications for remote sensing. *Earth-Science Reviews*, 103, 60–70.
- Hunt, G. R., & Salisbury, J. W. (1970). Visible and near-infrared spectra of minerals and rocks; I, Silicate minerals. *Modern Geology*, 1, 283–300.
- Hunt, G. R., & Salisbury, J. W. (1971). Visible and near-infrared spectra of minerals and rocks; II, Carbonates. *Modern Geology*, 2, 23–30.
- Hunt, G. R., & Salisbury, J. W. (1973). Visible and near infrared spectra of minerals and rocks; VI, Additional silicates. *Modern Geology*, 4, 85–106.
- Hunt, G. R., Salisbury, J. W., & Lenhoff, C. J. (1971). Visible and near-infrared spectra of minerals and rocks; III, Oxides and hydroxides. *Modern Geology*, 2, 195–205.

- Huntington, J. F., & Schodlok, M. C. (2009). Cadia East Phase 2 HyLogging Overview in Geometallurgical Mapping and Mine Modelling (AMIRA P843). GeMIII (AMIRA P843) Technical Report 3 (unpubl.). North Ryde NSW: CSIRO.
- Huntington, J. F., Whitbourn, L. B., Mason, P., Berman, M., & Schodlok, M. C. (2010). HyLogging – Voluminous industrial-scale reflectance spectroscopy of the earth's subsurface. Boulder, Colorado: Science and Application of Reflectance Spectroscopy Symposium (unpubl.).
- Johnson, J. R., Hoerz, F., & Staid, M. I. (2003). Thermal infrared spectroscopy and modeling of experimentally shocked plagioclase feldspars. *American Mineralogist*, 88, 1575–1583.
- Kirkland, L. E., Herr, K. C., & Salisbury, J. W. (2001). Thermal infrared spectral band detection limits for unidentified surface materials. *Applied Optics*, 40, 4852–4862.
- Kirkland, L. E., Herr, K. C., Salisbury, J. W., Keim, E. R., Adams, P. M., & Hackwell, J. A. (2002). Infrared remote sensing of Mars and the Mars astrobiology exploration strategy. In G. Hoover, G. V. Levin, R. Paepe, & A. Rozanov (Eds.), *SPIE Proceedings Vol. 4495, Instruments, Methods and Missions for Astrobiology IV* (pp. 158–169). San Diego, CA, USA.
- Lane, M. D., & Christensen, P. R. (1997). Thermal infrared emission spectroscopy of anhydrous carbonates. *Journal of Geophysical Research*, 102, 25 581–525 593.
- Lane, M. D., Glotch, T. D., Dyar, M. D., Pieters, C. M., Klima, R., Hiroi, T., ... Sunshine, J. (2011). Midinfrared spectroscopy of synthetic olivines: Thermal emission, specular and diffuse reflectance, and attenuated total reflectance studies of forsterite to fayalite. *Journal of Geophysical Research-Planets*, 116, E08010. doi:10.1029/2010JE003588, p 20
- Lyon, R. J. P. (1965). Analysis of rocks by spectral infrared emission (8 to 25 microns). *Economic Geology*, 60, 715–736.
- Lyon, R. J. P., & Burns, E. A. (1963). Analysis of rocks and minerals by reflected infrared radiation. *Economic Geology*, 58, 274–284.
- Michalski, J. R., Kraft, M. D., Diedrich, T., Sharp, T. G., & Christensen, P. R. (2003). Thermal emission spectroscopy of the silica polymorphs and considerations for remote sensing of Mars. *Geophysical Research Letters*, 30, 2008. doi:10.1029/2003GL018354, p.4
- Moersch, J. E., & Christensen, P. R. (1995). Thermal emission from particulate surfaces: A comparison of scattering models with measured spectra. *Journal of Geophysical Research – Planets*, 100, 7465–7477.
- Nash, D. B., & Salisbury, J. W. (1991). Infrared reflectance spectra (2.2–15  $\mu\text{m}$ ) of plagioclase feldspars. *Geophysical Research Letters*, 18, 1151–1155.
- Nicodemus, F. E. (1965). Directional reflectance and emissivity of an opaque surface. *Applied Optics*, 4, 767–775. doi: 10.1364/AO.4.000767
- Ninomiya, Y., Matsunaga, T., Yamaguchi, Y., Ogawa, K., Rokugawa, S., Uchida, K., ... Kaku, M. (1997). A comparison of thermal infrared emissivity spectra measured in situ, in the laboratory, and derived from thermal infrared multispectral scanner (TIMS) data in Cuprite, Nevada, USA. *International Journal of Remote Sensing*, 18, 1571–1581.
- Quigley, M., Huntington, J. F., Whitbourn, L. B., Munday, T., Yang, K., & Schodlok, M. C. (2009). HyLogging: Emerging core logging technologies heading to operational uptake. London, UK: Geological Remote Sensing Group (GRSG) Conference (unpubl.).
- Ramanaidou, E. R., & Cudahy, T. J. (1996). Application of field spectrometry to the characterisation of iron oxides: Hematite and goethite. *5th International congress on Applied Mineralogy in the Minerals Industry* (pp. 80–84). Warsaw, Poland.
