



# Geometrical analysis of laboratory soil spectra in the short-wave infrared domain: Clay composition and estimation of the swelling potential



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## ABSTRACT

This study presents a new laboratory reflectance spectroscopy method that characterizes soil spectra in terms of the positions, depths, asymmetries at half depth, and widths at half depth of the clay diagnostic absorption bands (1400 nm, 1900 nm, and 2200 nm). The calculation of the geometrical parameters, which is performed using continuum-removed spectra, is rapid and simply applicable to a large number of samples and, therefore, can be used to cover large areas. The illite, montmorillonite, and kaolinite contents in mixtures strongly influence the depths of the absorption bands at approximately 1400 nm ( $D_{1400}$ ), approximately 1900 nm ( $D_{1900}$ ), and approximately 2200 nm ( $D_{2200}$ ), respectively. The  $D_{1400}$ ,  $D_{1900}$ , and  $D_{2200}$  parameters are used to create 3D (using  $D_{1900}/D_{2200}$ ,  $D_{1400}/D_{1900}$ , and  $D_{2200}/D_{1400}$  as the axes) and 2D (using  $D_{1400}/D_{1900}$  and  $D_{1900}/D_{2200}$  as the axes) diagrams of synthetic mixtures. In the 3D and 2D diagrams, the plotted mixtures form a triangular shape. The mixtures composed of two clay minerals define the external envelope of the triangular shape, and the mixtures formed of three clay minerals are located inside the triangular shape. Using these 3D and 2D diagrams as standard templates, the clay compositions of natural soils were estimated from (i) the average clay compositions of the three closest mixtures when the soil samples were located inside the triangular distribution of mixtures and (ii) the closest mixture when the soil samples were located outside of the triangular distribution of mixtures. Comparison with X-ray diffraction demonstrates the reliability of the predictions of montmorillonite content, which were used to estimate the swelling potential of the soils. This method offers a simple, fast, and low-cost approach to classifying soils into four swelling classes based on comparison with the methylene blue test, and it could be used as a complementary or alternative method to traditional geotechnical analysis.

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## 1. Introduction

Expansive soils change in volume in response to water-content fluctuations caused by large climatic variations (Yitagesu et al., 2009a, and references therein) and thereby cause damage to infrastructures worldwide (Chen, 1988). The presence of clay minerals is a good indicator of the swelling and shrinking behavior of soils (Goetz et al., 2001; Yitagesu et al., 2012). Montmorillonite (i.e., the smectite group), illite, kaolinite, and interstratified minerals are the most common clay species (Galán, 2006) that are commonly involved in such processes. They have distinct compositions, structural arrangements, and physicochemical characteristics that affect their capacity to absorb water molecules into their structure (Brigatti et al., 2006). For example, montmorillonite, illite, and kaolinite content in soils indicates high, moderate, and low swelling potential, respectively, and can be considered to be indicators of the

swelling behavior (Goetz et al., 2001; Kariuki et al., 2004; Mitchell and Soga, 2005).

Conventional laboratory analyses (e.g., X-ray diffraction and geotechnical analyses) are traditionally used to determine clay mineralogical compositions to establish the swelling behavior of soils, even though such techniques are slow, expensive, and time consuming. These conventional analyses are therefore not well suited to large datasets or large-scale investigations, and an alternative method that may aid in identifying and targeting expansive soils is required.

In this respect, reflectance spectroscopy, i.e., the study of light reflected from materials, allows the rapid and low-cost measurement of soil properties via reflectance-spectra analysis (Clark, 1999). In the short-wave infrared spectral domain (SWIR: 1100–2500 nm), the montmorillonite, illite, and kaolinite spectra display absorption bands (Ben-Dor, 2002; Clark, 1999; Clark and Roush, 1984; Goetz et al., 2001; Kariuki et al., 2004) that result from vibrational processes that affect water molecules and hydroxyl (Clark, 1999; Farmer and Russell, 1964; Hunt, 1977), and these absorption bands can be used to identify these materials (Bourguignon et al., 2007; Chabrilat et al., 2002a; Goetz et al., 2001; Hauff et al., 1990; Kariuki et al., 2004; Lagacherie

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et al., 2008; Truche, 2011; van der Meer, 1999, 2004; Yitagesu et al., 2009a; Table 1):

- The montmorillonite spectrum exhibits a deep and generally asymmetric sharp absorption band at approximately 1400 nm and a deep absorption band at approximately 1900 nm. A sharp absorption band, shallower than the absorption band at approximately 1900 nm, is present at approximately 2200 nm.
- The illite spectrum exhibits deep absorption bands at approximately 1400 nm and approximately 1900 nm. The absorption band at approximately 1400 nm is generally sharper than the montmorillonite absorption band at approximately 1400 nm. The absorption band at approximately 1900 nm is shallower than the montmorillonite absorption band at approximately 1900 nm. The absorption band at approximately 2200 nm is deep, similar to the absorption band at approximately 1900 nm, and sharp. Two additional shallow absorption bands are present at 2340 nm and 2440 nm.
- The kaolinite spectrum exhibits a double absorption feature at approximately 1400 nm and a shallow absorption band at approximately 1900 nm. The kaolinite spectrum is also characterized by a double absorption feature at approximately 2200 nm that can also manifest as a shoulder at approximately 2170 nm. Three additional shallow absorption bands are present at 2310 nm, 2350 nm, and 2380 nm.