- Ramanaidou, E. R., Connor, P., Cornelius, A., & Fraser, S. (2002). Imaging Spectroscopy for iron ore mine faces. *Iron Ore 2002* (pp. 155–157). Perth, WA: AusIMM Publication Series.
- Ramanaidou, E. R., Wells, M., Belton, D., Verral, M., & Ryan, C. (2008). Mineralogical and microchemical methods for the characterization of high-grade BIF derived iron ore. *Reviews in Economic Geology*, 15, 129–156.
- Ruff, S. W., Christensen, P. R., Barbera, P. W., & Anderson, D. L. (1997). Quantitative thermal emission spectroscopy of minerals: A laboratory technique for measurement and calibration. *Journal of Geophysical Research*, 102, 14 899–814 913.
- Sabine, C., Realmuto, V. J., & Taranik, J. V. (1994). Quantitative estimation of granitoid composition from thermal infrared multispectral scanner (TIMS) data, Desolation Wilderness, northern Sierra Nevada, California. *Journal of Geophysical Research-Solid Earth*, 99, 4261–4271.
- Salisbury, J. W. (1993). Mid-infrared spectroscopy: Laboratory data. In C. Pieters & P. Englert (Eds.), *Remote geochemical analysis: Elemental and mineralogical composition* (p. 267). New York: Cambridge University Press.
- Salisbury, J. W., & D'Aria, D. M. (1992). Emissivity of terrestrial materials in the 8–14 atmospheric window. *Remote Sensing of Environment*, 42, 83–97.
- Salisbury, J. W., & Wald, A. (1992). The role of volume scattering in reducing spectral contrast of Reststrahlen Bands of powdered minerals. *ICARUS*, 96, 121–129.
- Salisbury, J. W., & Walter, L. S. (1989). Thermal Infrared (2.5–13.5  $\mu\text{m}$ ) Spectroscopic remote sensing of igneous rock types on particulate planetary surfaces. *Journal of Geophysical Research*, 94, 9192–9202.
- Salisbury, J. W., D'Aria, D. M., & Jarosewich, E. (1991a). Midinfrared (2.5–13.5  $\mu\text{m}$ ) reflectance spectra of powdered stony meteorites. *ICARUS*, 92, 280–298.
- Salisbury, J. W., Walter, L. S., Vergo, N., & D'Aria, D. M. (1991b). *Infrared (2.1–25  $\mu\text{m}$ ) Spectra of Minerals*. Baltimore and London: The Johns Hopkins University Press.
- Schodlok, M. C. (2004). Quantitative Analysen magmatischer Gesteine mittels reflexionsspektroskopischer Infrarot-Messungen (urn:nbn:de:kobv:b103-04100). Scientific Technical Report STR, 04/10. Potsdam, Germany: Deutsches GeoForschungs Zentrum GFZ; p. 127.
- Schodlok, M. C., Green, A. A., Huntington, J. F., & Whitbourn, L. B. (2009). A new library of thermal infrared reflectance spectra of rock-forming minerals and rocks. *6th Workshop on Imaging Spectroscopy: An Innovative Tool for Scientific and Commercial Applications*, Tel Aviv, Israel; p. 6.
- Schodlok, M. C., Whitbourn, L. B., Huntington, J. F., Mason, P., Green, A. A., Berman, B., ... Jolivet, J. et al. (2016). HyLogger-3, A visible to short-wave and thermal infrared reflectance spectrometer system for drill core logging: Functional description. *Australian Journal of Earth Sciences*, 63, doi 10.1080/08120099.2016.1231133
- Sherman, D. M., & Waite, T. D. (1985). Electronic-spectra of Fr<sup>3+</sup> Oxides and Oxide Hydroxides in the Near IR to Near UV. *American Mineralogist*, 70, 1262–1269.
- Spitzer, W. G., & Kleinman, D. A. (1961). Infrared lattice bands of quartz. *Physical Review*, 121, 1324–1335.
- Thomson, J. L., & Salisbury, J. W. (1993). The mid-infrared reflectance of mineral mixtures (7–14  $\mu\text{m}$ ). *Remote Sensing of Environment*, 45(1), 1–13.
- Wald, A. E., & Salisbury, J. W. (1995). Thermal infrared directional emissivity of powdered quartz. *Journal of Geophysical Research*, 100, 24 665–624 675.
- Walter, L. S., & Salisbury, J. W. (1989). Spectral characterization of igneous rocks in the 8– to 12- $\mu\text{m}$  region. *Journal of Geophysical Research – Solid Earth and Planets*, 94, 9203–9213.
- Wells, M., & Ramanaidou, E. R. (2007). Clay quantification of channel iron deposits (CID), Pilbara, Western Australia. *Iron Ore 2007* (pp. 203–207). Perth, WA: AusIMM Publication Series.
- Yang, K., Huntington, J. F., Browne, P. R. L., & Ma, C. (2000). An infrared spectral reflectance study of hydrothermal alteration minerals from the Te Mihi sector of the Wairakei geothermal system, New Zealand. *Geothermics*, 29, 377–392.
- Yang, K., Lian, C., Huntington, J. F., Peng, Q., & Wang, Q. (2005). Infrared spectral reflectance characterization of the hydrothermal alteration at the Tuwu Cu-Au deposit, Xinjiang, China. *Mineralium Deposita*, 40, 324–336.