Clay minerals in soils commonly occur in the form of mixtures with a variable amount of particular clay minerals; this variability complicates the direct identification and quantification of species. To predict various soil properties, including mineral composition and swelling potential, reflectance spectroscopy has thus been subjected to intensive research in the visible near-infrared (VNIR; 300–1100 nm) and SWIR wavelength domains (Bourguignon et al., 2007; Chabrilat et al., 2002b; Clark, 1999; Kariuki et al., 2003; Viscarra Rossel et al., 2009; Yitagesu et al., 2009b), and this research has also led to extensive investigation of the domain of wavelengths longer than 2500 nm (Yitagesu et al., 2011, 2012). Various techniques are commonly used to perform such spectral analyses (Viscarra Rossel et al., 2006). Visual interpretation of the clay mineralogical composition of a soil based on the similarities between the soil spectrum and the spectra of pure clay minerals is the simplest method (Clark and Roush, 1984; van der Meer, 1999). This approach is generally used as a first step for the estimation of mineralogical compositions, but it is highly imprecise, and the results can vary

depending on the operator who interprets the data. Furthermore, Ben-Dor et al. (1999) have demonstrated that the complexity of soils often prevents the use of simple spectral analyses or reference to generic spectral libraries to solve such problems. Multivariable regression analysis (also known as chemometric analysis), e.g., partial least-squares regression (PLSR; Ritz et al., 2010; Viscarra Rossel et al., 2006; Waiser et al., 2007; Yitagesu et al., 2009b), that exploits the potential covariables extracted from reflectance signals has been successfully used in various studies to predict the clay mineralogical compositions or swelling potentials of soils (Summers et al., 2011; Mulder et al., 2013). This approach is widely used but requires large datasets, extensive soil sampling for prediction and conventional soil analysis for calibration (Lagacherie et al., 2008), and it is not suitable for large-scale study. Alternatively, the continuum-removal method (see Section 3.1), which focuses on specific absorption features (Clark and Roush, 1984), constitutes a robust tool for characterizing spectral features and is frequently associated with chemometric analysis (Lagacherie et al., 2008). It has been successfully used by van der Meer (1999, 2004) and Kariuki et al. (2004) to characterize laboratory reflectance spectra in terms of the geometrical features of the absorption bands that correspond to (i) the position of the minimum value of the absorption band, (ii) its depth, (iii) its width, and (iv) its asymmetry. van der Meer (2004) has used these geometrical parameters of absorption bands to map key information regarding the surface mineralogy of a mining area in Nevada using AVIRIS images, and Kariuki et al. (2003, 2004) have established a link between these geometrical parameters of absorption bands and various geotechnical engineering parameters. These geometrical features (Table 1) are considered to be keys to the characterization of the clay mineralogical compositions of soils (Kariuki et al., 2004, 2006; van der Meer, 2004).

The common methods presented above, although they yield reliable estimations of various soil properties, are dependent on X-ray diffraction (XRD) analyses, geotechnical analyses, or airborne surveys, and therefore, these methods cannot be systematically applied or exported to new areas without performing costly analyses. Inspired by the efforts of van der Meer (1999, 2004), Kariuki (2003), and Kariuki et al. (2004), our study therefore aims to develop an alternative laboratory reflectance spectroscopy method that uses the geometrical parameters (depth, position, asymmetry, and width) of clay absorption bands in the SWIR domain to estimate the mineralogical compositions and swelling potentials of soils. We thus propose to use synthetic mixtures of montmorillonite, illite, and kaolinite (Truche, 2011; Fig. 1) to

**Table 1**  
Spectral characteristics of montmorillonite, illite, and kaolinite (Hauff et al., 1990; Kariuki, 2003; Yitagesu et al., 2009b).

Absorption band	Molecular origin	Diagnostic feature	Description	Clay minerals presence	Inferred swell risk
Approx. 1400 nm	OH	Asymmetry	<1 >1 Varied for illite	Montmorillonite Kaolinite	High Low
Approx. 1900 nm	H <sub>2</sub> O	Position of approx. 1900 nm minimum Depth of the absorption band	Minimum position is <1910 nm Minimum position is >1910 nm intense ↓ shallow	Montmorillonite Illite/kaolinite montmorillonite illite kaolinite	High Moderate/low high moderate low
Approx. 2200 nm	Al-OH	Position of approx. 2200 nm minimum Depth of the absorption band Double absorption band at approx. 2160 nm and approx. 2200 nm Asymmetry	Ineffective for discrimination of clay mineralogy Intense Shallow May be an inflection at approx. 2160 nm in clay mixture (identified using asymmetry)	Kaolinite Montmorillonite or illite Kaolinite	Low High/moderate Low
>2300 nm	Fe-OH (2340 nm) Mg-OH (2440 nm) Fe-OH	Absorption bands at approx. 2340 and approx. 2440 nm Absorption band at approx. 2380 nm Lack of absorption feature	<1 >1 Varied for illite Persist in mixed spectra Associated with absorption bands at approx. 2310 nm and approx. 2350 nm Small absorption variations complicate discrimination from kaolinite	Montmorillonite Kaolinite Illite Kaolinite Montmorillonite	High Low Moderate Low High

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